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*Lecture Notes in
Condensed Matter Physics*

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Chapter 1

Introduction

These lecture notes will be continuously updated and aim to give a pedagogical introduction at Master/Ph.D level to some of the most important topics in condensed matter physics, including recent research developments. Much of the text is adapted from various research articles, reviews, and lecture notes by other authors (which are cited in the text). Thus, the purpose of these lecture notes is educational use (it is primarily intended for the education of Master and Ph.D students at the host institution, NTNU) and should for the most part not be viewed as an original contribution from the author, although there are some places where original derivations are provided. Nor is this document to be distributed. These lecture notes can be viewed as a compilation of various key topics in condensed matter physics mostly extracted from scientific literature across the web.

Chapter 2

The importance of fundamental research

In recent years (currently 2015), there seems to be an increasing tendency toward a need to motivate ones research in terms of possible applications and technological advances. This is seen e.g. in criteria for grant proposals and an overall trend in scientific literature. Is this healthy? Is the fundamental research done on quantum condensed matter physics only justified by its potential to create new devices and technology?

The answer is a resounding no: gaining knowledge on how nature works has intrinsic value. There is nothing wrong with a long-term vision of technological applications emerging in the future from basic research, but discovering the solution to what is currently unknown and pushing the frontier of human knowledge forward, and disseminating these advances, is a key to the very understanding of the world around us.

With this in mind, it is interesting to note (and also an important argument for fundamental research that may not seem to have immediate prospects for applications) that there exist several examples of *major technological breakthroughs that originate from what at the time was considered fundamental research without any orientation toward applications*. Indeed, fundamental research has directly led to game-changing applications that were not anticipated when the research was undertaken. The challenge for investors is that since most applications arising in this way cannot be foreseen, the time interval between a basic research discovery and its application in technology may be years and decades. Some examples from e.g. *"The value of fundamental research"* by Cris dos Remedios (2006):

- Magnetic resonance imaging technology is now used widely for diagnosis (a non-invasive technique) and for research, with an increasingly wide variety of applications. Key developments include Carr and Purcell, who in 1954 described the use of magnetic field gradients to relate NMR frequencies to spatial position. Subsequently, magnetic resonance imaging became a multi-million industry although none of the early scientists had any idea that their work would lead to medical imaging technology of such practical significance.
- It is of course well known that fundamental studies of electromagnetic fields by Hertz and Maxwell underpin radio and television, developments that they clearly could not have imagined. The laser also falls into that category. The first working laser was built by Theodore Maiman in 1960. This idea came directly from atomic physics and, in particular, from princi-

ples of stimulated emission discovered by Einstein several decades before. With the subsequent development of gas lasers, these intense and coherent light sources found applications in experimental physics, enabled holographic and interferometric studies, and later were used for range finding and surveying. But the most important applications came with the development of solid state lasers and their use in fibre optic communications. Lasers are now used throughout the world in medicine, in consumer electronics, and in scanning and printing technology. Modern communications and data storage technologies depend on laser optics and in the next decade or so, optronic laser-based computers will supersede the electronic systems of today.

- The giant magnetoresistance effect is a good example of how an unexpected fundamental scientific discovery can quickly give rise to new technologies and commercial products, which is a strong argument for both public and private support of basic research. It has been noted that GMR can be considered one of the first real applications of the promising field of nanotechnology.
- The exactness of the quantized Hall conductance was discovered during routine resistance measurements. Actual measurements of the Hall conductance have been found to be integer or fractional multiples of e^2/h to nearly one part in a billion. It has allowed for the definition of a new practical standard for electrical resistance, based on the resistance quantum given by the von Klitzing constant. This is named after Klaus von Klitzing, the discoverer of exact quantization. Since 1990, a fixed conventional value RK-90 is used in resistance calibrations worldwide. The quantum Hall effect also provides an extremely precise independent determination of the fine structure constant, a quantity of fundamental importance in quantum electrodynamics.

Chapter 3

Central concepts related to quantum mechanics

3.1 Heisenberg's uncertainty principle

3.1.1 Position-momentum uncertainty

$$\Delta x \Delta p_x \geq \hbar/2. \quad (3.1)$$

3.1.2 Time-energy uncertainty: what it *really* means

Whereas the preceding uncertainty relation $\Delta x \Delta p_x \geq \hbar/2$ is well-defined mathematically and in terms of physical meaning, one often encounters a similar uncertainty relation involving time and energy in the literature. It has the form

$$\Delta E \Delta t \geq \hbar/2. \quad (3.2)$$

The problem with this relation is that it is not immediately clear how it is obtained or what it even means. For instance, while there is an energy operator in QM (the Hamiltonian $\hat{H}$), *there is no time operator $\hat{T}$* in QM. In fact, time is an independent variable in non-relativistic QM. Thus, from the very outset it is clear that we cannot derive Eq. (3.2) in the same way as Eq. (3.1), the latter requiring well-defined position and momentum operators. Moreover, what does Δt even mean? This has caused a lot of discussion regarding the existence and meaning of Eq. (3.2) and, unfortunately, some gross misinterpretations of it. Here, we will show (as was originally done in Ref. [30]) that Eq. (3.2) can be derived in non-relativistic QM as long as one properly defines the meaning of ΔE and Δt . Then, we will discuss its physical interpretation. We note in passing that one can also derive uncertainty principles of similar form as the well-known non-relativistic ones, albeit with relativistic corrections.

Before proceeding, let us briefly remind ourselves of the difference between stationary and non-stationary states. A stationary state Ψ_n solves both the time-dependent SE and is an eigenfunction of a time-independent H at the same time. It can be written as $\Psi_n = \psi_n e^{-iE_n t/\hbar}$ where ψ is an eigenfunction of H while E is the belonging eigenenergy. If the system is in a stationary state, all expectation values of observable quantities are time-independent.

Now, according to the superposition principle we also know that any linear combination of stationary states will also be a solution to the time-dependent SE, so that a general physical state of the system (still for a time-independent Hamiltonian) may be written as

$$\Psi = \sum_n c_n \Psi_n = \sum_n c_n \psi_n e^{-iE_n t/\hbar}. \quad (3.3)$$

The key point is that Ψ is no longer an eigenfunction of $\hat{H}$, meaning that Ψ is not a stationary state. Both the probability density $|\Psi|^2$ and the expectation value of physical observables may now depend on time, and energy is not sharply defined anymore ($\Delta E \neq 0$).

Let us now sketch the proof of Eq. (3.2). Let H be a time-independent Hamiltonian and let Ψ be the wavefunction of the system (but not necessarily stationary). In that case, we can show that in the Heisenberg picture (where the time-dependence is placed on the operators whereas the wavefunctions are time-independent), the expectation value of a quantity A that does not depend on time ($\partial A/\partial t = 0$) explicitly satisfies:

$$\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle \quad (3.4)$$

Let ΔA and ΔE denote the root-mean-square deviations (also known as standard deviations) of A and H , respectively:

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}. \quad (3.5)$$

One can then show that (see *e.g.* chapter 3 in Griffiths QM book) $\Delta A \cdot \Delta E \geq \frac{1}{2} |\langle [A, H] \rangle|$ using these definitions. Inserting our above expression for the commutator between A and H , one obtains:

$$\Delta E \cdot \frac{\Delta A}{|d\langle A \rangle/dt|} \geq \hbar/2. \quad (3.6)$$

which may be written precisely as

$$\Delta E \Delta t \geq \hbar/2, \quad (3.7)$$

if we define

$$\Delta t \equiv \frac{\Delta A}{|d\langle A \rangle/dt|}. \quad (3.8)$$

The crucial point regarding the physical interpretation of this uncertainty relation between ΔE and Δt is to recognize what Δt means. From its definition above, we see that Δt is the time required for the expectation value of A to change by an amount equal to its standard deviation ΔA . Put in more informal terms, it is the time required for the expectation value of A to change appreciably (with "appreciably" quantitatively being defined by the standard deviation).

If the system is in a stationary state, then we know that $d\langle A \rangle/dt = 0$ so that $\Delta t \rightarrow \infty$, but that is perfectly fine since $\Delta E \rightarrow 0$ then and the inequality is still valid. For a non-stationary state, however, $\Delta E \neq 0$ is the standard deviation of the Hamiltonian H and Δt can be thought of as the lifetime of the state Ψ with respect to the observable A , according to our above explanation. More precisely, it is the time interval after which the expectation value of A has changed appreciably (as

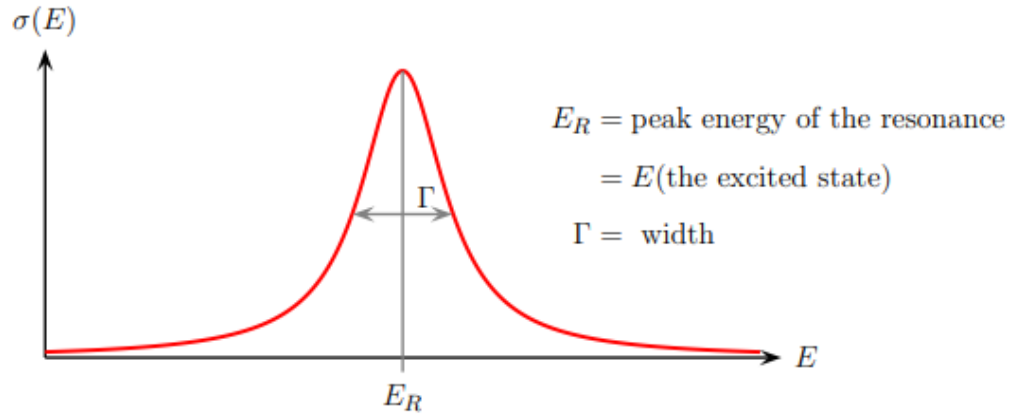


Figure 3.1: Sketch of energy-dependence of scattering cross section (or the number of detected events of a particular reaction) with a peak and corresponding linewidth that is inversely proportional to the lifetime of the decaying particle. Figure taken from <https://web2.ph.utexas.edu/~vadim/Classes/2019f/resonances.pdf>.

defined via the standard deviation of A).

How do we interpret this physically? One consequence is that a state that exists only for a short time cannot have a well-defined energy. For instance, an excited state in a condensed matter system that has a finite lifetime will then release a slightly different energy each time it decays, and the spread in this energy will be larger (meaning larger ΔE) the shorter its lifetime Δt . For a long-lived excitation $\Delta t \rightarrow \infty$, energy becomes well-defined $\Delta E \rightarrow 0$. This uncertainty in energy is reflected in the natural linewidth of the distribution of energies released by state that has decayed in this manner: fast-decaying states have a broad linewidth. The same principle also applies to fast-decaying particles in particle physics: the faster the particle decays, the shorter its lifetime and the less certain is its mass. We note that to detect particles with long lifetimes, one can simply observe the distance they propagate before decaying, which historically was done using *e.g.* bubble chambers. This no longer becomes possible for particles with lifetimes as short as for instance $\tau \rightarrow 10^{-20}$ s decaying via the strong interaction, since they propagate extremely short distances before disintegrating.

Quantum fluctuations

The above reasoning seems to suggest that there should be a strong link between the time-energy uncertainty relation and the concept of *quantum fluctuations*. A well-known example of a quantum fluctuation in particle physics is the bubble polarization diagram where a photon is converted into a temporary electron-positron pair which then collapses back into a photon. The fact that there exists confusing statements in the literature, such as that this can happen because the $e^- - e^+$ pair "borrows" energy from the environment, just underlines the importance of correctly interpreting what the time-energy uncertainty relation means. In fact, justifying the existence of virtual particles in Feynman diagrams from the energy-time uncertainty relation above is incorrect. The virtual particles arise as a result of a perturbative expansion of the path integral in QFT. At no point is energy-time uncertainty invoked as a requirement for their existence. Virtual particles do not represent a real particle that can be measured, but is a mathematical concept that is useful for the computation of cross-sections and lifetimes

3.1.3 Collapse of the wavefunction and superpositions

A quantum mechanical system may be in a superposition of states, $\Psi = \sum_n c_n \psi_n$. Assume that ψ_n are eigenstates of the operator $\hat{Q}$ with eigenvalues q_n . Upon measuring the physical quantity Q which has a quantum mechanical operator $\hat{Q}$, the only values we can obtain for this are q_n with probabilities $|c_n|^2$. Assume that we measure q_m at $t = t_0$. Immediately after the measurement has been performed, the system is in the state $\Psi = \psi_m$ and *no longer in a superposition of states*. Does it revert to a superposition of states? That depends: in fact, the time-dependence of the wavefunction Ψ will be governed by the time-dependent SE and thus by the Hamiltonian of the system, where one uses $\Psi(t = t_0) = \psi_m$ as the initial condition.

Performing a measurement on the system thus collapses the superposition of states into a single state and destroys effects such as the interference pattern in double-slit experiments (if one here detects the electron as it passes through a slit - if one does not detect the electron, the interference pattern is shown in the screen).

3.1.4 Boundary conditions for ψ : hard-wall versus periodic

One commonly encountered problem in introductory courses in QM is the particle-in-a-box scenario, where a particle is confined to a 1D box of length L . Since the potential is taken as infinitely high at $x < 0$ and $x > L$, the wavefunction must satisfy $\psi(x = 0) = \psi(x = L) = 0$. For a free particle inside the box, it is straightforward to show that this leads to the quantization condition

$$k = \frac{\pi n}{L}, \quad n = 1, 2, \dots \quad (3.9)$$

for the wavevector k of the wavefunction, which reads $\psi = \sqrt{2/L} \sin(kx)$. Mathematically, negative values of n should also be allowed since if $\sin(kx) = 0$, then clearly $\sin(-kx) = 0$ as well. However, negative values of k only changes ψ with an overall factor (-1) and thus physically corresponds to the same state since $|\psi|^2$ remains unchanged. That is why only positive integers n appear in the above quantization condition.

What is used more often than hard-wall boundary conditions, even when considering finite systems, is so-called *periodic boundary conditions*. What this means is that one demands that the wavefunction satisfies $\psi(x = 0) = \psi(x = L)$. Since the general solution of the wavefunction (just as in the particle-in-box case) reads

$$\psi = Ae^{ikx} + Be^{-ikx} \quad (3.10)$$

this imposes the quantization condition

$$k = \frac{2\pi n}{L}, \quad n = 0, \pm 1, \pm 2, \dots \quad (3.11)$$

which is different from Eq. (3.9). The main difference is that now also *negative values* of n are allowed. Why is this? The point is that since A and B are arbitrary complex coefficients [unlike the particle-in-box case where $\psi(x = 0)$ forces $A = -B$], a new ψ and $|\psi|^2$ is obtained when $k \rightarrow (-k)$ *unlike* the particle-in-box scenario. There are then twice as many solutions (pluss one since $n = 0$ also gives $\psi \neq 0$) in the periodic boundary condition case compared to the particle-in-box case.

Moreover, the periodic boundary conditions (PBC) allow us to describe propagating waves in both positive and negative directions with different weight A and B , unlike the particle-in-box case which only allows standing waves which is equivalent to counter-propagating waves $e^{\pm ikx}$ with equal weight. Choosing $A = -B$ in the PBC case of course reproduces the hard wall case.

Very well - but if we now have an isolated system, shouldn't we still use the hard wall boundary conditions to be accurate? Surely, the wavefunction must vanish at the vacuum edges. Strictly speaking, yes. However, there are at least two good reasons for using periodic boundary conditions:

- Usually, a material does not exist in isolation, but is rather connected to some contacts. In that case, we want to be able to describe the possibility of propagating electrons in either direction which is accomplished by using PBC. Note that even if we use PBC instead of hard wall boundary conditions, we can still count the number of electron modes k just fine.
- Even if a material does exist in strict isolation, we should not expect the boundary conditions to influence the physics substantially in the bulk of the material (far away from the boundaries) if the material is large enough. In that case, it should not matter which boundary conditions we use, and we may use whichever is more convenient, such as the PBC.

The strongest argument is, in the author's opinion, the first one. If one, for instance, is interested in discussing transport in a finite-sized system, it is clear that we must be able to describe propagating electrons in different directions. The hard wall condition should nevertheless be used if we want to identify edge-modes of a system which is truly terminated by vacuum.

Relevance to energy bands for electrons in solids.

When solving the SE for an electron in a periodic potential, such as in the Kronig-Penney model, one obtains a wavefunction of the form $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$ where $u_{\mathbf{k}}$ has the same periodicity as the lattice itself. The variable $\mathbf{k}$ is at this stage a continuous parameter which varies in the region $0 < k_i < 2\pi/a_i$ where a_i is the periodicity in direction i . However, $\mathbf{k}$ becomes discretized on a lattice when we introduce periodic boundary conditions. Periodic boundary conditions are useful because they in practice extend the lattice *ad infinitum* so that we maintain translational invariance. Consider for simplicity a 2D square lattice with periodicity a . The reciprocal lattice vectors are

$$\mathbf{a} = \frac{2\pi}{a}\mathbf{x}, \mathbf{b} = \frac{2\pi}{a}\mathbf{y}. \quad (3.12)$$

Let the position vector from the origin to atom n be $\mathbf{R}_n$ and assume that the wavefunction for neighbouring sites in the x and y direction differ by at most a constant phase factor A and B (with norm 1) since each site is supposed to be physically equivalent. The periodic boundary conditions then mean that the wavefunction satisfying the SE obeys

$$\psi(\mathbf{r} + N_1\mathbf{x}) = \psi(\mathbf{r}) = A^{N_1}\psi(\mathbf{r}), \psi(\mathbf{r} + N_2\mathbf{y}) = \psi(\mathbf{r}) = B^{N_2}\psi(\mathbf{r}) \quad (3.13)$$

when the lattice has N_1 sites in the x -direction and N_2 sites in the y -direction. The numbers A^{N_1} and B^{N_2} must both equal unity. Therefore, the solution for *e.g.* A is:

$$A = e^{2\pi i n_1/N_1}, \quad n_1 = 0, 1, 2, \dots, N_1. \quad (3.14)$$

This can be rewritten in the form

$$1 = e^{i\mathbf{k}\cdot N_1\mathbf{x}} \quad (3.15)$$

where $\mathbf{k}$ is precisely the reciprocal lattice-vector $\mathbf{k} = \frac{n_1}{N_1}\mathbf{a} + \frac{n_2}{N_2}\mathbf{b}$. From this, it follows that the wavefunction ψ is a Bloch function satisfying:

$$\psi(\mathbf{r} + \mathbf{R}_n) = e^{i\mathbf{k} \cdot \mathbf{R}_n} \psi_{\mathbf{k}}(\mathbf{r}) \quad (3.16)$$

which is equivalent to

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \psi_{\mathbf{k}}(\mathbf{r}). \quad (3.17)$$

Now, $\mathbf{k}$ is a discretized variable instead of continuous and its range is $[0, 2\pi]$, or equivalently $[-\pi/a, \pi/a]$.

The periodic boundary conditions used to make a finite size system translationally invariant in a specific direction means that the fermion operators c_i in second quantization should satisfy $c_1 = c_{1+N}$ where N is the lattice size. We can therefore write c_i as a Fourier-series and the periodic boundary conditions imply that $e^{ikN} = 1$, so that $k = 2\pi n/N$. According to our arguments above, we see that there exists as many k -values as sites. In the literature, the Fourier series

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{ikj} c_k \quad (3.18)$$

is often referred to simply as a Fourier transformation.

3.1.5 Normalization of eigenfunctions with discrete and continuous spectrum

Eigenfunctions with a discrete eigenvalue spectrum are normalizable whereas eigenfunctions with a continuous spectrum are only Dirac δ -function normalizable. This is a commonly used property, but few textbooks include a proof of this statement - it is usually taken for granted. However, it is possible to show this and we do so below.

The first thing to note is that for a Hermitian operator, let us call it $\hat{F}$, with eigenvalues f and eigenstates $|f\rangle$, all eigenstates belonging to different eigenvalues must be orthogonal. To see this, note first that

$$\langle l | \hat{F} | m \rangle = m \langle l | m \rangle, \quad (3.19)$$

but we also have

$$\langle l | \hat{F} | m \rangle = \langle m | \hat{F}^\dagger | l \rangle^* = l \langle m | \hat{F} | l \rangle^* = l \langle l | m \rangle. \quad (3.20)$$

Therefore, so long as $m \neq l$, we must have $\langle l | m \rangle = 0$. This is true regardless of whether $\{f\}$ is a discrete or continuous spectrum.

It then remains to clarify what happens with $\langle l | m \rangle$ when $l = m$.

Discrete spectrum

According to one of the fundamental postulates of QM, $|\psi\rangle$ is a normalizable state-vector satisfying the time-dependent SE. Since the eigenvectors of any Hermitian operator constitutes a complete set for the belonging Hilbert space, we can expand

$$|\psi\rangle = \sum_k c_k |k\rangle. \quad (3.21)$$

It then follows that

$$\langle \psi | \psi \rangle = 1 = \sum_{kk'} c_{k'}^* c_k \langle k' | k \rangle = \sum_k |c_k|^2 \langle k | k \rangle. \quad (3.22)$$

Since $\langle k | k \rangle$ is the norm of the state $|k\rangle$ in Hilbert space, and a norm in a linear vector space by definition must be positive and real, it is clear that $\langle k | k \rangle$ must be a finite number to satisfy the equality. This finite number may be chosen as, for instance, 1. Thus, $\{|k\rangle\}$ are normalizable. If they're chosen to be normalized to 1, $|c_k|^2$ has the meaning of the probability that the system will be found in state $|k\rangle$.

Continuous spectrum

In this case, $|\psi\rangle$ (which is normalizable) is expanded as

$$|\psi\rangle = \int df c(f) |f\rangle. \quad (3.23)$$

It then follows that

$$\langle \psi | \psi \rangle = 1 = \int \int df df' c^*(f') c(f) \langle f' | f \rangle. \quad (3.24)$$

We know that $\langle f' | f \rangle$ vanishes for all $f' \neq f$. But the only way an integral can give a finite value when the integrand is only non-zero in one particular point is if the integrand contains a δ -function. In other words, $\langle f | f \rangle$ cannot be finite in order for the above equality to be satisfied. Therefore, we are forced to conclude that

$$\langle f' | f \rangle = \delta(f' - f). \quad (3.25)$$

3.2 Scattering matrix S

The scattering matrix S is an important concept both in quantum mechanics, to describe the scattering of particles at barriers, and in quantum field theory, to describe the transition from an initial quantum mechanical state $|i\rangle$ to a final state $|f\rangle$.

3.2.1 S -matrix in quantum mechanics

The S -matrix relates the parts of a quantum mechanical wave incident toward a barrier with the parts of the quantum mechanical wave that moves away from the barrier. Due to conservation of the probability current, the S -matrix must be unitary: $SS^\dagger = 1$, which we prove below. If the system has additional symmetries, such as time-reversal symmetry, the S -matrix has additional properties.

Normal metal

To illustrate the S -matrix in action in the simplest possible case, consider a potential barrier $V(x)$ localized at $x = 0$. Particles are incident toward this barrier and can thus both reflect and transmit through it. These processes are described by the wavefunctions ψ_L and ψ_R on the left and right sides of the barrier:

$$\begin{aligned} \psi_L &= Ae^{ikx} + Be^{-ikx}, \\ \psi_R &= Ce^{ikx} + De^{-ikx}. \end{aligned} \quad (3.26)$$

Here, $k = \sqrt{2mE/\hbar^2}$. The waves A and D represent incoming waves toward the barrier whereas B and C represent waves moving away from the barrier. The scattering matrix is defined via the relation

$$\psi_{\text{out}} = S\psi_{\text{in}} \quad (3.27)$$

where

$$\psi_{\text{out}} = \begin{pmatrix} B \\ C \end{pmatrix}, \quad \psi_{\text{in}} = \begin{pmatrix} A \\ D \end{pmatrix}. \quad (3.28)$$

The scattering matrix is

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \quad (3.29)$$

and the elements S_{ij} characterize the scattering properties of the potential $V(x)$. The elements S_{ij} are thus directly related to reflection and transmission coefficients r and t and due to the unitary property of S one obtains $|r|^2 + |t|^2 = 1$.

To see how the unitarity property emerges, consider that the probability current J is defined as:

$$J = \frac{\hbar}{2mi}(\psi^* \partial_x \psi - \psi \partial_x \psi^*) \quad (3.30)$$

and conservation of probability requires that $J_L = J_R$. Therefore, we get

$$\begin{aligned} J_L &= J_R \\ \rightarrow |A|^2 - |B|^2 &= |C|^2 - |D|^2 \\ \rightarrow |B|^2 + |C|^2 &= |A|^2 + |D|^2 \\ \rightarrow \psi_{\text{out}}^\dagger \psi_{\text{out}} &= \psi_{\text{in}}^\dagger \psi_{\text{in}} \\ \rightarrow \psi_{\text{in}}^\dagger S^\dagger S \psi_{\text{in}} &= \psi_{\text{in}}^\dagger \psi_{\text{in}} \end{aligned} \quad (3.31)$$

It follows that $S^\dagger S = 1$. This proof can be generalized to *e.g.* spin-dependent situations.

The unitarity property can also be derived as follows. Let the wavefunctions for incoming and outgoing electrons be expressed as

$$\begin{aligned} \psi_{\text{in}} &= \sum_{\alpha} c_{\alpha}^{\text{in}} \phi_{\alpha}^{\text{in}}, \\ \psi_{\text{out}} &= \sum_{\beta} c_{\beta}^{\text{out}} \phi_{\beta}^{\text{out}}. \end{aligned} \quad (3.32)$$

Here, $\{\phi_{\alpha}^{\text{in}}\}$ and $\{\phi_{\beta}^{\text{out}}\}$ form an orthonormal basis. Since the Schrodinger equation is linear, the relation between the outgoing and incoming wavefunctions has to be linear. The coefficients are thus posited to fulfil:

$$c_{\beta}^{\text{out}} = \sum_{\alpha} S_{\beta\alpha} c_{\alpha}^{\text{in}}. \quad (3.33)$$

The matrix S is the scattering matrix which is determined by solving the Schrodinger equation in the scattering region and matching the solutions to the wavefunctions in the leads. Now, particle number conservation in the scattering process can be written as

$$\int d\mathbf{r} |\psi^{\text{in}}|^2 = \int d\mathbf{r} |\psi^{\text{out}}|^2, \quad (3.34)$$

which means that

$$\sum_{\alpha} |c_{\alpha}^{\text{in}}|^2 = \sum_{\alpha} |c_{\alpha}^{\text{out}}|^2. \quad (3.35)$$

Using Eq. (3.33), we obtain that

$$S^{\dagger} S = 1. \quad (3.36)$$

If the potential $V(x)$ is real, the system has time-reversal symmetry which means that if $\psi(x)$ solves the SE, then so does $\psi^*(x)$. The time-reversed solutions are

$$\begin{aligned} \psi_L^* &= A^* e^{-ikx} + B^* e^{ikx}, \\ \psi_R^* &= C^* e^{-ikx} + D^* e^{ikx}. \end{aligned} \quad (3.37)$$

Considering again which waves that are incident and outgoing, we obtain the relation

$$\begin{pmatrix} A^* \\ D^* \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} B^* \\ C^* \end{pmatrix}. \quad (3.38)$$

Using our definitions of ψ_{in} and ψ_{out} defined above, we now have two relations:

$$\psi_{\text{in}}^* = S \psi_{\text{out}}^*, \quad \psi_{\text{out}} = S \psi_{\text{in}}. \quad (3.39)$$

Together, they give $S^* S = 1$ which combined with $S^{\dagger} S = 1$ gives $S^T = S$. The scattering matrix thus satisfies $S = S^T$ if time-reversal symmetry is present.

How do we actually compute the S -matrix? Let us give a concrete example. Consider a potential barrier $V = V_0 \delta(x)$ separating two N regions. The corresponding wavefunctions are then given by Eq. (3.26). The boundary conditions $\psi_L = \psi_R$ and $\psi'_L - \psi'_R = 2mV_0 \psi_L$ at $x = 0$ gives us the equations:

$$A + B = C + D, \quad (A - B) - (C - D) = \frac{2mV_0}{ik}(A + B). \quad (3.40)$$

Let us define the dimensionless parameter $Z = 2mV_0/k$. To find the scattering matrix, we need to express B as a function of A and D and also express C as a function of A and D . The boundary conditions above allow us to do precisely this. We find

$$B = \frac{2i}{2i + Z} D - \frac{Z}{2i + Z} A, \quad C = \frac{2i}{2i + Z} A - \frac{Z}{2i + Z} D. \quad (3.41)$$

Therefore, we obtain

$$S = \frac{1}{2i + Z} \begin{pmatrix} -Z & 2i \\ 2i & -Z \end{pmatrix} \quad (3.42)$$

and one can verify directly that $S^{\dagger} S = 1$ is satisfied.

Superconductor

In order for $SS^\dagger = 1$ to express conservation of probability current, "incoming" and "outgoing" have to be defined in terms of group velocity and not in terms of momentum direction (which becomes an important distinction in the case of Andreev-reflected holes).

If we consider an NS interface and energies $E > \Delta$, so that quasiparticles can propagate inside the superconductor, we need to double the basis since we now can have reflection and transmission as holes in addition to electrons. We still consider the spin-degenerate case for simplicity. Let $I_{N,S}^{e,h}$ be the incoming amplitudes for electrons/holes from the normal/superconducting side, while $O_{N,S}^{e,h}$ is the same for outgoing amplitudes. We thus generally have the following wavefunctions

$$\begin{aligned}\psi_N &= I_N^e \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ikx} + I_N^h \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ikx} + O_N^e \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx} + O_N^h \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx}, \\ \psi_S &= I_S^e \begin{pmatrix} u \\ v \end{pmatrix} e^{-iqx} + I_S^h \begin{pmatrix} v \\ u \end{pmatrix} e^{iqx} + O_S^e \begin{pmatrix} u \\ v \end{pmatrix} e^{iqx} + O_S^h \begin{pmatrix} v \\ u \end{pmatrix} e^{-iqx}.\end{aligned}\quad (3.43)$$

The scattering matrix for the NS interface then takes the form

$$\begin{pmatrix} O_N^e \\ O_N^h \\ O_S^e \\ O_S^h \end{pmatrix} = S \begin{pmatrix} I_N^e \\ I_N^h \\ I_S^e \\ I_S^h \end{pmatrix}.\quad (3.44)$$

Keep in mind that if a different set of basis vectors is used, such as $(1,0)$ and $(0,1)$ in the N and (u,v) and (v,u) in the S, one has to make sure they are normalized in the same way in order for the particle number conservation to be valid and for the S -matrix to be unitary. However, it is unclear if this really works for supergap energies since Cooper pair transfer (Andreev reflection) can still occur, at least for E sufficiently close to Δ , and the scattering matrix might thus not be unitary due to lack of quasiparticle number conservation (since ψ does not account for Cooper pairs on the S side).

Considering instead an NS interface for energies $E < \Delta$ (interface at $x = 0$), we know that there are no propagating modes inside the superconductor. It is then possible to define an S -matrix for Andreev reflection which relates incident waves to outgoing waves in the N region alone. In effect,

$$\begin{pmatrix} c_e^- \\ c_h^+ \end{pmatrix} = S \begin{pmatrix} c_e^+ \\ c_h^- \end{pmatrix}\quad (3.45)$$

where $c_{e,h}^\pm$ denotes electron and hole particles with momentum $\pm \mathbf{k}$.

The scattering matrix formalism is useful to compute Andreev bound states in Josephson junctions. Consider an SXS Josephson junction where X is a scattering barrier which may contain *e.g.* magnetic elements. This can be modelled by Fig. ?? (taken from [49]).

We have here inserted "fictitious" normal-leads between the superconductor and the barrier region in order to be able to define simple modes in the normal region. The barrier can now contain impurity scattering, magnetic processes, and so forth. This idea was put forth in Ref. [50].

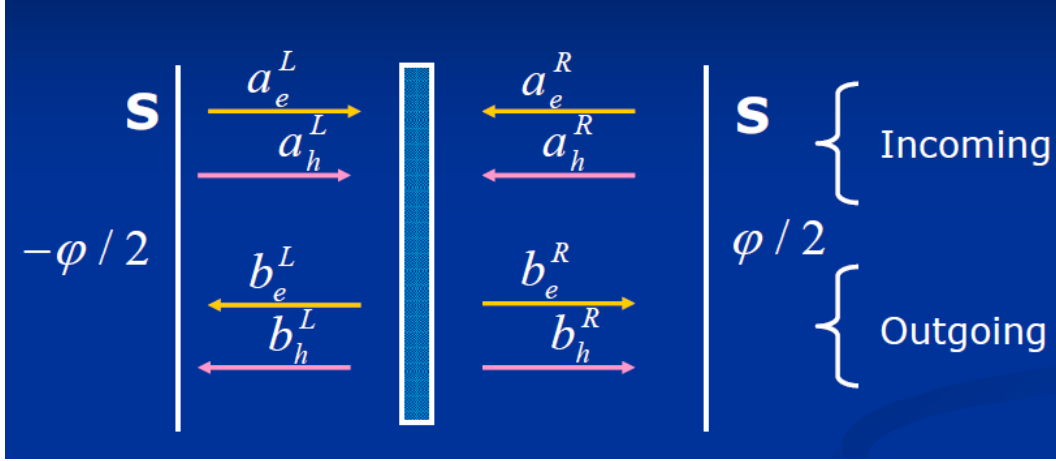


Figure 3.2: Scattering matrix treatment of an SXS junction where X is a barrier (the rectangular region in the middle)

The idea is then to first consider the scattering taking place at the barrier (the central blue rectangle in the figure). Since $\psi_{\text{out}} = S_N \psi_{\text{in}}$, we have that

$$\begin{pmatrix} b_e^L \\ b_h^L \\ b_e^R \\ b_h^R \end{pmatrix} = S_N \begin{pmatrix} a_e^L \\ a_h^L \\ a_e^R \\ a_h^R \end{pmatrix}. \quad (3.46)$$

Here, we denoted the scattering matrix of the central region by S_N and this has to be a block-diagonal matrix so long as the barrier region does not couple electron and hole excitations.

But we can also establish a relation between the amplitudes $\{a_{e,h}^{L,R}\}$ and $\{b_{e,h}^{L,R}\}$ through the scattering occurring at the S interfaces. Assuming for simplicity that there is no barrier region there (we can put all the barrier potential inside the scattering matrix S_N), Andreev reflection occurs with unit probability. We can then set up two separate scattering matrix equations for the left and right interface:

$$\begin{pmatrix} a_e^R \\ a_h^R \end{pmatrix} = s_R \begin{pmatrix} b_e^R \\ b_h^R \end{pmatrix} \quad (3.47)$$

where a straightforward computation gives (verify this):

$$s_R = \begin{pmatrix} 0 & e^{i\beta+i\phi_R} \\ e^{i\beta-i\phi_R} & 0 \end{pmatrix}. \quad (3.48)$$

Here, $\beta = \text{acos}(E/\Delta_0)$ and ϕ_R is the U(1) phase of the right superconductor. A similar equation holds at the left interface. We can combine the two scattering matrix equations at the two interfaces into one equation by writing:

$$\begin{pmatrix} a_e^L \\ a_h^L \\ a_e^R \\ a_h^R \end{pmatrix} = S_A \begin{pmatrix} b_e^L \\ b_h^L \\ b_e^R \\ b_h^R \end{pmatrix}, \quad S_A = \begin{pmatrix} 0 & 0 & e^{i\beta+i\phi_L} & 0 \\ 0 & 0 & 0 & e^{i\beta+i\phi_R} \\ e^{i\beta-i\phi_L} & 0 & 0 & 0 \\ 0 & e^{i\beta-i\phi_R} & 0 & 0 \end{pmatrix}. \quad (3.49)$$

By writing the equation in this way, we see that we have obtained a form

$$\psi_{\text{in}} = S_A \psi_{\text{out}} \quad (3.50)$$

according to our definitions above. Combining Eqs. (3.46) and (3.50), we get

$$\psi_{\text{out}} = S_N \psi_{\text{in}} = S_N S_A \psi_{\text{out}}. \quad (3.51)$$

Therefore, ψ_{out} is an eigenvector of the matrix $S_N S_A$ with the eigenvalue 1. This means that the condition

$$\det(S_N S_A - 1) = 0. \quad (3.52)$$

By solving this equation, one obtains the subgap Andreev bound state energies E that are allowed in the junction.

Note that if we had an SNS junction with energies where the gap in the left superconductor is smaller than the right, so that propagating states can exist there for $\Delta_L < E < \Delta_R$, it is possible to define a scattering matrix

$$\begin{pmatrix} O_L^e \\ O_L^h \end{pmatrix} = S \begin{pmatrix} I_L^e \\ I_L^h \end{pmatrix} \quad (3.53)$$

where S captures the scattering occurring in N and the right S, since there are no propagating states in the right S.

3.2.2 Scattering matrix for holes and relation to quasiclassical theory

When constructing boundary conditions for the quasiclassical Green function $\hat{g}$, several authors have previously employed the scattering matrix S in Nambu space. We here highlight a few key aspects of the scattering matrix used in this context and how it differs from the scattering matrix discussed above when it comes to the hole-part.

First, let us consider a calculation of a Nambu-space (particle-hole times spin) 4×4 scattering matrix for a normal metal/spin-orbit coupled barrier junction. The electron and hole parts for this problem are not coupled, so we may consider each separately. This means that the total scattering matrix should have the form

$$S = \begin{pmatrix} S_e & 0 \\ 0 & S_h \end{pmatrix} \quad (3.54)$$

where $S_{e,h}$ are 2×2 matrices in spin space. With the interface at $z = 0$, we consider the Hamiltonian

$$H = -\frac{1}{2m} \nabla^2 - \mu + (\mu + \epsilon_g + \beta \alpha (\hat{z} \times \nabla) \cdot \boldsymbol{\sigma}) \Theta(z). \quad (3.55)$$

We focus our attention on excitations close to the Fermi level of the normal metal, so that we set $E = 0$ in the BdG equation $H\psi = E\psi \simeq 0$. The eigenvalues in the SOC part are

$$E = \mathbf{k}^2/2m + \epsilon_g \pm \alpha |\mathbf{k}_{\parallel}| \quad (3.56)$$

where $\mathbf{k}_{\parallel} = (k_x, k_y, 0)$ and we have used a plane-wave ansatz for ψ . The general solutions in the N and barrier region B are then:

$$\phi(z) = \left[\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} e^{ik_z z} + \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} e^{-ik_z z} \right] e^{i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}} \quad (3.57)$$

for $z < 0$ whereas in the barrier region we have only evanescent waves

$$\phi(z) = C \begin{pmatrix} 1 \\ i e^{i\phi} \end{pmatrix} e^{-q_- z} + D \begin{pmatrix} 1 \\ -i e^{i\phi} \end{pmatrix} e^{-q_+ z} \quad (3.58)$$

where ϕ is the azimuthal angle $\tan \phi = k_y/k_x$. The momenta in the B region are obtained from the eigenvalues associated with each eigenstate:

$$q_{\pm} = \sqrt{\mathbf{k}_{\parallel}^2 + 2m(\epsilon_g \pm \alpha|\mathbf{k}_{\parallel}|)}. \quad (3.59)$$

The scattering matrix is found from the relation $B = SA$ which is obtained by using boundary conditions for $\phi(z)$ at $z = 0$, namely continuity of the wavefunction and its derivative. One finds

$$S = \frac{1}{(k_z + iq_+)(k_z + iq_-)} \begin{pmatrix} k_z^2 + q_+ q_- & e^{-i\phi} k_z (q_+ - q_-) \\ e^{i\phi} k_z (q_- - q_+) & k_z^2 + q_+ q_- \end{pmatrix}. \quad (3.60)$$

Since the scattering matrix is unitary, this can be parametrized for instance according to $S = e^{i\beta} e^{i\gamma(\hat{e} \cdot \boldsymbol{\sigma})}$ where $\hat{e}$ is a unit vector.

Now, what about the holes? The Hamiltonian for the holes is obtained from the electron one $H(\mathbf{k})$ by $-H(-\mathbf{k})^*$. The corresponding wavefunctions in each region are then:

$$\phi(z) = \left[\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} e^{ik_z z} + \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} e^{-ik_z z} \right] e^{i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}} \quad (3.61)$$

$$\phi(z) = G \begin{pmatrix} 1 \\ i e^{-i\phi} \end{pmatrix} e^{-q_- z} + H \begin{pmatrix} 1 \\ -i e^{-i\phi} \end{pmatrix} e^{-q_+ z}. \quad (3.62)$$

However, in order to describe incoming holes along the same trajectory as the electrons (meaning same group velocity direction), we have to reverse the sign of $\mathbf{k}_{\parallel}$ as well. The reason for this is that holes have opposite group velocity and momentum. The form of the wavefunction in N accounts for incoming holes already since it is a superposition of $e^{\pm ik_z z}$ waves, but to describe the same physical trajectory as the electron part S_e we have to reverse $\mathbf{k}_{\parallel}$ as well. This has the consequence $\phi \rightarrow \phi + \pi$ in the wavefunctions. The correct wavefunctions to consider are then:

$$\phi(z) = \left[\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} e^{ik_z z} + \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} e^{-ik_z z} \right] e^{-i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}} \quad (3.63)$$

$$\phi(z) = G \begin{pmatrix} 1 \\ -i e^{-i\phi} \end{pmatrix} e^{-q_- z} + H \begin{pmatrix} 1 \\ i e^{-i\phi} \end{pmatrix} e^{-q_+ z}. \quad (3.64)$$

We can now obtain the hole scattering matrix simply by comparing the system of equations obtained from the boundary conditions for $\phi(z)$ in the two cases. We see that if $B = S_e A$, then it immediately follows that

$$F = S_e [\phi \rightarrow (-\phi), q_{\pm} \rightarrow q_{\mp}] E. \quad (3.65)$$

But for the holes, it is E that are the outgoing waves. Therefore, S_h is defined via $E = S_h F$. Since S_e is unitary, we obtain from Eq. (3.65)

$$E = S_e^{\dagger} ([\phi \rightarrow (-\phi), q_{\pm} \rightarrow q_{\mp}] F) \quad (3.66)$$

which gives us

$$S_h = S_e^\dagger[\phi \rightarrow (-\phi), q_\pm \rightarrow q_\mp]. \quad (3.67)$$

A straight-forward calculation shows that

$$S_h = S_e^* \quad (3.68)$$

which is consistent with the relation $S_h(E) = S_e(-E)^*$ since we consider the case $E = 0$.

Relation to S used in quasiclassical theory.

Now, what about the S used in the boundary conditions for quasiclassical Green functions? Eschrig writes that

$$S = \begin{pmatrix} S_e(\mathbf{k}_\parallel) & 0 \\ 0 & S_e^T(-\mathbf{k}_\parallel) \end{pmatrix} \quad (3.69)$$

while Tokuyasu *et al.* and Millis *et al.* write

$$S = \begin{pmatrix} S_e(\mathbf{k}) & 0 \\ 0 & S_e^*(-\mathbf{k}) \end{pmatrix}. \quad (3.70)$$

Both of these give the same result for the hole part in *e.g.* the SOC-case discussed above. So they are internally consistent. But we obtained S_e^* for the hole part, not $S_e^*(-\mathbf{k})$. What is the reason for this?

The reason is rather subtle. We have to go back to consider the Gor'kov equation for the retarded Green function which looks like $[E\rho_3 + \hat{H}(1)]G(1, 2) = \delta(1 - 2)$. The point here is that the Hamilton-matrix $\hat{H}$ is *not* of the form $\text{diag}[H(\mathbf{k}), -H(-\mathbf{k})^*]$. Instead, it has an extra ρ_3 due to how the Green function matrix G is defined. Therefore, the hole part of $\hat{H}$ has an overall minus sign in difference compared to the hole Hamiltonian-matrix we used in the SOC-example above.

Which consequences does this have? Since we found the eigenfunctions from the equation $H_h\psi = 0$ with $H_h = -H(-\mathbf{k})^*$, an overall minus sign in difference for H_h has no consequence for the eigenfunctions. Thus, we should use the same wavefunctions as in Eq. (3.63), but with *one important modification*. Namely, the difference in overall minus sign for the hole part means that the "holes" in quasiclassical theory do *not* have opposite group velocity and momentum since they have the same normal dispersion as the electrons. Therefore, we must let $\mathbf{k} \rightarrow (-\mathbf{k})$ in Eq. (3.63) and consequently the same in the result for S_h . This proves that for the S used in the derivation of boundary conditions for the Green function in quasiclassical theory, the correct scattering matrix is

$$S = \begin{pmatrix} S_e(\mathbf{k}) & 0 \\ 0 & S_e^*(-\mathbf{k}) \end{pmatrix} \quad (3.71)$$

precisely as listed by Tokuyasu *et al.* .

3.2.3 S -matrix in quantum field theory

The S -matrix here describes the transition from an initial quantum mechanical state $|i\rangle$ to a final state $|f\rangle$. This transition is caused by scattering in the sense that the system interacts with some potential V that "scatters" the system between the two states.

Chapter 4

Theory of electromagnetism

The interaction between electromagnetic fields and matter is a pivotal topic in condensed matter physics. We here review some aspects of the theory of electromagnetism which are seldom discussed in full detail.

4.0.1 Relation between polarization of EM wave and spin polarization of photons

The polarization direction of an EM wave in classical physics is defined by the direction in which the electric field $\mathbf{E}$ is oriented. A linearly polarized wave has the electric field pointing along the same axis at all positions and times while a circularly polarized wave has an electric field which rotates in a circular fashion as one advances either position or time.

This seems like a straightforward definition. But in quantum mechanics, we learn that electromagnetic waves consist of photons. Photons are massless spin-1 particles and can be described by two spin-polarization states $|\psi_R\rangle$ and $|\psi_L\rangle$. The eigenvalues of the projection of the spin on the axis of propagation (say, $\hat{z}$) for these two states is $\pm\hbar$. These eigenvectors are known as right- and left-circularly polarized states.

Of course, a photon can also be in a superposition of these two states. For instance, a photon is linearly polarized if it is in a superposition (pure state) of the R and L circular polarization states where the belonging coefficients are equal in magnitude. Such a state has zero spin expectation value for the component projected along the axis of propagation, S_z , yet a measurement of the spin will always yield either $+\hbar$ or $-\hbar$. This is *different* from unpolarized light which is a quantum statistical mixture (mixed state) of equally many R and L polarized photons.

For instance, linearly polarized photons are in the state

$$\frac{1}{\sqrt{2}}(|\psi_R\rangle + e^{i\phi}|\psi_L\rangle), \quad (4.1)$$

where the polarization axis orientation is determined by ϕ . Depending on the choice of coordinate system, $\phi = 0$ can correspond to horizontally polarized photons whereas $\phi = \pi/2$ then corresponds to vertically polarized states.

The question is now: how does the classical definition of polarization (via $\mathbf{E}$) relate to the photon spin polarization? Since light is comprised of photons, a macroscopic EM wave must consist of a

tensor product of many photons. The number of photons required is determined by the energy of the wave (the magnitude of the electric field) and the energy quantum carried by each photon ($\hbar\omega$). Thus, if all the photon states that comprise this tensor product are circularly polarized, the EM wave is said to be circularly polarized and the electric field will rotate. Similarly, if the photons are all linearly polarized, the EM wave is linearly polarized.

To make the classical and quantum pictures consistent, this means that the orientation of the electric field associated with a quantum mechanical photon state is determined by the spin-polarization of that photon state. This can be seen mathematically from the quantization of the electromagnetic field. For instance, the vector potential $\mathbf{A}$ in its quantized version is written in terms of creation and annihilation operators and has a direction determined by the polarization vectors $\mathbf{e}_\mu$ ($\mu = 1, 2$). It is precisely these polarization vectors which mathematically define the spin operator acting on the photon field. Since the electric field $\mathbf{E} = -\partial\mathbf{A}/\partial t$, we see that the field direction is directly linked to the spin of the electromagnetic field.

Such a statement cannot immediately be generalized to other contexts, such as the electron. The electron spin has nothing to do with the direction of the electric field generated by the charge q of the electron.

The fact that the angular momentum operator is related to the electric field can be observed from the fact that an EM wave carries angular momentum $\mathbf{J}$:

$$\mathbf{J} = \epsilon_0 \int \mathbf{r} \times (\mathbf{E} \times \mathbf{B}) d\mathbf{r} \quad (4.2)$$

since the momentum of the wave is proportional to $\mathbf{E} \times \mathbf{B}$. We note that although a linearly polarized wave carries no spin angular momentum (since linearly polarized photons have zero spin expectation value) it does nevertheless have $\mathbf{J} \neq 0$, meaning that this so-called *orbital angular momentum* is related to the spatial distribution of the electric field (varying magnitude). The above formula (integral over angular momentum density) thus captures both the internal spin and the orbital angular momentum of the photon.

The *quantization* of the spin of a photon can only arise in quantum mechanics, but as far as spin being an internal angular momentum of the photon, this property is not quantum mechanical because it comes about due to the electric field carried by an EM wave (which is present already in the classical description).

Chapter 5

Central concepts related to symmetry and gauge-invariance

Symmetries, conservation laws, and gauge-theories are crucial in many branches of physics. It is important to have a clear idea of what is meant by these concepts and why they are so powerful. Below, we provide an introduction to them.

5.1 The origin of spin

Is the intrinsic spin of particles classical or quantum mechanical? Take for instance the electron. The Dirac Lagrangian is before quantization classical, if one accepts Grassmann numbers as a classical representation of fermionic anticommutation relations. In this classical Lagrangian, spinors are used as the fields, which do have a spin degree of freedom. Does this mean that the spin of particles is not a quantum mechanical property?

To answer this question, let us continue considering the electron for concreteness. There are two ways in which the origin of the electron spin can be understood. One way is through the quantum mechanical Dirac equation, where an internal angular momentum referred to as spin emerges even in the non-relativistic limit. This is the reason for why one often says that spin is a quantum variable.

But the other way to understand the origin of spin is by starting even with the classical field theory, namely the Dirac Lagrangian. Here, spin can be understood from the symmetry of the Lagrangian that emerges from the two ways in which a field can be rotated. It is this viewpoint which seemingly gives legitimacy to the question if spin can in fact be derived without quantum mechanics.

Let us explain this in more detail. A field ψ (in the present of an electron, more precisely a spinor) can be rotated by either moving all spatial positions around an axis, $\psi(\mathbf{r}) \rightarrow \psi(R\mathbf{r})$. Or it can be rotated by rotating the vector itself, $\psi(\mathbf{r}) \rightarrow U\psi(\mathbf{r})$. Here, R and U are rotation matrices acting on space and the spinor itself. We know that these are $SO(3)$ and $SU(2)$ matrices, respectively. The point is now that in general, the Dirac Lagrangian is only invariant under a rotation of *both* field and coordinate. This holds even in the non-relativistic limit. According to Noether's theorem,

there has to exist a conserved quantity. To see this, first note that

$$\begin{aligned} U(\mathbf{n}, \theta) &= e^{i\theta \mathbf{n} \cdot \boldsymbol{\sigma}/2}, \\ R(\mathbf{n}, \theta) &= e^{(\theta \mathbf{n} \cdot \boldsymbol{\Lambda})}, \\ \Lambda_x &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \dots \end{aligned} \quad (5.1)$$

for rotation an angle θ around an axis $\mathbf{n}$. For a small rotation, we then obtain the total transformation

$$\psi(\mathbf{r}) \rightarrow \psi(\mathbf{r}) + \theta \left[\frac{i}{2} \mathbf{n} \cdot \boldsymbol{\sigma} \psi(\mathbf{r}) + (\mathbf{n} \cdot \boldsymbol{\Lambda}) \mathbf{r} \cdot \nabla \psi(\mathbf{r}) \right] + \mathcal{O}(\theta^2). \quad (5.2)$$

The total Lagrangian

$$\mathcal{L} = \psi^\dagger \left[i\partial_t + \frac{\nabla^2}{2m} - U(\mathbf{r}, -\beta \nabla) + \mu \right] \psi \quad (5.3)$$

is then invariant up to a total gradient, and the corresponding conserved quantity $\rho(\mathbf{r})$ (generalized charge density) according to Noether's theorem is

$$\rho(\mathbf{r}) = \mathbf{n} \cdot [\mathbf{S}(\mathbf{r}) + \mathbf{L}(\mathbf{r})] \quad (5.4)$$

where

$$\begin{aligned} \mathbf{S}(\mathbf{r}) &= \frac{1}{2} \psi^\dagger(\mathbf{r}) \boldsymbol{\sigma} \psi(\mathbf{r}), \\ \mathbf{L}(\mathbf{r}) &= \psi^\dagger(\mathbf{r}) [\mathbf{r} \times (-i\nabla)] \psi(\mathbf{r}). \end{aligned} \quad (5.5)$$

We know that the above form for $\mathbf{L}(\mathbf{r})$ is an angular momentum (orbital). Hence, $\mathbf{S}(\mathbf{r})$ also has to be an angular momentum, and this is the intrinsic spin of the particle. As a sidenote, one can substantiate the fact that $\mathbf{S}$ is an angular momentum by using geometric algebra where spinors ψ define rotations of vectors. In this way, $\mathbf{S} = \frac{1}{2} \psi^\dagger(\mathbf{r}) \boldsymbol{\sigma} \psi(\mathbf{r})$ can be understood as the rotation of the vector $\boldsymbol{\sigma}$. The spinor defines a rotation to a coordinate system that is rotating around the axis which points in the direction given by $\mathbf{S}$. In this geometric algebra picture, one can then rightly interpret the electron field as rotating around its spin axis.

So we seem to have proven that particle spin arises without the need of quantum mechanics. However, this is not the case. Firstly, description of a particle as a field is in itself a quantum mechanical notion, even if we have not quantized the field yet. Secondly, the fact that the spinor components have to be treated as anticommuting variables (Grassmann numbers) rather than classical scalars suggests that something non-classical is at work. Finally, a point particle at rest has zero angular momentum according to the classical physics since $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, which is in contrast to the spin $\mathbf{S}(\mathbf{r})$ we identified from the Lagrangian treatment above.

In fact, one may take the viewpoint that the quantum mechanical Dirac equation (originally obtained by factorizing the Klein-Gordon equation) is the original observation that electrons have an internal spin. Then, one may construct a classical field equation corresponding to the Dirac equation by introducing Grassmann variables. This classical field theory then provides a suitable starting point to construct a quantum field theory for the Dirac field. When taking this viewpoint, it is clear

that particle spin should not be taken as something which exists in classical physics irrespective of quantum physics. With that said, we have shown above that spin emerges mathematically described in terms of the rotations of fields and their coordinates and the corresponding symmetries of the classical Lagrangian.

A similar reasoning applies to the photon described by the Proca Lagrangian, only that this field has spin 1, which follows from how it transforms under rotations of both space and the field itself. Note that the electromagnetic polarization of the photon is intimately related to the photon spin, but it is not the same. The polarization is described by how the electric and magnetic field directions evolve with space and time, which are described in a deterministic manner in classical physics. The polarization of the EM field determines the spin direction of the photons that make up the EM field along the quantization axis. However, a spin in quantum physics (more generally, an angular momentum) cannot have all components uniquely defined, unlike the classical description of electric and magnetic field components. So there are differences.

Note that one can also work with classical Hamiltonians like the Ising models where the binary variable is referred to as a classical spin. This analogy is probably based on the fact electron spins can take two values along the quantization axis, similar to the variables in the Ising model.

5.2 The Pauli principle and the spin-statistics theorem

Particles which have the same mass, charge, and spin in quantum mechanics, such as electrons, are considered to be identical. This means that they cannot be distinguished. Unlike in classical physics, where the trajectory of identical particles can be followed (making them in principle distinguishable), there is no such concept of a trajectory in QM and we thus have no way of distinguishing between *e.g.* two electrons.

Consider a state consisting of two particles. The state of the system is described by the total wavefunction $\Psi(\xi_1, \xi_2)$ where $\xi = (\mathbf{r}, \sigma)$ is the coordinate for the position $\mathbf{r}$ and z -component of the spin of each particles (assuming that the particle has spin - otherwise, the σ can simply be dropped). If the two particles are truly identical, then we should not be able to distinguish physically the state $\Psi(\xi_2, \xi_1)$ from the above. This means that

$$|\Psi(\xi_1, \xi_2)|^2 = |\Psi(\xi_2, \xi_1)|^2 \quad (5.6)$$

which in turn means that

$$\Psi(\xi_1, \xi_2) = e^{i\theta} \Psi(\xi_2, \xi_1). \quad (5.7)$$

By repeating the argument, we see that $e^{i\theta} = \pm 1$. The wavefunction describing two identical particles must thus be either symmetric or antisymmetric under exchange of the two particles, a statement which is described by the following theorem.

Spin-statistics theorem: systems of identical particles that have integer spin (bosons) must have a total wavefunction that is symmetric under exchange of any two particles. The wavefunction is said to obey Bose-Einstein statistics.

Conversely, systems of identical particles that have half-integer spin (fermions) must have a

total wavefunction that is antisymmetric under exchange of any two particles. In statistical mechanics, it is the Fermi-Dirac distribution function which governs the distribution of fermions: the latter are thus stated to obey Fermi-Dirac statistics.

Consider now fermions for concreteness. A two-electron wavefunction will have the general form

$$\Psi(\xi_1, \xi_2) = \psi(\mathbf{r}_1, \mathbf{r}_2) \times \chi(\sigma_1, \sigma_2) \quad (5.8)$$

as long as we can neglect spin-orbit coupling - otherwise, the orbital ψ and spin χ part cannot generally be factorized in this manner. There are two ways in which we can make the total wavefunction Ψ antisymmetric under exchange of ξ_1 and ξ_2 . One is that the spatial part $\psi(\mathbf{r}_1, \mathbf{r}_2)$ is symmetric under $\mathbf{r}_1 \leftrightarrow \mathbf{r}_2$ whereas the spin part is antisymmetric. The spin part must then be a singlet state $\uparrow\downarrow - \downarrow\uparrow$. The other possibility is that the spatial part is antisymmetric under exchange of the spatial coordinates, whereas the spin part is symmetric. The spin part is then in a triplet state $\uparrow\uparrow, \downarrow\downarrow, \uparrow\downarrow + \downarrow\uparrow$.

From the above considerations follows the so-called Pauli exclusion principle.

Pauli principle: no two fermions can be in exactly the same quantum state.

The state where the spatial part is symmetric (with the two electrons being in the same spatial quantum state) simultaneously as the spin part is symmetric (the spin of the two electrons is the same) is not allowed, which means that at least one quantum number must be different for the electrons (either a quantum number characterizing the spatial state or the spin quantum number).

5.2.1 Range of Pauli principle

Does the Pauli principle apply to any two electrons in the universe? Yes, the Pauli principle has an infinite range. However, it only has a practical consequence when the two electrons are close enough so that there is an overlap between their wavefunctions.

We know now that a wavefunction describing two electrons must be antisymmetric in their coordinates, including position. Neglect spin in what follows for brevity of notation. If we have two electrons 1 and 2 belonging to an atom where the eigenfunctions are labelled ψ_j where j is a quantum number describing the state, we can then antisymmetrize the total wavefunction in the following way to describe the total state:

$$\Psi(1, 2) = \psi_n(\mathbf{r}_1)\psi_m(\mathbf{r}_2) - \psi_m(\mathbf{r}_1)\psi_n(\mathbf{r}_2). \quad (5.9)$$

where (n, m) are a set of quantum numbers describing the state and $(1, 2)$ describes the electron coordinates. Clearly, the above satisfies $\Psi(1, 2) = -\Psi(2, 1)$. The generalization of this to N fermions is called a Slater determinant. We see from this expression that the two electrons should not be able to reside in exactly the same type of state ψ_n , even if they have different positions, because the wavefunction then vanishes:

$$\psi_n(\mathbf{r}_1)\psi_n(\mathbf{r}_2) - \psi_n(\mathbf{r}_2)\psi_n(\mathbf{r}_1) = 0. \quad (5.10)$$

It is important to distinguish such a scenario from a case where two electrons belong to different atoms separated in space. In that case, these electrons can be in the same quantum state because

their wavefunctions are separated in space and thus centered around different points (the core of each atom). Let the separation distance between the atoms be $\mathbf{R}$. Then, their wavefunction is

$$\Psi(1, 2) = \psi_n(\mathbf{r}_1)\psi_m(\mathbf{r}_2 - \mathbf{R}) - \psi_m(\mathbf{r}_1 - \mathbf{R})\psi_n(\mathbf{r}_2) \quad (5.11)$$

Now, we see that even if $m = n$, the wavefunction does not vanish. It only vanishes if $n = m$ and $\mathbf{r}_1 = \mathbf{r}_2$: the electrons cannot be at exactly the same position and in the same quantum state. This is the basic principle behind ferromagnetism: since electrons cannot be at the same position when they are in the same quantum state (both spins pointing in the same direction), they avoid the Coulomb interaction and lower the energy of the system.

A final note concerns Eq. (5.8). In light of how we wrote the antisymmetric wavefunction Eq. (5.9), one might be tempted to write a general two-electron wavefunction including spin on the form

$$\Psi(\xi_1, \xi_2) = \psi_n(\mathbf{r}_1)\chi(\sigma_1)\psi_m(\mathbf{r}_2)\chi(\sigma_2) - \psi_m(\mathbf{r}_1)\chi(\sigma_1)\psi_n(\mathbf{r}_2)\chi(\sigma_2) \quad (5.12)$$

by simply multiplying each wavefunction with a spin-part. However, we see that $\chi(\sigma_1)\chi(\sigma_2)$ can be factored out in the above equation, meaning that only an equal spin triplet state could be adequately described in this way since $\chi(\sigma_1)\chi(\sigma_2)$ is symmetric under the exchange $\sigma_1 \leftrightarrow \sigma_2$. Thus, Eq. (5.8) is more general.

5.2.2 Exchange energy from the Pauli principle: a quantum phenomenon

As mentioned previously, the antisymmetrization of the wavefunction has consequences when there is an overlap between the wavefunctions of the two quantum states ψ_n and ψ_m . To see this, consider as an example a Helium-like system where two electrons interact both with a nucleus Z and with each other. The total Hamiltonian is then

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{12} = \left(-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{Ze^2}{4\pi\epsilon_0 r_1} \right) + \left(-\frac{\hbar^2}{2m}\nabla_2^2 - \frac{Ze^2}{4\pi\epsilon_0 r_2} \right) + \frac{e^2}{4\pi\epsilon_0 r_{12}}. \quad (5.13)$$

The expectation value for the energy is then

$$\langle E \rangle = \int \int \Psi(1, 2)^* \hat{H} \Psi(1, 2) d^3 r_1 d^3 r_2 \quad (5.14)$$

where $\Psi(1, 2)$ is the wavefunction describing the two electrons. We know that this spatial part can be either symmetric or antisymmetric, depending on the spin state of the electrons. Let us therefore account for both possibilities by writing

$$\Psi(1, 2) = \frac{1}{\sqrt{2}} [\psi_n(\mathbf{r}_1)\psi_m(\mathbf{r}_2) \pm \psi_m(\mathbf{r}_1)\psi_n(\mathbf{r}_2)] \quad (5.15)$$

so that the $\pm$ corresponds to a singlet/triplet state. We don't need to write out the spin part explicitly because the Hamiltonian does not depend explicitly on spin, and thus this part plays no role in evaluating $\langle E \rangle$. However - it is important to emphasize that the *spin statistics* nevertheless will be seen to play a crucial role in that it determines the $\pm$ sign of the spatial part.

Inserting the above wavefunction into the expectation value, we obtain

$$\langle E \rangle = E_1 + E_2 + E_{12} \quad (5.16)$$

where E_{12} is the e-e Coulomb repulsion energy

$$E_{12} = \int \int \Psi(1, 2)^* \frac{e^2}{4\pi\epsilon_0 r_{12}} \Psi(1, 2) d^3r_1 d^3r_2. \quad (5.17)$$

Interestingly, the Coulomb energy can be further divided into two parts:

$$E_{12} = D_{nm} \pm J_{nm} \quad (5.18)$$

by inserting $\Psi(1, 2)$, namely the direct Coulomb energy D_{nm} and the *exchange energy* J_{nm} :

$$\begin{aligned} D_{nm} &= \frac{e^2}{4\pi\epsilon_0} \int \int \psi_n^*(\mathbf{r}_1) \psi_m^*(\mathbf{r}_2) \frac{1}{r_{12}} \psi_n(\mathbf{r}_1) \psi_m(\mathbf{r}_2) d^3r_1 d^3r_2, \\ J_{nm} &= \frac{e^2}{4\pi\epsilon_0} \int \int \psi_n^*(\mathbf{r}_1) \psi_m^*(\mathbf{r}_2) \frac{1}{r_{12}} \psi_m(\mathbf{r}_1) \psi_n(\mathbf{r}_2) d^3r_1 d^3r_2. \end{aligned} \quad (5.19)$$

To get this, we used that $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2| = r_{21}$. The direct Coulomb energy probes the repulsion due to an electron density at $\mathbf{r}_1$ and at $\mathbf{r}_2$. In the exchange energy integral, one instead effectively measures the overlap between the states ψ_n and ψ_m for the electrons 1 and 2, respectively, weighted by $1/r_{12}$ (the separation distance between the electrons). Its existence is a direct consequence of the fact that the wavefunction is a superposition of states. Moreover, it is seen that if the wavefunctions ψ_n and ψ_m have no overlap, meaning that one is zero when the other is non-zero for all positions $\mathbf{r}$, the exchange integral $J_{nm} \rightarrow 0$. This is in contrast to the Coulomb term D_{nm}

If $J_{nm} > 0$, it means that the energy of the system is minimized in the triplet configuration [the - sign in Eq. (5.18)]. Physically, this means that by aligning the spins of the electrons, they can maximize their separation distance and thus reducing the Coulomb repulsion energy. If $J_{nm} < 0$, the energy of the system is minimized in the singlet configuration. The exchange energy term is a purely quantum mechanical effect with no classical analogue.

The ground-state of a two-electron system with spin-independent $\hat{H}$ is always spin-singlet

It is shown in the textbook "Theory of magnetism" by Mattis that the ground-state (lowest energy level) of a two-fermion system with spin-independent Hamiltonian is always spin-singlet. We give this proof below.

However, we also note in passing that a simple two-fermion model can still give a ferromagnetic exchange interaction if one considers wavefunctions which are in an excited state and uses *e.g.* first-order perturbation theory. This is for instance the case for the He-example considered above. If one of the electrons is in the 1s ($n = 1$) state and the other is in an $n > 1$ state where n is the principal quantum number, then one can show that the triplet configuration for the electrons always has lower energy than the singlet configuration. This is demonstrated by evaluating the exchange integrals for the two configurations. However, the ground-state for He must be a spin-singlet state, just like for the H_2 molecule. When one considers *three or more electrons*, the ground-state can be ferromagnetic.

Therefore, we can state that simple two-fermion models can yield ferromagnetic coupling when using perturbation theory, but never in the ground-state: it will always be antiferromagnetically (singlet) coupled. We now give the proof for the latter statement following the textbook by D. C. Mattis.

Proof: Consider the two-fermion Schrödinger equation:

$$H\Psi(1, 2) = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\Psi(1, 2) + V(r_1, r_2)\Psi(1, 2) = E\Psi(1, 2). \quad (5.20)$$

Here, $1 = (r_1, s_1)$ and similarly for 2. The Hamiltonian is not separable, i.e. $H \neq H_1 + H_2$. Therefore, the solution Ψ cannot be a product of one-body eigenfunctions and the energy eigenvalues E cannot be written as the sum of the individual particles' energies.

We note that if spin does not explicitly enter in H , we can consider a simpler eigenvalue problem

$$H\Phi(r_1, r_2) = E\Phi(r_1, r_2) \quad (5.21)$$

where all spin labels have been removed, so that Φ is the spatial part of the wavefunction. If H is invariant under the interchange of spatial coordinates as it should be for identical particles. Moreover, we take Φ to be real without loss of generality since the wavefunction of the time-independent Schrödinger equation (for a stationary solution) can always be chosen to be real. Due to the overall antisymmetry of the wavefunction dictated by the Pauli principle, $\Phi(r_1, r_2)$ is *either* symmetric or antisymmetric under permutation of r_1 and r_2 . The belonging spin-part is then singlet or triplet. Let us moreover define a node as a point where a function crosses zero. Under these circumstances, we may state generally that:

The ground-state wavefunction will be a nodeless, symmetric function Φ . It is also unique (non-degenerate). Therefore, by the Pauli principle, the spin-part of the total particle wavefunction Ψ must be antisymmetric and singlet.

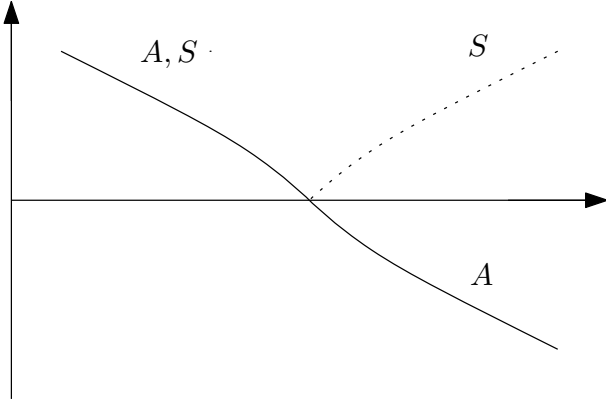
To see this, we use the principle of contradiction. Let us assume that the ground state is antisymmetric and see if there is some inconsistency. Suppose that the antisymmetric eigenstate $A(\mathbf{r}_1, \mathbf{r}_2) = -A(\mathbf{r}_2, \mathbf{r}_1)$ is unique and corresponds to the lowest energy eigenvalue E_0 . Its exact energy is:

$$E_0 = \frac{\int [\frac{\hbar^2}{2m}|\nabla_1 A(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\nabla_2 A(\mathbf{r}_1, \mathbf{r}_2)|^2 + V(\mathbf{r}_1, \mathbf{r}_2)A^2(\mathbf{r}_1, \mathbf{r}_2)]d^3r_1 d^3r_2}{\int A^2(\mathbf{r}_1, \mathbf{r}_2)d^3r_1 d^3r_2}. \quad (5.22)$$

Here, we used a partial integration to bring the ∇^2 term to a $|\nabla|^2$ term, which can be done since the surface term must vanish for a normalizable wavefunction. This wavefunction has nodes whenever $\mathbf{r}_1 = \mathbf{r}_2$ since it is antisymmetric: $A(\mathbf{r}_1, \mathbf{r}_1) = 0$.

Consider now instead a symmetric wavefunction $S(\mathbf{r}_1, \mathbf{r}_2) = |A(\mathbf{r}_1, \mathbf{r}_2)|$. This symmetric state cannot be an eigenstate of H for the following reason. In the perpendicular direction to the nodal surfaces defined by $A = 0$, the derivatives of S are discontinuous since S has a cusp at those surfaces. Thus, S has a discontinuous normal derivative to the nodal surface. But cusps are not allowed in the eigenfunction if the potential that enters the SE is non-singular. This can be seen by considering in 1D $\psi'' = (V - E)\psi$ which shows that if V is non-singular, ψ'' cannot be singular and hence ψ' cannot be discontinuous (*e.g.* derivative of step-function is Dirac delta).

The situation is illustrated in the figure below where A and S are plotted along a direction normal to a nodal surface of A .



If such an $S(\mathbf{r}_1, \mathbf{r}_2)$ is used to calculate the expectation value of H , we obtain a "variational" energy E_S which has to be higher than the ground-state since $S(r_1, r_2)$ does not satisfy the Schrödinger equation. Now, the variational energy obtained using S as a trial function is by definition given by:

$$E_S = \frac{\int [\frac{\hbar^2}{2m} |\nabla_1 S(\mathbf{r}_1, \mathbf{r}_2)|^2 + |\nabla_2 S(\mathbf{r}_1, \mathbf{r}_2)|^2 + V(\mathbf{r}_1, \mathbf{r}_2) S^2(\mathbf{r}_1, \mathbf{r}_2)] d^3 r_1 d^3 r_2}{\int S^2(\mathbf{r}_1, \mathbf{r}_2) d^3 r_1 d^3 r_2}. \quad (5.23)$$

This is true despite the fact that ∇S is not defined at the nodal surfaces defined by $A(\mathbf{r}_1, \mathbf{r}_2) = 0$, i.e. a 5-dimensional surface, for the following reason. We have that $|\nabla A|^2 = |\nabla |A||^2 = |\nabla S|^2$ everywhere *except* at the cusp points where ∇S is discontinuous in the direction normal to the surface. So why have we written the integral above over the entire region of space, i.e. integrating over all values of $\mathbf{r}_1$ and $\mathbf{r}_2$? Shouldn't we exclude the nodal surfaces?

Yes, we should, but here is the point: the contribution to the integral from those surfaces is exactly zero. This can be understood by noting that the contribution to an n -dimensional integral from a $(n-1)$ -dimensional surface is zero. Consider for instance the 1D integral $\int_a^b f(x) dx$. The contribution to this integral from one single point (0-dim surface) is zero since the point has no width. The only exception would be if the integrand is a Dirac δ -function at that point, but that is not the case for the system we consider: the normal derivative is discontinuous and not singular at the nodal surface. Similarly, consider a 2D integral $\int \int f(x, y) dx dy$. The contribution to this integral from a single curve $y = y(x)$ is zero, because the area of a 1D curve is zero. We can now generalize this all the way up to 6 dimensions. Just like a 2D surface has zero volume (in 3D), a 5D surface has zero volume in 6D and does not contribute to the integral.

Therefore, we have proven that

$$E_S = E_0. \quad (5.24)$$

But according to what we just stated concerning the variational principle, $E_S > E_0$. Yet the above equation shows that $E_S = E_0$. This is inconsistent and proves that an antisymmetric state A cannot be the ground state.

We close by mentioning that by similar argumentation one shows that the symmetric state of lowest energy, the true ground state, is nodeless. In that case, if we first assume that the true ground state is a nodeless function F , then the absolute value of F is either $+F$ or $-F$ and hence no contradiction appears when using the variational energy for $|F|$. Moreover, since two nodeless states cannot be orthogonal and the eigenfunctions of H should form an orthonormal complete set, the ground state

of the two-electron is non-degenerate and unique.

The take-home message here is then that even if $\hat{H}$ is spin-independent, the energy of the system depends on the spin-configuration of the particles.

5.2.3 What does choosing spin quantization axis mean?

One often reads the phrase that "the z -axis is chosen as the quantization axis", but what does this really mean?

We know that in quantum mechanics, only the length of the spin-vector and *one* of its components can be sharply defined simultaneously. In other words, the state of a spinful particle can only be an eigenstate of the spin operator and one of the components of the spins at the same time. All three components of the spin-vector cannot be precisely determined simultaneously.

We also know that spin is quantized, meaning that the length of the spin-vector and the value of each of its components can only take on discrete values. When we choose a quantization axis, it means that we choose a basis where the vectors are eigenstates of the spin projection operator for that particular axis. To be specific: if we choose z as the quantization-axis, it means that we have chosen a complete basis for our spin-wavefunctions that are the eigenfunctions of $\hat{S}_z$. Of course, there is nothing preventing us from choosing *e.g.* x as the quantization axis, in which case it means that our basis-vectors are $(1, 1)$ and $(1, -1)$, namely the eigenstates of $\hat{S}_x$.

5.3 Symmetries and conserved quantities

5.3.1 Time-reversal symmetry

Much of the material in this section is an adapted and somewhat rewritten version of chapter 2 in [?].

Classical physics

In classical physics, the existence of friction will in practice prevent time-reversal to be a true symmetry of most systems. However, at the level of modelling a system with a classical Hamiltonian $H(t)$, one says that $H(x, p)$ is time-reversal invariant (TRI) if

$$H(x, p) = H(x, -p) \quad (5.25)$$

since time-reversal means $t \rightarrow (-t)$ so that $x \rightarrow x$ and $p \rightarrow (-p)$. Time-reversal is not a canonical transformation since the Poisson bracket $\{p_j, x_j\} = \delta_{ij}$ is not left intact. A free particle $H = p^2/2m$ is thus described by a TRI Hamiltonian. A charged particle moving in an external magnetic field B is on the other hand not invariant under TR, since $H = (\mathbf{p} - e\mathbf{A})^2/2m$ contains linear term in $\mathbf{p}$ which changes sign upon $t \rightarrow (-t)$. However, note that if we include the field B as part of the system (thus characterizing it as *internal*), it would also change sign under TR so that $\mathbf{A} \rightarrow (-\mathbf{A})$ which would restore TRI of the Hamiltonian.

Quantum physics: spinless particles

In the quantum regime, a good starting point for discussing time-reversal symmetry (TRS) is to consider the Schrödinger equation

$$i\hbar\dot{\psi}(\mathbf{x}, t) = H\psi(\mathbf{x}, t). \quad (5.26)$$

An immediate difference from the classical case is that even if H is invariant under $t \rightarrow (-t)$, which also implies $\mathbf{x} \rightarrow \mathbf{x}$ and $\mathbf{p} \rightarrow (-\mathbf{p})$, the wavefunction $\psi(\mathbf{x}, -t)$ is *not* a solution of the resulting equation. This is due to the factor i . However, if we also complex conjugate ψ , it will satisfy the resulting equation. In other words, if $\psi(\mathbf{x}, t)$ satisfies the above SE and the Hamiltonian is time-reversal invariant, then $\psi^*(\mathbf{x}, -t)$ also solves the equation. This can be checked explicitly *e.g.* for

a spinless particle with a real Hamiltonian $H(\mathbf{x}, \mathbf{p}) = \mathbf{p}^2/2m + V(\mathbf{x})$ where $V(\mathbf{x}) = V^*(\mathbf{x})$ due to hermiticity. We then note for now that time-reversal in QM seems to involve complex conjugation as well and not only $t \rightarrow (-t)$.

For future reference, let us denote the operation of complex conjugation by K : $K\psi(\mathbf{x}) = \psi^*(\mathbf{x})$. It satisfies $K^2 = 1$. From its definition, we see that

$$K[a_1\psi_1(\mathbf{x}) + a_2\psi_2(\mathbf{x})] = a_1^*K\psi_1(\mathbf{x}) + a_2^*K\psi_2(\mathbf{x}) \quad (5.27)$$

which is a property known as antilinearity. In fact, antilinearity follows from the fact that the TR operator K is an *antiunitary operator* which is defined by the identity

$$\langle K\psi | K\phi \rangle = \langle \psi^* | \phi^* \rangle = \langle \psi | \phi \rangle^* = \langle \phi | \psi \rangle. \quad (5.28)$$

It is important to underline that the TR operator being K is the case specifically for the position representation and for spinless particles. In general, we shall denote the TR operator T , and we shall see that T can be more than the operation of the complex conjugation.

We consider as an example of the concrete operation of T the case of a rotationally symmetric potential $V(\mathbf{r}) = V(r)$ where the wavefunction ψ is written as

$$\psi(\mathbf{r}) = R_n(r)Y_l^m(\theta, \phi) = R_n(r)|l, m\rangle. \quad (5.29)$$

Since $T = K$ in the position representation for spinless particles, we see that

$$KY_l^m(\theta, \phi) = [Y_l^m(\theta, \phi)]^* = (-1)^m Y_l^{-m}(\theta, \phi) \quad (5.30)$$

Thus, it follows that

$$T|l, m\rangle = (-1)^m |l, -m\rangle. \quad (5.31)$$

We shall soon see a somewhat similar relation for spin-1/2 particles, but with the important exception that l and m are integer numbers above, which has consequences for what happens when T is applied twice.

Quantum physics: spin-1/2 particles

It is a general property of all TR operators T that they must be antiunitary:

$$\langle T\psi | T\phi \rangle = \langle \phi | \psi \rangle. \quad (5.32)$$

The product of two antiunitary operators is unitary, which can be verified from the definition of antiunitarity. As a result, we can actually write any time-reversal operator T on the form

$$T = UK \quad (5.33)$$

where U is a unitary operator and K is complex conjugation. To be clear, we should mention that the notation in Eq. (5.32) is to be understood as follows:

$$|T\phi\rangle \equiv T|\phi\rangle, \quad (5.34)$$

and $\langle T\phi|$ is the bra of the ket $|T\phi\rangle$. We do not further specify what the adjoint of T is since this is a non-trivial issue for an antiunitary/antilinear operator, but nor do we need to specify

what it is in the following calculations. We note for later use that the bra obtained from the ket $T^2|\phi\rangle = |T^2\phi\rangle = -|\phi\rangle$ (in the case of fermions where $T^2 = -1$, as we shall now prove) is then simply $-\langle\phi|$.

What should we expect happens if T is applied twice? Reversing time twice, we should be able to reproduce the original state, at least up to a phase factor. This means that $T^2 = \alpha$ with $|\alpha| = 1$. Using the standard form of T we get:

$$UKUK = UU^*K^2 = UU^* = \alpha \quad (5.35)$$

and since U is unitary we have $U^{-1} = U^\dagger$. Therefore, it follows that $U^* = \alpha U^\dagger$. Iterating this identity again provides $U^* = \alpha^2 U^*$, meaning $\alpha^2 = 1$ so that

$$T^2 = \pm 1. \quad (5.36)$$

The positive sign is valid for TR of spinless particles whereas we shall see that for half-integer spins, we must use $T^2 = -1$.

Can we now say something more specifically about what U is? We know that any angular momentum operator should change sign under time-reversal, both orbital and internal such as spin. Consider the latter, which in the standard representation takes the form

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z). \quad (5.37)$$

Since we must have

$$T\mathbf{S} = -\mathbf{S}T \quad (5.38)$$

which is equivalent to

$$T\mathbf{S}T^{-1} = -\mathbf{S} \quad (5.39)$$

it follows by inserting $T = UK$ that U must be a unitary matrix satisfying

$$\begin{aligned} T\sigma_x T^{-1} &= U\sigma_x U^{-1} = -\sigma_x, \\ T\sigma_y T^{-1} &= -U\sigma_y U^{-1} = -\sigma_y, \\ T\sigma_z T^{-1} &= U\sigma_z U^{-1} = -\sigma_z. \end{aligned} \quad (5.40)$$

In other words, U should commute with σ_y , but anticommute with σ_x and σ_z . In order to identify which U that satisfies this, we note that any 2×2 matrix can be written as

$$U = \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z + \delta. \quad (5.41)$$

One verifies that $\alpha = \delta = \gamma = 0$, whereas β is unrestricted by Eq. (5.40). The unitarity of U , however, imposes a restriction on β , namely that $|\beta| = 1$. This means that we can only determine the TR operator T up to a phase-factor $\beta = e^{i\phi}$. Different conventions are (unfortunately) found in the literature, but one of the most common choices is to set $\beta = i$ so that

$$T = i\sigma_y K = e^{i\pi\sigma_y/2} K. \quad (5.42)$$

Keep in mind that K is the complex conjugation operator which acts on both the position representation (orbital part of the wavefunction) and the spin representation. We see from Eq. (5.42) that

$$T^2 = i\sigma_y K i\sigma_y K = (i\sigma_y)^2 = -1 \quad (5.43)$$

as previously announced.

The effect of time-reversal on a spinor state for $\uparrow$ and $\downarrow$ electrons (having chosen z as the quantization axis) is then inferred as follows:

$$T|\uparrow\rangle = T\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -|\downarrow\rangle, \quad (5.44)$$

while

$$T|\downarrow\rangle = T\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle, \quad (5.45)$$

Thus, in general,

$$T|\sigma\rangle = -\sigma|\sigma\rangle. \quad (5.46)$$

We see that this is equivalent to how T operated on an angular momentum state of a spinless particle in the position representation, Eq. (5.31). We can also check that this statement is consistent with the eigenvalue equation for the spin operator S_z :

$$S_z|\sigma\rangle = \sigma|\sigma\rangle. \quad (5.47)$$

Applying T to this equation and using that $TS_z = -S_zT$, we obtain

$$S_zT|\sigma\rangle = -\sigma T|\sigma\rangle. \quad (5.48)$$

This means that $T|\sigma\rangle$ must be an eigenstate of S_z with eigenvalue $(-\sigma)$, which is precisely what is expressed by Eq. (5.46).

If we are considering a system of N spin-1/2 particles, the matrix U becomes the direct product of N single-particle matrices:

$$T = (i\sigma_{1y})(i\sigma_{2y}) \dots (i\sigma_{Ny})K = e^{i\frac{\pi}{2}(\sigma_{1y} + \dots + \sigma_{Ny})}K = e^{i\pi s_Y/\hbar}K \quad (5.49)$$

where S_y is the y -component of the total spin operator $\mathbf{S}$. The square of T now depends on whether the number of particles is odd or even, so that

$$\begin{aligned} T^2 &= 1 \text{ if } N \text{ is even} \\ T^2 &= -1 \text{ if } N \text{ is odd.} \end{aligned} \quad (5.50)$$

This is reasonable since an even number of spin-1/2 particles must have integer spin and thus behave in the same way under T^2 as spinless particles.

When a Hamiltonian has time-reversal symmetry, $[H, T] = 0$. Moreover, if $T^2 = +1$, one can show that a H with TR-symmetry can always be given by a real matrix representation.

Kramer's degeneracy for spin-1/2 particles

For any Hamiltonian invariant under TR, Kramer's degeneracy theorem states that if ψ is an eigenfunction with eigenvalue E , then $T\psi$ is an eigenfunction of H with the same eigenvalue. In other words, if $|\psi\rangle$ and $T|\psi\rangle$ are different, then each energy state of H is doubly degenerate. We now show this specifically for spin-1/2 particles where $T^2 = -1$.

Due to $[H, T] = 0$, it is straightforward to show from $H\psi = E\psi$ that both ψ and $T\psi$ are eigenfunctions of H with the same eigenvalue E . The remaining part of the proof is just to show that ψ and $T\psi$ are indeed different states, i.e. orthogonal. This can be done as follows. If they are orthogonal, then $\langle\psi|T\psi\rangle = 0$. Due to the antiunitarity property of T , we have

$$\langle\psi|T\psi\rangle = \langle T\psi|T^2\psi\rangle^* = -\langle T\psi|\psi\rangle^* = -\langle\psi|T\psi\rangle. \quad (5.51)$$

The only possible solution to this equation ($x = -x$ where $x = \langle\psi|T\psi\rangle$) is that $\langle\psi|T\psi\rangle = 0$, proving the theorem. As a corollary, we note that it follows that the dimension of the Hilbert space must be even (assuming that it is finite). This agrees with our previous statement that $T^2 = -1$ for an odd number of spin-1/2 particles, because the total spin quantum number S is then a half-integer and $2S + 1$ (the number of spin configurations) is then even.

Summarizing thus far, we have defined time-reversal via an antiunitary operator T satisfying (for any pair of states ψ and ϕ)

$$\begin{aligned} \langle T\phi|T\psi\rangle &= \langle\psi|\phi\rangle, \\ T^2 &= \pm 1, \end{aligned} \quad (5.52)$$

in addition to

$$\begin{aligned} T\mathbf{x}T^{-1} &= \mathbf{x}, \\ T\mathbf{p}T^{-1} &= -\mathbf{p}, \\ T\mathbf{J}T^{-1} &= -\mathbf{J}. \end{aligned} \quad (5.53)$$

Bogoliubov-de Gennes Hamiltonians

A particularly interesting class of Hamiltonians are the so called BdG Hamiltonians which are used to describe various types of superconducting systems. Using mean-field theory to describe such a system provides an effective single-particle theory. The second-quantized BCS Hamiltonian is expressed via annihilation and creation operators c_α and $c_\alpha^\dagger$, where the index α represents N available orbital single-particle states and the two spin states. This means that $\alpha = 1, 2, \dots, 2N$. They satisfy $\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha\beta}$.

A very general form of the BCS Hamiltonian then reads

$$H = \sum_{\alpha\beta} \left(h_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \Delta_{\alpha\beta} c_\alpha^\dagger c_\beta^\dagger + \frac{1}{2} \Delta_{\alpha\beta}^* c_\beta c_\alpha \right). \quad (5.54)$$

Here, the matrix h describes the non-superconducting part of the Hamiltonian, i.e. kinetic energy, single-particle potentials, magnetic fields, spin-orbit coupling, and so forth. The superconducting order parameters $\Delta_{\alpha\beta}$ account for electron pairing in the system (Cooper pairs) as well as the electron-hole coupling in quasiparticles of the system. Because H must be Hermitian and since the

second quantized operators satisfy Fermi statistics, one finds that the elements of the matrices h and Δ (which are scalars) must satisfy

$$\begin{aligned} h_{\alpha\beta} &= h_{\beta\alpha}^*, \\ \Delta_{\alpha\beta} &= -\Delta_{\beta\alpha}. \end{aligned} \quad (5.55)$$

One can rewrite the Hamiltonian as:

$$H = H_0 + \frac{1}{2}(c^\dagger \ c) \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \quad (5.56)$$

where $H_0 = \frac{1}{2}\text{Tr}(h)$ is a constant while h^T is the transpose matrix of h . We here defined $c = (c_1, c_2, \dots, c_{2N})$. Thus, the total BCS Hamiltonian is expressed via the Hermitian $4N \times 4N$ matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^T \end{pmatrix} \quad (5.57)$$

known as the Bogoliubov-de Gennes Hamiltonian. The conditions of Eq. (5.55) can now be compactly expressed via

$$\mathcal{H} = -\Sigma_x \mathcal{H}^* \Sigma_x \text{ where } \Sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (5.58)$$

It also follows that if ψ is an eigenvector of $\mathcal{H}$ with eigenvalue E , then $\Sigma_x \psi^*$ is an eigenvector of $\mathcal{H}$ with eigenvalue $-E$. This shows that there exists a symmetry of the energy spectrum of $\mathcal{H}$ around $E = 0$ since the existence of a state with energy $E_0 > 0$ guarantees that there exists a state with energy $-E_0$. This fact is usually referred to as a particle-hole symmetry of the Hamiltonian.

The entire BCS Hamiltonian, including second-quantized operators, is invariant under the combined operation of $c \leftrightarrow c^\dagger$ and complex conjugation. Note that complex conjugation does not affect the $\{c, c^\dagger\}$ operators: it only acts on the elements of $\mathcal{H}$. This particle-hole symmetry can be expressed in terms of $\mathcal{H}$ by defining an antiunitary charge conjugation operator C

$$C = \Sigma_x K, \ C^2 = 1. \quad (5.59)$$

This satisfies $\{C, \mathcal{H}\} = 0$, meaning that it is not a symmetry in the usual sense since $\mathcal{H}$ and C anticommute instead of commuting. However, it is a symmetry in the sense that if $\mathcal{H}$ satisfies this, then the *full* Hamiltonian including the second quantized operators has particle-hole symmetry.

BdG Hamiltonians that are time-reversal invariant belong to the so-called symmetry class DIII and satisfy $[\mathcal{H}, T] = 0$. In order for $\mathcal{H}$ to satisfy this, the individual matrices h and Δ must be time-reversal invariant, i.e. $[\mathbf{i}\sigma_2 K, h] = [\mathbf{i}\sigma_2 K, \Delta] = 0$. If they do, then one can show that $[\mathcal{H}, T] = 0$ is satisfied with

$$T = \begin{pmatrix} \mathbf{i}\sigma_2 & 0 \\ 0 & \mathbf{i}\sigma_2 \end{pmatrix} K. \quad (5.60)$$

We underline that the $\mathbf{i}\sigma_2$ is meant to act on the spin part of the matrices, while it is independent on channel space.

But how do the second-quantized operators themselves transform under TR T ? We should expect T to change both the sign of spin and momentum of these operators, but let us be more specific. A

first thing to note is that the complex conjugation part of T does not affect creation or annihilation operators. One way to see this is to consider the definition of such operators using $\hat{x}$ and $\hat{p}$ for a harmonic oscillator, in which case

$$\begin{aligned} c &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}, \\ c^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega}}\hat{p}. \end{aligned} \quad (5.61)$$

Since $\hat{x} = x$ and $\hat{p} = -i\partial_x$, it is clear that complex conjugating c or $c^\dagger$ has no effect. Now, consider a vacuum state where we create a spin at position i :

$$c_{i\sigma}^\dagger|0\rangle = |i, \sigma\rangle. \quad (5.62)$$

Applying T to this equation, we know from our earlier treatment that $T|i, \sigma\rangle = -\sigma|i, -\sigma\rangle$. It is then clear that in order for $(Tc_{i,\sigma}^\dagger)$ to produce this state, we need

$$Tc_{i,\sigma}^\dagger = -\sigma c_{i,-\sigma}^\dagger. \quad (5.63)$$

Had we instead considered $c_{k,\sigma}^\dagger$, then k would have been reversed as well so that

$$Tc_{k,\sigma}^\dagger = -\sigma c_{-k,-\sigma}^\dagger. \quad (5.64)$$

Therefore, overall we may write that the transformation of the second quantized operator under TR is:

$$T(zc_{\mathbf{k}\alpha}^\dagger) = z^*(-i\sigma_y)_{\alpha\beta}c_{-\mathbf{k}\beta}^\dagger T \quad (5.65)$$

where z is an arbitrary complex scalar. Note that we included a T after the operator on the right hand side for the sake of generality: this is necessary if there is some additional operator following $c_{\mathbf{k}\alpha}^\dagger$, which T also has to act on *after* having acted on $c_{\mathbf{k}\alpha}^\dagger$. The same relation holds for the annihilation operator:

$$T(zc_{\mathbf{k}\alpha}) = z^*(-i\sigma_y)_{\alpha\beta}c_{-\mathbf{k}\beta}T \quad (5.66)$$

Let us confirm that this kind of transformation correctly transforms a given Hamiltonian H (rather than just $\mathcal{H}$) under the TR operation. Consider for instance a system of electrons under the influence of a Zeeman effect from an external field $\mathbf{h}$:

$$H = \sum_{\mathbf{k}\alpha\beta} c_{\mathbf{k}\alpha}^\dagger [\epsilon_{\mathbf{k}} + (\mathbf{h} \cdot \boldsymbol{\sigma})]_{\alpha\beta} c_{\mathbf{k}\beta} \quad (5.67)$$

where $\epsilon_{\mathbf{k}}$ is the normal-state dispersion satisfying $\epsilon_{\mathbf{k}} = \epsilon_{-\mathbf{k}}$. Since $[\dots]_{\alpha\beta}$ is a scalar quantity, we obtain

$$\begin{aligned} TH &= \sum_{\mathbf{k}\alpha\beta} Tc_{\mathbf{k}\alpha}^\dagger T^{-1}T[\epsilon_{\mathbf{k}} + (\mathbf{h} \cdot \boldsymbol{\sigma})]_{\alpha\beta}T^{-1}Tc_{\mathbf{k}\beta}T^{-1}T \\ &= \sum_{\mathbf{k}\alpha\beta} (-\alpha c_{-\mathbf{k},-\alpha}^\dagger)[\dots]_{\alpha\beta}^*(-\beta c_{-\mathbf{k},-\beta})T = \sum_{\mathbf{k}\alpha\beta} \alpha\beta c_{\mathbf{k},-\alpha}^\dagger[\dots]_{\alpha\beta}^*c_{\mathbf{k},-\beta}T \end{aligned} \quad (5.68)$$

where we used that the summation is over both positive and negative $\mathbf{k}$, so that we could replace $-\mathbf{k}$ with $\mathbf{k}$ inside the summation. Now, since

$$[\epsilon_{\mathbf{k}} + (\mathbf{h} \cdot \boldsymbol{\sigma})]_{\alpha\beta} = \begin{pmatrix} \epsilon_{\mathbf{k}} + h_z & h_x - ih_y \\ h_x + ih_y & \epsilon_{\mathbf{k}} - h_z \end{pmatrix}_{\alpha\beta}, \quad (5.69)$$

we see that the part involving $\epsilon_{\mathbf{k}}$ transforms differently under T than the part including $\mathbf{h}$. The part including $\epsilon_{\mathbf{k}}$ satisfies $[\dots]_{\alpha\beta} = [\dots]_{-\alpha, -\beta}$ whereas the part including $\mathbf{h}$ satisfies $[\dots]_{\alpha\beta} = -\alpha\beta[\dots]_{-\alpha, -\beta}^*$. Using this, we finally obtain

$$TH = \sum_{\mathbf{k}\alpha\beta} c_{\mathbf{k}\alpha}^\dagger [\epsilon_{\mathbf{k}} - (\mathbf{h} \cdot \boldsymbol{\sigma})]_{\alpha\beta} c_{\mathbf{k}\beta} T \quad (5.70)$$

where we used that the summation goes over both positive and negative $\{\alpha, \beta\}$. As seen, the part of the Hamiltonian involving the external field $\mathbf{h}$ breaks time-reversal symmetry and ensures that H is not invariant under T .

But hang on - what if $\mathbf{h}$ had been an *internal* field instead? Shouldn't the Hamiltonian then be time-reversal invariant, since any internal field would change sign along with the spin of the electrons? Yes, it should. However, in that case we would have to write down the full Hamiltonian H which included the source of the field $\mathbf{h}$ produced internally in the system, such as localized spins. Since those spins should be reversed under T , the net result is that the $\mathbf{h}$ appearing in H after TR must be understood as the internal field produced after TR which is opposite to before the T operation, meaning that the total Hamiltonian indeed remains invariant.

We can also consider the Hamiltonian describing the surface states of a topological insulator:

$$H = \sum_{\mathbf{k}\alpha\beta} c_{\mathbf{k}\alpha}^\dagger (\mathbf{k} \cdot \boldsymbol{\sigma})_{\alpha\beta} c_{\mathbf{k}\beta} \quad (5.71)$$

We see that

$$(\mathbf{k} \cdot \boldsymbol{\sigma})_{\alpha\beta} = -\alpha\beta(\mathbf{k} \cdot \boldsymbol{\sigma})_{-\alpha, -\beta}^*, \quad (5.72)$$

which means that (following the same procedure as the example with the Zeeman field):

$$TH = \sum_{\mathbf{k}\alpha\beta} c_{-\mathbf{k}\alpha}^\dagger (-\mathbf{k} \cdot \boldsymbol{\sigma})_{\alpha\beta} c_{-\mathbf{k}\beta} T \quad (5.73)$$

But the summation over $\mathbf{k}$ itself includes both positive and negative momenta, so we have $\sum_{\mathbf{k}} = \sum_{-\mathbf{k}}$. In effect, $[H, T] = 0$ and the total Hamiltonian is time-reversal invariant. More generally, writing a Hamiltonian as

$$H = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \psi_{\mathbf{k}} \quad (5.74)$$

where $\psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k}\uparrow}^\dagger, c_{\mathbf{k}\downarrow}^\dagger)$, then TRS of the complete Hamiltonian H can be expressed through how T acts on $\mathcal{H}$, for instance that for certain types of Hamiltonians time-reversal invariance means that $T\mathcal{H}(\mathbf{k})T^{-1} = \mathcal{H}(-\mathbf{k})$.

5.3.2 Inversion symmetry

The transform of the second quantized operator under inversion is:

$$c_{\mathbf{k}\sigma}^\dagger \rightarrow c_{-\mathbf{k}\sigma}^\dagger. \quad (5.75)$$

5.3.3 Rotational symmetry

The second quantized operators transform as follows under a point group operation g such as rotation [28]:

$$c_{\mathbf{k}\alpha}^\dagger \rightarrow c_{g\mathbf{k},\beta}^\dagger U_{\beta\alpha}(g) \quad (5.76)$$

with

$$U = e^{-i\theta(\mathbf{n}\cdot\boldsymbol{\sigma})/2} \quad (5.77)$$

being the rotation matrix about a direction $\mathbf{n}$ by an angle θ .

5.3.4 Mirror symmetry

Let us consider the effect of a mirror operation on spin. The spin expectation value $\langle \mathbf{S} \rangle$ is a pseudovector, like magnetic field. This means that it transforms as a vector under rotation, but it is unaffected by inversion symmetry. Hence, it is parity-even.

Now consider a mirror operation with respect to a plane. Let us consider the xy -plane for concreteness. A mirror operation is defined as the combined effect of inversion and a π rotation around the axis normal to the plane. Vectors and pseudovectors thus transform differently under a mirror operation since they transform differently under parity. A vector $\mathbf{A}$ would have the following transformation of its components upon mirroring with respect to the xy -plane (which means the rotation is around the z -axis):

$$A_z \rightarrow -A_z, A_x \rightarrow A_x, A_y \rightarrow A_y. \quad (5.78)$$

A pseudovector would have the opposite sign for all components.

But we must distinguish the transformation of the spin expectation value (which is a pseudovector) from the transformation of a *spin eigenstates* (which is a spinor). A spinor has to transform differently from a pseudovector: for instance, we know that a pseudovectors returns to its original state upon a 2π rotation, but a spinor requires a 4π rotation to return to its original state.

If we then consider π rotation around the z -axis, we know that the correct operator $U = e^{-i\theta\hat{n}\cdot\boldsymbol{\sigma}}$ that applies this transformation to a spinor is $\pm i\sigma_z$ since $\hat{n} = \hat{z}$ in this case and $\theta = \pm\pi$. The $\pm$ is for whether we rotate counterclockwise or clockwise. We then see that applying a mirror operation to a spin-up state $\uparrow = (1, 0)$ gives $\uparrow \rightarrow i\uparrow$. A similar argument can be performed for any mirroring plane.

Applying this to $\downarrow$ gives $-i\downarrow$. Then, we see that a singlet state is invariant under a mirror operation. We underline again that transformations of the spin expectation value is in general different (transforms like a pseudovector) than transformation of a spinor itself.

5.4 Explicit vs. spontaneous symmetry breaking

5.5 Elitzur's theorem

The theorem by Shmuel Elitzur, proposed in 1975, was proven for Abelian gauge fields on a lattice, but was realized later to hold more generally in QFT and quantum statistical/condensed matter physics. It is stated as:

Elitzur's theorem: Local gauge symmetry cannot be spontaneously broken in a quantum gauge theory in that the expectation values of arbitrary gauge-dependent combinations of fields are always zero.

Elitzur's theorem thus claims that local gauge symmetries cannot be spontaneously broken. Let us recall that a spontaneously broken symmetry means that there exists a finite expectation value for a field which value changes depending on which gauge one chooses whereas the Lagrangian (or equations of motion) are invariant under different gauge choices. Therefore, Elitzur's theorem in practice means that only locally gauge-invariant quantities can have non-zero expectation values: any gauge-variant quantity will have expectation value zero. As a consequence of this, one can show that it is not possible to define a *local* order parameter in a gauge-theory.

Using a superconductor as an example, it is clear that the order parameter Δ is not local when the gauge-field is included if we try to write Δ in a gauge-invariant way. The order parameter would be

$$\Delta = |\Delta| e^{i\theta + i \int_{r_0}^r \mathbf{A} \cdot d\mathbf{l}} \quad (5.79)$$

and this is a non-local object due to the integral over $\mathbf{A}$.

Note that a gauge theory is a type of field theory in which the Lagrangian, and hence the dynamics of the system itself, does not change under local transformations. The transformation is most often continuous, but there also exists discrete gauge theories. The term gauge refers to any specific mathematical formalism to regulate redundant degrees of freedom in the transformation of the Lagrangian.

5.6 Higgs mechanism

The Higgs mechanism is a process in which a gauge boson, such as the photon, gains mass. To see how this works, we first recall the known result that the spontaneous symmetry breaking of a global, continuous symmetry results in a set of massless Goldstone bosons. An example of a Lagrangian with a global, continuous symmetry is

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)^* \partial^\mu \phi + \frac{1}{2}\mu^2 \phi^* \phi - \frac{1}{4}\lambda^2 (\phi^* \phi)^2. \quad (5.80)$$

The Lagrangian thus depends on the complex field ϕ . It is invariant under the continuous transformation $\phi \rightarrow e^{i\theta} \phi$ where θ is a real scalar and thus has a global U(1) symmetry.

Now, $\mathcal{L}$ can be made invariant under local continuous transformations $\phi \rightarrow e^{i\theta(x)} \phi$ if we introduce a gauge-field A_μ via minimal coupling:

$$D_\mu = \partial_\mu + iqA_\mu. \quad (5.81)$$

As detailed in the Griffiths textbook, we can now perform spontaneous symmetry breaking (SSB) on this new $\mathcal{L}$ which has local symmetry (rather than a global symmetry), and then choose a specific gauge where the gauge-field has become massive and the Goldstone modes are gone.

However, this is somewhat misleading. There is something else going besides SSB, namely *gauge-fixing*. Namely, we utilized the gauge-symmetry of the Lagrangian to make the complex field $\phi = \phi_1 + i\phi_2$ purely real. Thus, there is initially SSB by selecting a particular ground-state. But in analyzing the perturbative deviation from the GS, the gauge is fixed by keeping it real (fixing $\phi_2 = 0$ so that the fluctuation field denoted ξ in Griffiths vanishes). Then, the theory we are analyzing no longer has gauge-symmetry in the complex field ϕ since we have fixed the gauge. Had we allowed for fluctuation fields in both ϕ_1 and ϕ_2 when looking at deviations from the selected ground-state when doing the perturbation theory, we would still have a gauge-invariant theory. It is, however, after fixing the gauge that the Higgs mechanism arises. So in the usual (Griffiths) treatment of Higgs, we need SSB and gauge fixing.

One can also view this as follows. After the gauge-fixing, the fields no longer have the freedom to transform under gauge transformations, because the representation ϕ being purely real, with its real component $\phi_1(x) = v + \eta(x)$, where $\eta(x)$ is the fluctuation field, is now fixed. The ground-state of the Lagrangian where we have fixed the gauge is then uniquely defined: it is v . So one can argue that in the theory we are analyzing, there is no SSB any longer because the ground-state is unique. To get to that point, however, we first did perform an SSB and then fixed the gauge.

We underline that if one writes out the possible ground-state configurations for ϕ before fixing the gauge and then re-express the Lagrangian in terms of deviations from a particular ground-state, then the Lagrangian still has the original gauge-symmetry with respect to ϕ . It does not, however, have that symmetry with respect to the fluctuation fields. Moreover, for some gauge theories, fixing the gauge still leaves a remnant global symmetry in the Lagrangian. This can still break spontaneously without violating Elitzur's theorem.

What about Elitzur's theorem, which states both that local symmetries can never be SSB and as a result that gauge-dependent quantities cannot have finite vacuum expectation value? It depends on whether you view fixing the freedom to select the gauge as a symmetry or not. There are different opinions on this in the literature. If you view a gauge-transformation in a classical local gauge field theory as a symmetry of the Lagrangian, then the treatment in the Griffith's book is indeed spontaneous symmetry breaking of a local symmetry. If you make a distinction between a global field theory having a true symmetry and a local gauge-theory where gauge-transformations are viewed as something separate from a symmetry-transformation, then the Griffith's treatment is not related to SSB.

If one takes the viewpoint that the gauge-transformation is a symmetry so that we indeed perform SSB to begin with in the Higgs mechanism, it is unclear how this can be reconciled with Elitzur's theorem. There is no obvious mathematical error in the treatment in Griffiths. However, fortunately the Higgs mechanism can however be reformulated entirely in a gauge invariant way which does not require any form of SSB, so that there is no potential conflict with Elitzur's theorem. For an alternative way to prove the Higgs mechanism, namely via gauge-invariant fields so that local gauge symmetry need not be discussed, see [66]. So spontaneous symmetry breaking is not required for the Higgs mechanism. Instead, both the approach with gauge-fixing and the gauge-invariant approach have one crucial element in common: the non-zero vacuum expectation value of the Higgs field.

5.7 Gauge-theories and gauge-invariance

Performing a unitary transformation on a Hamiltonian H so that $H' = UHU^\dagger$ does not change the eigenvalues: H' has the same eigenvalues as H , but it also has a new set of eigenfunctions ψ . We must have $\psi' = U\psi$. The same physics is described by $\{H', \psi'\}$ as $\{H, \psi\}$. It is important to note that although the same physics is described, it does not mean that H' is *the same* as H : they are different, but changing the wavefunctions as well gives the same excitation spectrum. On the other hand, a Hamiltonian which is *invariant* under a given transformation is said to have a symmetry corresponding to that transformation.

Consider for instance a charged particle moving in an EM field described by a vector potential $\mathbf{A}$, we know that the system has a local U(1) symmetry corresponding to the transformation $e^{i\theta}$. The Hamiltonian is invariant under this transformation. It is also invariant under a local U(1) transformation $e^{i\theta(x)}$ if we introduce a gauge-field $\mathbf{A}$ via the minimal coupling scheme, contingent on that the gauge-field itself also transforms: $\mathbf{A} \rightarrow \mathbf{A} + \nabla\theta(x)$. The corresponding conserved quantity is electric charge. So in this case, we have a Hamiltonian that is actually invariant under a gauge-transformation, meaning not only that the transformed Hamiltonian obviously describes the same physics as the original one (since they are the same) but that there also exists a conserved quantity (charge).

Now let us contrast this with another example. In the presence of antisymmetric SOC which is linear in momentum, it is possible to formally include the SOC field as a vector gauge field $\mathcal{A}$ with components being SU(2) matrices in the same way as a magnetic vector potential $\mathbf{A}$ would be included, namely $\mathbf{p} \rightarrow \mathbf{p} - \mathcal{A}$. Such a Hamiltonian is invariant if one simultaneously makes an SU(2) transformation of it, $UHU^\dagger$, while transforming also the gauge field $\mathcal{A}$. However, transforming the gauge field actually alters the spin-orbit coupling since the latter is *not* invariant under a transformation of $\mathcal{A}$. We know from above that applying only a unitary transformation to H must give the same eigenvalues as before. A unitary transformation on a Hamiltonian including homogeneous magnetism and SOC can remove the SOC at the expense of making the magnetization spatially inhomogeneous instead (up to lowest order in the SOC coefficient, at least). Thus, we should expect the same physics for a homogeneous ferromagnet with SOC as an inhomogeneous magnet without SOC for the right type of spatial profile of $\mathbf{M}(\mathbf{r})$.

However, an important difference between the present case where SOC is treated as an SU(2) gauge field and the former case where the system had a U(1) symmetry, is that the gauge $\mathcal{A}$ cannot be freely chosen without altering the SOC. This is unlike the magnetic vector potential gauge $\mathbf{A}$ which can be altered without changing $\mathbf{B}$. Thus, the so-called SU(2) gauge symmetry that the Hamiltonian has when treating the spin-orbit coupling as a gauge field does describe a physically different spin-orbit coupling after the SU(2) transformation has taken place, and the *spin physics*, associated with *e.g.* the spin current or spin density operator, is not invariant.

Transforming the Usadel equation to a rotated Green function may thus bring the equation to a form where the terms can be more easily interpreted, but it is important to keep in mind that the Green function now has a different spin structure which is not equivalent to the original spin carriers. All of the physics is thus *not invariant* under an SU(2) SOC gauge transformation.

5.8 Neumann's principle

It is intuitively reasonable that the physical properties of an environment should somehow reflect the environment itself. This is formalized through Neumann's principle.

Neumann's principle: Any physical property of a crystal lattice must have the same symmetries as the crystal lattice itself.

More formally, if a crystal is invariant with respect to certain symmetry operations, any of its physical properties must also be invariant with respect to the same symmetry operations. Note that the physical properties can in principle have additional symmetries which the lattice does not, but the properties must have at least the symmetries of the underlying lattice.

To see how this works, it is useful to introduce three related quantities: response (R), property (P), and drive (D). They are symbolically related through $R = PD$, meaning that the response of a system when a driving force is applied is determined by the coupling property P. An example of this could be how a current is produced by an electric field. The link between these quantities is the conductivity tensor (in fact, physical properties of the lattice are often tensor-quantities). We have

$$\mathbf{j} = \sigma \mathbf{E} \quad (5.82)$$

where σ is a tensor, making possible in principle the induction of a current in the x -direction when a field is applied in the y -direction. It is σ which is the physical property of the lattice, and this quantity must thus be invariant with respect to the same operations that keep the lattice itself invariant.

Another example is the magnetic anisotropy tensor of a crystal lattice. For a cubic ferromagnet, the three perpendicular axes must have the same value for the anisotropy (the physical property of the lattice) according to Neumann's principle.

5.9 Do vortex patterns in superconductors have the same symmetries as the geometry?

In the superconducting case, the attractive interaction $V_{\mathbf{k}\mathbf{k}'}$ causing superconductivity must have the same symmetries as the crystal lattice itself. Mathematically, one can then use basis functions $\{\phi_\eta(\mathbf{k})\}$ (labelled by the subscript η) for the appropriate symmetry group of the lattice to construct the attractive interaction $V_{\mathbf{k}\mathbf{k}'}$. The order parameter may then in turn be expanded via the basis functions:

$$\Delta(\mathbf{k}) = \sum_{\eta} c_{\eta} \phi_{\eta}(\mathbf{k}). \quad (5.83)$$

Note, however, that Neumann's principle does not mean that the superconducting order parameter itself must be invariant under the same symmetry operations as the lattice. An example of this is the d -wave superconducting order parameter for the square lattice, which changes sign upon a $\pi/2$ rotation. It can also be seen from the fact that a *particular* basis function $\phi_{\eta}(\mathbf{k})$ can change sign upon perform a symmetry operation of the lattice.

Very well, but must $|\Delta|$ at least be invariant under the same symmetry operations as the lattice? The d -wave order parameter satisfies this. In general, the answer is actually no. The order parameter can display a spontaneous symmetry breaking in space, beyond the spontaneously broken $U(1)$ gauge symmetry. An example of this is a superconducting square and an applied magnetic field. When vortices nucleate in such a geometry, one would expect a vortex pattern which respects the square symmetry. For a flux magnitude of two elementary flux quanta, symmetry then demands that a giant $n = 2$ vortex nucleates in the middle of the sample in order to be consistent with the square symmetry. However, if two $n = 1$ vortices were to appear on the x -axis instead, the energy would actually have been lower since the kinetic energy of a vortex scales as n^2 . Such a pattern nevertheless breaks the square symmetry operations since it is not invariant under a $\pi/2$ rotation. In other words, the realized solution of $|\Delta|$ does not contain all symmetry operations of the system geometry. However, and importantly, the free energy of the system should remain invariant if the symmetry operations of the lattice are applied to Δ , even if Δ itself is not invariant. If now the aforementioned solution of $|\Delta|$ consisting of two $n = 1$ vortices positioned along the x -axis is rotated $\pi/2$, we get two $n = 1$ vortices positioned along the y -axis. The free energy, computed by integrating the free energy density over the system, is identical in the two configurations.

From the above reasoning, we must conclude that a particular realization of the order parameter Δ and its magnitude $|\Delta|$ do not have to obey the same symmetries as the system geometry, i.e. the underlying lattice geometry. The $|\Delta|$ can thus not be considered as a "physical property of the lattice" in the context of Neumann's principle. However, performing a symmetry operation on the order parameter which belongs to the symmetry operations of the lattice must give rise to a state which is physically equivalent (same free energy) as the original state. In this sense, von Neumann's principle is still preserved.

This is in fact similar to the case of different solutions of the hydrogenic Schrodinger equation with a rotationally invariant Coulomb-potential. Here, one can obtain a solution which is a p_x -wave orbital. This clearly does not respect rotational symmetry on its own. However, rotating the solution with $\pi/2$ produces a p_y -wave which is also a solution. In fact, rotating it with an arbitrary angle produces a linear combination of p -wave orbitals along different directions, and such a superposition is also a solution of the SE. Thus, analogous to the discussion of Δ above, Neumann's principle is still conserved even though one particular solution can break the symmetry of the Hamiltonian.

This paper <https://arxiv.org/abs/1102.1212> shows specifically that there exist multiple solution branches for Δ when a subject is placed in an external field. These branches can have a different number of vortices, even at a fixed flux. Dependent on which gauge $\mathbf{A}$ and initial guess for Δ that one chooses, the numerical self-consistent solver can end up in different branches.

See in particular section 6.1 and figure 5, as well as the beginning of section 6.2 and figure 7. There, μ is the field strength. The figures show the free energy for different solution branches of Δ , and the true ground-state will be the one that has the lowest free energy.

For a given flux of N elementary flux quanta, it thus seems possible to obtain stable solutions with a net vorticity $n \leq N$. It should be possible to nudge the numerical solver towards solutions with $n = N$ by giving the initial guess a vorticity of n . Note that one can also in principle find more exotic things like giant vortices or antivortices, which allow for a vortex pattern that respect the geometry of the sample itself, see <https://journals.aps.org/prl/pdf/10.1103/PhysRevLett.120.207001>. One can also think of what is the "physical property" of the lattice qualitatively in a way analogous

to the equation:

$$\mathbf{j} = \sigma \mathbf{E}. \quad (5.84)$$

Here, the magnetic field takes the role of $\mathbf{E}$ whereas the vortices takes the role of $\mathbf{j}$. The physical property of the lattice, which must respect the lattice symmetries, is the tensor which connects the field and the vortices. The vortex pattern, then, does not have to have the same symmetries as the lattice.

The same goes for the magnetic order parameter $\mathbf{m}$ in a ferromagnet. For instance, consider the striped phase with a textured antiferromagnetic-like magnetization on a square lattice. This magnetization direction realized in the ground-state is not invariant under the symmetry operations of the underlying square lattice. Thus, the magnetization spontaneously breaks the underlying symmetry of the lattice. The free energy, however, must be invariant if we apply a symmetry operation of the lattice to the magnetization: just imagine taking the material sample and turning it 90 degrees by hand, which will not change the free energy.

Note that the magnetic anisotropy produced by the lattice must still obey the lattice symmetries, since this is a tensor which can be probed by applying an external magnetic field: all physical response tensors of a lattice must respect the lattice symmetry.

Alternative explanation: Peierls transition

Incommensurate spin- or charge density wave phases break the translational symmetry of the lattice. Does this violate Neumann's principle? If we think of the realized density wave state as spontaneously breaking the symmetry of the lattice and that the actual magnetization pattern that is realized cannot be viewed as a physical property of the lattice itself, then there is no contradiction. However, an alternative explanation is as follows. The formation of CDW and SDW states can sometimes be associated with a change in the periodicity of the lattice itself, see *e.g.* Peierls transition. In Cr, the formation of an incommensurate SDW state coincides with a lattice strain wave, which means a periodic modulation of the lattice distance. Seen from this perspective, one might posit that if the formation of SDW and lattice distortions coincide. The mean-field result of incommensurate density waves should then, in a more accurate model, also produce a lattice distortion which removes the incommensurateness and thus restores the magnetic texture as compatible with the lattice discrete translational symmetry. A weakness with this argument is nevertheless the appearance of striped phases, as discussed above.

Chapter 6

Non-interacting fermions: holes, distribution functions and other key concepts

6.1 Hole excitations

Excitations can occur both as electrons or holes: absence of electrons. At $T = 0$, an excited electron should find its place outside the Fermi sphere whereas a hole (an unoccupied state) corresponds to removing an electron occur inside the sphere. In the latter case, it might appear at first glance that we are actually removing energy from the system. It is then unclear how this can be considered an excitation. The resolution lies in the fact that the remaining state with the vacant electron state is actually an excited state compared to the ground-state of the remaining electrons. The hole may be formally considered as a quasiparticle, and we here consider its properties more carefully.

A good place to start in terms of understanding how hole excitations behave is energy balance. The excitation energy of the system is:

$$E - E_0 = \sum_k E(k) f_k - \sum_{k < k_F} E(k), \quad (6.1)$$

where E_0 (the last term) is the energy of the system at $T = 0$ with all states below k_F being occupied. We have omitted the spin index in the argument above for simplicity. The quantities $E(k)$ and f_k represent the energies of electrons with momentum k and the distribution function (takes a value between 0 and 1, the probability that a state $E(k)$ will be occupied by an electron), respectively. We can rewrite this equation as

$$E - E_0 = \sum_{k > k_F} E(k) f_k - \sum_{k < k_F} E(k) (1 - f_k) = \sum_{k > k_F} \epsilon(k) f_k + \sum_{k < k_F} |\epsilon(k)| (1 - f_k), \quad (6.2)$$

where we have defined the relative excitation energy with regard to the Fermi level $\epsilon(k) = E(k) - E_F$. To get this equation, we made use of the fact that

$$\sum_k f_k = \sum_{k < k_F} 1 \quad (6.3)$$

due to conservation of particle number. Thus, the total excitation energy of the system can be written as the sum of the energies of all electrons and holes, these energies being defined as the

positive energy difference between the energy $E(k)$ of the particle and the Fermi energy.

Let us now explain why creating a hole, corresponding to removing an electron below the Fermi level, requires energy even though it actually looks like we are removing energy from the system. Consider first a normal metal at $T = 0$. The ground-state consists of all states up to k_F filled with electrons. Let us denote the total energy of this system as E_0 , as above. We now add an extra electron to the metal, which will occupy one of the states $k > k_F$ since the others are filled. The ground-state of the system with this extra electron is

$$E_g = E_0 + k_F^2/2m \quad (6.4)$$

since the lowest energy-state of the system with an extra electron would have been to put that electron at the Fermi level. To be very accurate, we would have to put it at $k = k_F^+$, but we assume that next available state is infinitesimally close to k_F so that we can set $k_F^+ = k_F$. Instead, with the electron put at $k > k_F$ the energy of the system is

$$E_{\text{syst}} = E_0 + k^2/2m. \quad (6.5)$$

The excitation energy of the system is now the difference in energy between the energy of the system and the ground-state of the system:

$$E_{\text{ex}} = E_{\text{syst}} - E_g = k^2/2m - E_F, \quad (6.6)$$

where $E_F = k_F^2/2m$. This energy increase is equal to the energy of the elementary excitation and the system's momentum will be k , namely the momentum of the elementary excitation. Thus, adding an electron at $k > k_F$ is a positive excitation with energy E_{ex} relative the ground-state.

Now we turn to the hole excitation case. Consider again the ground-state of the normal metal, but this time we remove an electron from $k < k_F$. The resulting state can also be treated as an elementary excitation, because its energy is greater than the ground-state energy of the *remaining* electrons. The energy of the system after removing the electron is

$$E_{\text{syst}} = E_0 - k^2/2m. \quad (6.7)$$

But the ground-state of the remaining electrons (after we have removed the electron at $k < k_F$) is:

$$E_g = E_0 - k_F^2/2m. \quad (6.8)$$

This can be understood by taking an electron at the Fermi level and putting it into the place of the missing electron in order to obtain the ground-state for the remaining electrons. Now, just like in the electron case, we obtain the excitation energy of the system by subtracting the ground-state energy from the system energy:

$$E_{\text{ex}} = E_{\text{syst}} - E_g = E_F - k^2/2m. \quad (6.9)$$

This is an energy increase (since $k < k_F$) and it is equal to the energy of the elementary hole excitation. The system's momentum will be $-k$ since we removed an electron, and $-k$ is then the momentum of the elementary hole excitation. Thus, removing an electron at $k < k_F$ is a positive excitation with energy E_{ex} relative the ground-state.

Note that the total crystal momentum $\sum_k k f_k$ is not a conserved quantity as one increases temperature in an out of equilibrium situation. Increasing temperature changes the distribution function and increases the total momentum of the gas. This can be understood from the fact that increasing temperature increases the kinetic energy of the particles in the system, corresponding to an increase in total momentum for a free electron gas. However, if $f_k = f_{-k}$, then the total crystal momentum is still zero.

Properties of holes

A hole is a quasiparticle representing a missing electron. Consider a normal metal. If the electron has mass m , momentum $\mathbf{k}$, charge $-e$, and spin σ , the hole has the following properties:

- Opposite mass, $-m$.
- Opposite momentum, $-\mathbf{k}$.
- Opposite spin, $-\sigma$.
- Opposite charge, $+e$.

An Andreev-reflected hole, which thus represents a missing spin- $\downarrow$ electron with momentum $-\mathbf{k}$, has momentum $\mathbf{k}$ (thus moving physically in the left direction) and spin- $\uparrow$. Note that the fact that the hole has the opposite momentum of the empty electron state is demanded by momentum conservation: either we can describe a missing electron at $\mathbf{k}$ by subtracting $+\mathbf{k}$ from the total crystal momentum or we can describe it by adding a hole particle with momentum $-\mathbf{k}$. In both cases, we get the same total crystal momentum.

What about the spin magnetic moment $\boldsymbol{\mu}$ of holes, which determines their Zeeman-energy in a magnetic field $\mathbf{B}$ via $E = -\boldsymbol{\mu} \cdot \mathbf{B}$? We know that the spin magnetic moment of a particle is given by

$$\boldsymbol{\mu} = g \frac{(-e)}{2m} \mathbf{S} \quad (6.10)$$

where g is the g -factor and $\mathbf{S}$ is the electron spin. Since the charge and the mass of the hole are opposite to an electron, a hole with spin $\mathbf{S}$ has the same spin magnetic moment as an electron with spin $\mathbf{S}$ and thus experiences the same Zeeman-energy.

6.2 Distribution function in the presence of voltage

6.2.1 Derivation of shift in Fermi-Dirac distribution function for holes

We know that the distribution function for an electron under equilibrium conditions is given by the Fermi-Dirac function:

$$f(\epsilon) = \frac{1}{1 + e^{\beta\epsilon}}, \quad (6.11)$$

where $\epsilon \equiv E - \mu$ is the energy of the electron measured relative the Fermi level. The probability to find an electron at energy ϵ is then given by $f(\epsilon)$. Now, since mathematically

$$f(\epsilon) = 1 - f(-\epsilon) \quad (6.12)$$

it follows that $f(-\epsilon)$ must be the probability that there is no electron at energy ϵ . Similarly, $f(\epsilon)$ is the probability to find that there is no electron at energy $-\epsilon$. It is clear that $f(\epsilon)$ is the distribution function for holes with energy ϵ (which means a missing electron at $-\epsilon$). For instance, if $\epsilon < 0$ it means that we are computing the probability to have a missing electron below the Fermi level. As discussed above, a hole below the Fermi level has positive energy $\epsilon > 0$.

Imagine that we now apply a voltage to the system which raises the entire electron band by $+eV$. The new distribution function for electrons with energy ϵ relative the old Fermi level μ then reads

$$f(\epsilon - eV) = \frac{1}{1 + e^{\beta(\epsilon - eV)}}. \quad (6.13)$$

In effect, this is the probability to find an electron with energy ϵ relative the reference level μ (which is still the Fermi level on the other side of the interface in a bilayer when a voltage is applied across the interface). Since the band has been raised, we see that the probability to find an electron at ϵ increases since the electron moves deeper inside the Fermi sea.

What about the distribution function for holes in the presence of a voltage? We have that $1 - f(\epsilon - eV)$ is the probability to find a missing electron at energy ϵ , so that

$$f(-\epsilon + eV) = 1 - f(\epsilon - eV) \quad (6.14)$$

must be the probability of finding a hole at that electron energy. But as we have stated above, the energy of a hole excitation corresponding to a missing electron at ϵ is $-\epsilon$ when the reference level is μ . A key point here is that this reference level does not change just because we apply a voltage. Therefore, the probability distribution for a hole with energy ϵ is $f(\epsilon + eV)$. This is what enters in the distribution function for holes in the BTK-treatment, for instance.

Let us check if this statement makes sense. For instance, imagine we want to find the probability to find a hole with energy $\epsilon = 0$. The probability for this has to be 1 minus the probability to find a missing electron with energy $\epsilon = 0$, so that the probability becomes:

$$1 - f(0 - eV) = 1 - (f - eV) = f(eV). \quad (6.15)$$

This makes perfect sense since the holes lies a distance eV under the local Fermi level $\mu + eV$ on the left side and thus the probability for it to exist at $\epsilon = 0$ is obtained by evaluating it as an excitation with energy eV .

If we want to compute the probability of finding a hole with energy $\epsilon > 0$ (again, relative the Fermi level on the right side), this is equal to 1 minus the probability to find a missing electron at $-\epsilon$. Therefore, the hole distribution is:

$$1 - f(-\epsilon - eV) = f(\epsilon + eV). \quad (6.16)$$

Note that even if the left side is raised by eV , we can still talk about the possibility of finding an electron with energy $\epsilon = 0$ because ϵ is well-defined: it is the energy relative μ , thus measured relative the Fermi level on the right side. That does not mean that the electron has energy $\epsilon = 0$ relative the local Fermi level on the left side (which has been altered due to the voltage), but that is ok since we have defined the energy reference level as μ (right side).

In the same way, we can speak about a hole with excitation energy ϵ relative μ . Again, that does not mean the hole has the same energy relative the local Fermi level on the left side, but this is still ok. As pointed out above, the fact that it does not have energy ϵ relative the left side local Fermi level is manifested by the fact that the probability to find *e.g.* an $\epsilon = 0$ hole is $f(eV)$, precisely because the $\epsilon = 0$ state is eV below the local left side fermi level (thus energy $+eV$).

We therefore conclude that when describing the distribution function for electron and hole excitations with energy ϵ , an applied voltage causes the net distribution function to be $f(\epsilon - eV)$ for electrons and $f(\epsilon + eV)$ for holes.

6.2.2 Relation to Ref. [34]

The above result is consistent with the statement in Ref. [34] that for e and h leads, the distribution functions are the same except that the sign of the voltage (or local chemical potential relative the reference level) is changed.

6.2.3 Relation to quasiclassical theory and distribution matrix

It is useful to also compare the above reasoning with the distribution function matrix $\hat{h}$ in the quasiclassical theory which is written as:

$$\hat{h} = \begin{pmatrix} \tanh[\beta(\epsilon - eV)/2] & 0 \\ 0 & \tanh[\beta(\epsilon + eV)/2] \end{pmatrix} \quad (6.17)$$

in Ref. [35]. This is consistent with the distribution function for holes that we derived above if:

$$\hat{h} = \begin{pmatrix} 1 - 2f_{\text{electron}} & 0 \\ 0 & 1 - 2f_{\text{hole}} \end{pmatrix} \quad (6.18)$$

which also agrees with the text below Eq. (7.3) in this book.

That the hole distribution is indeed obtained by swapping the sign of eV compared to the electron distribution is also consistent with *e.g.* eq. (26) in Phys. Rev. B **61**, 8125 (2000). If this is then correct, ϵ has to be interpreted as the excitation energy of the hole: it is positive if the hole corresponds to a missing electron below the Fermi level and it is negative otherwise.

It is also useful to check if this interpretation of what the ϵ -quantity means for holes is consistent with the quasiclassical expression for heat current. Write more ...

6.2.4 Distribution function modes and their kinetic equations

The distribution functions for electrons and holes can be used to construct new linear combinations which instead of expressing the distribution of electrons and holes express the distribution of charge, energy, and spin in the system.

In the spin-degenerate case, it is common to write

$$\hat{h} = f_L + f_T \hat{\tau}_3 \quad (6.19)$$

where f_L is the *energy mode* that determines the effective temperature in the system whereas f_T is the *charge mode* which arises in the presence of an effective chemical potential shift. Comparing Eqs. (6.18) and (6.19), we see that they are defined as:

$$\begin{aligned} f_T &= f_{\text{hole}} - f_{\text{electron}}, \\ f_L &= 1 - f_{\text{hole}} - f_{\text{electron}}. \end{aligned} \quad (6.20)$$

The charge mode f_T then measures the excess distribution of electrons or holes in the system at a given energy ϵ since holes and charges have opposite charge. A charge mode can be created by inducing an electric potential difference in the system [44] which causes an imbalance between electron and hole occupation probabilities for a given energy relative a fixed reference level. The charge mode is symmetric in energy ϵ .

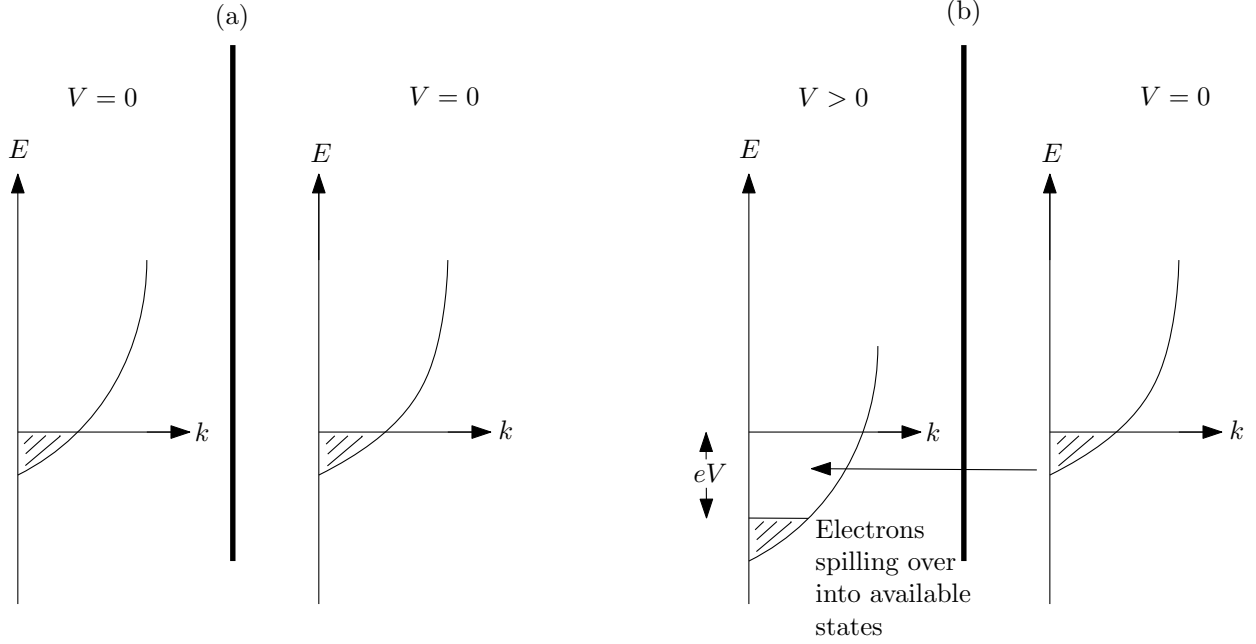
On the other hand, the energy mode f_L is a measure of the distribution of energy in the system. Note that such an energy mode exists even in equilibrium, since the existing particles in the system have a Fermi-Dirac distribution describing the occupation of energy levels ϵ . For instance, an electron in the filled Fermi sea that is excited to a state ϵ above the Fermi level leaves behind a hole below the Fermi level. Such a process contributes to changing the equilibrium energy mode. Such excitations can be obtained via temperature or radiation. If the electron is taken from a state that lies equally far below the Fermi level as the state the electron ends up in lies above the Fermi level, the charge-mode f_T in the system remains zero according to its definition. If the energy is not equally far below as above the Fermi level, a charge mode appears in addition to the energy mode. In both of these cases, the equilibrium energy mode changes from its equilibrium value $\tanh(\beta\epsilon/2)$. The energy mode is antisymmetric in energy ϵ . This can be seen from the fact that $f_{\text{hole}}(E) = 1 - f_{\text{electron}}(-E)$, regardless of what f_{electron} is (non-equilibrium or equilibrium). Inserted into f_L , it is immediately seen that it is antisymmetric in E .

To understand what the specific form $f_L = 1 - f_{\text{hole}} - f_{\text{electron}}$ at a given energy ϵ expresses, we first note that $f_{\text{hole}} + f_{\text{electron}}$ measures how likely it is that an energy excitation exists at energy ϵ , regardless of whether the excitation is of electron or hole type. If $f_L = 1$, the probability that an excitation exists at that energy is zero. The more f_L deviates from 1 (more specifically, the closer it becomes to -1), the stronger the probability that electron or hole excitations exist at an energy ϵ .

In a superconductor, the charge mode f_T usually decays quickly away from the interfaces over a distance comparable to the superconducting coherence length, but strictly speaking energy-dependent. In contrast, the energy mode f_L relaxes only due to inelastic processes. If such are neglected, f_L remains constant throughout the superconductor.

Spin-generalized versions of the above energy mode can be straight-forwardly obtained, and one may similarly define spin modes which arise in the presence of an effective spin accumulation. For the holes, one has to be careful with the meaning of the spin index. For instance, if you apply a voltage eV to the spin-up electron band, the distribution function matrix in quasiclassical theory takes the form

$$\begin{aligned} \hat{h} &= \text{diag}(1 - 2f_{e\uparrow}, 1 - 2f_{e\downarrow}, 1 - 2f_{h\uparrow}, 1 - 2f_{h\downarrow}) \\ &= \text{diag}\left(\tanh[\beta(E + eV_{\uparrow}/2)], \tanh(\beta E), \tanh[\beta(E - eV_{\uparrow}/2)], \tanh(\beta E)\right). \end{aligned} \quad (6.21)$$



The spin accumulation mode is given by $h_{\text{spin}} = \text{Tr}(\rho_3 \hat{\sigma}_3 \hat{h})/4$, meaning

$$h_{\text{spin}} \propto f_{e\uparrow} - f_{e\downarrow} - f_{h\uparrow} + f_{h\downarrow}. \quad (6.22)$$

From the above, we see that $f_{h,\uparrow}$ actually describes the occupation of missing electrons with spin $\uparrow$. Therefore, it represents spin- $\downarrow$ excitations. This is the reason for why $f_{h\uparrow}$ contributes with the opposite sign of $f_{e\uparrow}$ to the spin accumulation. The σ subscript on the hole occupation functions thus describe the spin of the corresponding missing electron, and the actual excitation has reversed spin.

6.2.5 Tunneling between normal metals and direction of current

Consider an N/N junction. No bias voltage is applied to the system. The situation then looks like Fig. 6.2.5(a). The energy bands are given by

$$E = k^2/2m - \mu \quad (6.23)$$

with energy measured from the electrochemical potential μ . The occupation of electrons is described by the Fermi-Dirac function

$$f(E) = \frac{1}{1 + e^{\beta E}} \quad (6.24)$$

and the highest occupied state lies at $E = 0$ at $T = 0$.

Now apply a positive voltage $V > 0$ to the left part of the system. We know that charged particles moving in a potential V has a potential energy qV where q is the charge of the particle. Therefore, the potential energy of the electrons on the left part of the system is $-eV$ where $e > 0$ since $q = -e$ is the electron charge. Their energy is modified to

$$E = k^2/2m - \mu - eV. \quad (6.25)$$

The voltage thus lowers the entire energy band. However, it does not change the number of electrons. This means that the highest occupied electron state, which previously was at $E = 0$, now must reside at $E = -eV$.

Which distribution function should we then use on the left side? The distribution function should correctly give the highest occupied state occurring at $E = -eV$, meaning that the argument of Fermi-Dirac has to vanish when $E = -eV$. This is satisfied by $f(E + eV)$.

This can also be viewed differently. The electrochemical potential is generally given by $qV + \mu$ where μ is the chemical potential, so for electrons it is $-eV + \mu$. The distribution function for the electrons without the voltage is then $f(k^2/2m - \mu)$, i.e. the energy minus the electrochemical potential. So the highest filled state has $k = \sqrt{2m\mu}$, as dictated by $k^2/2m - \mu = 0$. We now apply a voltage. Then, both the electrochemical potential and the energy of the particle changes. So we get $f(k^2/2m - eV - (\mu - eV)) = f(k^2/2m - \mu)$. We see that the distribution function is the same as without voltage! In effect, the highest occupied state still has $k = \sqrt{2m\mu}$. This is consistent with the above figure, where we have just displaced the entire band downwards without changing the number of electrons. Note that when we write the Fermi-Dirac distribution function on the left and right side of the junction in terms of a common energy reference level E , namely energy measured from μ , we must adjust the left hand side precisely according to $f(E + eV)$ since the electrochemical potential there lies a distance eV from μ .

Electrons can now spill over from the right N to the left N since there are available states in the energy window of size eV in the left N. This is consistent with electrons moving from low to high potential V . Moreover, such an electron flow means that a positive current is flowing from left to right.

Finally, note that if we wanted to actually increase the number of electrons on the left side of the system, and not merely shift the energy band, we would change only the electrochemical potential in the Fermi-Dirac distribution, so that we would obtain $f(k^2/2m - \mu - eV)$. Now, the highest occupied state would lie at momentum $k = \sqrt{2m(\mu + eV)}$, i.e. have a higher kinetic energy than before. This corresponds to keeping the bands on both sides identical, but just increasing the hatched area on the left side to indicate that more states are filled. This would also give rise to a current flow, but this time from left to right since the distribution function on the left side would be $f(E - eV)$.

6.3 Scattering wavefunctions and currents in hybrid structures: electron vs hole excitations

When describing currents of charge and spin in heterostructures, one can use a Landauer-Buttiker formalism with scattering wavefunctions (BTK formalism if superconductors are involved). Without superconductivity, it is not needed to include hole excitations and it is sufficient to use only electron wavefunctions. However, if we like, we should be able to describe transport using holes instead of electrons: it is just a mathematically different description (of missing electrons) which must give physically exactly the same result.

Consider then an N/N junction with identical normal metals. A voltage eV is applied so that the distribution function is $f(E - eV)$ and $f(E)$ on the left and right side, respectively. The electron

energy dispersion in a simple free electron model is

$$E = k^2/2m - \mu. \quad (6.26)$$

and thus runs from $-\mu$ to ∞ . The total current from left to right is

$$\int_{-\mu}^{\infty} j_e(E) f(E - eV) dE \quad (6.27)$$

where $j_e(E)$ is the expression for quantum mechanical current in the right normal metal obtained using the scattering (transmission) coefficient.

Similarly, the total current from right to left is:

$$- \int_{-\mu}^{\infty} j_e(E) f(E) dE \quad (6.28)$$

Note the overall minus sign (since tunneling is in the opposite direction) and that we use $f(E)$ now instead of $f(E - eV)$. The same expression for $j_e(E)$ is valid for right to left tunneling as left to right, since the metals are identical.

So, the total current in the junction is the left-right current minus the right-left current:

$$\int_{-\mu}^{\infty} j_e(E) [f(E - eV) - f(E)] dE \quad (6.29)$$

This is the standard expression (although the integral limits are usually taken as $-\infty$ to ∞ , although the minimum energy is $-\mu$): think of $j_e(E)$ as essentially the transmission coefficient $T(E)$.

Let's then instead say that we for some reason wanted to describe the electric current through the system using holes. The holes have energy dispersion

$$E = \mu - k^2/2m \quad (6.30)$$

so their energies run from $-\infty$ to μ for real (propagating) values of k . We can now set up expressions for current from left to right and right to left, with only a few changes compared to the above expressions. One is that we should use $j_h(E)$ instead. Looking at the wavefunctions, one finds the relation

$$j_h(E) = -j_e(-E) \quad (6.31)$$

This is reasonable since the holes have opposite energy compared to the electrons and since they carry opposite charge. The other change is that the distribution function for holes on the N side with voltage eV is $f(E + eV)$ instead of $f(E - eV)$ [which can be derived using that the hole distribution function at a given energy is equal to unity minus the distribution function for electrons at the negative of that energy].

We thus get the total current:

$$\int_{-\infty}^{\mu} j_h(E) [f(E + eV) - f(E)] dE \quad (6.32)$$

However, physically we should obtain exactly the same total current flowing regardless of if we choose to describe the problem with electron or hole excitations. Fortunately, this can be shown by using that $j_h(E) = -j_e(-E)$ and changing variable from $E \rightarrow (-x)$, which gives an identical expression as the current obtained using electrons.

So all is good. However, now comes an apparent problem. Consider an I/N junction where I is an insulator. There is no voltage applied. We can only have incoming particles from the N side toward the I side. There can be no electric current, but there can be a spin-current flowing if the insulator is magnetic and thus can provide spin-flip scattering. Consider then the spin current in the junction obtained using electrons as our excitations. We get

$$\int_{-\mu}^{\infty} j_{S,e}(E) f(E) dE \quad (6.33)$$

where $j_{S,e}(E)$ is the quantum mechanical expression for spin current obtained using the wavefunctions and scattering coefficients. Now we can use holes instead of electrons and expect to get exactly the same physical spin current. In that case, we get

$$\int_{-\infty}^{\mu} j_{S,h}(E) f(E) dE \quad (6.34)$$

One verifies, similarly to the charge current case, that the relation $j_{S,h}(E) = -j_{S,e}(-E)$ holds. Inserting this and changing variable from $E \rightarrow (-x)$, I would have hoped to get the same expression for the spin current (since it shouldn't matter if I use electrons or holes). But instead, I get

$$\int_{-\mu}^{\infty} j_{S,e}(E) f(E) dE - \int_{-\mu}^{\infty} j_{S,e}(E) dE \quad (6.35)$$

The first term is exactly the same expression as the spin-current obtained using electrons. But there is a second term which is non-zero. The presence of this term makes the spin-current different, depending on whether I choose electrons or holes to describe the transport. This must be unphysical.

Density of state effects have been ignored here by considering 2D (so that the free electron/hole DOS is constant, independent of energy). The problem seems to be that we only have particles incoming from one side now, which prevents the electron and hole expressions for the total spin current to become equal. This problem is present to begin with also in the example shown initially for the charge current: in effect, if we only the left-to-right current, the expression depends on whether we consider incoming electrons or incoming holes. But the problem is resolved when computing the total current, thus including the right-to-left current, making the expressions identical.

The solution: the reason for the discrepancy is that we have neglected a background contribution to the spin current when using the hole description. The fact that such a background contribution exists can be seen by noting that when going from an electron Hamiltonian $H = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}$ to a hole Hamiltonian, one using anticommutation $c^\dagger c = 1 - cc^\dagger$. The latter term describes the hole excitations and is used to construct the hole wavefunctions. The constant term 1 has no impact on the hole wavefunctions and is usually disregarded. But the solution lies in considering this 1 term seriously. Namely, it mathematically gives rise to a constant term $\sum_{k\sigma} \epsilon_{k\sigma}$ in H which has clear physical meaning: all electron energy levels are filled as a background term. This means that to describe the current in the I/N case using hole excitations, one cannot only consider incoming hole wavefunctions, but the contribution to the spin current from the background term corresponding to all electron levels being filled must also be accounted for. This corresponds precisely to a current

term $+\int_{-\mu}^{\infty} j_S, e(E) dE$, without any distribution function since all levels are filled, and this term cancels exactly the difference between the currents in the electron and hole description above.

To exaggerate the picture: say you would have a chemical potential below the band edge (i.e. completely empty band), then there are no particles trying to squeeze their spin into the insulator. In the hole picture, the band is then suddenly completely filled with particles that talk to the insulator, which is unphysical. That is indeed taken care of by that 1 that pops out from the transformation.

6.4 Spin-battery and spin-energy battery

We here discuss how it is possible to generate spin-modes and spin-energy modes out of equilibrium in magnetic heterostructures. First, it is instructive to consider a voltage-biased normal metal and look at how the charge and energy distribution modes behave there. We disregard for simplicity inelastic processes such as $e-e$ scattering here. We have two reservoirs coupled to a normal metal at its left and right interface. When the reservoirs have a voltage $+V$ and $-V$, respectively, the distribution matrices read

$$\hat{h}_{L,R} = \begin{pmatrix} T_{\mp} & 0 & 0 & 0 \\ 0 & T_{\mp} & 0 & 0 \\ 0 & 0 & T_{\pm} & 0 \\ 0 & 0 & 0 & T_{\pm} \end{pmatrix} \quad (6.36)$$

where we defined $T_{\pm} = \tanh[\beta(E \mp eV)/2]$. We know that the charge mode is obtained by $\text{Tr}(\rho_3 \hat{h})/4 = (T_{\mp} - T_{\pm})/2 \equiv h_4$ while the energy mode is $\text{Tr}(\hat{h})/4 = (T_{\mp} + T_{\pm})/2 \equiv h_0$. The kinetic equation governing the spatial evolution of these modes in the normal metal reads (in the absence of inelastic processes):

$$\partial_x^2 h_{0,4} = 0. \quad (6.37)$$

The solution reads $h_j = A_j x + B_j$ where A_j and B_j are constants. Let the normal metal have a length L and interfaces at $x = -L/2$ and $x = L/2$. Assuming for simplicity continuous boundary conditions, we have at $x = -L/2$ the boundary conditions

$$h_0 = (T_- + T_+)/2, \quad h_3 = (T_- - T_+)/2. \quad (6.38)$$

At $x = L/2$, we have the boundary conditions

$$h_0 = (T_+ + T_-)/2, \quad h_3 = (T_+ - T_-)/2. \quad (6.39)$$

It is clear that the solutions for h_j then give a constant energy mode over the entire normal region ($A_0 = 0$) in order to satisfy the boundary conditions and an antisymmetric and linear charge mode over the normal region ($B_4 = 0$). In the middle of the structure, $x = 0$, it follows that only an energy mode is present and no charge mode.

With this in mind, we now discuss a structure known as a *spin-battery*. This structure is used to electrically create a spin-accumulation (spin-mode) without any belonging charge-mode: thus a source of pure spin diffusion. The way to accomplish this is to make the reservoirs ferromagnetic. Let us for simplicity consider half-metallic ferromagnets so that only one spin-band is conducting. The main result in the argument below, namely that a spin-mode exists in the middle of the junction without any accompanying charge-mode holds even in the non-halfmetallic case. We consider now

an F/N/F junction with voltage $\pm V$ on left and right reservoir as before and let both magnets point in opposite directions. We write this as F($\uparrow$)/N/F($\downarrow$).

The spin and spin-energy modes are given as $h_7 = \text{Tr}(\rho_3 \hat{\sigma}_3 \hat{h})/4$ and $h_3 = \text{Tr}(\hat{\sigma}_3 \hat{h})/4$. They satisfy the same kinetic equations as $h_{0,3}$ did in the normal metal when inelastic scattering and spin-flip scattering processes are neglected. The distribution functions at the left and right interfaces are now

$$h_L = \text{diag}(T_-, 0, T_+, 0), h_R = \text{diag}(0, T_+, 0, T_-). \quad (6.40)$$

Using continuous boundary conditions again, we find that the spin-mode is constant throughout the junction and the spin-energy mode varies linearly with position, thus being absent at $x = 0$. Interestingly, by aligning the ferromagnets to create a F($\uparrow$)/N/F($\uparrow$) junction we create a *spin-energy* battery. The distribution functions in the reservoirs now take the form

$$h_L = \text{diag}(T_-, 0, T_+, 0), h_R = \text{diag}(T_+, 0, T_-, 0). \quad (6.41)$$

The same line of reasoning gives a spin-energy mode constant throughout N whereas the spin-mode is antisymmetric and vanishes in the middle at $x = 0$, thus leaving a pure spin-energy mode at the center.

6.4.1 Inequivalence between half-metallic reservoirs and normal reservoirs with fully polarized barrier

The spin-battery setup described above also works if we replace the half-metals with normal metals and fully polarized interfaces in an AP alignment (see Eschrig boundary conditions). In that case, we find a constant energy and spin mode in the normal metal. There is no charge mode anywhere, since neither spin up or spin down can pass through both interfaces. Thus the charge current is zero.

If the interfaces are partially polarized, then in the middle there is still only an energy and spin mode since the charge mode vanishes in the middle.

However, the spin-energy battery described above is *not equivalent* to a N/N/N structure with fully polarized interfaces in a P alignment. One finds a constant energy mode and antisymmetric charge and spin modes (vanishing in the middle of the junction). Thus, it acts in the same way as the half-metallic case except that the spin-energy mode is zero! It is worth remarking that to obtain this result, one actually has to include spin-flip scattering in the kinetic equations and then take the limit $\tau_{\text{sf}} \rightarrow \infty$. If one does not include spin-flip scattering, a non-unique solution is found of the form $h_0 = H_0 - C$ and $h_3 = C$ where H_0 is the energy mode in the N reservoirs and C is an undetermined constant.

The fact that the half-metallic case and normal case with $P = 1$ interfaces are inequivalent is surprising at first glance. Although the energy, charge, and spin modes behave qualitatively the same in the two models, the *spin-energy mode* does not: it is always absent in the normal case with $P = 1$ interfaces. The reason for this is that in our model for the half-metallic reservoir, a finite spin-energy mode exists in the reservoir itself. In our model with N/N/N, the distribution function matrix in the N reservoirs, where both spin bands exist, does not have any spin-energy mode. However, we'll now show how we can get a spin-energy mode without accompanying spin-mode in a normal metal by using ferromagnetic reservoirs instead of normal reservoirs.

6.4.2 How to get pure spin-energy mode in middle of a normal metal without any accompanying spin- or charge-mode

We consider an FNF junction with weakly polarized ferromagnets. Such F's can be described quasiclassically, assuming that the exchange field is much smaller than the Fermi level. We should thus be allowed to consider polarizations of the ferromagnets of up to say 15% ($P = 0.15$).

Note that this is different from considering NNN with polarized interfaces, in effect really N/FI/N/FI/N, where P can be arbitrary even with quasiclassical formalism due to Eschrig's boundary conditions. If we now instead consider FNF, then P comes from the splitting of the spin bands in the ferromagnets and must be weak according to the quasiclassical criterion.

It is important that we consider FNF rather than N/FI/N/FI/N, which we tried above, for the following reason. When an electric current flows through a ferromagnet, it becomes spin-polarized. There are more spin-up carriers than spin-down. When a current flows through an FN junction, it therefore goes from being spin-polarized in the bulk of F to being unpolarized in the bulk of N. But the polarization does not vanish abruptly as soon as the current enters N. Instead, the polarization decays over the spin relaxation length in N, which is dictated by *e.g.* magnetic impurities. Therefore, the spin-polarization of the current must persist for a short while inside N. This occurs via the concept of spin accumulation, illustrated in the figure below (taken from <https://physics.aps.org/articles/v8/83>).

The polarization is made possible by a non-equilibrium shift of the chemical potentials of $\mu_\uparrow$ and $\mu_\downarrow$. This shift also exists close to the interface on the ferromagnetic side, as seen from the figure. In the picture, the chemical potentials for each spin are continuous at the boundary if one neglects interface resistance. If interface resistance is included, however, the chemical potentials μ_σ are not continuous. In that case, there is a net jump $\Delta\mu$ in the average chemical potential, as shown in the figure below. In the F and N, respectively, the average chemical potential μ drops linearly according to Ohm's law (dotted line).

Here is the key observation: the proper distribution function matrix $\hat{h}$ that should be used on the F side does not only have an electric voltage, but also a *spin voltage* due to the spin accumulation. This is clear since $\mu_\uparrow \neq \mu_\downarrow$ on the F side.

We will see that it is this fact, which we have not taken into account in the simulations, which provides our constant spin-energy mode in the N region. Fortunately, it is easy to include since the only change that has to be made is to change the distribution function matrices (see below).

Analytical solution of kinetic equations for weakly polarized FNF

We consider an electric voltage applied across an $F_L/N/F_R$ structure. According to the above description, the distribution function matrix in F_L should have both a voltage and spin-voltage near the F_L/N interface. In general, we have

$$\hat{h} = \begin{pmatrix} \tanh[\beta(E + eV_\uparrow)/2] & 0 & 0 & 0 \\ 0 & \tanh[\beta(E + eV_\downarrow)/2] & 0 & 0 \\ 0 & 0 & \tanh[\beta(E - eV_\uparrow)/2] & 0 \\ 0 & 0 & 0 & \tanh[\beta(E - eV_\downarrow)/2] \end{pmatrix} \quad (6.42)$$

Let us introduce electric voltage $V = (V_{\uparrow} + V_{\downarrow})/2$ and spin-voltage $V_s = (V_{\uparrow} - V_{\downarrow})/2$. Introducing the notation

$$T_{\alpha\beta} = \tanh[\beta(E + \alpha eV + \beta eV_s)/2], \quad \alpha, \beta = \pm 1, \quad (6.43)$$

we can then write for the left reservoir:

$$\hat{h}_L = \text{diag}(T_{++}, T_{+-}, T_{--}, T_{-+}). \quad (6.44)$$

For the right reservoir, we have the opposite electric voltage: $V \rightarrow (-V)$. This means we have to let $V_{\uparrow} \rightarrow -V_{\uparrow}$ and $V_{\downarrow} \rightarrow -V_{\downarrow}$. As a consequence, we must also let $V_s \rightarrow -V_s$ at the right reservoir. Therefore, the distribution function matrix takes the form

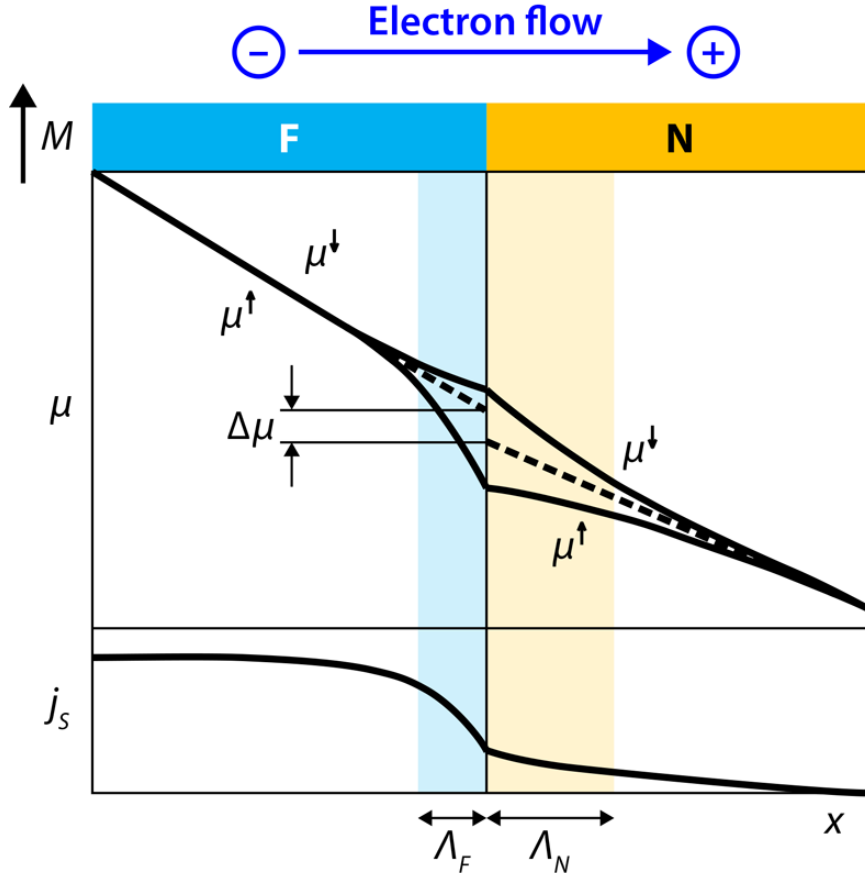
$$\hat{h}_R = \text{diag}(T_{--}, T_{-+}, T_{++}, T_{+-}) \quad (6.45)$$

there. Let us write the distribution function matrix in the normal metal as follows

$$\hat{h} = \text{diag}(h_1, h_2, h_3, h_4). \quad (6.46)$$

Here, h_3 does therefore not mean the spin-energy mode: it is the 33 element of the matrix. Instead, we have

$$\begin{aligned} h_{\text{energy}} &= (h_1 + h_2 + h_3 + h_4)/4, \\ h_{\text{spin-energy}} &= (h_1 - h_2 + h_3 - h_4)/4, \\ h_{\text{charge}} &= (h_1 + h_2 - h_3 - h_4)/4, \\ h_{\text{spin}} &= (h_1 - h_2 - h_3 + h_4)/4. \end{aligned} \quad (6.47)$$



Now, we just need the boundary conditions at the interfaces. These are obtained from the KL boundary conditions. We can take into account a weak polarization P to account for different transmission probabilities due to the spin-splitting of the bands in the ferromagnets.

The boundary conditions at the left interface ($x = -L$)

$$\check{g}\partial_x\check{g} = (G_0\check{1} + 2G_1\check{M}_L + G_{MR}\check{1})[\check{g}_L, \check{g}], \quad (6.48)$$

and at the right interface ($x = L$):

$$\check{g}\partial_x\check{g} = -(G_0\check{1} + 2G_1\check{M}_R + G_{MR}\check{1})[\check{g}_R, \check{g}], \quad (6.49)$$

The normal metal has a total length $2L$. The quantities G_0, G_1, G_{MR} depend on P . The Green function in N is $\check{g}$. The matrices $\check{M}_{L,R} = \text{diag}(\mathbf{m}_{L,R} \cdot \hat{\boldsymbol{\sigma}}, \mathbf{m}_{L,R} \cdot \hat{\boldsymbol{\sigma}})$ and $\hat{\boldsymbol{\sigma}} = \text{diag}(\boldsymbol{\sigma}, \boldsymbol{\sigma}^*)$. In the parallel configuration, which we are concerned with here, $\vec{m}_L = \vec{m}_R$.

Writing out the boundary conditions in terms of the distribution function matrix $\hat{h}$, we get at the left interface

$$\partial_x\hat{h} = (G_0 + G_{MR} + 2G_1\mathbf{m}_L \cdot \hat{\boldsymbol{\sigma}})(\hat{h} - \hat{h}_L), \quad (6.50)$$

while

$$\partial_x\hat{h} = (G_0 + G_{MR} + 2G_1\mathbf{m}_R \cdot \hat{\boldsymbol{\sigma}})(\hat{h}_R - \hat{h}) \quad (6.51)$$

at the right interface. Let $G_{\pm} \equiv G_0 + G_{MR} \pm 2G_1$. The equations of motion for the elements of $\hat{h}$ are

$$\partial_x^2 h_i = 0 \rightarrow h_i = A_i x + B_i. \quad (6.52)$$

The boundary conditions can then be written in matrix form:

$$M\mathbf{x} = \mathbf{V} \quad (6.53)$$

where I defined

$$\mathbf{x} = (A_0, B_0, A_1, B_1, \dots)^T, \quad \mathbf{V} = (G_+T_{++}, G_-T_{+-}, G_+T_{--}, G_-T_{-+}, -G_+T_{--}, -G_-T_{-+}, -G_+T_{++}, -G_-T_{+-})^T \quad (6.54)$$

and the matrix

$$M = \begin{pmatrix} -1 - G_+L & G_+ & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 - G_-L & G_- & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 - G_+L & G_+ & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 - G_-L & G_- \\ -1 - G_+L & -G_+ & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 - G_-L & -G_- & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 - G_+L & -G_+ & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 - G_-L & -G_- \end{pmatrix}. \quad (6.55)$$

Solving this system of equation in Maple, I get the following solutions for the various modes

$$\begin{aligned}
 h_{\text{energy}} &= \sum_{\alpha\beta} T_{\alpha\beta}, \\
 , h_{\text{spin-energy}} &= \sum_{\alpha\beta} \alpha\beta T_{\alpha\beta}, \\
 h_{\text{charge}} &= xF_1(L, G_{\pm}, T_{\alpha\beta}), \\
 h_{\text{spin}} &= xF_2(L, G_{\pm}, T_{\alpha\beta}).
 \end{aligned} \tag{6.56}$$

The charge and spin modes are antisymmetric and vanish in the middle $x = 0$. Their slope in real space is determined by the functions F_1 and F_2 (their exact expression isn't relevant here, although it is straightforward to obtain from solving the above system of equations).

The energy and spin-energy modes are constant and exist in the middle $x = 0$. Note that the $h_{\text{spin-energy}} \neq 0$ so long as a spin-voltage is included in the F reservoirs.

The spin-energy and energy modes are both antisymmetric in energy E and thus vanish at $E = 0$. But they are in general finite for $E \neq 0$ and both exist in the middle of the junction.

In other words: including a spin-voltage in the reservoirs $\hat{h}_{L,R}$, which we can justify physically, can provide a pure spin-energy mode in the center of the normal metal. Coupling this with a supercurrent can then give a supercurrent-induced spin accumulation, since a spin mode is induced from a spin-energy mode in the presence of a spectral supercurrent (see JP Morten thesis).

A relevant question is if V_s is just another input parameter or if it can be related to the applied electric voltage and polarization of the ferromagnet. In general, it should be, since the spin accumulation, and thus V_s , vanish if there is no electric voltage or if the ferromagnet is not polarized (i.e. a normal metal). So even though the analytical expression for $h_{\text{spin-energy}}$ does not depend on P explicitly, it does so implicitly through its dependence on V_s . It is possible to analytically estimate how $eV_s = \mu_{\uparrow} - \mu_{\downarrow}$ at an FN interface depends on P and the applied electric voltage eV .

6.4.3 Microscopic mechanism for thermal-gradient induced charge accumulation in a superconductor

Insert a picture here of the quasiparticle band structures including the Doppler-shift due to a supercurrent, and show how charge accumulates when a temperature-gradient ∇T is applied (see review by Heikkilä et al.).

6.5 Distribution function for quasiparticles in second quantization

6.5.1 Fermions

Consider a Hamiltonian H which we have diagonalized to yield

$$H = H_0 + \sum_{\mathbf{k}} E_{\mathbf{k}} \gamma_{\mathbf{k}}^{\dagger} \gamma_{\mathbf{k}}. \tag{6.57}$$

This is *e.g.* the case for a mean-field superconductor here $\gamma_{\mathbf{k}}$ are linear combinations of electrons and holes. The fact that the above Hamiltonian has a free electron gas form means that

$$\langle \gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} \rangle = f(E_{\mathbf{k}}) \quad (6.58)$$

which we now prove. We assume that the chemical potential μ was already included in the original Hamiltonian and is thus part of $E_{\mathbf{k}}$. In the above example, we would have had $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta|^2}$. Thus, we are dealing with a grand canonical ensemble [fixed (T, V, μ)] and the grand canonical partition function is

$$Z = \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle \quad (6.59)$$

where $\sum_n$ is a sum over all eigenstates of $\hat{H}$. Note that $|n\rangle$ is in general a many-particle state so that $\{n\}$ represents a set of indices. This is commonly written as $Z = \text{Tr}\{e^{-\beta \hat{H}}\}$ in the literature, where the trace then should be understood as taking the expectation value of the operator $e^{-\beta \hat{H}}$ in the state $|n\rangle$ and then performing a summation over all n .

We again underline that the above is consistent with the standard definition $Z = \sum_n \langle n | \{e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle$ since our $\hat{H}$ already includes the subtraction of the chemical potential term. The actual derivation of the above formula can be done following similar arguments as in classical statistical mechanics, but with the density matrix $e^{-\beta E_n}/Z$ taking the role of the probability p_n for different microstates in classical statistical mechanics.

More specifically, we can have that:

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}. \quad (6.60)$$

This expression can be understood as follows. A quantum system in a pure state can be described by a single state $|\psi\rangle$, which in turn can be expanded in terms of the eigenstates $|n\rangle$ of the Hamilton-operator $\hat{H}$. The corresponding density matrix operator is as usual

$$\hat{\rho} = |\psi\rangle\langle\psi|. \quad (6.61)$$

This density matrix now provides us with a convenient way to extend our considerations to finite temperature where we expect the system to be described by a statistical mixture of states due to thermal fluctuations. By following the principles of statistical mechanics, we put our system in contact with a heat bath and assign probabilities (weight-factors) p_n for each of the eigenstates $|n\rangle$, leading to a thermal density operator:

$$\hat{\rho} = \sum_n p_n |n\rangle\langle n|. \quad (6.62)$$

At a temperature T , the probabilities are given by the Boltzmann factor $p_n = e^{-\beta E_n}/Z$ with $\beta = 1/k_B T$. Thus, the density operator now reads

$$\hat{\rho} = \frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle\langle n| = \frac{e^{-\beta \hat{H}}}{Z}. \quad (6.63)$$

The last equality is verified by multiplying with $|m\rangle$ from the right side.

The density matrix in the representation with Hamilton-operator energy eigenstates as basis vectors takes the form:

$$\rho_{nn'} = \langle n | \hat{\rho} | n' \rangle. \quad (6.64)$$

The probability (statistical weight-factor) for a particular state $|n\rangle$ being occupied at a given temperature is given by

$$p_n = e^{-\beta E_n} / Z \quad (6.65)$$

which is seen to satisfy $\sum_n p_n = 1$, as it should. The expectation value of an operator $\hat{A}$ is obtained as

$$\langle \hat{A} \rangle = \frac{1}{Z} \sum_{nn'} \langle n | \hat{A} | n' \rangle \langle n' | e^{-\beta \hat{H}} | n \rangle = \frac{1}{Z} \text{Tr}\{A\rho\}. \quad (6.66)$$

With the above definition of Z , we obtain:

$$\begin{aligned} Z &= \sum_{n_1, n_2, \dots, n_\infty} \langle n_1, n_2, \dots, n_\infty | e^{-\beta H} | n_1, n_2, \dots, n_\infty \rangle \\ &= \sum_{n_1, n_2, \dots, n_\infty} \langle n_1, n_2, \dots, n_\infty | e^{-\beta \sum_i E_i n_i} | n_1, n_2, \dots, n_\infty \rangle. \end{aligned} \quad (6.67)$$

Here, the index i labels the allowed $\mathbf{k}$ -values and $n_\infty \equiv n_{\mathbf{k}_{\max}}$ where $\mathbf{k}_{\max}$ is the last value of the allowed $\mathbf{k}$. For fermions, n_i takes the value 0 or 1 due to the Pauli principle. Since many-fermion states in the occupation number representation (Fock basis) is a product:

$$|n_1, n_2, \dots, n_\infty\rangle = |n_1\rangle |n_2\rangle \dots |n_\infty\rangle, \quad (6.68)$$

we can factorize

$$Z = \left(\sum_{n_1} e^{-\beta E_1 n_1} \right) \left(\sum_{n_2} e^{-\beta E_2 n_2} \right) \dots \quad (6.69)$$

and we obtain the final result

$$Z = \prod_{i=1}^{\infty} (1 + e^{-\beta E_i}). \quad (6.70)$$

The free energy $F = -\frac{1}{\beta} \ln(Z)$ is then obtained by

$$F = -\frac{1}{\beta} \sum_i \ln(1 + e^{-\beta E_i}). \quad (6.71)$$

Relation Helmholtz free energy and grand potential

We underline here that although the terminology *free energy* is often used in the literature for the above quantity when Z is the grand canonical partition function, it is really the *grand potential* of the system. Just like the Helmholtz free energy is the appropriate thermodynamic free energy to minimize in order to obtain the ground state for a canonical ensemble [fixed (T, V, N)], the minimized

grand potential determines the ground state for the grand canonical ensemble [fixed (T, V, μ)]. The reason for why the grand potential is sometimes referred to as the free energy is that some authors use the terminology *Landau free energy* for the grand potential. The relation between the grand potential F (more commonly denoted Φ) and the Helmholtz free energy F_H , which are arguably the two most important thermodynamical potentials in statistical mechanics for condensed matter systems, is

$$F = F_H - \mu N. \quad (6.72)$$

A specific example of this can be found in Phys. Rev. B 98, 024521 (2018) where the authors state that a term μN must be added to the free energy they minimize to find the ground state of the system when the particle number (filling fraction of the system) is fixed. Namely, for an isolated system with fixed T and V , the Helmholtz free energy F_H is minimized in equilibrium. Since the system is isolated, the particle number N is fixed. Therefore, $F_H = F_H(T, V, N)$.

On the other hand, for an open system with fixed T and V , the particle number N can change. Instead, the system is now characterized by the chemical potential μ which gives us information about how much energy it costs to change the particle number. For such a system, the grand potential F described above is minimized in equilibrium. In this case, chemical potential is fixed rather than particle number, so $F = F(T, V, \mu)$.

This is explained in section 10.1 and 10.2 here: https://itp.uni-frankfurt.de/~gros/Vorlesungen/TD/10_Grand_canonical_ensemble.pdf

See also eqs 8-11 and chapter 7 here: https://schwartz.scholars.harvard.edu/sites/g/files/omnuum7046/files/schwartz/files/8-freeenergy_0.pdf

In the Hamiltonian of the above PRB, the authors have subtracted μ in the single-particle dispersion energy. Therefore, the free energy that we compute from the partition function based on this Hamiltonian is the grand potential F . As shown in the above notes, the relation between F and F_H is

$$F = F_H - \mu N. \quad (6.73)$$

Therefore, if we want to consider a system with fixed particle number N , we have to minimize F_H . We see that

$$F_H = F + \mu N. \quad (6.74)$$

This is exactly the formula in the PRB.

Gibbs free energy

Let us in passing also briefly comment on the importance of the Gibbs free energy. Whereas the Helmholtz free energy and grand potential minimize the equilibrium state when the volume and temperature are fixed, we have to use the Gibbs free energy when the pressure and temperature are fixed. This occurs precisely when we apply an external force (in effect, pressure) to the system, like we do when we apply an external magnetic field (Lorentz force). Therefore, one has to use

the Gibbs free energy in a system where the external magnetic field $\mathbf{H}$ is the independent variable (applied field) whereas the Helmholtz free energy is used to minimize the energy in a system where the total magnetic field $\mathbf{B}$ is the independent variable.

Thus, to find the preferred state of the system in equilibrium in the presence of a magnetic field, it is the Gibbs free energy that should be minimized. It is obtained as

$$G(p, T) = F + pV \quad (6.75)$$

in contrast to the Helmholtz free energy

$$F(V, T) = -\frac{1}{\beta} \ln Z, \\ Z[p] = \text{Tr}\{e^{-\beta H}\}. \quad (6.76)$$

In the case of a magnetic field dependence, one has instead the Gibbs free energy (density) $G/V = F/V - BM$.

We can now evaluate the average fermion number, i.e. $\langle \gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} \rangle$, by using that any operator $\hat{O}$ has expectation value

$$\langle \hat{O} \rangle = \text{Tr}(\rho O) \quad (6.77)$$

as stated above. The expectation value for the operator $\hat{O} = \gamma_s^\dagger \gamma_s$, where s is one of the allowed $\mathbf{k}$ -values, is then:

$$\langle \gamma_s^\dagger \gamma_s \rangle = \frac{\left(\sum_{n_1} e^{-\beta E_1 n_1} \right) \left(\sum_{n_2} e^{-\beta E_2 n_2} \right) \dots \left(\sum_{n_s} n_s e^{-\beta E_s n_s} \right) \dots}{\prod_{i=1}^{\infty} (1 + e^{-\beta E_i})}. \quad (6.78)$$

All factors in the nominator and denominator cancel except for the term with n_s , and thus we get:

$$\langle \gamma_s^\dagger \gamma_s \rangle = \frac{e^{-\beta E_s}}{1 + e^{-\beta E_s}} = \frac{1}{1 + e^{\beta E_s}} \equiv n_F(E_s) \quad (6.79)$$

where n_F is the Fermi-Dirac distribution function.

The internal energy of the system is obtained as $U = \langle H \rangle = -\partial \ln(Z) / \partial \beta$, as can be shown straightforwardly. However, the actual ground-state of the system will be the one that minimizes the free energy F and not the internal energy U , since at finite temperatures there is a competing entropy term $-TS$, namely $F = U - TS$.

Actually, there exists a very general formula which will help us identify the effective field entering the LLG equation later on. Assume our $\hat{H}$ depends on a parameter h . It does not have to be a magnetic field, but can be any scalar parameter. We then have

$$\begin{aligned} \left\langle \frac{\partial \hat{H}}{\partial h} \right\rangle &= \frac{1}{Z} \text{Tr} \left\{ \frac{\partial \hat{H}}{\partial h} e^{-\beta \hat{H}} \right\} \\ &= -\frac{1}{\beta Z} \frac{\partial}{\partial h} \text{Tr} \{ e^{-\beta \hat{H}} \} \\ &= \frac{\partial}{\partial h} \left(-\frac{1}{\beta} \ln(Z) \right). \end{aligned} \quad (6.80)$$

Thus, we see that

$$\left\langle \frac{\partial \hat{H}}{\partial h} \right\rangle = \frac{\partial F}{\partial h}. \quad (6.81)$$

Note that the differential operator and taking the expectation value do not commute:

$$\left\langle \frac{\partial \hat{H}}{\partial h} \right\rangle \neq \frac{\partial}{\partial h} \langle \hat{H} \rangle \quad (6.82)$$

This can be directly verified using a free electron gas in a Zeeman-field, $\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$ with $\epsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} - \sigma h$.

6.5.2 Minimize free energy at finite temperature?

The free energy is generally given by $F = U - TS$ and can also be computed from the partition function Z of the system via $F = -\frac{1}{\beta} \ln(Z)$. The partition function is in turn given as a sum or integral over all possible states of the system weighted by their Boltzmann factor.

Consider a system of two interacting spins. At $T = 0$, the ground-state is found by minimizing the free energy. This is only the internal energy at zero temperature. In a Heisenberg model, one finds either P or AP spins depending on the sign of the prefactor.

At finite temperature, one could attempt the same procedure. However, there is seemingly a problem. The partition function is no longer dependent on the spin configuration of the system, in contrast to the internal energy U at $T = 0$. This is because upon increasing the temperature, the probability for the system to be in any spin configuration $\{\mathbf{S}_i\}$ is given by the Boltzmann factor $e^{-\beta \mathcal{H}_{\text{eff}}(\{\mathbf{S}_i\})}/Z$, and we are supposed to perform a summation over all possible spin configurations. Therefore, at a finite temperature that exceeds the magnitude of the highest excited state of the Hamiltonian, all spin configurations are sampled in the partition function in the sense that they have a significant probability to occur. The more separated the $T = 0$ ground-state energy is from higher excited states, the more robust the ground state spin configuration against thermal fluctuations. In effect, at finite temperature we cannot speak of the system being in one particular state with a given spin configuration.

But this seems different from the usual procedure at finite temperature when identifying the thermodynamically preferred state of a superconductor. In that case, one minimizes the free energy with respect to the order parameter Δ . We do not speak about the system being in all possible states with all possible values of Δ . The point is that we have now performed a mean-field approximation. If we do not perform such a mean-field approximation, i.e. an exact approach, the partition function is independent on Δ just like it was independent on the spin configuration in the previous example. In the mean-field approximation, however, the partition function is given by the action S at a *single value* as the only contributor to the integral over the order parameter configurations:

$$Z_{\text{mf}} = e^{-S_{\text{mf}}(\Delta_{\text{mf}}^\dagger, \Delta)}. \quad (6.83)$$

In this case, there is still one particular state that minimizes the free energy at finite temperature, namely the particular value of Δ which causes the action to be stationary: $\partial S_{\text{mf}}/\partial \Delta = 0$.

In summary, in a mean-field treatment there is one particular value of the order parameter, and thus one particular state, that is realized even at finite temperature. This stems from the approximation

that the partition function is no longer a sum over all possible states with a probability factor. Instead, Z is assumed to be completely dominated by the state with the energetically preferred value of Δ . In an exact treatment, such as the interacting spins without a mean-field approximation, this is no longer the case and the system probes all possible states with a probability dependent on the Boltzmann weight.

6.5.3 Bosons

For bosonic quasiparticles like phonons and magnons, the distribution function describing the occupation of states in equilibrium is the Bose-Einstein distribution

$$n_B(E_{\mathbf{k}}) = \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} - 1} \quad (6.84)$$

where $E_{\mathbf{k}}$ is the dispersion relation of the quasiparticles. From this form, it is immediately clear that μ must always be smaller than the lowest value of $E_{\mathbf{k}}$:

$$\mu < E_{\mathbf{k}} \quad (6.85)$$

Otherwise, the occupation number would be able to take on negative or infinite values.

Given this restriction, we can discuss further which specific values that μ can take. The allowed values for μ depends crucially on whether or not the number of quasiparticles is conserved.

Thus, as stated below eq. 76 in <https://pubs.aip.org/aip/jap/article/126/15/151101/994488/Introduction-to-antiferromagnetic-magnons>, the occupation number of magnons in thermal equilibrium is given by a Bose-Einstein distribution with zero chemical potential.

6.6 Role of chemical potential in lattice models

6.6.1 Tune filling fraction

Consider a lattice with N lattice sites which we describe using a tight-binding lattice Hamiltonian without any chemical potential. If we are considering a closed system with a fixed number of electrons N_e , we must have $N_e \leq 2N$ due to the Pauli principle. The occupation numbers of an eigenstate with N_e electrons must satisfy the constraint:

$$\sum_{i\sigma} \langle n_{i\sigma} \rangle = N_e. \quad (6.86)$$

The ground state of this system is obtained by filling the N_e states labelled by (i, σ) that give the smallest total energy of the system. If we Fourier-transform to $\mathbf{k}$ -space, it becomes more transparent what this means since the equivalent condition is to fill the N_e states labelled by $(\mathbf{k}, \sigma)$ that have the smallest energies $\varepsilon_{\mathbf{k}}$.

The point is that a chemical potential term in the Hamilton-operator, $-\mu \sum_{i,\sigma} n_{i\sigma}$, gives us a way to adjust the *filling fraction* N_e/N of the system. In effect, tuning μ determines the average number of electrons per lattice site (N_e/N) by means of the self-consistency equation Eq. (6.86). This happens as follows. If we change μ , we change the expectation value $\langle c_{i\sigma}^\dagger c_{i\sigma} \rangle = \langle n_{i\sigma} \rangle$, and we thus change what N_e is. Alternatively, we can demand that we want a fixed value of N_e , and then find what μ has to be in order to satisfy Eq. 6.86).

Therefore, one role of the μ -term is that it controls the electron filling in the system. We next discuss another role this term has.

6.6.2 Understanding LDOS relative chemical potential: position of Fermi level and superconducting gap

Another role of the μ -term in the Hamilton-operator is that it controls where the normal-state Fermi level is located, and thus also what the density of states (DOS) is at the Fermi level.

The Fermi energy is defined as the energy at which the occupation of electrons changes abruptly from 1 to 0 at $T \rightarrow 0$. In equilibrium, the distribution function for the quasiparticles in the diagonalized Hamiltonian is the Fermi-Dirac function $f(E)$ where E is the energy of the quasiparticles measured from the Fermi-level. More specifically, if a particle has energy $\epsilon_{\mathbf{k}}$ and the chemical potential of the system is μ , then

$$f(\epsilon_{\mathbf{k}}) = \frac{1}{1 + e^{\beta(\epsilon_{\mathbf{k}} - \mu)}}. \quad (6.87)$$

Introducing the quasiparticle energy measured from the Fermi level, $E = \epsilon_{\mathbf{k}} - \mu$, we see that we may write this as $f(E) = 1/(1 + e^{\beta E})$. We automatically measure energies relative μ when the $-\mu \sum_{i,\sigma} n_{i\sigma}$ term is included in the Hamilton-operator.

For free electrons, the quasiparticles are the original electrons themselves, and thus E is just the normal-state dispersion $\epsilon_{\mathbf{k}}$ minus the chemical potential μ , as explained above. It is clear that at $T = 0$, corresponding to $\beta \rightarrow \infty$, the highest occupied energy state of the system is $\epsilon_{\mathbf{k}} = \mu$ since $f(E)$ changes abruptly at $E = 0$. In other words, $E = 0$ corresponds to particles located at the Fermi surface. When we say that μ is the Fermi level of the system, what we mean is that the highest occupied energy level $\epsilon_{\mathbf{k}}$ equals μ .

The DOS for a free-electron model (such as square lattice or graphene) will give a DOS that is centered around $E = 0$ if $\mu = 0$ because the spectrum is particle-hole symmetric in the absence of μ . When $\mu \neq 0$, the entire DOS curve will instead be shifted to the side - it is no longer centered around $E = 0$.

For instance, in the graphene case the Dirac point, which has zero DOS, will be shifted so that it occurs at $E = -\mu$. This can be understood by first looking at the band structure E vs. k , since the crossing of the energy bands then occurs at $E = -\mu$. This has the consequence that in the DOS vs. E plot, the V-shaped DOS will be centered around $E = -\mu$ instead of $E = 0$. A finite DOS then appears at the Fermi level $E = 0$.

If one introduces superconductivity, the gap in the DOS is *always* centered at $E = 0$ irrespective of the chemical potential. This is in contrast to *e.g.* the V-shape of the DOS in the graphene case, which is centered around $E = -\mu$.

The reason is because of the energy dispersion $E = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta|^2}$. Below the gap, $E < |\Delta|$, there are no available states. Therefore, the DOS has to be zero in an interval centered around $E = 0$ irrespective of what the normal-state Fermi level μ is. In fact, $E = 0$ is the energy of particles located at the normal-state Fermi level in our model, since we are subtracting μ .

6.7 Kinetic energy and curvature of wavefunction

From the Schrodinger equation, we see that the kinetic energy associated with a wavefunction ψ depends on its second derivative with respect to position. This poses an apparent paradox.

Imagine that you have a highly localized wavefunction, meaning that the position of the particle is determined very accurately. Such a wavefunction is necessarily sharply centered around some point x_0 and thus has a very large second derivative - just think of *e.g.* the derivative of a Dirac δ -function. We thus arrive at the conclusion that localized particles have very high kinetic energies, quantum mechanically speaking. How can a *localized* particle have a high kinetic energy? The solution is obtained by considering the Heisenberg uncertainty principle $\Delta x \cdot \Delta p \geq \hbar/2$. The more localized the particle is, the smaller the uncertainty Δx in position is. Consequently, the larger the uncertainty in momentum Δp becomes. Localized particles thus have a much larger spread in the value of their momentum expectation value, and as a result the average kinetic energy can become huge.

Chapter 7

Important theorems and mathematical relations in condensed matter physics

7.1 Fluctuation-dissipation theorem

For a detailed review of the fluctuation-dissipation theorem, see [46]: we follow mainly this article below.

7.1.1 Definition and heuristic argument

The FD theorem states a general relationship between the response of a system to an external disturbance/force and the internal fluctuations of that system in the absence of the disturbance/force. The response is typically characterized by a function such as an admittance or impedance whereas the fluctuations are characterized by a correlation function for the physical quantities that fluctuate in thermal equilibrium. The FD theorem can then be used in two ways:

- It can predict the correlation function characterizing the fluctuations/noise intrinsic to the system if one knows the admittance/impedance.
- It can be used to derive the admittance/impedance of the system if one knows the mathematical form of the thermal fluctuations in the system.

The theorem connects the linear response relaxation of a system from a prepared non-equilibrium state to its statistical fluctuation properties in equilibrium. Often the linear response takes the form of one or more exponential decays. Recall that linear response essentially means that if a macroscopic system variable $\mathcal{X}$ is displaced by a quantity $\Delta\mathcal{X}$, there will act a restoring force $F = -c\Delta\mathcal{X}$ which is proportional to the displacement where c is a constant.

There is a heuristic way of thinking about why the FD theorem "works": in other words, why there should be a relation between the dissipation and the fluctuations. It is best illustrated with a concrete example. Imagine a small glass container with colloidal particles. These particles undergo irregular motion even in the absence of any driving force, as is experimentally well-known. This is due to thermal fluctuations which microscopically originates with the particles colliding with molecules in the liquid due to their finite thermal energy. The molecules thus provide a random driving force on the particles.

Now imagine that an external force is applied as a driving force. The particles undergoing Brownian motion due to thermal fluctuations now undergo forced motion which inevitably will suffer from friction (resistive force). The origin of the friction is again, just as for the thermal fluctuations, impacts of molecules in the liquid with the particles. The impacts with the molecules are random, but a number of collisions will nevertheless produce a systematic result proportional to the velocity of the particles.

We can then conclude that the random impacts of surrounding molecules cause *two kinds of effects*: they act as a random driving force causing irregular motion (thermal fluctuations) and also give rise to a frictional force for forced motion. Since both effects, random force and frictional force, come from the same origin, it is natural that they are related. The internal relationship between these two parts of microscopic forces is manifested via the FD theorem.

7.1.2 Examples

The FD theorem was originally formulated by Harry Nyquist in 1928 and it is useful to illustrate the FD theorem with two examples (from Wiki).

Drag and Brownian motion

If an object is moving through a fluid, it experiences drag (air resistance or fluid resistance). Drag dissipates kinetic energy, turning it into heat. The corresponding fluctuation is Brownian motion. An object in a fluid does not sit still, but rather moves around with a small and rapidly-changing velocity, as molecules in the fluid bump into it. Brownian motion converts heat energy into kinetic energy - the reverse of drag. Thus, the FD theorem establishes a quantitative relation between the drag and the Brownian motion.

Resistance and Johnson noise

If electric current is running through a wire loop with a resistor in it, the current will rapidly go to zero because of the resistance. Resistance dissipates electrical energy, turning it into heat (Joule heating). The corresponding fluctuation is Johnson noise. A wire loop with a resistor in it does not actually have zero current, it has a small and rapidly-fluctuating current caused by the thermal fluctuations of the electrons and atoms in the resistor. Johnson noise converts heat energy into electrical energy - the reverse of resistance. Thus, the FD theorem establishes a quantitative relation between the resistance and the Johnson noise.

Johnson-Nyquist noise is the electronic noise caused by thermal motion of the charge carriers in a conducting material at equilibrium. This motion thus takes place even without any applied voltage. The statistical derivation of this noise is achieved via the FD theorem when a generalized impedance is used to characterize the medium. In passing, we note that thermal noise in an ideal resistor is approximately white. This means that the power spectral density is almost constant throughout the frequency spectrum: in other words, white noise is a random signal having equal intensity at different frequencies.

Physically, the fluctuation-dissipation theorem is thus a statement that the return to equilibrium is governed by the same laws, whether the perturbation was created by an external field or by a spontaneous fluctuation.

7.2 Kramers-Konig relation

Kramers-Konig relations connect the real and imaginary part of a complex function that is analytic in the upper half-plane. Such relations are frequently used to compute the real part from the imaginary part, or the other way around, of response functions in physical systems. This is made possible from the observation that for stable systems, causality implies analyticity and vice versa [56].

Let $f(\omega) = f_1(\omega) + i f_2(\omega)$ be a complex function of a complex variable ω where $f_{1,2}$ are real. Assume that f is analytic in the closed upper half-plane of ω and vanishes like $1/|\omega|$ or faster when $|\omega| \rightarrow \infty$. If so, the following relations are satisfied

$$f_1(\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{f_2(\omega')}{\omega' - \omega} d\omega', \quad f_2(\omega) = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{f_1(\omega')}{\omega' - \omega} d\omega', \quad (7.1)$$

where $\mathcal{P}$ denotes Cauchy's principal value. The full function f can thus be reconstructed given just f_1 or f_2 .

The proof of this relation makes use of Cauchy's residue theorem and the Sokhotski-Plemelj theorem.

7.3 Analytic continuation

In simple terms, analytic continuation is a method to extend the domain of an analytic function. Considering a function $f(x)$ for simplicity, the domain of the function are the x -values for which the function converges and thus remains analytic.

A standard example is to consider $f(x) = 1 + x + x^2 + x^3 + \dots$ which only converges for $|x| < 1$. For such x , $f(x)$ equals $1/(1 - x)$. However, the function $F(x) = 1/(1 - x)$ is defined and analytic for all x except $x = 1$. Since $F(x) = f(x)$ for all $|x| < 1$, we can thus say that $F(x)$ is an analytic continuation of $f(x)$ from a domain $|x| < 1$ to the domain of all numbers except $x = 1$.

To put this into a physics context, consider the Matsubara Green function for non-interacting fermions:

$$G^M(\mathbf{k}, \omega_n) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}. \quad (7.2)$$

Here, ω_n is a real number. The Green function G^M is often stated to be analytically continued to the real axis by setting $i\omega_n \rightarrow \omega \pm i\delta$ where δ is a positive, infinitesimal quantity. In this way, the resulting Green function $G^{R,A}(\omega)$ is defined for ω -values on the entire real axis. For $+$, this can be called an analytic continuation in the upper complex half-plane in the sense that we are going from a function $1/(z - \epsilon_{\mathbf{k}})$ (which is defined for all z in the upper half-plane except the real line) to a function $1/(z - \epsilon_{\mathbf{k}} + i\delta)$ (which is defined for all z in the upper half-plane including the real line). We are thus going from the Matsubara Green function G^M to the retarded Green function G^R . The former is defined everywhere in the upper half-plane except the real line, whereas the latter is defined everywhere in the upper half-plane including the real line. The operation $i\omega_n \rightarrow \omega \pm i\delta$ can nevertheless not be called an analytic continuation if we also include the lower half-plane, since the Green function obtained afterwards (G^R) is not defined at every point where the initial Green function (G^M) is defined in the lower plane.

Similarly, $i\omega_n \rightarrow \omega - i\delta$ gives us the advanced Green function G^A . This operation defines an analytic continuation in the lower complex half-plane.

7.4 Symmetry-analysis of currents and bias: cause and effect

See detailed discussion in section II in <https://www.sciencedirect.com/science/article/pii/S0375960119311703>.

7.5 Diagonalization of fermion and boson Hamiltonian

When analyzing systems with electrons and magnons, one often encounters second-quantized Hamiltonians of the form

$$H = \sum_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} M_{\mathbf{k}} \alpha_{\mathbf{k}} \quad (7.3)$$

where $M_{\mathbf{k}}$ is a matrix and α contains the quasiparticle operators. Generally, it may be written

$$\alpha_{\mathbf{k}}^{\dagger} = [\gamma_{\mathbf{k}}^{\dagger}, \beta_{\mathbf{k}}], \quad \alpha_{\mathbf{k}} = \begin{pmatrix} \gamma_{\mathbf{k}} \\ \beta_{\mathbf{k}}^{\dagger} \end{pmatrix}. \quad (7.4)$$

7.5.1 Bosonic case

Consider first the boson case. Then, γ and β are boson operators individually satisfying the appropriate commutation relations, which we can express as

$$\alpha \alpha^{\dagger} - [(\alpha^{\dagger})^T \alpha^T]^T = \sigma_3. \quad (7.5)$$

Here, we dropped the momentum subscript for brevity of notation. Note that $\alpha_{\mathbf{k}}^{\dagger}$ can in general be a vector itself containing additional subspecies of boson operators: $\alpha_{\mathbf{k}}^{\dagger} = [\gamma_{\mathbf{k}}^{1,\dagger}, \gamma_{\mathbf{k}}^{2,\dagger}, \dots, \beta_{\mathbf{k}}^1, \beta_{\mathbf{k}}^2, \dots]$. Note that for the above relation to hold, β does not have to be different from γ in general. We could have for instance $\beta_{\mathbf{k}} = \gamma_{-\mathbf{k}}$. However, what is important is that the upper half of the operator vector contains operators that are distinct from the lower half, which is guaranteed above by having $\dagger$ on the upper half and no $\dagger$ on the lower half.

We now want to find a transformation T of the operators α which diagonalizes the Hamiltonian for each $\mathbf{k}$. Skipping the summation over $\mathbf{k}$ and considering one specific $\mathbf{k}$, we then have:

$$H = \alpha^{\dagger} M \alpha = \alpha^{\dagger} T^{\dagger} (T^{\dagger})^{-1} M T^{-1} T \alpha = A^{\dagger} D A. \quad (7.6)$$

Here, $D = (T^{\dagger})^{-1} M T^{-1} = \text{diag}(\epsilon_1, \epsilon_2, \dots)$ is a diagonal matrix while $A = T \alpha$ is a vector containing the new boson operators. In order to ensure that the new operators A , which are the long-lived excitations of the system, are still bosonic operators, we require that

$$A A^{\dagger} - [(A^{\dagger})^T A^T]^T = \sigma_3. \quad (7.7)$$

Inserting $A = T \alpha$, we get

$$T \left(\alpha \alpha^{\dagger} - [(\alpha^{\dagger})^T \alpha^T]^T \right) T^{\dagger} = \sigma_3 \quad (7.8)$$

which gives $T \sigma_3 T^{\dagger} = \sigma_3$. This can be rewritten as $\sigma_3 T^{\dagger} = T^{-1} \sigma_3$ or $T^{\dagger} \sigma_3 = \sigma_3 T^{-1}$. Using this relation in $D = (T^{\dagger})^{-1} M T^{-1}$, we get

$$M T^{-1} = \sigma_3 T^{-1} \sigma_3 D. \quad (7.9)$$

If we now define the new diagonal matrix

$$\sigma_3 D = \text{diag}(\lambda_1, \lambda_2, \dots) \quad (7.10)$$

we see that what we have at hand in Eq. (7.9) is really an eigenvalue problem for the matrix $\sigma_3 M$. We have

$$\sigma_3 M w_\rho = \lambda_\rho w_\rho \quad (7.11)$$

where w_ρ are the column vectors of T^{-1} and λ_ρ are the eigenvalues of the matrix $\sigma_3 D$. Note that the eigenvalue problem only determines the eigenvectors up to a multiplicative coefficient. This coefficient is determined from the fact that the condition $T \sigma_3 T^\dagger = \sigma_3$ has to be satisfied.

Summarizing, we want to find the transformation matrix T and the eigenvalues D that enter the Hamiltonian. The way to find this, for bosonic excitations, is the following. T^{-1} is the matrix that diagonalizes the matrix $\sigma_3 M$, with eigenvalues $\sigma_3 D$.

To avoid matrix inversion, one can note that Eq. (7.9) is completely equivalent to

$$M \sigma_3 T^\dagger = T^\dagger D \sigma_3 \quad (7.12)$$

so that we can instead solve the eigenvalue problem

$$M \sigma_3 E_\rho = E_\rho x_\rho \quad (7.13)$$

where x_ρ are the column vectors of $T^\dagger$ and E_ρ are the eigenvalues of the matrix $D \sigma_3$.

7.5.2 Fermionic case

We now consider how this changes for a fermionic Hamiltonian. In that case, α and β satisfy fermionic anticommutation relations, meaning $\alpha \alpha^\dagger + [(\alpha^\dagger)^T \alpha^T]^T = 1$. Inserting again $A = T \alpha$, we get

$$T \left(\alpha \alpha^\dagger + [(\alpha^\dagger)^T \alpha^T]^T \right) T^\dagger = 1 \quad (7.14)$$

which means that $T T^\dagger = 1$. It follows that T must be unitary: $T^{-1} = T^\dagger$. Therefore, from the general equation $(T^\dagger)^{-1} M T^{-1} = D$, we get in the fermionic case that

$$M T^{-1} = T^{-1} D \quad (7.15)$$

or alternatively

$$M w_\rho = \epsilon_\rho w_\rho. \quad (7.16)$$

For fermionic excitations, T^{-1} is the matrix that diagonalizes the matrix M , with eigenvalues D . Note that an eigenvalue problem only determines the eigenvectors up to a multiplicative constant. But in order to satisfy $T^\dagger = T^{-1}$, these eigenvectors must be normalized. This is because the columns of a unitary matrix are orthonormal. So when diagonalizing the matrix, one has to ensure that the eigenvectors are normalized before one inserts them as column vectors in T^{-1} (T^{-1} is also a unitary matrix if T is).

The essential difference between the bosonic and fermionic case is then that in the bosonic case, we must diagonalize $\sigma_3 M$ to find the transformation matrix that takes the old boson operators to the new boson operators, whereas in the fermionic case we can diagonalize M directly.

7.5.3 A practical example

We here consider the example shown in section 1.3.1 here <https://d-nb.info/1044195223/34>. We start with a Hamiltonian

$$H = \sum_{\mathbf{k}} A_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \frac{B_{\mathbf{k}}}{2} (b_{\mathbf{k}} b_{-\mathbf{k}} + b_{-\mathbf{k}}^{\dagger} b_{\mathbf{k}}^{\dagger}). \quad (7.17)$$

We allow for $A_{\mathbf{k}}$ which is not necessarily symmetric in $\mathbf{k}$, and write generally $A_{\mathbf{k}} = A_{\mathbf{k}}^{+} + A_{\mathbf{k}}^{-}$ where $A_{\mathbf{k}}^{\pm} = \pm A_{-\mathbf{k}}^{\pm}$. In contrast, $B_{\mathbf{k}} = B_{-\mathbf{k}}$ must be fulfilled, as follows from commuting operators in Eq. 1.25.

We now consider two issues in more detail.

- We show why not splitting the $\sum_{\mathbf{k}} A_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$ into $\frac{1}{2} \sum_{\mathbf{k}} (A_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + A_{-\mathbf{k}} b_{-\mathbf{k}} b_{-\mathbf{k}}^{\dagger} - A_{\mathbf{k}})$ gives a problem when diagonalizing the Hamiltonian which is related to internally consistent relations for the new boson operators. In effect, we cannot matrix-diagonalize the above H as it stands.
- How to diagonalize the problem if the Hamiltonian above acquires an additional momentum-shift in the boson operators.

Consider the first point. The standard procedure is now to split the $a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$ term into

$$a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} = \frac{1}{2} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{1}{2} a_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} - \frac{1}{2}. \quad (7.18)$$

This allows us to write the Hamiltonian compactly in matrix form

$$H = \frac{1}{2} \sum_{\mathbf{k}} \phi_{\mathbf{k}}^{\dagger} M_{\mathbf{k}} \phi_{\mathbf{k}} - \frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}} \quad (7.19)$$

where

$$\phi_{\mathbf{k}} = \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix}, \quad M_{\mathbf{k}} = \begin{pmatrix} A_{\mathbf{k}} & B_{\mathbf{k}} \\ B_{\mathbf{k}} & A_{-\mathbf{k}} \end{pmatrix}. \quad (7.20)$$

This can be diagonalized by introducing a new basis

$$\psi_{\mathbf{k}} = \begin{pmatrix} \alpha_{\mathbf{k}} \\ \alpha_{-\mathbf{k}}^{\dagger} \end{pmatrix} = P_{\mathbf{k}} \phi_{\mathbf{k}}, \quad (7.21)$$

so that

$$H = \frac{1}{2} \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} D_{\mathbf{k}} \psi_{\mathbf{k}} - \frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}} \quad (7.22)$$

where the entries of the diagonal matrix $D_{\mathbf{k}}$ are determined from the eigenvalues $D_{\mathbf{k}} \sigma_3$ of the matrix $M_{\mathbf{k}} \sigma_3$. The eigenvalues of the matrix $M_{\mathbf{k}} \sigma_3$ are

$$E_{\mathbf{k}}^{\pm} = \frac{1}{2} (A_{\mathbf{k}} - A_{-\mathbf{k}}) \pm \frac{1}{2} \sqrt{(A_{\mathbf{k}} + A_{-\mathbf{k}})^2 - 4B_{\mathbf{k}}^2}, \quad (7.23)$$

and therefore our Hamiltonian is

$$\begin{aligned} H &= -\frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}} \left(\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} E_{\mathbf{k}}^{+} - \alpha_{-\mathbf{k}} \alpha_{-\mathbf{k}}^{\dagger} E_{\mathbf{k}}^{-} \right) \\ &= -\frac{1}{2} \sum_{\mathbf{k}} (A_{\mathbf{k}} + E_{\mathbf{k}}^{-}) + \frac{1}{2} \sum_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} (E_{\mathbf{k}}^{+} - E_{-\mathbf{k}}^{-}) \\ &= -\frac{1}{2} \sum_{\mathbf{k}} (A_{\mathbf{k}} + E_{\mathbf{k}}^{-}) + \frac{1}{2} \sum_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \Omega_{\mathbf{k}}. \end{aligned} \quad (7.24)$$

We thus have arrived at a theory where the long-lived magnon excitations have dispersion relation

$$\begin{aligned}\Omega_{\mathbf{k}} &= E_{\mathbf{k}}^+ - E_{-\mathbf{k}}^- \\ &= A_{\mathbf{k}} - A_{-\mathbf{k}} + \sqrt{(A_{\mathbf{k}} + A_{-\mathbf{k}})^2 - 4B_{\mathbf{k}}^2}.\end{aligned}\quad (7.25)$$

This is consistent with the result in the above link. We now specify the transformation matrix which diagonalizes the problem. This matrix needs to be such that the new boson operators satisfy proper boson commutation relations. If we then write

$$\begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \alpha_{-\mathbf{k}}^\dagger \end{pmatrix}\quad (7.26)$$

we get bosonic statistics for the new operators, i.e. $[\beta_{\mathbf{k}}, \beta_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'}$ and $[\beta_{\mathbf{k}}, \beta_{\mathbf{k}'}] = 0$, if the coefficients in the matrix fulfill

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1. \quad (7.27)$$

Moreover, the above relation between the old and new boson operators will diagonalize the problem if they satisfy

$$\begin{aligned}u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 &= \frac{A_{\mathbf{k}}^+}{\epsilon_{\mathbf{k}}}, \\ 2u_{\mathbf{k}}v_{\mathbf{k}} &= \frac{B_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\end{aligned}\quad (7.28)$$

where $\epsilon_{\mathbf{k}} = \sqrt{(A_{\mathbf{k}}^+)^2 - B_{\mathbf{k}}^2}$. This can be shown via the general diagonalization procedure explained in the previous section. The solution for these coefficients, demanding that they are real, is found to be

$$\begin{aligned}u_{\mathbf{k}} &= \sqrt{\frac{A_{\mathbf{k}}^+ + \epsilon_{\mathbf{k}}}{2\epsilon_{\mathbf{k}}}}, \\ v_{\mathbf{k}} &= \frac{B_{\mathbf{k}}}{|B_{\mathbf{k}}|} \sqrt{\frac{A_{\mathbf{k}}^+ - \epsilon_{\mathbf{k}}}{2\epsilon_{\mathbf{k}}}}.\end{aligned}\quad (7.29)$$

Compare this now with a method where we do not split the $A_{\mathbf{k}}$ term initially, so that we instead are faced with the matrix

$$\phi_{\mathbf{k}} = \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix}, \quad N_{\mathbf{k}} = \begin{pmatrix} 2A_{\mathbf{k}} & B_{\mathbf{k}} \\ B_{\mathbf{k}} & 0 \end{pmatrix}. \quad (7.30)$$

The matrix $N_{\mathbf{k}}$ can be diagonalized, but it *cannot* be diagonalized by a transformation matrix which has the form in Eq. (7.26) if we demand that the new boson operator basis should be $[\alpha_{\mathbf{k}}, \alpha_{-\mathbf{k}}^\dagger]$. If we instead assume a more general basis $[\alpha_{\mathbf{k}}, \beta_{\mathbf{k}}^\dagger]$, the above matrix with zero in the right corner can be diagonalized in a way that fulfills the bosonic commutation relations for the new operators, but we can then no longer state that the β operator is related to the α operator. In effect, we have seemingly introduced a new degree of freedom, which cannot be correct. Another reason for why this cannot be correct is that one ends up with a diagonalized Hamilton-operator

$$H \frac{1}{2} \sum_{\mathbf{k}} \left(E_{\mathbf{k}}^+ \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} - E_{\mathbf{k}}^- \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} - E_{\mathbf{k}}^- \right) \quad (7.31)$$

where $E_{\mathbf{k}}^{\pm} = A_{\mathbf{k}} \pm \sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}$. Since $-E_{\mathbf{k}}^{-} < 0$, we have a magnon-mode with negative energy, which indicates an instability.

Put differently, if we set the diagonalized boson operators to generally equal $[\alpha_{\mathbf{k}}, \beta_{\mathbf{k}}^{\dagger}]$, then we can only prove that $\beta_{\mathbf{k}} = \alpha_{-\mathbf{k}}$ in the first approach where we split the $A_{\mathbf{k}}$ term by looking at the eigenvectors which form the transformation matrix. We cannot prove it in the case where we do not split the $A_{\mathbf{k}}$ term.

To be able to state that $\psi_{\mathbf{k}} = P_{\mathbf{k}}\phi_{\mathbf{k}}$ with $\psi_{\mathbf{k}} = [\alpha_{\mathbf{k}}, \alpha_{-\mathbf{k}}^{\dagger}]$, we must have

$$P_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & v_{-\mathbf{k}}^* \\ v_{\mathbf{k}} & u_{-\mathbf{k}}^* \end{pmatrix}. \quad (7.32)$$

This can be proven to hold for the matrix $M_{\mathbf{k}}$ where we split $A_{\mathbf{k}}$. Namely, it can be shown by defining an operator K such that

$$K \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} v_{-\mathbf{k}}^* \\ u_{-\mathbf{k}}^* \end{pmatrix} \quad (7.33)$$

and then noting that $M_{\mathbf{k}}$ satisfies:

$$M_{\mathbf{k}}\sigma_3K \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = -KM_{\mathbf{k}}\sigma_3 \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}. \quad (7.34)$$

It follows that if $[u_{\mathbf{k}}, v_{\mathbf{k}}]$ is an eigenvector, then so is $[v_{-\mathbf{k}}^*, u_{-\mathbf{k}}^*]$. However, for $N_{\mathbf{k}}$ no such relation exists. In this case, the $P_{\mathbf{k}}$ matrix instead takes the form:

$$P_{\mathbf{k}} = [e_1|e_2] \quad (7.35)$$

with column vectors

$$e_i = \frac{v_i}{\sqrt{|v_i^{\dagger}\sigma_3v_i|}}, \quad (7.36)$$

where v_1 belongs to the eigenvalue E^{+} and reads

$$v_1 = \begin{pmatrix} \frac{B_{\mathbf{k}}}{A_{\mathbf{k}} - \sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}} \\ 1 \end{pmatrix} \quad (7.37)$$

while v_2 belongs to the eigenvalue E^{-} and reads:

$$v_2 = \begin{pmatrix} \frac{B_{\mathbf{k}}}{A_{\mathbf{k}} + \sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}} \\ 1 \end{pmatrix}. \quad (7.38)$$

Now consider the second point. Adding a momentum-shift, our Hamiltonian has the form

$$H = \sum_{\mathbf{k}} A_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \frac{B_{\mathbf{k}}}{2} (b_{\mathbf{k}} b_{-\mathbf{k}-\mathbf{Q}} + b_{-\mathbf{k}-\mathbf{Q}}^{\dagger} b_{\mathbf{k}}). \quad (7.39)$$

Here, $A_{\mathbf{k}}$ is in general asymmetric in $\mathbf{k}$, whereas $B_{\mathbf{k}}$ must satisfy $B_{-\mathbf{k}-\mathbf{Q}}$.

Now we need a transformation which preserves the bosonic commutation relations for the new operators $\beta_{\mathbf{k}}$ and which also makes the Hamiltonian diagonal. First, rewrite our Hamiltonian to

$$H = -\frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}} A_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + A_{-\mathbf{k}-\mathbf{Q}} b_{-\mathbf{k}-\mathbf{Q}} b_{-\mathbf{k}-\mathbf{Q}}^{\dagger} + B_{\mathbf{k}} (b_{\mathbf{k}} b_{-\mathbf{k}-\mathbf{Q}} + b_{-\mathbf{k}-\mathbf{Q}}^{\dagger} b_{\mathbf{k}}) \quad (7.40)$$

so that the Hamiltonian can be written in matrix form with

$$\begin{pmatrix} A_{\mathbf{k}} & B_{\mathbf{k}} \\ B_{\mathbf{k}} & A_{-\mathbf{k}-\mathbf{Q}} \end{pmatrix} \quad (7.41)$$

We look for a transformation

$$\begin{pmatrix} b_{\mathbf{k}} \\ b_{-\mathbf{k}}^\dagger \end{pmatrix} = \begin{pmatrix} C_{\mathbf{k}} & D_{\mathbf{k}} \\ E_{\mathbf{k}} & F_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \beta_{\mathbf{k}} \\ \beta_{-\mathbf{k}}^\dagger \end{pmatrix} \quad (7.42)$$

To make these relations between operators internally consistent, we must have that $E_{\mathbf{k}} = B_{-\mathbf{k}-\mathbf{Q}}$ and $F_{\mathbf{k}} = C_{-\mathbf{k}-\mathbf{Q}}$. We want to write this in a similar form as the above link, so that the results become the same when $\mathbf{Q} = 0$. Thus, the transformation matrix

$$T_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ -v_{-\mathbf{k}-\mathbf{Q}} & u_{-\mathbf{k}-\mathbf{Q}} \end{pmatrix} \quad (7.43)$$

will satisfy the bosonic commutation relations if the relations

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1 \quad (7.44)$$

and

$$u_{\mathbf{k}} = u_{-\mathbf{k}-\mathbf{Q}}, \quad v_{\mathbf{k}} = v_{-\mathbf{k}-\mathbf{Q}} \quad (7.45)$$

are satisfied. This reduces to the expressions in the above link for $\mathbf{Q} = 0$, since in that case one also has $u_{\mathbf{k}} = u_{-\mathbf{k}}, v_{\mathbf{k}} = v_{-\mathbf{k}}$. Note also that our above transformation matrix satisfies $T_{\mathbf{k}} = T_{\mathbf{k}}^\dagger = T_{\mathbf{k}}^{-1}$, just like in the above link.

We can now follow the same steps as in the link above. In order to obtain a diagonal Hamiltonian, we have to fulfill

$$(A_{\mathbf{k}} + A_{-\mathbf{k}-\mathbf{Q}})u_{\mathbf{k}}v_{\mathbf{k}} = B_{\mathbf{k}}(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2). \quad (7.46)$$

Note that this is completely equivalent to eq 1.32a,b in the above link, because $(A_{\mathbf{k}} + A_{-\mathbf{k}-\mathbf{Q}})$ is symmetric under the operation $\mathbf{k} \rightarrow -\mathbf{k} - \mathbf{Q}$, just like the expressions in the link are symmetric under $\mathbf{k} \rightarrow -\mathbf{k}$. Hence, the solutions in eq 1.34a,b should be the same, just replacing $A_{\mathbf{k}}^+$ with $(A_{\mathbf{k}} + A_{-\mathbf{k}-\mathbf{Q}})/2$. The final Hamiltonian and eigenvalues are obtained in the same way. One verifies from these final expressions that our assumption about

$$u_{\mathbf{k}} = u_{-\mathbf{k}-\mathbf{Q}}, \quad v_{\mathbf{k}} = v_{-\mathbf{k}-\mathbf{Q}} \quad (7.47)$$

are indeed correct due to the symmetry properties of $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$.

7.6 Schrieffer-Wolff transformation

Use for studying interactions in the low-energy sector perturbatively

State-of-the-art experiments allow for studies of many-body Hamiltonians, such as Hubbard-models or Ising-models, with atoms. In order to obtain systems which are computationally manageable and can be treated theoretically, one typically considers only a small subspace of atomic states, such as the low-energy sector of the system's spectrum, and describes the interaction between them by an effective Hamiltonian. The *Schrieffer-Wolff transformation* [Phys. Rev. 149, 491 (1966), Ann.

Phys. 326, 2793 (2011)] accomplishes this aim.

The basic idea is to consider a system with a Hamiltonian $H = H_0 + \Delta H$ where H_0 describes an uncoupled low- and high-energy sector while the small perturbation ΔH couples these two sectors. Mathematically, one can thus think of H_0 as a diagonal matrix while ΔH is off-diagonal. If one wishes to determine how the coupling influences only the low-energy part of the spectrum, it is not straight-forward to immediately project out the low-energy part in H when the off-diagonal part ΔH is present. However, by performing a unitary transformation on H , this projection becomes much easier. The S-W transformation consists of precisely such a unitary transformation of H which allows one to capture the effect of ΔH in the low-energy sector to any desired order in the perturbation ΔH . The validity of this procedure requires that the separation between the low- and high-energy parts of the spectrum in H_0 is much larger than the coupling term ΔH . This is the same as the criterion in standard second-order perturbation theory.

The transformation has the form $H' = e^{iS} H e^{-iS}$ where S is Hermitian. This unitary transformation does not change the eigenvalues of H . Using the Baker-Campbell-Hausdorff formula, we get

$$H' = H_0 + \Delta H + i[S, H_0] + i[S, \Delta H] - \frac{1}{2}[S, [S, H_0]] + \mathcal{O}(\lambda^3) \quad (7.48)$$

where λ is the strength of the perturbation. By choosing S so that

$$\Delta H + i[S, H_0] = 0 \quad (7.49)$$

the transformed Hamilton-operator reduces to

$$H' = H_0 + \frac{i}{2}[S, \Delta H] + \mathcal{O}(\lambda^3). \quad (7.50)$$

Since H_0 is diagonal and ΔH is off-diagonal, it is clear that S must be off-diagonal to fulfill Eq. (7.49). The goal of the approach is to construct an effective Hamiltonian H_{eff} which has a form allowing us to identify what the correction to the low-energy part of the spectrum is due to the perturbation. We have now accomplished this since

$$H_{\text{eff}} = H_0 + \frac{i}{2}[S, \Delta H] \quad (7.51)$$

is diagonal since both S and ΔH are off-diagonal. Note that since we discarded higher order terms in λ , H_{eff} no longer has exactly the same eigenvalues as H despite S still being unitary.

We can now evaluate the expectation value of H_{eff} using the unperturbed low-energy states to get the energy of the system. This can be justified by considering $\frac{i}{2}[S, \Delta H]$ as a perturbation of its own and applying first order perturbation theory to it. The energy correction to the groundstate of the system is then $\langle 0 | \frac{i}{2}[S, \Delta H] | 0 \rangle$ where $|0\rangle$ is the groundstate of H_0 . In other words, we have used a canonical transformation to consider the effect of the original perturbation ΔH on the space of eigenstates of H_0 via an effective interaction term H_{eff} instead of the original perturbation.

The first order correction (in ΔH) to H_{eff} vanished since we assumed that ΔH was purely off-diagonal. If it is not, then the diagonal contribution gives a first-order correction. This can be seen explicitly by taking the matrix element of ΔH between two states n and m of the unperturbed Hamiltonian with eigenvalues E_n and E_m . Using Eq. (7.49):

$$\langle n | \Delta H | m \rangle + i \langle n | S H_0 - H_0 S | m \rangle = 0 \quad (7.52)$$

which is rearranged to

$$\langle n|S|m\rangle = \frac{1}{i} \frac{\langle n|\Delta H|m\rangle}{E_n - E_m}. \quad (7.53)$$

Now, we can compute the expectation value of H_{eff} taken in the ground-state, as described above. By inserting a completeness relation $\sum_j |j\rangle\langle j|$, we get:

$$\begin{aligned} \langle 0|H_{\text{eff}}|0\rangle &= E_0 + \langle 0|\frac{i}{2}[S, \Delta H]|0\rangle \\ &= E_0 + \frac{i}{2} \sum_j \left(\langle 0|S|j\rangle\langle j|\Delta H|0\rangle - \langle 0|\Delta H|j\rangle\langle j|S|0\rangle \right) \\ &= E_0 + \frac{1}{2} \sum_j \langle 0|\Delta H|j\rangle\langle j|\Delta H|0\rangle \left(\frac{1}{E_0 - E_j} - \frac{1}{E_j - E_0} \right) \\ &= E_0 + \frac{1}{2} \sum_j \frac{|\langle 0|\Delta H|j\rangle|^2}{E_0 - E_j}. \end{aligned} \quad (7.54)$$

This is the standard result for the second-order correction in perturbation theory. Special attention should be taken for the $j = 0$ contribution, causing a divergence, which can be resolved by excluding it from the sum by grounds of maintaining normalization of the eigenstates. Note that the eigenvalues E_j are not $\varepsilon_{\mathbf{k}}$ in the free electron gas case, since the states $|n\rangle$ are the eigenstates of the *full* Hamiltonian $H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$.

Therefore, in the case of a purely off-diagonal coupling ΔH (with no matrix elements between intra-low-energy states or intra-high-energy states) the S-W transformation allows us to get an effective Hamiltonian that gives the second-order correction to the energy eigenstates right away when computing the expectation value of the effective Hamiltonian in an unperturbed state. One can think of this as removing the effect of part of the system on the energy via the canonical transformation that we make and keeping only a part that we are interested in.

This procedure is useful since the resulting transformed Hamilton-operator can be used to project out certain subspaces of the eigenstates, such as high-energy excitations, and thus obtain an effective low-energy model, even when the high-energy and low-energy excitations are coupled to begin with. Alternatively, one might be interested in a high-energy model: both limits can be projected out. Historically, the S-W transformation has played an important part in obtaining a systematic perturbative approach to the strong coupling regime of quantum-many body Hamiltonians. For instance, the S-W transformation shows that the Kondo model lies in the strong coupling regime of the Anderson impurity model.

Use for obtaining effective interactions

The S-W transformation is also useful for another purpose, namely identifying effective interactions between particles that are mediated by other particles, even when we are not interested in computing energy expectation values via perturbation theory. This is what is done in BCS theory, where one uses a S-W transformation to obtain an effective electron-electron interaction mediated by phonons. When this is done, one does not proceed to evaluate the correction to the energy of the electron part of the spectrum by computing the expectation value of H_{eff} , as above. This is because the superconducting state cannot be found via perturbation theory - it is a qualitatively different state compared to the normal Fermi sea. Instead, we use the effective Hamiltonian to build up an entirely

new ground-state for that Hamiltonian. One does take the expectation value with respect to the ground-state of the phonons in order to integrate out/average out the phonon part, so that one is left with only an effective interaction between electrons:

$$H_{\text{eff}}(c, c^\dagger) = \langle H_{\text{eff}}(c, c^\dagger, a, a^\dagger) \rangle_{\text{phonons}} \quad (7.55)$$

7.6.1 Löwdin partitioning

The above procedure may be recast into matrix element form using the unperturbed eigenstates $\{\psi_l\}$ of H_0 as the basis, see Winkler 2003. In this case, it is often referred to as a Löwdin partitioning or downfolding. Assume the unperturbed eigenstates of H_0 are separated into low-energy ones and high-energy ones, separated by a gap. The procedure then consists of choosing S so that matrix elements of H' between low- and high-energy states vanish up to a desired order in the perturbation ΔH . One may now write down the matrix representation of H' in the eigenbasis $\{\psi_l\}$ of H_0 and observe that it is block-diagonal. We have then evaluated in an approximative manner the effect of the perturbation on the low-energy states and the high-energy states. At this point, since there is no coupling anymore between the low- and high-energy states, the latter may simply be discarded and we are left with an effective low-energy theory.

We note that the eigenenergies obtained from H_{eff} indeed are a good approximation to the eigenenergies of the original Hamiltonian which treats ΔH non-perturbatively. This is the case since H_{eff} is obtained from a unitary transformation of $H = H_0 + \Delta H$. Similarly, the eigenstates of H_{eff} can be used as an approximation for the eigenstates of H . However, it should be noted that the eigenstates ψ_{eff} of H_{eff} are not exactly the same as the eigenstates ψ for H . In fact, they are related via the unitary transformation $\psi_{\text{eff}} = e^{iS}\psi$. For instance, the exact low-energy eigenstates of H will contain a small coupling to the high-energy states. However, the point is that we neglect this coupling to construct an effective theory for only the low-energy states. For the purpose of obtaining *e.g.* band-structure (eigenvalues) for the low-energy states, the above procedure is excellent since the eigenvalues are preserved in the unitary transformation (up to a given order in ΔH).

To illustrate the complete procedure, consider then a tight-binding Hamiltonian which originally reads $\phi^\dagger(H_0 + \Delta H)\phi$ where ϕ is some basis of second-quantized fermion operators. Now diagonalize H_0 to D and let $\tilde{\phi}$ be the eigenstates of H_0 . Then we have $\tilde{\phi}^\dagger(D + \Delta\tilde{H})\tilde{\phi}$ since the matrix-representation of ΔH also changes when we change basis from ϕ to $\tilde{\phi}$. We now identify low- and high-energy sectors of D and then perform a unitary transformation $e^{iS}(D + \Delta\tilde{H})e^{-iS}$ with S chosen to remove the off-diagonal parts of $\Delta\tilde{H}$ (which may also contain diagonal parts after transforming from ϕ to $\tilde{\phi}$). The eigenvalues of the Hamiltonian $H_{\text{eff}} = e^{iS}(D + \Delta\tilde{H})e^{-iS}$ are then an approximative result for the exact eigenvalues of the original full Hamiltonian H . Note that they are easily read out since H_{eff} is now diagonal. Moreover, the eigenstates of H_{eff} are an approximative result for the exact eigenstates of the original full Hamiltonian H . The low- and high-energy bands of H_{eff} are easily read out and projected out if desired since there is no coupling anymore.

7.6.2 Application: RKKY interaction

We can use a Schrieffer-Wolff transformation to obtain the RKKY interaction both in the normal and superconducting state.

Normal metal

Consider a second-quantized Hamilton-operator $H = H_0 + \Delta H$ with an exactly solvable part H_0

and a small perturbation ΔH . In our context, let us consider a free electron gas with impurity classical spins $\mathbf{S}_j$ that interacts with the conduction electron spins:

$$H = \sum_{\langle i,j \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + J \sum_j \mathbf{S}_j \cdot \mathbf{s}_j \quad (7.56)$$

Moreover, we know that the spin operator for conduction spin is:

$$\mathbf{s}_j = \frac{1}{2} \sum_{\alpha\beta} c_{j\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{j\beta} \quad (7.57)$$

It should be clear which part is H_0 and which part is ΔH . Let us also do a Fourier-transformation according to

$$a_j = \frac{1}{\sqrt{N}} \sum_k a_k e^{-ikr_j}. \quad (7.58)$$

Here, I've just considered 1D (k instead of $\mathbf{k}$) for simplicity, but we should consider at least 2D in the paper. Our full Hamiltonian is then:

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{J}{N} \sum_j \mathbf{S}_j \cdot \sum_{kk'\alpha\beta} e^{i(k-k')r_j} c_{k\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{k'\beta}. \quad (7.59)$$

If we perform a unitary transformation on H , we know that its eigenvalues do not change. We can then perform such a unitary transformation U and obtain a new Hamiltonian which shows the spin-spin interaction (RKKY) explicitly. A unitary transformation is obtained via

$$\tilde{H} = e^{iS} H e^{-iS} \quad (7.60)$$

where $S = S^\dagger$ is a hermitian matrix. Now, let ΔH be characterized by a small quantity λ since it is a perturbation: $\Delta H \propto \lambda$. We let S be proportional to that same small quantity λ , so that it is also small. By expanding $e^{iS} = 1 + iS + \dots$, we see that

$$\tilde{H} = H_0 + \Delta H + i[S, H_0] + i[S, \Delta H] - \frac{1}{2}[S, [S, H_0]] + \mathcal{O}(\lambda^3) \quad (7.61)$$

Here, we see that by choosing S appropriately, we can get rid off all first-order terms in the small quantity. Namely, if we choose S so that

$$\Delta H + i[S, H_0] = 0 \quad (7.62)$$

the effective Hamiltonian $\tilde{H}$ above becomes

$$\tilde{H} = H_0 + \frac{i}{2}[S, \Delta H] + \mathcal{O}(\lambda^3). \quad (7.63)$$

By keeping only the first two terms (since λ is small), we will see how this gives an effective spin-spin RKKY interaction.

The only challenging step is how to find S so that Eq. (7.62) is satisfied. To do so, we can use a general ansatz for S which is capable of producing the terms in ΔH after commuting S with H_0 , as required in Eq. (7.62). In general, it is a good strategy to choose an S which has the same type of operator-combinations as ΔH . Indeed, choosing an S with the same operator-combination

as H_0 will be of no use, since those will just commute with S . Put colloquially, S needs to have off-diagonal terms compared to H_0 . This will become more clear in the superconducting case. Thus, we write

$$S = \sum_{kk'\alpha\beta} c_{k\alpha}^\dagger A_{kk'\alpha\beta} c_{k'\beta} \quad (7.64)$$

where $A_{kk'\alpha\beta}$ are unknown coefficients that we need to determine in order to satisfy Eq. (7.62). We first compute $[S, H_0]$. After some straightforward algebra, using fermion anticommutation rules, we get:

$$[S, H_0] = \sum_{kk'\alpha\beta} A_{kk'\alpha\beta} (\epsilon_{k'} c_{k\alpha}^\dagger c_{k'\beta} - \epsilon_k c_{k\alpha}^\dagger c_{k'\beta}). \quad (7.65)$$

This is supposed to equal $i\Delta H$ where ΔH is given in Eq. (7.59). Comparing the two, it is clear that

$$A_{kk'\alpha\beta} = i \frac{J}{N} \sum_j \mathbf{S}_j \boldsymbol{\sigma}_{\alpha\beta} \frac{e^{i(k-k')r_j}}{\epsilon_{k'} - \epsilon_k}. \quad (7.66)$$

Please note that $\boldsymbol{\sigma}_{\alpha\beta}$ is matrix element (α, β) in the Pauli-matrix vector $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. One can directly verify that with this $A_{kk'\alpha\beta}$, S is indeed hermitian.

Here, we must be a bit careful with the case where $\epsilon_{k'} = \epsilon_k$ which seemingly cause a divergence in Eq. (7.66). The resolution is to note that the value of $A_{kk'\alpha\beta}$ in Eq. (7.66) does not cause a divergence in the effective Hamiltonian because it will appear as a product with Fermi-Dirac distribution functions in the form $A_{kk'\alpha\beta} [f(\epsilon_{k'}) - f(\epsilon_k)]$. For the problematic case $\epsilon_k = \epsilon_{k'}$, the point is that the expression

$$A_{kk'\alpha\beta} [f(\epsilon_{k'}) - f(\epsilon_k)] = i \frac{J}{N} \sum_j \mathbf{S}_j \boldsymbol{\sigma}_{\alpha\beta} \frac{e^{i(k-k')r_j} [f(\epsilon_{k'}) - f(\epsilon_k)]}{\epsilon_{k'} - \epsilon_k} \quad (7.67)$$

has a finite value. To see this, we can use L'Hopital's rule that for $\lim_{x \rightarrow c} f(x) = \lim_{x \rightarrow c} g(x) = 0$, then

$$\lim_{x \rightarrow c} \frac{f(x)}{g(x)} = \lim_{x \rightarrow c} \frac{f'(x)}{g'(x)}. \quad (7.68)$$

Therefore, we have

$$\lim_{x \rightarrow c} \frac{f(x) - f(c)}{x - c} = \lim_{x \rightarrow c} \frac{d}{dx} \left(\frac{1}{1 + e^{\beta x}} \right) = \frac{-\beta}{4 \cosh^2(\beta c/2)}. \quad (7.69)$$

This is a finite number. Therefore, using the solution for $A_{kk'\alpha\beta}$ in Eq. (7.66) ensures that both $\Delta H + i[S, H_0] = 0$ is satisfied even for $\epsilon_k = \epsilon_{k'}$, since

$$\lim_{\epsilon_k \rightarrow \epsilon_{k'}} A_{kk'\alpha\beta} (\epsilon_{k'} - \epsilon_k) = i \frac{J}{N} \sum_j \mathbf{S}_j \boldsymbol{\sigma}_{\alpha\beta} e^{i(k-k')r_j}, \quad (7.70)$$

and that we do not have any divergent terms in the effective Hamiltonian: there, we must use Eq. (7.69) whenever we encounter a term in the summation for which $\epsilon_{k'} = \epsilon_k$.

Now that we have found S , we can obtain the new Hamiltonian in Eq. (7.63): we just have to compute $\frac{i}{2}[S, \Delta H]$ where both S and ΔH are now known. We get after straight-forward algebra

$$\frac{i}{2}[S, \Delta H] = -\frac{1}{2} \frac{J^2}{N^2} \sum_{ijkk'qq'\alpha\beta\gamma\delta} \frac{e^{i(k-k')r_i}}{\epsilon_{k'} - \epsilon_k} \mathbf{S}_i \cdot \boldsymbol{\sigma}_{\alpha\beta} \left(-c_{q\gamma}^\dagger c_{k'\beta} e^{i(q-k)r_j} \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\gamma\alpha} + c_{k\alpha}^\dagger c_{q'\delta} e^{i(k'-q')r_j} \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\beta\delta} \right). \quad (7.71)$$

We have thus found an effective Hamiltonian describing the RKKY interaction:

$$H_{\text{eff}} = H_0 - \frac{1}{2} \frac{J^2}{N^2} \sum_{ijkk'qq'\alpha\beta\gamma\delta} \frac{e^{i(k-k')r_i}}{\epsilon_{k'} - \epsilon_k} \mathbf{S}_i \cdot \boldsymbol{\sigma}_{\alpha\beta} \left(-c_{q\gamma}^\dagger c_{k'\beta} e^{i(q-k)r_j} \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\gamma\alpha} + c_{k\alpha}^\dagger c_{q'\delta} e^{i(k'-q')r_j} \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\beta\delta} \right). \quad (7.72)$$

To compute the RKKY energy, we need to find the expectation value of H_{eff} . The lowest-order approximation will be to compute the expectation value by using the unperturbed eigenstates, i.e. the eigenstates of H_0 . In effect, we are applying first order perturbation theory to H_{eff} with the second term as the perturbation. As described earlier, this gives us the second-order correction to the energy-values from the perturbation, but not the first-order correction. We have discarded the effect of ΔH on part of the total Hilbert space described by H . This is fine for our purposes, because we are here interested precisely in the second-order correction which physically describes the interaction between spins in the system.

We know that H_0 describes a free-electron gas. Therefore, only terms in the operator H_{eff} which leave the free-electron gas invariant will contribute when taking the expectation value of it. For instance, the term

$$-c_{q\gamma}^\dagger c_{k'\beta} \quad (7.73)$$

will then only contribute when $q = k'$ and $\gamma = \beta$ so that we get $-c_{k'\beta}^\dagger c_{k'\beta}$. Similarly for $c_{k\alpha}^\dagger c_{q'\delta}$. Taking this into account, and using

$$f_k = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle \quad (7.74)$$

where f_k is the Fermi-Dirac distribution function, as well as

$$\sum_{\alpha\beta} (\mathbf{S}_i \cdot \boldsymbol{\sigma}_{\alpha\beta}) (\mathbf{S}_j \cdot \boldsymbol{\sigma}_{\beta\alpha}) = 2\mathbf{S}_i \cdot \mathbf{S}_j, \quad (7.75)$$

we get:

$$\langle H_{\text{eff}} \rangle = E_0 + \sum_{ij} I(r_{ij}) \mathbf{S}_i \cdot \mathbf{S}_j \quad (7.76)$$

where the interaction $I(r_{ij})$, with $r_{ij} \equiv r_i - r_j$, is equal to

$$I(r_{ij}) = -\frac{J^2}{N^2} \sum_{kk'} e^{i(k-k')(r_i-r_j)} \frac{f_k - f_{k'}}{\epsilon_{k'} - \epsilon_k}. \quad (7.77)$$

This term can now be either numerically evaluated or actually also analytically computed by converting the k -sum to integrals over k . The sign of I thus determines of P or AP configuration is

avored and it is the quantity we are interested in.

Thus, we have kept only the state of the localized spins from the entire Hilbert space and integrated out the degrees of freedom of the electrons by taking the ground-state expectation value with respect to the electrons.

Let us show how I can be analytically evaluated in 3D. First, we have:

$$\begin{aligned} I &= -\frac{J^2}{N^2} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}_{ij}} \frac{f_{k'} - f_k}{\epsilon_k - \epsilon_{k'}} \\ &= -\frac{J^2}{N^2} (2\pi)^2 \frac{V^2}{(2\pi)^6} \int \int dk dk' k^2 (k')^2 \sin \theta \sin \theta' d\theta d\theta' \frac{f_{k'} - f_k}{\epsilon_k - \epsilon_{k'}} e^{ikR \cos \theta} e^{-ik'R \cos \theta'} \end{aligned} \quad (7.78)$$

where we defined $\mathbf{R}_{ij}$ to lie along the z -axis. We are free to make this choice for a normal metal since all spatial directions are equivalent. There is no azimuthal angle dependence, giving the $(2\pi)^2$ prefactor.

We will evaluate the integral containing $f_{k'}$ and the integral containing $-f_k$ separately. In that case, there is seemingly a singularity occurring at $k = k'$ due to the denominator vanishing at such a value. However, we saw that the contribution to the effective Hamiltonian (and thus I above) from this value still gives a finite value. We deal with this mathematically by taking the principal value $\mathcal{P}$ of the integral, and treating the $\mathbf{k} = \mathbf{k}'$ in the original sum separately. Since

$$\lim_{k \rightarrow k'} \frac{f_{k'} - f_k}{\epsilon_k - \epsilon_{k'}} = -df_k/d\epsilon_k, \quad (7.79)$$

we get

$$I = \frac{J^2}{N^2} \sum_{\mathbf{k}} \frac{df_k}{d\epsilon_k} - \frac{J^2}{N^2} \frac{V^2}{(2\pi)^4} \mathcal{P} \int \int dk dk' k^2 (k')^2 \sin \theta \sin \theta' d\theta d\theta' \frac{f_{k'} - f_k}{\epsilon_k - \epsilon_{k'}} e^{ikR \cos \theta} e^{-ik'R \cos \theta'}. \quad (7.80)$$

For $T = 0$, we know that $f_k = \theta(\mu - \epsilon_k)$ so that $df_k/d\epsilon_k = -\delta(\mu - \epsilon_k)$. Then, the first term in I , which is the $\mathbf{k} = \mathbf{k}'$ contribution, is essentially the DOS $D(\mu)$ at the Fermi level:

$$\frac{J^2}{N^2} \sum_{\mathbf{k}} \frac{df_k}{d\epsilon_k} = -\frac{J^2 V}{N^2} D(\mu), \quad (7.81)$$

since generally we have the density of states at energy E being:

$$D(E) = \frac{1}{V} \sum_j \delta(E - \epsilon_j) \quad (7.82)$$

where ϵ_j are the allowed energy states of the system. For instance, in 3D one has $D(E = \mu) = mk_F/\pi^2$ for a free electron gas. The prefactor is crucial here, because if we now consider the thermodynamic limit of a large system, then $V/N^2 \rightarrow 0$ since N is the number of sites, so that $V \propto N$. This means that this term can be neglected in the thermodynamic limit. Thus, we can focus on computing I from the principal value of the remaining integral.

Now let $x = kR \cos \theta$ and $x' = k'R \cos \theta'$ which gives

$$I = -\frac{J^2}{N^2} \frac{V^2}{(2\pi)^4} \mathcal{P} \int \int dk dk' k^2 (k')^2 \frac{1}{kR} \frac{1}{k'R} dx dx' e^{ix} e^{-ix'} \frac{f_{k'} - f_k}{\epsilon_k - \epsilon_{k'}}. \quad (7.83)$$

and use that

$$\int_{kR}^{-kR} e^{ix} dx = -2 \sin kR. \quad (7.84)$$

This gives

$$I = -\frac{4J^2}{N^2} \frac{V^2}{(2\pi)^4} \mathcal{P} \int \int dk dk' k^2 (k')^2 \frac{\sin(kR)}{kR} \frac{\sin(k'R)}{k'R} \frac{f_{k'} - f_k}{\epsilon_k - \epsilon_{k'}}. \quad (7.85)$$

Now set $T = 0$. This makes $f_{k'} = \theta(k_F - k')$. At non-zero temperatures, one can find a correction to this result by expanding the Fermi-Dirac distributions in T . Now look at the contribution from $f_{k'}$ above. It gives

$$I_1 = -\frac{4J^2}{N^2} \frac{V^2}{(2\pi)^4} \mathcal{P} \int_0^\infty \int_0^\infty dk dk' k^2 (k')^2 \frac{\sin(kR)}{kR} \frac{\sin(k'R)}{k'R} \frac{\theta(k_F - k')}{\epsilon_k - \epsilon_{k'}}. \quad (7.86)$$

The contribution from f_k gives exactly the same result as can be seen by renaming $k \leftrightarrow k'$ in that term. Thus, $I = 2I_1$, so that

$$I = -\frac{8J^2}{N^2} \frac{V^2}{(2\pi)^4} \mathcal{P} \int_0^{k_F} dk \int_0^{k_F} dk' k^2 (k')^2 \frac{\sin(kR)}{kR} \frac{\sin(k'R)}{k'R} \frac{1}{\epsilon_k - \epsilon_{k'}}. \quad (7.87)$$

Using a free-electron dispersion $\epsilon_k = k^2/2m - \mu$, we want to perform the integral over k first:

$$I = -\frac{8J^2}{N^2} \frac{V^2}{(2\pi)^4} \mathcal{P} \int_0^{k_F} dk' (k')^2 \frac{\sin(k'R)}{k'R} \int_0^\infty dk k^2 \frac{\sin(kR)}{kR} \frac{1}{\epsilon_k - \epsilon_{k'}}. \quad (7.88)$$

We write this as

$$\begin{aligned} I &= -\frac{8J^2}{N^2} \frac{V^2}{(2\pi)^4} \int_0^{k_F} dk' (k')^2 \frac{\sin(k'R)}{k'R} \times K, \\ K &= \mathcal{P} \int_0^\infty dk k^2 \frac{\sin(kR)}{kR} \frac{1}{\epsilon_k - \epsilon_{k'}}. \end{aligned} \quad (7.89)$$

The integral is even in k , thus can we extend the integration to $-\infty$. Do this and rewrite $\sin(kR)$ using Euler's formula to get:

$$K = \frac{1}{4i} \mathcal{P} \int_{-\infty}^\infty dk k^2 \frac{(e^{ikR} - e^{-ikR})}{kR} \frac{1}{\epsilon_k - \epsilon_{k'}}. \quad (7.90)$$

Using that

$$\frac{1}{k^2 - (k')^2} = \frac{1}{(k - k')(k + k')} = \frac{1}{2k} \left(\frac{1}{k - k'} + \frac{1}{k + k'} \right) \quad (7.91)$$

we obtain

$$K = \frac{m}{4Ri} \mathcal{P} \int_{-\infty}^\infty dk \left(\frac{e^{ikR}}{k - k'} + \frac{e^{ikR}}{k + k'} - \frac{e^{-ikR}}{k - k'} - \frac{e^{-ikR}}{k + k'} \right) \quad (7.92)$$

Shifting integration variable at a fixed value of k' , such as $y = k - k'$, we rewrite this as

$$K = \frac{m}{4Ri} \mathcal{P} \int_{-\infty}^\infty dy \left(\frac{e^{i(y+k')R}}{y} + \frac{e^{i(y-k')R}}{y} - \frac{e^{-i(y+k')R}}{y} - \frac{e^{-i(y-k')R}}{y} \right) \quad (7.93)$$

Now, we can use the Sokhotski-Plemelj theorem which states that

$$\mathcal{P} \int_{-\infty}^{\infty} \frac{f(y)}{y} dy = \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{f(y)}{y \pm i\epsilon} dy \pm i\pi f(0) \quad (7.94)$$

when $f(y)$ is a complex-valued function that is defined and continuous along the real axis. In our case, we have $f(y) = e^{\pm i(y \pm k')R}$ which satisfies this criterion. Let us consider the first term in Eq. (7.93) above. Here, $f(y) \rightarrow 0$ for large y in the upper complex half-plane for y . Therefore, we evaluate $\lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{f(y)}{y \pm i\epsilon} dy$ for this term by choosing the $+$ sign so that the pole of the integrand occurs in the lower half-plane. Then, we close the contour in the upper half-plane so that the integral vanishes due to the residue-theorem (as the contour does not enclose any poles). We are then left with only the $+i\pi f(0)$ term which for the first term equals $i\pi e^{ik'R}$.

We then repeat this procedure for the rest of the terms in Eq. (7.93), choosing each time a sign for ϵ and a contour which allows us to discard the integral since no poles are enclosed. This gives

$$K = \frac{m\pi}{R} \cos(k'R). \quad (7.95)$$

We are allowed to consider this integral for a fixed k' , since k' is always finite (due to the integration over k' going only up to k_F at $T = 0$). Instating this expression for K into our expression for I gives:

$$\begin{aligned} I &= -\frac{8m\pi J^2}{RN^2} \frac{V^2}{(2\pi)^4} \int_0^{k_F} dk' (k')^2 \frac{\sin(k'R) \cos(k'R)}{k'R} \\ &= -\frac{8m\pi J^2}{R^2 N^2} \frac{V^2}{(2\pi)^4} \int_0^{k_F} dk' k' \sin(k'R) \cos(k'R). \end{aligned} \quad (7.96)$$

The integral gives

$$\int_0^{k_F} dk' k' \sin(k'R) \cos(k'R) = \frac{1}{8R^2} [\sin(2k_F R) - 2k_F R \cos(2k_F R)]. \quad (7.97)$$

Thus, we arrive at the final result

$$\begin{aligned} I &= -\frac{8m\pi J^2}{R^2 N^2} \frac{V^2}{(2\pi)^4} \frac{1}{8R^2} [\sin(2k_F R) - 2k_F R \cos(2k_F R)] \\ &= -\frac{m\pi J^2}{(2\pi)^4 R^4} \frac{V^2}{N^2} [\sin(2k_F R) - 2k_F R \cos(2k_F R)]. \end{aligned} \quad (7.98)$$

Superconducting case

In the superconducting case, the method is the same. The only difference is that we have to use a different ansatz for the generator S in order to satisfy

$$\Delta H + i[S, H_0] = 0 \quad (7.99)$$

since now H_0 is not just a free-electron gas, but it also contains the superconducting term Δ . Before proceeding, however, we should first diagonalize H_0 with a diagonalizing matrix P that has the eigenvectors as columns. This will make it easier to choose a good ansatz for S . We start with a superconductor including a spin-splitting field (Meservey-Tedrow):

$$H_0 = \frac{1}{2} \sum_{k\sigma} \phi_{k\sigma}^\dagger M_{k\sigma} \phi_{k\sigma}, \quad (7.100)$$

where

$$\phi_{k\sigma} = \frac{1}{2} \begin{pmatrix} c_{k\sigma} \\ c_{-k,-\sigma}^\dagger \end{pmatrix}, \quad M_k = \begin{pmatrix} \epsilon_{k\sigma} & \sigma\Delta \\ \sigma\Delta & -\epsilon_{k,-\sigma} \end{pmatrix} \quad (7.101)$$

where $\epsilon_{k\sigma} = \epsilon_k - \sigma h$. It is diagonalized to

$$H = \sum_{k\sigma} E_{k\sigma} \gamma_{k\sigma}^\dagger \gamma_{k\sigma} \quad (7.102)$$

where

$$E_{k\sigma} = \sqrt{\epsilon_k^2 + (\sigma\Delta)^2} - \sigma h. \quad (7.103)$$

The relation between the original fermions and the new quasiparticles is:

$$\begin{pmatrix} \gamma_{k\sigma} \\ \gamma_{-k,-\sigma}^\dagger \end{pmatrix} = P_{k\sigma}^\dagger \begin{pmatrix} c_{k\sigma} \\ c_{-k,-\sigma}^\dagger \end{pmatrix} \quad \text{where} \quad P_{k\sigma}^\dagger = \begin{pmatrix} u_k^* & \sigma v_k^* \\ -\sigma v_k^* & u_k^* \end{pmatrix}. \quad (7.104)$$

The matrix elements are

$$u_k = \sqrt{\frac{1}{2} \left(1 + \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}} \right)}, \quad v_k = \sqrt{\frac{1}{2} \left(1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}} \right)}. \quad (7.105)$$

Note how the coherence factors are invariant under parity reversal and also independent on spin. The perturbation is

$$\Delta H = \sum_{kk'\alpha\beta} T_{kk'\alpha\beta} c_{k\alpha}^\dagger c_{k'\beta} \quad (7.106)$$

with

$$T_{kk'\alpha\beta} = \sum_j \frac{J}{N} e^{i(k-k')r_j} \mathbf{S}_j \cdot \boldsymbol{\sigma}_{\alpha\beta}. \quad (7.107)$$

After expressing the c -operators in terms of γ -operators via:

$$\begin{aligned} c_{k\sigma}^\dagger &= \gamma_{k\sigma}^\dagger u_k^* - \gamma_{-k,-\sigma} \sigma v_k^*, \\ c_{k\sigma} &= \gamma_{k\sigma} u_k - \gamma_{-k,-\sigma}^\dagger \sigma v_k, \end{aligned} \quad (7.108)$$

we obtain the expression:

$$\Delta H = \sum_{kk'\alpha\beta} T_{kk'\alpha\beta} [u_k^* u_{k'} \gamma_{k\alpha}^\dagger \gamma_{k'\beta} - u_k^* v_{k'} \beta \gamma_{k\alpha}^\dagger \gamma_{-k',-\beta}^\dagger - v_k^* u_{k'} \alpha \gamma_{-k,-\alpha} \gamma_{k',\beta} + v_k^* v_{k'} \alpha \beta \gamma_{-k,-\alpha} \gamma_{-k',-\beta}^\dagger]. \quad (7.109)$$

The next step is to find S so that

$$i[H_0, S] = \Delta H, \quad (7.110)$$

which allows us to find the effective Hamiltonian

$$H_{\text{eff}} = H_0 + \frac{i}{2} [S, \Delta H]. \quad (7.111)$$

To find this S , the point is to choose an ansatz for it that has the same operator-structure as ΔH , as we reasoned previously. Therefore, we choose the ansatz

$$\sum_{kk'\alpha\beta} [A_{kk'\alpha\beta}\gamma_{k\alpha}^\dagger\gamma_{k'\beta} + B_{kk'\alpha\beta}\gamma_{k\alpha}^\dagger\gamma_{-k',-\beta}^\dagger + C_{kk'\alpha\beta}\gamma_{-k,-\alpha}\gamma_{k',\beta} + D_{kk'\alpha\beta}\gamma_{-k,-\alpha}\gamma_{-k',-\beta}^\dagger] \quad (7.112)$$

Inserted into Eq. (7.110), we identify

$$A_{kk'\alpha\beta} = \dots \quad (7.113)$$

$$B_{kk'\alpha\beta} = \dots \quad (7.114)$$

$$C_{kk'\alpha\beta} = \dots \quad (7.115)$$

$$D_{kk'\alpha,\beta} = \dots \quad (7.116)$$

$$(7.117)$$

Note that $E_{k,\sigma} = E_{-k,\sigma}$.

Now, it should be possible to use S to compute H_{eff} and finally take the expectation value $\langle H_{\text{eff}} \rangle$ in the ground-state (where only terms like $\gamma_{k\alpha}^\dagger\gamma_{k\alpha}$ will contribute since H_0 is diagonal) to get an expression for the RKKY interaction. We get: ...

7.6.3 Application: Anderson and Kondo model

7.7 Kubo formula: linear response

The Kubo formula, named for Ryogo Kubo who first presented the formula in 1957, is an equation which expresses the linear response of an observable quantity due to a time-dependent perturbation. The Kubo formula is extremely useful and can be used to compute conductivities and charge and spin susceptibilities of systems of electrons in response to applied electric and magnetic fields. Responses to external mechanical forces and vibrations can be calculated as well. Below, we present a detailed derivation of this formula, including some finer points which are usually excluded in other textbooks or lecture notes. We also explain why conductivities and susceptibilities can be complex and what the physical meaning of the real and imaginary terms are (both are measurable).

In thermodynamic equilibrium, the expectation value of an observable A is evaluated according to

$$\langle A \rangle = \text{Tr}\{\rho_S(t)A_S\} = \frac{1}{Z} \sum_n \langle n(t) | A | n(t) \rangle e^{-\beta E_n} \quad (7.118)$$

since

$$\rho = \frac{e^{-\beta H_0}}{Z} = \frac{1}{Z} \sum_n |n(t)\rangle \langle n(t)| e^{-\beta E_n}. \quad (7.119)$$

Here, ρ is the density operator and $Z = \text{Tr}\{e^{-\beta H_0}\}$. The states $|n(t)\rangle$ are the eigenstates of H_0 and E_n its eigenenergies.

The time evolution of the states in the Schrödinger picture are given as $|n(t)\rangle = |n(t=0)\rangle e^{-iE_n t}$ for a time-independent Hamiltonian. The time-dependence in the above expression then cancels, and we have that $\langle A \rangle$ is time-independent. However, if a time-dependent perturbation is turned on

at $t = t_0$, the time-evolution is governed by the time-dependent $H(t)$ and the states are no longer stationary.

Above, we have used the Schrodinger picture to evaluate the expectation value. However, the expectation value is independent on which picture we use, and we could also write it in the Heisenberg or interaction picture generally as:

$$\langle A \rangle = \text{Tr}\{\rho_H A_H(t)\} = \text{Tr}\{\rho_I(t) A_I(t)\} \quad (7.120)$$

For a time-independent Hamilton-operator $H = H_0 + H'$, we have

$$\begin{aligned} \rho_S(t) &= -e^{-iHt} \rho_S(t=0) e^{iHt}, \\ \rho_H &= e^{iHt} \rho_S(t) e^{-iHt}, \\ \rho_I(t) &= e^{iH_0 t} \rho_S(t) e^{-iH_0 t}. \end{aligned} \quad (7.121)$$

We note that if $H = H_0$, then all density matrices $\rho_S(t), \rho_H, \rho_I(t)$ are equal for all times up to $t = t_0$ since they are time-independent.

Having established some basic relations, consider now a time-dependent Hamiltonian $H(t) = H_0 + H'(t)\theta(t - t_0)$ where the system is in equilibrium up to and including t_0 whereas a time-dependent perturbation starts acting infinitesimally after t_0 . The system will then start to evolve according the full $H(t)$ after t_0 and so reside in a non-equilibrium state. The Kubo formula relates the expectation value in the non-equilibrium state to a time-dependent commutator evaluated in the equilibrium state. This is advantageous since equilibrium state expectation values are easier to evaluate and can also be decomposed into 2-point Green functions using Wick's theorem.

In the interaction picture, one derives from the above definition of $\rho_I(t)$ and the equation of motion for the density matrix in the Schrodinger picture,

$$\frac{\partial \rho_S(t)}{\partial t} = -\frac{i}{\hbar} [H, \rho_S(t)], \quad (7.122)$$

that

$$\frac{\partial \rho_I(t)}{\partial t} = -\frac{i}{\hbar} [H'_I(t), \rho_I(t)]. \quad (7.123)$$

This is integrated to yield

$$\begin{aligned} \rho_I(t) &= \rho_I(t_0) - \frac{i}{\hbar} \int_{t_0}^t dt' [H'_I(t'), \rho_I(t')] \\ &\simeq \rho_I(t_0) - \frac{i}{\hbar} \int_{t_0}^t dt' [H'_I(t'), \rho_I(t_0)]. \end{aligned} \quad (7.124)$$

Above, we reinserted $\rho_I(t)$ on the right hand side and truncated at linear order in the perturbation H'_I . This is the linear response approach. Thus, the expectation value of an observable A is then:

$$\begin{aligned} \langle \hat{A}(t) \rangle &= \text{Tr}\{\rho_I(t) A_I(t)\} \\ &\simeq \text{Tr}\{\rho_I(t_0) A_I(t)\} - \frac{i}{\hbar} \int_{t_0}^t dt' \text{Tr}\{[H'_I(t'), \rho_I(t_0)] A_I(t)\} \\ &= \text{Tr}\{e^{-iH_0 t} \rho_S(t_0) e^{iH_0 t} A_S\} - \frac{i}{\hbar} \int_{t_0}^t dt' \text{Tr}\{\rho_I(t_0) [A_I(t), H'_I(t')]\} \end{aligned} \quad (7.125)$$

where we used that $\rho_I(t_0) = \rho_S(t_0)$ and also $\text{Tr}\{H\rho A - \rho H A\} = \text{Tr}\{\rho[O, H]\}$ via the cyclic property of trace. Now, the term inside the first trace is now $\rho_S(t_0)O_S$ since ρ_S is time-independent up to t_0 so that $\rho_S(t_0)$ commutes with H_0 . We obtain

$$\begin{aligned}\langle \hat{A}(t) \rangle &= \langle \hat{A}(t) \rangle_0 - \frac{i}{\hbar} \int_{t_0}^t dt' \text{Tr} \left\{ \rho_I(t_0) [A_I(t), H'_I(t')] \right\} \\ &= \langle \hat{A}(t) \rangle_0 - \frac{i}{\hbar} \int_{t_0}^t dt' \langle [A_I(t), H'_I(t')] \rangle_0.\end{aligned}\quad (7.126)$$

We here used that in the term $\text{Tr} \left\{ \rho_I(t_0) [A_I(t), H'_I(t')] \right\}$, $\rho_I(t_0) = \rho_H$ while $A_I(t)$ and $H'_I(t')$ are Heisenberg operators in the unperturbed system since their time dependence is determined by H_0 . Therefore, the trace is the definition of the expectation value of the product of two Heisenberg operators in the equilibrium case, which permits us to make the transition to the second line.

Now consider the specific observable $\hat{A} = \hat{J}^Q$. We have

$$\hat{J}_x^Q(\mathbf{r}_i, t) = e\hat{J}_x^P(\mathbf{r}_i) + e^2\hat{K}_x(\mathbf{r}_i)A_x(\mathbf{r}_i, t) \quad (7.127)$$

where $\hat{J}_x^P$ is the particle current flowing in the x -direction

$$\hat{J}_x^P = it \sum_{\sigma} (c_{i+\hat{x},\sigma}^{\dagger} c_{i\sigma} - c_{i\sigma}^{\dagger} c_{i+\hat{x},\sigma}) \quad (7.128)$$

while $\hat{K}_x(\mathbf{r}_i)$ is the kinetic energy associated with x -oriented hopping, namely

$$\hat{K}_x(\mathbf{r}_i) = -t \sum_{\sigma} (c_{i+\hat{x},\sigma}^{\dagger} c_{i\sigma} + c_{i\sigma}^{\dagger} c_{i+\hat{x},\sigma}). \quad (7.129)$$

Finally, e is the electron charge while A_x is the x -component of the vector potential. Note that a time-dependent vector potential can model an applied electric field. The field is assumed weak and enters the lattice model via a Peierls substitution on the hopping elements. All of the above is derived in a lattice model in the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, setting the scalar potential $\phi = 0$, in the textbook *Bogoliubov-de Gennes Method and Its Applications* by J.-X. Zhu.

The expectation value of the current is an observable and thus has to be real. Therefore, A_x must be a real scalar. However, we can still work with a complex vector potential $A_x(\mathbf{r}_i, t) = \frac{1}{i\omega} E_x e^{i(\mathbf{q} \cdot \mathbf{r}_i - \omega t)}$ since $\mathbf{E} = -\partial_t \mathbf{A} = E_x e^{i(\mathbf{q} \cdot \mathbf{r}_i - \omega t)} \hat{\mathbf{x}}$ if we write $\hat{J}_x^Q = e\hat{J}_x^P(\mathbf{r}_i) + e^2\hat{K}_x(\mathbf{r}_i)\text{Re}\{A_x(\mathbf{r}_i, t)\}$.

We note that, generally, if an electric field $E = E_0 \cos \omega t$ is applied, the electric current response can be out of phase:

$$J^Q = \sigma_1 E_0 \cos \omega t + \sigma_2 E_0 \sin \omega t = J_0 \cos(\omega t - \delta). \quad (7.130)$$

This relation can be expressed as $J^Q = \text{Re}(\sigma E_0 e^{-i\omega t})$ where $\sigma = \sigma_1 + i\sigma_2$ is a complex conductivity. In the end, we will see that this is exactly the type of relation we will obtain. Note that the out-of-phase contribution can occur even if we work with purely real quantities all the way, due to the integral over dt' with an integrand that depends on $H'_I(t')$ (which in turn will turn depends on the perturbing electric field).

General frequency symmetry for complex conductivity

On general grounds, we should be able to write a current $J(t)$ as

$$J(t) = \int dt' \sigma(t-t') E(t') \quad (7.131)$$

where all quantities are real. Here, $E(t)$ is an electric field and $\sigma(t-t')$ is the response function. This equation takes into account that the current $J(t)$ not necessarily follows the electric field instantaneously, but that the current at time t may depend on the behavior of the electric field at any time smaller than t .

To preserve causality, we must demand that $\sigma(t-t') = 0$ if $t' > t$. Thus, σ must be a retarded response function. Now assume a harmonically varying electric field. As noted previously in these notes, the response of the current can in general be out of phase with the electric field input, so that it may have both a cos and sin part. We can then write $E(t)$ as a complex quantity, $E(t) = E_0 e^{-i\omega t}$, so long that we take the real part of the expression for the current in the end:

$$J(t) = \text{Re} \int dt' \sigma(t-t') E(t') \quad (7.132)$$

But we may write this as

$$J(t) = \text{Re} \int dt' \sigma(t-t') e^{i\omega(t-t')} E(t). \quad (7.133)$$

Now switch variable to $\tau = t - t'$, and we see that this is a Fourier-transformation of $\sigma(t-t')$ [we consider t to be a fixed variable where the current is evaluated]. Therefore,

$$J(t) = -\text{Re}\{\sigma(\omega) E_0 e^{-i\omega t}\} \quad (7.134)$$

where $\sigma(\omega)$ is the complex conductivity, which is the FT of the real quantity $\sigma(t-t')$. This is where the frequency symmetry of $\sigma(\omega)$ can be discussed. If $\sigma(t-t')$ is real, we see from

$$\sigma(t) = \int d\omega e^{-i\omega t} \sigma(\omega) \quad (7.135)$$

that the FT quantity generally must satisfy

$$\sigma(\omega) = \sigma^*(-\omega). \quad (7.136)$$

It follows that

$$\text{Re } \sigma(\omega) = \text{Re } \sigma(-\omega) \quad (7.137)$$

and

$$\text{Im } \sigma(\omega) = -\text{Im } \sigma(-\omega) \quad (7.138)$$

The real part of the the complex conductivity thus has to be symmetric to guarantee that the conductivity in the time-domain is real and thus physical.

Identifying an expression for $\sigma(\omega)$

Now, we have $H \simeq H_0 - ea \sum_i A_x(\mathbf{r}_i, t) J_x^P(\mathbf{r}_i) \equiv H_0 + H'$. In $\langle \hat{A}(t) \rangle_0$, only $e^2 \hat{K}_x(\mathbf{r}_i) A_x(\mathbf{r}_i, t)$ survives since there is no current without external field in equilibrium (a bulk system). Thus, we have

$$\langle \hat{J}_x^Q(\mathbf{r}_i, t) \rangle = \langle e^2 \hat{K}_x(\mathbf{r}_i) A_x(\mathbf{r}_i, t) \rangle - \frac{i}{\hbar} \int_{t_0}^t dt' \langle [e \hat{J}_x^P(\mathbf{r}_i, t), (-ea) \sum_i A_x(\mathbf{r}_i, t') J_x^P(\mathbf{r}_i, t')] \rangle_0. \quad (7.139)$$

The expectation value of $\hat{J}_x^P$ has to be real. Moreover, $i \langle [\hat{J}_x^P(\mathbf{r}_i, t), \hat{J}_x^P(\mathbf{r}_i, t')] \rangle$ has to be real since $\hat{J}_x^P$ is a Hermitian operator. We can now use the complex representation of A_x if we everywhere replace A_x with $\text{Re}\{A_x\}$. But it turns out that we can extract the $\text{Re}\{\dots\}$ operation to act on the entire expression by noting the following. If $\langle \hat{f} \rangle$ is real, then for a complex scalar c (here c includes A_x and other prefactors) we have $\langle \text{Re}\{c\} \hat{f} \rangle = \text{Re}\{c\} \langle \hat{f} \rangle = \text{Re}\{c \langle \hat{f} \rangle\} = \text{Re}\{\langle c \hat{f} \rangle\}$ and this can also be used for each time-step in the integral, since the expectation value of the integrand is always real. This is valid since we can assume that $t - t_0$ is infinitesimal and then gradually increase it: for each step, it has to be real. We can apply this trivially to the first term and also to the second term in Eq. (7.139) by letting $\hat{f} = -\frac{i}{\hbar} [\hat{J}_x^P(\mathbf{r}_i, t), J_x^P(\mathbf{r}_i, t')] \rangle$ while $\text{Re}\{c\} = -ea \text{Re}\{A_x(\mathbf{r}_i, t')\}$. Inserting now the complex representation for A_x in the expression for H' gives:

$$\begin{aligned} H' &= -ea \sum_i A_{x0} e^{-i\omega t} e^{i\mathbf{q} \cdot \mathbf{r}_i} J_x^P(\mathbf{r}_i) \\ &= -ea A_{x0} e^{-i\omega t} J_x^P(-\mathbf{q}) \\ &= -\frac{ea E_{x0}}{i\omega} e^{-i\omega t} J_x^P(-\mathbf{q}) \\ &= \frac{iea E_{x0}}{\omega} e^{-i\omega t} J_x^P(-\mathbf{q}). \end{aligned} \quad (7.140)$$

Thus:

$$\begin{aligned} \langle \hat{J}_x^Q(\mathbf{r}_i, t) \rangle &= \text{Re} \left\{ e^2 A_x(\mathbf{r}_i, t) \langle \hat{K}_x(\mathbf{r}_i) \rangle + \frac{e^2 a E_{x0}}{\hbar \omega} \int_{t_0}^t dt' \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle_0 e^{-i\omega t'} \right\} \\ &= \text{Re} \left\{ e^2 A_x(\mathbf{r}_i, t) \langle \hat{K}_x(\mathbf{r}_i) \rangle + \frac{e^2 a E_x(\mathbf{r}_i, t) e^{-i\mathbf{q} \cdot \mathbf{r}_i}}{\hbar \omega} \int_{t_0}^t dt' \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle_0 e^{i\omega(t-t')} \right\} \end{aligned} \quad (7.141)$$

In this way, we obtain:

$$\langle \hat{J}_x^Q(\mathbf{r}_i, t) \rangle = \text{Re} \left\{ \frac{-ie^2}{\omega} E_x(\mathbf{r}_i, t) \langle \hat{K}_x(\mathbf{r}_i) \rangle + \frac{e^2 a E_x(\mathbf{r}_i, t) e^{-i\mathbf{q} \cdot \mathbf{r}_i}}{\hbar \omega} \int_{t_0}^t dt' e^{i\omega(t-t')} \langle J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t') \rangle_0 \right\} \quad (7.142)$$

We can now write this in term of a complex conductivity which gives both the reactive and dissipative response of the current to the applied electric field:

$$\langle \hat{J}_x^Q(\mathbf{r}_i, t) \rangle = \text{Re}\{\sigma E_x\} \quad (7.143)$$

where we defined

$$\sigma(\mathbf{q}, \omega, \mathbf{r}_i) \equiv -\frac{ie^2}{\omega} \langle \hat{K}_x(\mathbf{r}_i) \rangle + \frac{e^2 a e^{-i\mathbf{q} \cdot \mathbf{r}_i}}{\hbar \omega} \int_{t_0}^t dt' e^{i\omega(t-t')} \langle J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t') \rangle_0. \quad (7.144)$$

Physical interpretation of real and imaginary part of a susceptibility or transport coefficient

Note that for a given generalized susceptibility that provides a relation between a response and an input, such as the magnetization due to an external field $M = \chi B$ or as in the present case the current due to an electric field $J = \sigma E$ (χ and σ thus being the generalized susceptibilities in these cases), it is the symmetry-properties under time-reversal for the observable (M, J) and stimulus (E, B) that determines whether the real and imaginary parts of the response function are reactive or dissipative. We will give a mathematical proof of this below.

Consider first the dc case where there is no time-dependence. For instance, since both M and B are odd under time-reversal, χ has to be even under time-reversal. This is different for spin and charge currents. If a spin current is driven by an electric field, as it can be due to spin-orbit coupling, one has $J_s = \sigma_s E$ where J_s and E both are time-reversal symmetric. Thus, σ_s has to be time-reversal symmetric. This is in sharp contrast to Ohm's law $J = \sigma E$ since the charge current is time-reversal odd. Then, σ (conductivity) also has to be time-reversal odd, and describes dissipation due to Joule heating. Note that in the case of a superconductor where $J = \sigma A$ with the vector potential A , σ becomes even under time-reversal and correctly describes a reactive transport that does not dissipate energy. For dc transport, reactive in general then refers to a response function which is even under time-reversal, whereas dissipative refers to the part which is odd under time-reversal.

Note that Hall currents are dissipationless, as can be seen from the following argument. **<insert Landau and Nagaosa arguments>**

Consider now the ac case where the stimulus and observable response are time-dependent. In this case, it is useful to work with a complex representation of the observable, response function, and stimulus, as we noted in Eq. **INSERT**. Note how we saw in the case of current and electric field that both the real and imaginary part of the conductivity can contribute to the current response. This happens even if the real part of the conductivity describes a dissipative process and the imaginary part describes a dissipationless process. A concrete example of a dissipationless process contributing to the current response is inductance in a circuit, which describes stored energy that is returned to the system.

The part of the susceptibility, or response function, that leads to dissipation can be calculated by computing the energy loss in the system when applying a generalized "force" such as B or E . This can be either the real or imaginary part, depending on which specific observable-stimulus pair we consider. We now give two concrete examples of computation of the dissipation in a system expressed in terms of the response function.

Let us first show how the energy change (dissipation) in the system can be computed quantum mechanically. The change in energy is the time-derivative of the expectation value of the Hamiltonian:

$$\frac{dW}{dt} = \frac{d}{dt} \text{Tr}(\rho H) \quad (7.145)$$

where ρ is the density matrix of the system. Note that the Hamiltonian includes a time-dependent perturbation in the form of a source term

$$H_{\text{source}}(t) = \phi(t) \mathcal{O}(t). \quad (7.146)$$

This could be for instance a magnetic field coupling to spin ($\phi = B, \mathcal{O} = S$) or a magnetic vector potential coupling to charge current ($\phi = A, \mathcal{O} = J$). Now we can evaluate the above trace, and thus

dW/dt , in either the Heisenberg or Schrodinger picture: it does not matter which one we choose, since the answer must be the same. Let us choose the Schrodinger picture. In this case, the density matrix satisfies

$$i\dot{\rho} = [H, \rho] \quad (7.147)$$

whereas we note in passing that in the Heisenberg picture, the density matrix is a constant since states are time-independent. This means that $\text{Tr}(\dot{\rho}H) = 0$ as can be seen by writing out the commutator. In the Schrodinger picture, only the source-term has a time-dependence and so we get $\dot{H} = \mathcal{O}\dot{\phi}(t)$. This gives us the change in energy:

$$\frac{dW}{dt} = \text{Tr}(\rho\mathcal{O}\dot{\phi}) = \langle\mathcal{O}\rangle_{\phi}\dot{\phi} = [\langle\mathcal{O}_{\phi=0} + \delta\langle\mathcal{O}\rangle]\dot{\phi} \quad (7.148)$$

where $\langle\mathcal{O}\rangle_{\phi}$ is the expectation value of $\mathcal{O}$ using the time-dependent Hamiltonian eigenstates. Looking at a periodically varying source

$$\phi(t) = \text{Re}(\phi_0 e^{-i\omega t}) \quad (7.149)$$

and we can then compute average work done over a complete cycle:

$$\frac{d\bar{W}}{dt} = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \frac{dW}{dt}. \quad (7.150)$$

Inserting Eq. (7.148) into this equation, the contribution from $\langle\mathcal{O}_{\phi=0}$ vanishes when integrated over a full cycle since $\dot{\phi}$ gives the only time-dependence and has zero average. We are left with

$$\frac{d\bar{W}}{dt} = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \int_{-\infty}^{\infty} dt' \chi(t-t') \phi(t') \dot{\phi}(t). \quad (7.151)$$

Here we used that the change in the observable $\delta\langle\mathcal{O}\rangle$, which enters dW/dt , can be written in terms of the response function χ according to

$$\delta\langle\mathcal{O}\rangle(t) = \int dt' \chi(t-t') \phi(t'). \quad (7.152)$$

This holds for systems that are time-translation invariant without the perturbation, so that the linear response function $\chi(t-t')$ only depends on the relative time-coordinate. Now Fourier-transform the response function χ and write out the source terms explicitly to get:

$$\begin{aligned} \frac{d\bar{W}}{dt} &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \int_{-\infty}^{\infty} dt' \int \frac{d\omega'}{2\pi} \chi(\omega) e^{-i\omega(t-t')} \\ &\quad \times \frac{1}{4} [\phi_0 e^{-i\omega t'} + \phi_0^* e^{i\omega t'}] [-i\omega \phi_0 e^{-i\omega t} + i\omega \phi_0^* e^{i\omega t}] \\ &= \frac{1}{4} [\chi(\omega) - \chi(-\omega)] |\phi_0|^2 i\omega. \end{aligned} \quad (7.153)$$

The ϕ^2 and $(\phi^*)^2$ terms cancel out after performing the $\int dt$. To arrive at the final result, we only need to use the fact that the real part of a response function $\chi(\omega) = \chi' + i\chi''$ must always be symmetric in ω and that the imaginary part is antisymmetric. This follows from the fact that the response function $\chi(t)$ expressed in real-time must be purely real. Thus, only the imaginary part survives and we get the final result

$$\frac{d\bar{W}}{dt} = -\frac{1}{2} \omega \chi''(\omega) |\phi_0|^2. \quad (7.154)$$

This proves that the imaginary part of the response function is what determines the dissipation in the system.

At first glance it looks like we are contradicting what we wrote earlier. There, we stated that it is the real part of the response function (conductivity) which is dissipative, not the imaginary part. The resolution lies in considering what the source term ϕ is. We wrote the perturbation as $\mathcal{O}\phi$. If the observable is an electric current, then ϕ is the magnetic vector potential since these enter in the Hamiltonian precisely as $-\mathbf{J} \cdot \mathbf{A}$. In effect, in the particular case of electrical conductivity we have $\phi = -\mathbf{A}$. Since the response function was defined via $\delta\langle\mathcal{O}\rangle(t) = \int dt' \chi(t-t')\phi(t')$, it means that the χ in Eq. (7.154) is not the conductivity σ . Instead, we can find the relation between σ and χ as follows. We have

$$J(t) = \int \sigma(t-t')E(t') \quad (7.155)$$

and $E = -\dot{A} = \dot{\phi}$. We assume here for simplicity that we're dealing with just one component of $\mathbf{E}$ and $\mathbf{A}$ to not have to write vectors all the way (this does not detract any generality from the proof). We know that $\sigma(t-t') = 0$ for $t' > t$ due to causality, so that σ is a retarded response function. Moreover, we assume that the source term in the Hamiltonian is turned on adiabatically so that $\phi(t' \rightarrow -\infty) = 0$. These two conditions ensure that the surface term in a partial integration on Eq. (7.155) vanishes, leaving us with

$$J(t) = - \int \frac{d\sigma(t-t')}{dt'} \phi(t') dt'. \quad (7.156)$$

We have proven that $\chi(t-t') = -d\sigma(t-t')/dt'$. Let us now go back to the rate of energy change (dissipation) and insert this expression for χ into Eq. (7.151). Performing a partial integration on the $\int dt'$ integral, the surface term vanishes due to the two conditions mentioned above, and we are left with

$$\begin{aligned} \frac{d\bar{W}}{dt} &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \int_{-\infty}^{\infty} dt' \sigma(t-t') \dot{\phi}(t) \dot{\phi}(t') \\ &= \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt \int d\omega' \sigma(\omega') e^{-i\omega' t} \frac{1}{4} [-\omega^2 \phi_0^2 e^{-i\omega t} \delta(\omega' - \omega) \\ &\quad + \omega^2 |\phi_0|^2 e^{i\omega t} \delta(\omega' - \omega) + \omega^2 |\phi_0|^2 e^{-i\omega t} \delta(\omega' + \omega) - \omega^2 (\phi_0^*)^2 e^{i\omega t} \delta(\omega' + \omega)]. \end{aligned} \quad (7.157)$$

The terms with ϕ_0^2 and $(\phi_0^*)^2$ will cancel upon performing the $\int dt$ integral since they will be proportional to $e^{\pm 2i\omega t}$ after doing the Dirac-delta function integrals, and thus cancel upon averaging over one period. What remains is

$$\frac{d\bar{W}}{dt} = \frac{1}{4} \omega^2 |\phi_0|^2 [\sigma(\omega) + \sigma(-\omega)]. \quad (7.158)$$

Any response function has a real part that is even in frequency, so we are left with just the real part σ' of $\sigma = \sigma' + i\sigma''$. Moreover, since $|\phi_0| = |A| = |E/\omega|$, we end up with

$$\frac{d\bar{W}}{dt} = \frac{1}{2} |E|^2 \sigma'(\omega) \quad (7.159)$$

which agrees with the textbook result.

Note that if an electric field is given an explicit time-dependence, such as $E = E_0 \sin \omega t$, it can break time-reversal symmetry. This does not change the fact that the real part of the conductivity describes dissipation and the imaginary part dissipationless processes such as inductance, since we did take the time-dependence of the applied field into account in our derivation.

Can also add fluctuation-dissipation theorem derivation from Tong here.

To get rid of atomic fluctuations in the expressions, we average over the lattice sites via $(1/N) \sum_i$ and obtain

$$\begin{aligned} \sigma(\mathbf{q}, \omega) &= \frac{1}{N} \sum_i \sigma(\mathbf{q}, \omega, \mathbf{r}_i) \\ &= -\frac{ie^2}{\omega} \langle \hat{K}_x \rangle + \frac{e^2 a}{\hbar \omega N} \int_{t_0}^t dt' e^{i\omega(t-t')} \langle [J_x^P(\mathbf{q}, t), J_x^P(-\mathbf{q}, t')] \rangle_0. \end{aligned} \quad (7.160)$$

The current-current correlation function is actually dependent on $t - t'$ alone (relative time). This is physically reasonable since we are performing the average in the equilibrium system before the perturbation is applied, but let us also show this formally. For two general operators A and B in the interaction picture, we showed above that

$$\begin{aligned} \langle [\hat{A}_I(t), \hat{B}_I(t')] \rangle_0 &= \text{Tr} \{ \rho_I(t_0) [\hat{A}_I(t), \hat{B}_I(t')] \} \\ &= \text{Tr} \{ e^{-iH_0 t'} \rho_S(t_0) e^{iH_0 t} \hat{A}_S e^{-iH_0(t-t')} \hat{B}_S \\ &\quad - e^{-iH_0 t} \rho_S(t_0) e^{iH_0 t'} \hat{B}_S e^{-iH_0(t'-t)} \hat{A}_S \}. \end{aligned} \quad (7.161)$$

The point is now that

$$e^{-iH_0 t} \rho_S(t_0) = \rho_S(t_0) e^{-iH_0 t}, \quad (7.162)$$

as can be seen from the definition of the Schrodinger picture density matrix:

$$\rho_S(t_0) = \sum_n |n(t_0)\rangle \langle n(t_0)| e^{-\beta E_n}. \quad (7.163)$$

Note that $e^{-iH_0 t} \rho_S(t) \neq \rho_S(t) e^{-iH_0 t}$ for $t > t_0$, on the other hand, since $|n(t)\rangle$ are not eigenstates of H_0 for $t > t_0$, but rather of $H = H_0 + H'$. Making use of the commutation between $\rho_S(t_0)$ and H_0 , we see that there is only a dependence on $t - t'$ above. Since in general

$$\int_{t_0}^t f(t-t') dt' = - \int_{t-t_0}^0 f(\tau) d\tau = \int_0^{t-t_0} f(\tau) d\tau, \quad (7.164)$$

where $\tau = t - t'$, we see that we may write

$$\begin{aligned} \sigma(\mathbf{q}, \omega) &= -\frac{ie^2}{\omega} \langle \hat{K}_x \rangle + \frac{e^2 a}{\hbar \omega N} \int_0^{t-t_0} e^{i\omega\tau} \langle [J_x^P(\mathbf{q}, \tau), J_x^P(-\mathbf{q}, 0)] \rangle_0 d\tau \\ &= -\frac{ie^2}{\omega} \langle \hat{K}_x \rangle + \frac{e^2 a}{\hbar \omega N} \int_{-\infty}^{t-t_0} \theta(\tau) e^{i\omega\tau} \langle [J_x^P(\mathbf{q}, \tau), J_x^P(-\mathbf{q}, 0)] \rangle_0 d\tau. \end{aligned} \quad (7.165)$$

At this point, we let $\omega \rightarrow \omega + i\eta$ where $\eta \rightarrow 0^+$ everywhere in the above equation. This is mathematically equivalent to letting our electric field $\mathbf{E} = E_x e^{\eta t} e^{i(\mathbf{q} \cdot \mathbf{r}_i - \omega t)}$ from the start, since that is where ω comes from. The physical meaning of this is that we are turning on the electric field adiabatically, rather than abruptly. At $t_0 \rightarrow -\infty$, where the field is turned on from an equilibrium state where

it is zero, the magnitude of the electric field is slowly increased from zero to E_x at $t = 0$. We want to evaluate the response function at $t = 0$ where the field adiabatically has been ramped up to its final value.

This procedure is necessary for several reasons. One reason is mathematical: it ensures that the integral converges since the integrand goes to zero for large τ (keep in mind that the upper limit of the integral is $-t_0 \rightarrow \infty$ when we evaluate the conductivity at $t = 0$) due to the factor $e^{-\eta\tau}$. However, secondly, this also has physical meaning. It means that the influence of the perturbation H' at a time t' (in effect, the contribution of the integrand at t') to the response of the observable at time t should vanish when $t \gg t'$. Put differently, the physical significance of turning the field on slowly is that it causes the influence of the electric field at t' to have no influence on the value of the current at $t \gg t'$. This is reasonable physically since any form of relaxation mechanism, even if it is small, should prevent a perturbation to affect an observable at a much later time (longer than the relaxation time).

Therefore, by turning on the field gradually, our model takes into account that even though we have not included impurity scattering, we are in fact including some other unspecified relaxation mechanism (arbitrarily small, but not zero) which prevents the retarded effect of the perturbation to affect the physical observable to have an infinite range in time. The time-scale of turning on the electric field is thus not short compared to the duration of the the perturbation itself, as would have been the case for a field $\mathbf{E}$ that is abruptly switched on, and the system should have time to enter a stationary state at the time of evaluation $t = 0$.

Thirdly, it ensures that the response function (conductivity) in this case does not become purely imaginary, which is forbidden due to Kramers-Konig relations: a finite imaginary part implies a finite real part. We will see in the next subsection why the conductivity becomes purely imaginary for a normal metal if one does not include the η -factor coming from turning the field on gradually.

Thus, setting $t_0 \rightarrow -\infty$ and evaluating the conductivity at $t = 0$ where the field has been completely turned on, we may write:

$$\sigma(\mathbf{q}, \omega) = \lim_{\eta \rightarrow 0^+} \frac{e^2}{i(\omega + i\eta)} [-\Pi(\mathbf{q}, \omega) + \langle \hat{K}_x \rangle], \quad (7.166)$$

where we defined

$$\Pi(\mathbf{q}, \omega) = -\frac{ia}{\hbar N} \int_{-\infty}^{\infty} d\tau e^{i(\omega + i\eta)\tau} \theta(\tau) \langle [J_x^P(\mathbf{q}, \tau), J_x^P(-\mathbf{q}, 0)] \rangle_0. \quad (7.167)$$

This expression is consistent with the original papers by Scalapino *et al.* in 1992 and the BdG textbook by Zhu in his Eq. (2.92) (where the appearance of the $i\eta$ in the denominator is never explained). If impurities are added to the lattice model, however, it seems like it is not necessary to turn the field on gradually since the impurity scattering ensures that there is momentum relaxation in the system and thus a finite resistance and conductivity - there is no need to introduce any additional relaxation mechanism. The $i\eta$ in the denominator is not needed, but the $i\eta$ in the exponent in the integral still is needed to get guarantee a convergent integral, and thus turning the correlation function into the retarded one. This is consistent with the treatment in Rammer and Smith, Rev. Mod. Phys. (1986). However, we note that we *can* include the $i\eta$ in the denominator as well and still obtain the same result when impurities are treated in the Born approximation so that $G^{R/A}(\omega) = \frac{1}{\omega + i\eta - \xi_{\mathbf{k}} \pm i/\tau}$. The reason for this is that one can prove analytically (see the calculation by

Erik Hodt for altermagnets and the S^{RA} term specifically)) that the calculation of the conductivity includes a factor

$$\frac{1}{\omega + i\eta} \frac{1}{\omega + i/\tau} \quad (7.168)$$

which is identical to

$$\frac{1}{\omega + i\eta} \frac{1}{\omega + i/\tau} = \frac{1}{\omega^2 + i(\eta + 1/\tau)\omega - \eta/\tau} \simeq \frac{1}{\omega} \frac{1}{\omega + i/\tau} \quad (7.169)$$

so long that $1/\tau \gg \eta$. In practice, however, it is simpler just to keep the infinitesimal positive quantity in the exponent.

Let us first comment on the different behavior of the complex optical conductivity in the clean limit and when elastic impurity scattering is present.

Ballistic limit

Firstly, consider the clean limit and a normal metal. In that case, the standard textbook result for the evaluation of the above general expression for complex conductivity gives in the long-wavelength limit $\mathbf{q} = 0$ that

$$\sigma(0, \omega) = \frac{ne^2\pi}{m}\delta(\omega) + \frac{ine^2}{m\omega}. \quad (7.170)$$

The second term is referred to as the diamagnetic term. We see that as $\omega \rightarrow 0$, the both the real and imaginary part diverge. This is unphysical, but simply a result of the fact that we have an idealized situation with no scattering and thus no source of resistance in the system. A stationary state is achieved due to the relaxation time $\lim_{\eta \rightarrow 0^+} 1/\eta$, but this is extremely long and produces no resistance at $\omega = 0$.

Let us see how we get this form from the treatment in T. Yanagisawa and H. Shibata, *Optical properties of unconventional superconductors*, Frontiers in Superconductivity Research (Nova Science Publishers, 2004). The optical conductivity is given by Eq. (2.36):

$$\sigma(\mathbf{q}, \omega) = \frac{i}{\omega + i\delta} [\Pi(\mathbf{q}, \omega) - \Pi(\mathbf{q}, 0)] \quad (7.171)$$

where $\Pi(\mathbf{q}, \omega)$ is the current-current correlation function. We now consider the dc limit $\mathbf{q} = 0$. Taking $\Pi(\mathbf{q} \rightarrow 0, \omega = 0)$ in the last term gives the diamagnetic contribution to the optical conductivity (their Eq. 2.43):

$$\Pi(0, 0) = -\frac{ne^2}{m}. \quad (7.172)$$

On the other hand, taking the limit $\mathbf{q} \rightarrow 0$, then $\omega \rightarrow 0$ in the $\Pi(\mathbf{q}, \omega)$ term gives zero, as can be verified from their Eq. 2.45 (or Scalapino's Eq. 24). Therefore, we are left with

$$\sigma(\mathbf{q}, \omega) = \frac{i}{\omega + i\delta} \frac{ne^2}{m}. \quad (7.173)$$

We know that $\delta \rightarrow 0^+$ according to our above discussion regarding turning the field on gradually and ensuring that the perturbation does not have an effect for an infinite amount of time. Taking

this limit gives us

$$\begin{aligned}
\sigma(\mathbf{q}, \omega) &= \frac{i}{\omega + i\delta} \frac{ne^2}{m} \frac{\omega - i\delta}{\omega + i\delta} \\
&= \frac{i(\omega - i\delta)}{\omega^2 + \delta^2} \frac{ne^2}{m} \\
&= \frac{\delta}{\omega^2 + \delta^2} \frac{ne^2}{m} + \frac{i\omega}{\omega^2 + \delta^2} \frac{ne^2}{m} \\
&= \frac{ne^2}{m\pi} \delta(\omega) + \frac{i}{\omega} \frac{n^2}{m}.
\end{aligned} \tag{7.174}$$

The diamagnetic term thus survives (is not cancelled) and the real part is a δ -function. This is consistent with Scalapino's PRB 1993 where the $\langle -k_x \rangle$ term is the diamagnetic term and Λ_{xx} is the auto-correlation function which vanishes when $\mathbf{q} \rightarrow 0$ for a normal metal, leaving us again with a real part which has a delta-function and an imaginary part scaling like $1/\omega$.

Impurity scattering

Consider the case where impurity scattering τ is present. The textbook result is (obtained using Green functions that include the effect of elastic impurity scattering):

$$\sigma(0, \omega) = \frac{ne^2}{m} \frac{1}{1/\tau - i\omega} = \frac{ne^2\tau}{m(1 + \omega^2\tau^2)} + \frac{ine^2\omega\tau^2}{m(1 + \omega^2\tau^2)}. \tag{7.175}$$

Now, the real part is finite, but still has a strong peak at $\omega = 0$ so long that τ is large (close to clean limit). This is physical since we get a finite conductivity. The peak is called the Drude peak. The imaginary (dissipationless) part is absent at $\omega = 0$ so long that impurity scattering exists.

Consider some limiting cases. We see that we reproduce exactly the results for the ballistic case above if $\tau \rightarrow \infty$. In the opposite extremely diffusive limit of frequent impurity scattering, $\tau \rightarrow 0$, we may neglect the $\omega^2\tau^2$ term in the denominator and obtain a frequency-independent real part of the conductivity which is simply the Drude conductivity: $\text{Re}\{\sigma\} = ne^2\tau/m$. This is consistent with the normal-state limit of the Mattis-Bardeen formula in the sense that they also obtain a frequency independent real part of the conductivity and they do consider the diffusive limit.

The above result for the complex conductivity can be understood by the following simple physical argument. When an electric field $\mathbf{E}$ is applied, conduction electrons experience a force $-e\mathbf{E}$. In the presence of elastic impurity scattering, the electrons also experience a friction force which can be written $-(m/\tau)d\mathbf{r}/dt$. As usual the friction force is modelled to be proportional to the velocity of the particles. The mass is there because we can think of the friction force as ma_{friction} where a_{friction} is the deceleration provided by the impurity scattering. This deceleration should then be determined by the velocity and the inverse scattering time $1/\tau$. The more frequently the electrons scatter on impurities, the smaller the time τ between scattering events and thus the larger the damping of the electron motion. The total equation of motion then becomes

$$m \frac{d^2 \mathbf{r}(t)}{dt^2} = -e\mathbf{E} - \frac{m}{\tau} \frac{d\mathbf{r}(t)}{dt}. \tag{7.176}$$

We can write this in the Fourier representation by multiplying with $e^{i\omega t}$ and integrating over all t . This gives

$$-im\omega v(\omega) = -eE(\omega) - \frac{m}{\tau} v(\omega). \tag{7.177}$$

Solving for the velocity:

$$v(\omega) = \frac{-eE}{m} \frac{1}{1/\tau - i\omega}. \quad (7.178)$$

The current density is $j = -nev$ where n is the electron density. We can write this precisely as $j = \sigma(\omega)E$ with the complex conductivity

$$\sigma(\omega) = \frac{ne^2}{m} \frac{1}{1/\tau - i\omega}. \quad (7.179)$$

Hence, in the DC case $\omega \rightarrow 0$, we get the Drude conductivity $\sigma = \frac{ne^2\tau}{m}$ where an electric field drives a current whose magnitude is determined by the momentum relaxation τ . In the ballistic case $\omega \gg 1/\tau$, the conductivity instead becomes increasingly imaginary (non-dissipative). This is reasonable since the electric field now varies on a time-scale that is much smaller than the scattering time, and so the electrons behave as if there were no impurities, but cannot produce any net dissipate current flow due to the rapid variation of the field: they do not have sufficient time to respond to the field.

When impurity scattering is taken into account, the divergence $1/\omega$ of the diamagnetic term $\langle K_x \rangle$ is cancelled (which is proven analytically in Erik's approach or even in Altland's textbook) and one is left with Eq. (7.175) for a normal metal. Note how we regain the $\delta(\omega)$ behavior for the real part of σ in the limit $\tau \rightarrow \infty$ which can be seen by dividing nominator and denominator of the real part of Eq. (7.175) on $1/\tau^2$ and taking the limit $\tau \rightarrow \infty$. In the lattice case, using the inhomogeneous BdG equations, impurities can be straightforwardly incorporated, and since there is no delta-function behavior in the presence of impurities one may consider directly $\text{Re } \sigma$ and $\text{Im } \sigma$ without extracting any Drude weight explicitly.

For a general analytical derivation of the complex optical conductivity beyond a normal metal, including *e.g.* altermagnetism, see Erik Hodt's paper. For a superconductor, optical conductivity can be evaluated exactly as a function of frequency, temperature and impurity concentration: see <https://journals.aps.org/prl/pdf/10.1103/PhysRevLett.71.2304>.

Limiting cases of complex optical conductivity

Now we can start taking limits to obtain conductivities in various scenarios.

- The frequency-dependent, uniform conductivity is obtained via $\mathbf{q} \rightarrow 0$, corresponding to the application of a spatially uniform, time-dependent electric field.
- The dc conductivity corresponding to a constant electric field is obtained by first taking the limit $\mathbf{q} \rightarrow 0$ and then $\omega \rightarrow 0$, in that order. The order is important, because taking $\omega \rightarrow 0$ first corresponds to a different physical situation. In this case, one sets up a long wavelength static potential in which the electrons will find a new equilibrium position where no current flows. Thus, by taking $\omega \rightarrow 0$ first and then $\mathbf{q} \rightarrow 0$, one finds a purely imaginary conductivity corresponding to a non-dissipative response which is precisely the rearrangement of the electrons. In contrast, taking $\mathbf{q} \rightarrow 0$ first and then $\omega \rightarrow 0$, one sets up a uniform electric field which oscillates slowly with frequency, and thus gives rise to a current with a real component of the conductivity (dissipative).
- A zero-resistance state (which is *not* the same as a symmetry breaking superconductor in general) can according to Scalapino *et al.* PRL (1992) be identified if $\langle \hat{K}_x \rangle - \Pi(\mathbf{q} = 0, \omega) \neq 0$

when $\omega \rightarrow 0$. In this case, one defines the Drude weight $D \equiv \lim_{\omega \rightarrow 0} [\langle \hat{K}_x \rangle - \Pi(0, \omega)]$. However, as discussed in detail above, it is unclear to what extent this is justified from the derivation where the $i\delta$ factor is seemingly inserted without any reason. If correct, however, such behavior is acceptable in a metal without impurities and at zero temperature. Thus, one distinguishes between a metal ($D \neq 0$) and an insulator ($D = 0$) when the system has no impurities and is at zero temperature. At $T \neq 0$ or in the presence of disorder, $D(\omega \rightarrow 0) = 0$ while $\sigma \neq 0$ (but does not diverge) for a metallic system.

Superfluid density

Remarkably, we can also take a limit of the momentum and frequency to obtain the superfluid density of the system, which indicates a Meissner response in the system. This is the hallmark of superconductivity, and not a resistanceless current.

The superfluid density D_S is the proportionality factor between the current density and the vector potential. To see this, London showed that the Meissner effect follows if the current response to a static $\omega = 0$ and transverse gauge potential $\nabla \cdot \mathbf{A} = 0$ is

$$j_x = -\frac{1}{4\pi^2\lambda^2}A_x \quad (7.180)$$

in the long wavelength limit $q_y \rightarrow 0$. Keep in mind that $\mathbf{q}$ is the momentum characterizing the spatial variation of the applied magnetic field. In the gauge chosen above, we need $q_x = 0$ since $\nabla \cdot \mathbf{A} = 0$ gives $q_x A_x = 0$ for $A_x(\mathbf{r}_i) = A_x e^{i\mathbf{q} \cdot \mathbf{r}_i}$. Moreover, taking the $q_y \rightarrow 0$ limit is required since the EM response of a clean superconducting system is in general non-local [of the form $j(z) \propto \int f(z, z') A(z') dz'$, see discussion in the next paragraph]. Therefore, we get direct proportionality between j and A only when it is so slowly varying that it can be taken outside of the integral.

Following the same steps as before, but expressing $\langle \hat{j}_x^Q \rangle$ with $A_x(\mathbf{r}_i) = A_x e^{i\mathbf{q} \cdot \mathbf{r}_i}$ rather than $\mathbf{E}(\mathbf{r}_i, t)$, we get at large times:

$$\langle \hat{j}_x^Q \rangle = \text{Re}\{\tilde{D}_S A_x(\mathbf{r}_i)\} \quad (7.181)$$

where we have

$$\tilde{D}_S = -e^2 \langle K_x(\mathbf{r}_i) \rangle - ie^2 a e^{-i\mathbf{q} \cdot \mathbf{r}_i} \int_{-\infty}^{\infty} \theta(\tau) e^{i(\omega + i\eta)\tau} \langle [J_x^P(\mathbf{q}, \tau), J_x^P(-\mathbf{q}, 0)] \rangle_0 d\tau. \quad (7.182)$$

where $\eta \rightarrow 0^+$. From this, we may define the spatially averaged superfluid density

$$D_S = \lim_{\omega=0, q_x=0, q_y \rightarrow 0} \frac{1}{N} \sum_i \tilde{D}_S = \lim_{\omega=0, q_x \rightarrow 0, q_y \rightarrow 0} -e^2 \langle K_x \rangle + \Pi(\mathbf{q}, \omega). \quad (7.183)$$

If $D_S \neq 0$, we have a superconducting state. Note the difference in order in which $\omega \rightarrow 0$ and $\mathbf{q} \rightarrow 0$ for the Drude weight D and the superfluid density D_S . Importantly, there is no problem having $\omega = 0$ and $q \neq 0$ for a vector potential $\mathbf{A}$, which provides a physically acceptable $\mathbf{B}$, unlike the situation that arose in the $\mathbf{E}$ field case.

Finally, note that superfluid stiffness and density are often used synonymously in the literature, but they are in fact different quantities. The stiffness measures the energy cost of having a spatially varying superconducting U(1) phase. The density measures the density of Cooper pairs in the system, which in turn decides how large supercurrent that can be transported through the superconductor. The stiffness and density are proportional via the effective mass of the charge carriers,

which is probably the reason for why they are referred to as one another interchangeably, but they can be very different in magnitude for instance in heavy-fermion systems where the effective electron mass can be thousands of bare electron masses.

To understand why it is necessary to take the long wavelength limit of the superfluid density, one should note that the electromagnetic response of a clean superconductor is in general non-local: instead of $\mathbf{j}(x) = -K(x)\mathbf{A}(x)$ in the diffusive limit (local relation), one has $\mathbf{j}(x) = -\int K(x, x')\mathbf{A}(x')$ in the clean limit. A detailed discussion of this is given in Pippard's original paper from 1952 and was motivated by the experimental observation that changing the impurity concentration in superconducting indium by just 3% nearly doubled the penetration depth λ without changing thermodynamic quantities like T_c . In fact, the variation in λ commenced at an impurity concentration which rendered the mean free path and λ to be comparable in size.

This cast doubt on the phenomenological theory of London where the penetration depth $\lambda \propto \sqrt{m/n}$ depends only on constants that do not depend on the amount of impurity scattering present, such as the n number of superconducting electrons per unit volume or electron mass m . Such an expression for λ was inconsistent with the experimental findings.

This prompted a new description where the current is related to a spatial average of the vector potential over the superconductor. More precisely, to determine the current response at a point, one averages the vector potential over a region of size comparable to the coherence length ξ which does depend on the impurity concentration. Phenomenologically, one can think of this as the Cooper pairs having a spatial extent of ξ (which can be analytically shown by computing the Cooper pair correlator in real space). Therefore, when ξ becomes long enough that the vector potential varies significantly within the size of a given Cooper pair, the effective vector potential felt by them is a spatial average over $\mathbf{A}$. In contrast, for a slowly varying magnetic vector potential in real space (which corresponds precisely to the long wavelength limit), one recovers from Pippard's equation the London equation since the vector potential can be taken outside of the integral.

We also note that this has an analogy in the context of the skin effect in conductors. So long as l_{mfp} is short, so that the electric field is constant over a region comparable to l_{mfp} , one can use $\mathbf{j} = \sigma\mathbf{E}$. However, as the material gets so clean that l_{mfp} is comparable to the spatial variation of $\mathbf{E}$, one must use a non-local relation in which the current is related to an appropriate average of $\mathbf{E}$. This yields the anomalous skin effect.

7.8 Time-reversal symmetry for conductivity tensor and currents

Above, we explained the physical meaning of the real and imaginary parts of the conductivity tensor. In the literature, one often speaks about T -even and T -odd currents, for instance for spin currents in various systems. We now clarify what this means.

We consider the dc limit. It then follows from $J = \sigma E$ that σ must be T -odd for a charge current. In real time, σ is real, but after Fourier-transformation $\sigma = \sigma(\omega)$ is complex. The real part is thus T -odd, while the imaginary part is T -even. This is always true for any system.

Similarly, for spin current $J_s = \sigma_s E$, σ_s must be T -even for a spin current. The real part is thus dissipationless and T -even while the imaginary part is T -odd.

Then why does the literature refer to things like T -even and T -odd spin currents? The explanation follows.

T -even spin conductivity refers to a contribution that can be nonzero even when the system preserves time-reversal symmetry. T -odd spin conductivity refers to a contribution that vanishes in time-reversal symmetric systems and therefore requires explicit time-reversal symmetry breaking. Thus, the “ T -odd spin conductivity” discussed in the literature is not the imaginary part of σ_s . Rather, it is a real dc contribution which is zero in systems that are invariant under time-reversal. Such terms typically originate from Berry-curvature-like quantities, which become explicit after manipulations such as partial integration, as done *e.g.* in the Methods section of <https://www.nature.com/articles/s41467-024-45318-8>.

Thus, “ T -odd” characterizes whether a given contribution survives or vanishes under the time-reversal symmetry of the material, not the time-reversal parity of the linear-response tensor σ or σ_s itself.

We note that a quantum Hall current may therefore be said to be a T -odd charge current, because it only appears when T -symmetry is broken in the material by an external magnetic field. It does not appear in the absence of a field. Same goes for the anomalous quantum Hall effect in ferromagnets. This can be proven using Onsager relations, see Sec. III A in <https://arxiv.org/pdf/0904.4154>. A longitudinal charge current in a normal metal induced by an electric field should in contrast be referred to as a T -even charge current.

However, a key point requires clarification here regarding dissipation. Earlier, we stated that the real part of electric conductivity σ is odd under T , and thus describes dissipative transport. This only holds for the longitudinal component, since it is only current along the electric field which produces a voltage drop. This can be seen by considering that dissipation is computed from $\langle dH/dt \rangle$ where H is the Hamiltonian and the coupling between current and vector potential in the Hamiltonian is $\mathbf{J} \cdot \mathbf{A}$. Since $\mathbf{A} \parallel \mathbf{E}$, there is no coupling between the Hall current and the electric field and hence no dissipation contributing to $\langle dH/dt \rangle$. In other words, a component of the current transverse to the electric field does not produce any Joule heating since $\mathbf{J} \cdot \mathbf{E} = 0$ for such a current. Now, the Hall (or quantum Hall) current is precisely such a transverse current, but the Hall conductivity σ must still be odd under T . This means that the transverse current changes sign if we reverse the direction of the magnetic field, but this current is *still* dissipationless even if σ is real and odd under T .

Thus, the real part of σ is only dissipative for longitudinal currents. This can be seen mathematically by generalizing our earlier derivation of dissipation in the system to a case where σ is a tensor. In that case, we find that (see Sec. III A in <https://arxiv.org/pdf/0904.4154>)

$$\begin{aligned} \frac{d\bar{W}}{dt} &= \sum_{ab} \frac{1}{4} (\sigma_{ab}^* + \sigma_{ba}) E_a E_b^* \\ &= \frac{1}{4} \sum_{ab} [\text{Re}(\sigma_{ab} + \sigma_{ba}) \text{Re}(E_a E_b^*) + \text{Im}(\sigma_{ab} - \sigma_{ba}) \text{Im}(E_a E_b^*)]. \end{aligned} \quad (7.184)$$

Note that if we have an electric field in only one direction, it follows that only the longitudinal part of the conductivity contributes to dissipation, as we wrote above. In general, we see that $\text{Re}(\sigma_{ab} - \sigma_{ba})$, which is the intrinsic Hall response, thus does not contribute to dissipation, even if

we have components of the electric field in several directions. Notably, $\text{Im}(\sigma_{ab} - \sigma_{ba})$ does contribute to dissipation *if* we have a phase-lag between the field components.

The main message is thus that we have to be careful about stating that a part of the conductivity tensor is dissipative or not based on its time-reversal symmetry.

7.8.1 General expression spin Hall conductivity

The following derivation follows the Methods section of <https://www.nature.com/articles/s41467-024-45318-3>

The spin current generated by electric field can to linear response be written as

$$j_a^c = \sigma_{\text{spin},ab}^c E_b \quad (7.185)$$

where j_a^c is the spin current along the a -direction polarized in the c -direction. The spin current density is generally given as

$$\mathbf{j}^c = \sum_n \int \frac{d^2k}{(2\pi)^2} f_n(\mathbf{k}) \mathbf{j}_n^c(\mathbf{k}) \quad (7.186)$$

where n and $\hbar\mathbf{k}$ are band index and crystal momentum, whereas

$$\mathbf{j}_n^c(\vec{\gamma}) = \langle u_n(\mathbf{k}) | \frac{1}{2} \{ \hat{v}, \hat{s}^c \} | u_n(\mathbf{k}) \rangle \quad (7.187)$$

is the momentum-resolved spin current operator. In the relaxation time approximation, we know that

$$f_n - f_0 = -\frac{e}{\hbar} \tau \mathbf{E} \cdot \partial_{\mathbf{k}} f_0. \quad (7.188)$$

Performing a partial integration (in order to bring out the dependence on Berry-curvature, as previously mentioned), we obtain:

$$\sigma_{ab}^c = \frac{e}{\hbar} \tau \sum_n \int \frac{d^2k}{(2\pi)^2} f_0 \partial_{\mathbf{k}_b} j_{a,n}^c(\mathbf{k}). \quad (7.189)$$

7.9 Tunnel Hamiltonian formalism

A common perturbative technique to compute transport of various quantities is the tunnel Hamiltonian formalism. To consider its simplest form, we write it down for two normal metals coupled via tunneling:

$$\hat{H} = H_L + H_R + \sum_{\mathbf{k}\mathbf{k}'} T_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}}^\dagger d_{\mathbf{k}'} + \text{h.c.} \quad (7.190)$$

where c/d are fermion operators on the left and right side of the junction. The Hamiltonians $H_{L,R}$ describe the left and right regions and take the form $H_L = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$ and similarly for H_R .

We now derive this second-quantized Hamilton-operator starting from a 1st quantized Hamiltonian. We follow the book "Quantum kinetic theory and applications", appendix H.

Consider parabolic electrons moving in 3D in the presence of a 1D potential energy $U(z)$ which creates a barrier separating L and R regions. We also include a random scattering potential $V(\mathbf{x}, z)$

modelling impurities. Choose $z = 0$ as the interface region where the potential is maximal and then it decays into the L and R regions. Let $\mathbf{x} = (x, y)$ be the coordinates in the plane of the interface. We then have

$$\hat{H}\Psi(\mathbf{x}, z) = E\psi(\mathbf{x}, z), \quad \hat{H} = \frac{\hat{p}_z^2 + \hat{p}_{\mathbf{x}}^2}{2m} + U(z) + V(\mathbf{x}, z). \quad (7.191)$$

We consider here energies E which are smaller than the maximum value of $U(z)$, so that the barrier is classically impenetrable. We now decompose $U(z)$ into two parts:

$$U(z) = U_L(z) + U_R(z) \quad (7.192)$$

so that

$$U_L(z) = \begin{cases} U(z), & z < 0 \\ 0, & z > 0 \end{cases} \quad (7.193)$$

and oppositely for $U_R(z)$. In this way, $U_{L,R}$ represent impenetrable potential walls for electrons in the left and right regions, respectively. For each region $j = L, R$ we introduce the basis functions $F_{jk} = \langle z|jk\rangle$ satisfying the 1D Schrodinger equation

$$\left[\frac{\hat{p}_z^2}{2m} + U_j(z) \right] F_{jk}(z) = \epsilon_{jk} F_{jk}(z). \quad (7.194)$$

Generally, these basis functions and their eigenvalues ϵ_{jk} may depend on a variable k with specific allowed values arising from the boundary conditions (just like a particle-in-a-box wavefunction depends on a wavevector k_n and has energy eigenvalues E_n). These functions form complete sets for each region j and we let k be a discrete variable by adding a hard wall boundary condition at $z \rightarrow -\infty$ for the L region and vice versa for R (the spacing between each k -value can nevertheless be very small). The functions F_{jk} are guaranteed to be orthogonal (due to different eigenvalues) and also taken to be normalized:

$$\int_{-\infty}^{\infty} F_{jk'}^*(z) F_{jk}(z) dz = \delta_{kk'}. \quad (7.195)$$

Functions from different regions, however, are not guaranteed to be orthogonal since they belong to different Hamilton-operators. Their overlap is denoted

$$S_{j'k',jk} = \langle j'k'|jk\rangle = \int_{-\infty}^{\infty} F_{j'k'}^*(z) F_{jk}(z) dz, \quad j' \neq j. \quad (7.196)$$

Let us compute the matrix elements of Eq. (7.191) in the basis $|jk\rangle$. This will allow us to ultimately write down the second quantized Hamiltonian. The diagonal elements in j are:

$$\langle jk'|\hat{H}|jk\rangle = \delta_{kk'} \left(\frac{\hat{p}_x^2}{2m} + \epsilon_{jk} \right) + \langle jk'|V(\mathbf{x}, z)|jk\rangle + \langle jk'|U_{j'}(z)|jk\rangle_{j' \neq j}. \quad (7.197)$$

The last term in this expression contains an exponential smallness of second order with respect to the overlap factors S above. This is because this term is formed as an integral over a product of two wavefunctions of the region j over the region $j' \neq j$, where these functions decrease exponentially. We neglect such terms in the following. The remaining part of Eq. (7.197) then represents the matrix element that enters the second quantized Hamiltonian of region j .

The non-diagonal elements of $\hat{H}$ ($j' \neq j$) are computed as

$$\langle j'k'|\hat{H}|jk\rangle = S_{j'k',jk} \left[\frac{\hat{p}_x^2}{2m} + \frac{\epsilon_{jk} + \epsilon_{j'k'}}{2} \right] + t_{j'k',jk} + \langle j'k'|V(\mathbf{x}, z)|jk\rangle + \frac{1}{2} \langle j'k'|U_{j'}(z) - U_j(z) - \epsilon_{j'k'} + \epsilon_{jk}|jk\rangle, \quad (7.198)$$

where we have defined

$$t_{j'k',jk} = \frac{1}{2} \langle j'k'|U_L(z) + U_R(z)|jk\rangle = \frac{1}{2} \langle j'k'|U(z)|jk\rangle. \quad (7.199)$$

This is called the tunnel matrix element. The last term in Eq. (7.198) is zero. This is seen by writing:

$$\begin{aligned} & -\frac{1}{2} \langle j'k'|U_j(z) - \epsilon_{jk}|jk\rangle + \frac{1}{2} \langle j'k'|U_{j'}(z) - \epsilon_{j'k'}|jk\rangle \\ & = -\frac{1}{4m} \int_{-\infty}^{\infty} dz [F_{j'k'}^*(z) \hat{p}_z^2 F_{jk}(z) - F_{jk}(z) \hat{p}_z^2 F_{j'k'}^*(z)]. \end{aligned} \quad (7.200)$$

Performing an integration by parts and using that $F_{jk}(z \rightarrow \infty) = 0$ and $F_{j'k'}(z \rightarrow -\infty) = 0$, the proof is completed.

Now we want to look for solutions $\psi(\mathbf{x}, z)$ of the Schrodinger equation. We look for solutions of the form

$$\psi(\mathbf{x}, z) = \frac{1}{L^2} \sum_{j'k'\mathbf{p}} A_{j'k'\mathbf{p}} e^{i\mathbf{p}' \cdot \mathbf{x}} F_{j'k'}(z). \quad (7.201)$$

Note that the summation over $\mathbf{p}$ gives an arbitrary function depending on $\mathbf{x}$, determined by the expansion coefficients $A_{jk\mathbf{p}}$, as required due to the impurity potential. We now take the SE $(\hat{H} - E)\Psi = 0$ and perform the operation $\int dz d\mathbf{x} F_{jk}^*(z) e^{-i\mathbf{p} \cdot \mathbf{x}}$. We note that

$$\frac{1}{L^2} \sum_{\mathbf{x}} e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}} = \delta_{\mathbf{p}\mathbf{p}'}. \quad (7.202)$$

The above operation gives

$$\int dz d\mathbf{x} F_{jk}^*(z) (\hat{H} - E) \frac{1}{L^2} \sum_{j'k'\mathbf{p}'} A_{j'k'\mathbf{p}'} e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}} F_{j'k'}(z) = 0. \quad (7.203)$$

Split the summation over j' into $j' = j$ and $j' \neq j$:

$$\begin{aligned} & \int d\mathbf{x} \sum_{k'\mathbf{p}'} \left(\langle jk|\hat{H}|jk'\rangle - \delta_{kk'} E \right) \frac{1}{L^2} A_{jk'\mathbf{p}'} e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}} F_{jk'}(z) \\ & + \int d\mathbf{x} \sum_{j' \neq j, k'\mathbf{p}'} \left(\langle jk|\hat{H}|j'k'\rangle - S_{j'k',jk} E \right) \frac{1}{L^2} A_{j'k'\mathbf{p}'} e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}} F_{j'k'}(z) = 0. \end{aligned} \quad (7.204)$$

Now our previous results for the matrix elements in these equations come in handy. Inserting them gives:

$$\begin{aligned} & (\epsilon_{jk\mathbf{p}} - E) A_{jk\mathbf{p}} + \sum_{j'k'\mathbf{p}'} A_{j'k'\mathbf{p}'} \frac{1}{L^2} \int d\mathbf{x} \langle j'k'|V(\mathbf{x}, z) e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}} |jk\rangle \\ & + \sum_{j' \neq j, k'} A_{j'k'\mathbf{p}'} \left[t_{jk,j'k'} + S_{jk,j'k'} \left(\frac{\epsilon_{j'k'\mathbf{p}} - \epsilon_{jk\mathbf{p}}}{2} - E \right) \right] = 0. \end{aligned} \quad (7.205)$$

Here, we defined $\epsilon_{jk\mathbf{p}} \equiv \epsilon_{jk} + \mathbf{p}^2/2m$. We see that it is the Fourier-transform of the impurity potential that enters the equations:

$$V(\mathbf{p}' - \mathbf{p}, z) = \frac{1}{L^2} \int d\mathbf{x} V(\mathbf{x}, z) e^{i(\mathbf{p}' - \mathbf{p}) \cdot \mathbf{x}}. \quad (7.206)$$

To proceed, we make a number of approximations to this expression, which so far is exact except for the one term neglected in the matrix elements due to higher order exponential smallness. Firstly, it is reasonable to neglect the non-diagonal term in j (i.e. the one coupling the two sides of the interface) for the impurity potential, since the barrier potential $U \gg V$ in the region where the wavefunctions for $j = L, R$ overlap. Secondly, we make the following observation for the last term in the above equation. From its definition, we see that $t_{jk,j'k'} \sim U_0 S_{jk,j'k'}$ where U_0 is a characteristic energy scale for $U(z)$ near the interface region (note that the main contribution to $S_{jk,j'k'}$ is precisely for a region close to $z = 0$). Therefore, by assuming that the energies involved for particles tunneling across the barrier U_0 are much smaller than the barrier itself, in effect

$$|E - \frac{\epsilon_{j'k'\mathbf{p}} - \epsilon_{jk\mathbf{p}}}{2}| \ll U_0, \quad (7.207)$$

we can neglect the contribution proportional to $S_{jk,j'k'}$ in Eq. (7.205). With all these approximations, we are left with the following equation for the coefficients $A_{jk\mathbf{p}}$:

$$(\epsilon_{jk\mathbf{p}} - E)A_{jk\mathbf{p}} + \sum_{k'\mathbf{p}'} \langle jk | V(\mathbf{p}' - \mathbf{p}, z) | j'k' \rangle A_{jk'\mathbf{p}'} + \sum_{j \neq j', k'} t_{jk,j'k'} A_{j'k'\mathbf{p}}. \quad (7.208)$$

This is formally the matrix representation of a Schrodinger equation for an effective tunneling Hamiltonian. This can be seen as follows. Recall that for a SE written using the general formulation of quantum mechanics, $H|\psi\rangle = E|\psi\rangle$, we can expand $|\psi\rangle$ in a particular basis $|k\rangle$ using $|\psi\rangle = \sum_k A_k |k\rangle$. Assuming this is an orthonormal basis, we now insert this in the SE, take the inner product of the SE with the bra $\langle n|$, and obtain

$$\sum_k \langle n | H | k \rangle A_k = A_n E. \quad (7.209)$$

This is precisely a matrix equation

$$(H_{\text{eff}} - E)A = 0 \quad (7.210)$$

where A is a column vector containing the coefficients A_k and H_{eff} is a matrix with elements $\langle n | H | k \rangle$. This is the SE in the matrix representation using the basis $|k\rangle$. Looking back now on Eq. (7.208), we see that this also has the form

$$(H_T - E)A = 0 \quad (7.211)$$

where A is a column vector containing all the coefficients $A_{jk\mathbf{p}}$ and H_T is the matrix representation of the Hamiltonian with matrix elements

$$\langle j'k'\mathbf{p}' | H_T | jk\mathbf{p} \rangle = \delta_{jj'} \left(\delta_{kk'} \delta_{\mathbf{p}\mathbf{p}'} \epsilon_{jk\mathbf{p}} + V_{k'k}^j(\mathbf{p}' - \mathbf{p}) \right) + \delta_{\mathbf{p}\mathbf{p}'} t_{j'k',jk}. \quad (7.212)$$

Here, $V_{k'k}^j(\mathbf{q}) = \langle jk' | V(\mathbf{q}, z) | jk \rangle$. The form of these matrix elements is read out from Eq. (7.208). In effect, we have expanded the statevector $|\psi\rangle$ precisely in a basis $|jk\mathbf{p}\rangle$ which has wavefunctions $\langle \mathbf{x}, z | jk\mathbf{p} \rangle = L^{-2} e^{i\mathbf{p} \cdot \mathbf{x}} F_{jk}(z)$. This is consistent with the form of the wavefunctions we looked for in

terms of solutions for the SE: we have expanded the wavefunction in the basis $L^{-2}e^{i\mathbf{p}\cdot\mathbf{x}}F_{jk}(z)$ using expansion coefficients $A_{jk\mathbf{p}}$.

We now have everything we need to write down the second quantized version of our effective Hamiltonian that has emerged after a series of justified approximations, namely

$$\begin{aligned}
 H_T = & \sum_{jk\mathbf{p}} \epsilon_{jk\mathbf{p}} c_{jk\mathbf{p}}^\dagger c_{jk\mathbf{p}} + \sum_{jkk'\mathbf{p}\mathbf{p}'} V_{k'k}^j(\mathbf{p}' - \mathbf{p}) c_{jk'\mathbf{p}'}^\dagger c_{jk\mathbf{p}} \\
 & + \sum_{kk'\mathbf{p}} (t_{Lk',Rk} c_{Lk'\mathbf{p}}^\dagger c_{Rk\mathbf{p}} + t_{Rk,Lk'} c_{Rk\mathbf{p}}^\dagger c_{Lk'\mathbf{p}})
 \end{aligned} \tag{7.213}$$

where $c^\dagger, c$ are creation and annihilation operators for an electron in state $|jk\mathbf{p}\rangle$. We verify from the definition of the tunnel matrix elements that $t_{Lk',Rk} = t_{Rk,Lk'}^*$, which ensures that H_T is Hermitian. Through this derivation we see that a second quantized tunnel Hamiltonian can be written down even when momentum is not conserved due to translational symmetry breaking (because of the interface). In effect, even though momentum perpendicular to the interface is not a conserved quantity, we can write the second quantized Hamiltonian above (at no point in the derivation did we rely on conservation of k). The reason is simply that k is not a momentum variable: it is a quantum index labelling the allowed wavefunction-solutions on each side of the interface (*e.g.* standing waves if we also introduce a barrier at $\pm\infty$).

Note that reflection at the barrier has been taken into account in H_T via the type of quantum states that $c_k^\dagger$ and c_k create and annihilate, because the k -value here characterizes the allowed states precisely when we have an impenetrable interface at the barrier region. We can therefore perform a summation over positive and negative k without worrying about them being coupled.

Thus: a key point is that even if our system does not have translational invariance, and momentum is not conserved, we can still write the Hamilton-operator on the second-quantized form of H_T above. However, we have to keep in mind what kind of states the $c_{jk\mathbf{p}}$ -operators correspond to, namely the eigenstates of the system without translational invariance: standing waves characterized by a wavevector k .

Chapter 8

Fermi liquid theory: adding interactions to the free electron gas

8.0.1 Phonons

As electrons move through a crystal lattice, they interact electromagnetically with the atomic cores that are positively charged. At finite temperature, the atoms that make up the crystal lattice are not completely stationary: their finite thermal energy causes them to have vibrational motion as well. In turn, this slightly modifies the electric potential landscape that the electrons move through when compared to an ideal crystal lattice structure where the atoms are fully at rest.

If we assume that the atoms behave as harmonic oscillators for small deviations from equilibrium, it is clear the deviation u of the atoms from their $T = 0$ equilibrium position can be quantized by expressing u as a superposition of bosonic creation and annihilation operators $a^\dagger$ and a . This is completely analogous to how the position operator q in the standard harmonic oscillator treatment is expressed via a and $a^\dagger$.

We take a moment here to reflect on what *quantized* means in this context. In the English language, quantized is a synonym to discretized, meaning that a quantity can only take discrete values. However, in physics one must be aware of the fact that quantized can also mean "treated quantum mechanically". Importantly, quantized therefore *does not necessarily mean that something is discretized*: it just means that we have replaced the classical description of a quantity, such as a lattice vibrational mode, with a quantum mechanical treatment, namely the phonon quasiparticle. *Sometimes*, this results in a discrete energy spectrum, but it does not have to. For instance, in the case of magnons (the quantized version of a spin-wave, i.e. the quantum mechanical treatment of a spin-wave) the dispersion relation is essentially identical in the classical and quantum case. The magnon energy dispersion, $\omega_q \propto q^2$ in the ferromagnetic case and $\omega_q \propto q$ in the antiferromagnetic case, is thus not discretized so long as the system is large enough that we can disregard the quantization (meaning actual discretization) of the momentum q . On the other hand, one could say that a phonon represents a quantum of a lattice vibration and in this sense is an abstract, discrete quantity.

Getting back to the phonons, each quantized normal mode of oscillation of the lattice corresponds to a harmonic oscillator with momentum $\mathbf{q}$ and energy ω_q where the displacement $u_{\mathbf{q}}$ takes the

form:

$$u_{\mathbf{q}} = i\sqrt{\frac{\hbar}{2\omega_{\mathbf{q}}}}(a_{\mathbf{q}} - a_{\mathbf{q}}^{\dagger}). \quad (8.1)$$

Since the electrons couple to these deviations via their charge density coupling to the crystal potential, one obtains interaction terms in the Hamiltonian of the form

$$H_I = \sum_{\mathbf{k}, \mathbf{q}} (V_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}} a_{\mathbf{q}} + \text{h.c.}) \quad (8.2)$$

where the potential energy $V_{\mathbf{q}} \propto i\mathbf{q}\sqrt{\hbar/2\omega_{\mathbf{q}}}$. This is the so-called Frölich Hamiltonian. The interaction can be visualized as a phonon being absorbed (emitted) by an electron and at each vertex we have momentum conservation.

In effect: the interaction between the electrons and the vibrating lattice of atoms can be described as a quasi-mechanical collision between electrons and the quasiparticles described by a and $a^{\dagger}$. These quasiparticles (also called collective excitations since they are bosons) are *phonons*. The phonons carry zero charge, but have energy and momentum. More specifically, the phonons we have implicitly considered above are longitudinal phonons which generate a charge density variation felt by the electrons. These have zero spin.

Note that even though the phonons represent the coupling between charged electrons and the charged atom lattice, the phonons are themselves electrically neutral. This is similar to how the *photon* represent the electromagnetic coupling between charged electrons despite being electrically neutral itself. The phonon number does not have to be conserved in an interaction.

Chapter 9

Hubbard model

Second quantization is described in the Appendix of these notes. An important point is that the physics described by the second quantized Hamiltonian should not depend on which orthonormal basis set we use, be it discrete or continuous.

9.1 Half-filling

This corresponds to a mean value of one electron per lattice site. The value of μ which gives half-filling depends on how we write the interaction term. If the interaction term is written $U \sum_i n_{i\uparrow} n_{i\downarrow}$, $\mu = 0$ does not correspond to half-filling: instead, the value of μ that gives half-filling depends on the value chosen for U . Instead, if the interaction term is written as $U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$, $\mu = 0$ corresponds to half-filling. This is true despite the fact that one obtains an effective chemical potential term $\propto U$ by writing the interaction term in this way. It is reasonable that the factors of $1/2$ make the model particle-hole symmetric around $\langle n_{i\sigma} \rangle = \frac{1}{2}$ since $\langle n_i \rangle = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle$.

9.2 Density-wave states

In the Hubbard model, charge density-wave and spin density-wave states can occur as ground-states of the model. These are characterized by a spatially modulated charge or spin density (magnetization). One distinguishes between commensurate and incommensurate density waves:

- Commensurate density-wave: the ratio between the period λ of the modulated state and the size of the unit cell a (in other words, the periodicity of the crystal lattice) is a rational number p/q where p and q are integers. Alternatively, one can express this by saying that the wave-vector Q characterizing the density-wave is one of the allowed k -values in the 1BZ.
- Incommensurate density-wave: the ratio λ/a is not a rational number. In other words, there is no way to fit p density-wave periods inside q unit cells. For such a state, the model has completely lost all translational symmetry. The lattice itself has a discrete translational symmetry on its own.

But consider now Neumann's principle:

Neumann's principle: Any physical property of a crystal lattice must have the same symmetries as the crystal lattice itself.

and Curie's principle:

Curie's principle: The symmetry characteristic of a phenomenon is the highest compatible with the existence of the phenomenon; the phenomenon may exist in a medium which possesses that symmetry or that of a subgroup of that symmetry.

These principles at first glance seem to forbid that incommensurate density-wave states should appear on a crystal lattice described by a Hamilton-operator that does not contain explicitly symmetry-breaking terms with respect to translational symmetry. In other words, the standard Hubbard model on a lattice with periodic boundary conditions should not be able to give incommensurate density-wave states according to the two above principles.

However, as discussed earlier in these lecture notes, the SDW state cannot be considered a physical property of the lattice itself, analogously to the vortex pattern of a superconducting triangle which can break the triangular symmetry as one gradually increases the field from zero to one flux quantum: the vortex enters from *one* of the triangle sides. Instead, the free energy of the entire system, which is a functional of the magnetic texture $\mathbf{M}(\mathbf{r})$ of the system state, is a property of the lattice. So if we apply a symmetry operation (such as $\pi/2$ rotation or mirroring) to the SDW magnetic texture $\mathbf{M}(\mathbf{r})$, the free energy of the resulting system must be exactly the same as for the original SDW magnetic texture. In this way, the actual SDW texture that is realized does not have the same symmetries of the lattice, and thus the state cannot be considered a property of the lattice in the context of the Neumann principle. Instead, the realized magnetic texture spontaneously breaks the symmetries of the lattice. An example of this is the striped antiferromagnetic-like phase that can occur in the cuprates on a square lattice. The magnetization texture does not respect the lattice symmetry, but instead spontaneously breaks it.

9.3 Discretization of derivation operator

We start by discussing how derivative operators can be treated on a lattice.

Consider a function $F = F(x)$ defined on a lattice. This means that x takes on discrete values $x_j \equiv ja$ where j is an integer. The first derivative can then be naturally defined in several ways. The forward difference approximation gives

$$\left. \frac{dF}{dx} \right|_{x_j} = \frac{1}{a} [F|_{x_{j+1}} - F|_{x_j}] \quad (9.1)$$

according to the fundamental definition of the derivative. However, we could have used a backward difference (x_j and x_{j-1} instead) or even a central difference method:

$$\left. \frac{dF}{dx} \right|_{x_j} = \frac{1}{2a} [F|_{x_{j+1}} - F|_{x_{j-1}}] \quad (9.2)$$

One can show that the central difference approximation for the first derivative is actually the most accurate one and so we will stick with it. We have now expressed the first derivative at a lattice point exclusively in terms of the function values at other lattice points. This will come in handy when second quantizing Rashba spin-orbit coupling.

As for the second derivative, we use an intermediate step as follows:

$$\left. \frac{dF}{dx} \right|_{x_{j+1/2}} = \frac{1}{a} [F|_{x_{j+1}} - F|_{x_j}]. \quad (9.3)$$

The function F isn't really defined on $x = (j + 1/2)a$, but we won't evaluate anything between lattice points in the end: it is just an intermediate step. Now use this result to evaluate:

$$\begin{aligned} \frac{d^2 F}{dx^2} \Big|_{x_j} &= \frac{1}{a} \left[\frac{dF}{dx} \Big|_{x_{j+1/2}} - \frac{dF}{dx} \Big|_{x_{j-1/2}} \right] \\ &= \frac{1}{a^2} [F_{j+1} - 2F_j + F_{j-1}]. \end{aligned} \quad (9.4)$$

We thus have an expression for the second derivative at a lattice point exclusively in terms of function values at other lattice points. This will come in handy when second-quantizing the kinetic energy.

9.3.1 Deriving second-quantized Hamiltonian with different basis-choices

Let us start by second-quantizing the Hamiltonian for an electron moving in a crystal potential:

$$H = T + U = \sum_i \left(\frac{-\nabla_i^2}{2m} + U(\mathbf{r}_i) \right). \quad (9.5)$$

Here, U is the crystal potential and $U(\mathbf{r}_i)$ is thus a periodic function. As we shall discuss later, which orthonormal basis we use to second quantize this Hamiltonian does not impact the physics, but a smart choice of basis for a given Hamiltonian might make the math easier. We will illustrate the effect of choosing different bases here.

If we expect that the Hamiltonian will describe electrons that are tightly bound to the ions and only occasionally tunnel between lattice sites, it is natural to use atomic orbitals as our basis. We thus write the single-particle wavefunction satisfying the single-particle SE as:

$$\psi_{n,\sigma}(\mathbf{r} - \mathbf{R}) = \phi_n(\mathbf{r} - \mathbf{R})\chi_\sigma, \quad (9.6)$$

where $\phi_n(\mathbf{r} - \mathbf{R})$ solves the SE:

$$\left(\frac{-\nabla^2}{2m} + U_0(\mathbf{r} - \mathbf{R}) \right) \phi_n(\mathbf{r} - \mathbf{R}) = E_n \phi_n(\mathbf{r} - \mathbf{R}) \quad (9.7)$$

and χ_σ is a spinor which is not important for our discussion here. The index n denotes the atomic orbital (principal quantum number) and any other relevant quantum numbers. We mention in passing that while $\{\phi_n\}$ constitutes a complete set and thus a basis for Hilbert space (meaning they are linearly independent), this does not mean that they are necessarily orthogonal. Simple illustration 2D: the vectors $(1, 0)$ and $(1, 1)$ are linearly independent, but not orthogonal.

We can write the total crystal potential as

$$U = \sum_i U(\mathbf{r}_i), \quad U(\mathbf{r}_i) = \sum_j U_0(\mathbf{r}_i - \mathbf{R}_j). \quad (9.8)$$

Here, $U_0(\mathbf{r}_i - \mathbf{R}_j)$ is the electrostatic interaction between an electron at position $\mathbf{r}_i$ and an ion at position $\mathbf{R}_j$. With our choice of basis, the second-quantized Hamiltonian would be diagonal if it were not for the off-site contribution to the crystal potential, $\sum_{i,j \neq i} U_0(\mathbf{r}_i - \mathbf{R}_j)$. We will see that this results in tunneling of electrons from one site to another. Using the standard prescription for setting up the second-quantized Hamiltonian, we see that (dropping spin and orbital indices for simplicity):

$$H = \sum_{i,j} \langle i | H | j \rangle c_i^\dagger c_j, \quad (9.9)$$

where H is the single-particle Hamiltonian. We therefore obtain:

$$\begin{aligned} \langle i|H|j\rangle &= \int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i)^* \left[-\frac{\nabla^2}{2m} + U_0(\mathbf{r} - \mathbf{R}_j) \right] \phi(\mathbf{r} - \mathbf{R}_j) \\ &+ \int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i)^* \left[\sum_{m \neq j} U_0(\mathbf{r} - \mathbf{R}_m) \right] \phi(\mathbf{r} - \mathbf{R}_j). \end{aligned} \quad (9.10)$$

We split the Hamiltonian H in this way for every i and j so that the first integral can be evaluated by using Eq. (9.14) according to:

$$\int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i)^* \left[-\frac{\nabla^2}{2m} + U_0(\mathbf{r} - \mathbf{R}_j) \right] \phi(\mathbf{r} - \mathbf{R}_j) = E \int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i)^* \phi(\mathbf{r} - \mathbf{R}_j). \quad (9.11)$$

The second integral is:

$$\int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i)^* \left[\sum_{m \neq j} U_0(\mathbf{r} - \mathbf{R}_m) \right] \phi(\mathbf{r} - \mathbf{R}_j). \quad (9.12)$$

However, since the atomic orbitals ϕ_l and ϕ_k should be centered around different atoms l and k , we do expect both above integrals to vanish for atoms that are far apart. We can now write the Hamiltonian as:

$$\begin{aligned} H &= \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i,j \neq i} t_{ij} c_i^\dagger c_j, \\ \epsilon_i &= E + \int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i)^* \left[\sum_{m \neq i} U_0(\mathbf{r} - \mathbf{R}_m) \right] \phi(\mathbf{r} - \mathbf{R}_i), \\ t_{ij} &= E \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) \phi(\mathbf{r} - \mathbf{R}_j) + \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) \left[\sum_{m \neq j} U_0(\mathbf{r} - \mathbf{R}_m) \right] \phi(\mathbf{r} - \mathbf{R}_j) \end{aligned} \quad (9.13)$$

where we have assumed that $\phi(\mathbf{r} - \mathbf{R})$ are normalized. The largest contribution to t_{ij} should come from when i and j are nearest neighbors and corresponds precisely to tunneling between lattice sites. Note that we have not made use of any orthogonality assumption for the atomic wavefunctions. If they are orthogonal, the term $\propto E$ in t_{ij} vanishes and the tunneling is then solely due to the offsite Coulomb potential.

Physics invariant of basis

Let us now use a different basis than $\phi(\mathbf{r} - \mathbf{R}_i)$. Consider the basis $\psi(\mathbf{r})$ satisfying the single-particle SE:

$$H\psi(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U(\mathbf{r}) \right) \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (9.14)$$

where the difference from Eq. (9.14) is that we have now used the full crystal potential U instead of just the onsite part. Therefore, $\psi(\mathbf{r})$ must be a Bloch function since $U(\mathbf{r})$ is a periodic potential (whereas U_0 is not necessarily periodic). There is no ' i ' dependence in the basis function anymore since the potential does not originate from one specific atom i , but is instead the sum from all atoms i . Instead, we know that ψ will depend on a momentum index $\mathbf{k}$ and a band index, so that the eigenfunctions can be written in the form

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}). \quad (9.15)$$

This means that the Bloch wavefunctions are characterized by a quantum number n and a wavevector parameter $\mathbf{k}$, and the same goes for the eigenvalues $E = E_{n,\mathbf{k}}$. If now $\{\psi_{n,\mathbf{k}}\}$ is our basis set, the second quantized Hamiltonian is immediately diagonal:

$$H = \sum_{n,n',\mathbf{k},\mathbf{k}'} \langle n', \mathbf{k}' | H | n, \mathbf{k} \rangle c_{n',\mathbf{k}'}^\dagger c_{n,\mathbf{k}} = \sum_{n,\mathbf{k}} E_{n,\mathbf{k}} c_{n,\mathbf{k}}^\dagger c_{n,\mathbf{k}}, \quad (9.16)$$

since

$$H|\mathbf{r}|n, \mathbf{k}\rangle = H\psi_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r}). \quad (9.17)$$

The physics described by the Hamiltonian in this basis-choice must be identical to our previous basis-choice. Although we did not obtain an hopping term with the basis $\{\psi_{n,\mathbf{k}}\}$, *the physics is in fact still the same* since the above Hamiltonian describes itinerant electrons moving with momentum $\mathbf{k}$ (just as the first Hamiltonian describes electron moving due to hopping).

Wannier functions

When working with a localized basis, a common choice is to use Wannier functions. These functions provide a natural extension from atomic orbitals into solids as they bridge the gap between chemists, who speak of chemical bonds and localized atomic orbitals, and physicists, who speak of delocalized Bloch waves in a periodic solid.

The Wannier functions are Fourier-transforms of the Bloch functions. In this way, it makes sense that they are localized since the Bloch functions are delocalized. Consider a lattice with atoms at positions $\mathbf{R}$ and momenta $\mathbf{k}$. The Wannier functions are then defined as:

$$w_n(\mathbf{r} - \mathbf{R}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}} \psi_{n,\mathbf{k}}(\mathbf{r}), \quad (9.18)$$

and the set $\{w_n\}$ is an orthonormal basis set as can be shown from the above definition and using that the Bloch functions form an orthonormal set. The inverse transformation reads

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} w_n(\mathbf{r} - \mathbf{R}). \quad (9.19)$$

They are characterized by a band index n and lattice site positions $\mathbf{R}$. The coordinate $\mathbf{r}$ is the position of the electron and the Wannier functions form an orthonormal set in the sense that:

$$\int d\mathbf{r} \phi_n^*(\mathbf{r} - \mathbf{R}_i) \phi_n(\mathbf{r} - \mathbf{R}_j) = \delta_{ij} \quad (9.20)$$

The difference between the Wannier functions and the atomic orbitals is that they can be expressed as linear combinations of each other. Specifically, the Wannier functions are a linear combinations of atomic orbitals in such a manner that the Wannier functions become orthogonal. One can thus think of the construction of Wannier functions as a Gram-Schmidt type of procedure for the atomic orbitals.

We also introduce the corresponding Fourier-transformed creation and annihilation operators:

$$\begin{aligned} c_j &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_j}, \\ c_{\mathbf{k}} &= \frac{1}{\sqrt{N}} \sum_j c_j e^{-i\mathbf{k} \cdot \mathbf{R}_j}. \end{aligned} \quad (9.21)$$

Let us now write down the second-quantized Hamiltonian in a Wannier basis. Inserting Eq. (9.19) into Eq. (9.16), we obtain

$$H = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{R}, \mathbf{R}', j, j'} e^{-i\mathbf{k} \cdot \mathbf{R}' + i\mathbf{k} \cdot \mathbf{R}} \int d\mathbf{r} w^*(\mathbf{r} - \mathbf{R}') H w(\mathbf{r} - \mathbf{R}) c_j^\dagger c_{j'} e^{i\mathbf{k} \cdot \mathbf{R}_j - i\mathbf{k} \cdot \mathbf{R}_{j'}}. \quad (9.22)$$

We now use that

$$\frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} = \delta_{\mathbf{R}, \mathbf{R}'}. \quad (9.23)$$

to obtain

$$\begin{aligned} H &= \sum_{\mathbf{R}, \mathbf{R}', j, j'} \delta_{\mathbf{R} - \mathbf{R}' + \mathbf{R}_j - \mathbf{R}_{j'}} \int d\mathbf{r} w^*(\mathbf{r} - \mathbf{R}') H w(\mathbf{r} - \mathbf{R}) c_j^\dagger c_{j'} \\ &= \sum_{\mathbf{R}, \mathbf{R}', j} \int d\mathbf{r} w^*[\mathbf{r} - \mathbf{R} + (\mathbf{R} - \mathbf{R}')] H w(\mathbf{r} - \mathbf{R}) c_j^\dagger c_{j+\mathbf{R}-\mathbf{R}'}. \end{aligned} \quad (9.24)$$

Since the Wannier functions $w(\mathbf{r} - \mathbf{R})$ are localized around $\mathbf{r} = \mathbf{R}$, it is a reasonable assumption to say that the integral only gives a contribution when $\mathbf{R} - \mathbf{R}' = 0$ in addition to when $\mathbf{R}$ and $\mathbf{R}'$ are nearest neighbor atoms. In this case, we obtain

$$\begin{aligned} H &= \sum_j \left(\sum_{\mathbf{R}} \int d\mathbf{r} w^*(\mathbf{r} - \mathbf{R}) H w(\mathbf{r} - \mathbf{R}) \right) c_j^\dagger c_j \\ &\quad + \sum_{j, \delta} \left(\sum_{\mathbf{R}} \int d\mathbf{r} w^*(\mathbf{r} - \mathbf{R} + \delta) H w(\mathbf{r} - \mathbf{R}) \right) c_j^\dagger c_{j+\delta}. \end{aligned} \quad (9.25)$$

where δ is the distance between j and a nearest-neighbor atom. This can be rewritten as

$$H = \sum_j \epsilon_0 c_j^\dagger c_j + \sum_{j, \delta} t_\delta c_j^\dagger c_{j+\delta}. \quad (9.26)$$

We have here defined the onsite energy

$$\epsilon_0 = \sum_{\mathbf{R}} \int d\mathbf{r} w^*(\mathbf{r} - \mathbf{R}) H w(\mathbf{r} - \mathbf{R}) \quad (9.27)$$

and the hopping term

$$t_\delta = \sum_{\mathbf{R}} \int d\mathbf{r} w^*(\mathbf{r} - \mathbf{R} + \delta) H w(\mathbf{r} - \mathbf{R}). \quad (9.28)$$

We see that we have arrived at the tight-binding model where ϵ_0 is an on-site energy whereas $t(\delta)$ describes hopping of electrons between sites. Such a model also suggests a natural generalization

to the case where disorder is included, so that $\epsilon_0 \rightarrow \epsilon_{0,j}$, and to where the hopping may be site-dependent, $\sum_{j,\delta} t_\delta c_j^\dagger c_{j+\delta} \rightarrow \sum_{ij} t_{ij} c_j^\dagger c_i$.

This generalization also emerges by directly Fourier-transforming the operators in Eq. (9.16) to

$$H = \frac{1}{N} \sum_{\mathbf{k}jj'} E_{\mathbf{k}} c_j^\dagger c_{j'} e^{i\mathbf{k} \cdot \mathbf{R}_j - i\mathbf{k} \cdot \mathbf{R}_{j'}} = \sum_{jj'} t_{jj'} c_j^\dagger c_{j'} \quad (9.29)$$

where

$$t_{jj'} = \frac{1}{N} \sum_{\mathbf{k}} E_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_{j'})}. \quad (9.30)$$

9.4 Second quantization of Rashba spin-orbit coupling

The first quantized single-particle form of the Rashba SOC term is

$$H_{\text{SOC}} = \alpha \mathbf{n} \cdot (\boldsymbol{\sigma} \times \mathbf{p}). \quad (9.31)$$

Here α is the strength of the SOC and $\mathbf{n}$ is a unit vector characterizing the direction of inversion symmetry breaking. The second quantized takes the following form when using atomic orbital states $|i\sigma\rangle$ as our complete set of basis functions:

$$H = \sum_{ij\sigma\sigma'} \langle i\sigma | H_{\text{SOC}} | j\sigma' \rangle c_{i\sigma}^\dagger c_{j\sigma'}. \quad (9.32)$$

Here $|i\sigma\rangle$ are eigenstates of a Hamiltonian $\hat{H}_{\text{localized}}$ describing a single-particle bound to an atom at site $\mathbf{R}_i$ by its potential:

$$\hat{H}_{\text{localized}} |i\sigma\rangle = E_{i\sigma} |i\sigma\rangle. \quad (9.33)$$

By multiplying at left from $\langle x|$, we arrive at the corresponding SE in the position representation since $\langle x|i\sigma\rangle = \phi(\mathbf{r} - \mathbf{R}_i)$ and

$$\langle x | \hat{H}_{\text{localized}} | i\sigma \rangle = \int dq \langle x | \hat{H}_{\text{localized}} | q \rangle \langle q | i\sigma \rangle = \hat{H}_{\text{localized}} \left(\frac{\hbar}{i} \nabla, \mathbf{r} \right) \phi(\mathbf{r} - \mathbf{R}_i). \quad (9.34)$$

as shown in detail *e.g.* in the QM II lecture notes. To evaluate the matrix element in the second quantized version, we see that it is equal to

$$\langle i\sigma | H_{\text{SOC}} | j\sigma' \rangle = \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) \chi_\sigma^\dagger \alpha \mathbf{n} \cdot (\boldsymbol{\sigma} \times \mathbf{p}) \phi(\mathbf{r} - \mathbf{R}_i) \chi_{\sigma'}. \quad (9.35)$$

To see what comes out of this, let us for concreteness choose $\mathbf{n} = \mathbf{x}$. This gives

$$\begin{aligned} \langle i\sigma | H_{\text{SOC}} | j\sigma' \rangle &= \chi_\sigma^\dagger \sigma_z \chi_{\sigma'} \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) (-i\hbar \partial_y) \phi(\mathbf{r} - \mathbf{r}_j) \\ &\quad - \chi_\sigma^\dagger \sigma_y \chi_{\sigma'} \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) (-i\hbar \partial_z) \phi(\mathbf{r} - \mathbf{R}_j). \end{aligned} \quad (9.36)$$

The values of the overlap integrals depend on the relation between the sites i and j . Our first approximation will be to neglect overlap integrals between orbitals on sites that are not nearest

neighbors. Now, let the system be three-dimensional (so that all momentum components exist). If i and j are nearest neighbors in the y direction, we would expect the two overlap integrals to take different values. The overlap integral is appreciably changed by the y derivative, since $\partial_y \phi(\mathbf{r} - \mathbf{R}_j)$ will extend further into the neighboring site than $\phi(\mathbf{r} - \mathbf{R}_j)$ does, but it is hardly changed at all by the z derivative. We will therefore approximate the overlap integrals as a constant $i\gamma$ when i and j are nearest neighbors along the momentum direction, and as zero otherwise. Notice in particular that we expect the onsite contribution $i = j$ to vanish if the atomic orbital functions have a definite parity around their respective atoms, since the derivative changes the parity and causes the integrand to be antisymmetric in $\mathbf{r}$.

Alternatively, we can also show mathematically that the above integrals behave as explained if we use Wannier functions $w(\mathbf{r} - \mathbf{R})$ as our basis in addition to a discretization scheme for the derivation operator. This is motivated by the fact that the electrons after all reside on a lattice, so that it is reasonable to approximate

$$\partial_x w(\mathbf{r} - \mathbf{R}_i) \simeq \frac{1}{a} [w(\mathbf{r} + a\mathbf{x} - \mathbf{R}_i) - w(\mathbf{r} - a\mathbf{x} - \mathbf{R}_i)] \quad (9.37)$$

Using the orthogonality property of the Wannier functions, we then obtain for instance

$$\begin{aligned} \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) (-i\hbar \partial_y) \phi(\mathbf{r} - \mathbf{r}_j) &= \frac{-i\hbar}{a} \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) [\phi(\mathbf{r} + a\mathbf{y} - \mathbf{R}_j) - \phi(\mathbf{r} - a\mathbf{y} - \mathbf{R}_j)] \\ &= -\frac{i\hbar}{a} (\delta_{i,j-az} - \delta_{i,j+az}). \end{aligned} \quad (9.38)$$

Using now for the spin-part that:

$$\chi_\sigma^\dagger \sigma_i \chi_{\sigma'} = (\sigma_i)_{\sigma, \sigma'}, \quad (9.39)$$

we obtain for a general $\mathbf{n}$ that:

$$\langle i\sigma | \alpha_R \mathbf{n} \cdot (\boldsymbol{\sigma} \times \mathbf{p}) | j\sigma' \rangle = i\alpha_R \mathbf{n} \cdot (\boldsymbol{\sigma} \times \mathbf{d}_{ij}), \quad (9.40)$$

where α_R is a real coefficient where we've absorbed all prefactors into it while $\mathbf{d}_{ij} = -\mathbf{d}_{ji}$ is the vector between nearest neighbor sites i and j . In the end, we thus have the following second quantized form for the Rashba SOC:

$$H = i\alpha_R \sum_{\langle i,j \rangle, \sigma, \sigma'} [\mathbf{n} \cdot (\boldsymbol{\sigma} \times \mathbf{d}_{ij})]_{\sigma, \sigma'} c_{i\sigma}^\dagger c_{j\sigma'}. \quad (9.41)$$

Finally, we note that one can also write down a second quantized form of the Rashba Hamiltonian with field operators, as done *e.g.* in quasiclassical theory. This simply corresponds to using the position eigenfunctions $\{|x\rangle\}$ as basis vectors so that the second quantized operators become field operators $\psi(x)$ and $\psi^\dagger(x)$. The above lattice form can then be recovered by expanding the field operators in a Wannier basis:

$$\psi(\mathbf{r}) = \sum_i w_i(\mathbf{r}) c_i \quad (9.42)$$

Chapter 10

Green functions and matrices

10.1 Bogoliubov-de Gennes diagonalization on a lattice

I here analytically show how the diagonalization of the BdG Hamiltonian can be done in a manner that

- Does not overcount the number of independent operators, so that the number of degrees of freedom is preserved.
- Does not require eigenvalues to be sorted in any special way in the numerical code, thus making the procedure compatible with MATLAB.

To begin with, I consider the case with translational invariance along two out of the three directions in space (as in Lina's papers). Afterwards, I explain how the procedure can also be used when we do not use periodic boundary conditions in any direction (as in Atousa's papers).

Periodic boundary conditions

For concreteness, consider here the Hamilton-operator used in the papers where we have superconductivity, ferromagnetism, and spin-orbit coupling (corresponding to the Hamiltonian in Lina's master-thesis). Lina: you can then apply the procedure below to the AFM case to check that it holds also there.

The starting point is the Hamilton-operator

$$H = H_0 + \frac{1}{2} \sum_{k_y, k_z} W_{k_y, k_z}^\dagger H_{k_y, k_z} W_{k_y, k_z}. \quad (10.1)$$

Here, we have

$$W_{k_y, k_z} = \begin{pmatrix} B_{1, k_y, k_z} \\ B_{2, k_y, k_z} \\ \dots \\ B_{N_x, k_y, k_z} \end{pmatrix}, \quad B_{i_x, k_y, k_z} = \begin{pmatrix} c_{i_x, k_y, k_z, \uparrow} \\ c_{i_x, k_y, k_z, \downarrow} \\ c_{i_x, -k_y, -k_z, \uparrow}^\dagger \\ c_{i_x, -k_y, -k_z, \downarrow}^\dagger \end{pmatrix}. \quad (10.2)$$

We have defined

$$H_{k_y, k_z} = \begin{pmatrix} H_{1, 1, k_y, k_z} & \dots & H_{1, N_x, k_y, k_z} \\ H_{2, 1, k_y, k_z} & \dots & \dots \\ \dots & \dots & \dots \\ H_{N_x, 1, k_y, k_z} & \dots & \dots \end{pmatrix} \quad (10.3)$$

and the 4×4 matrix:

$$H_{i_x, j_x, k_y, k_z} = \begin{pmatrix} \epsilon_k + \delta[h_{i_x}^z - \lambda_{i_x} \sin(k_y)] & \delta[h_{i_x}^x - i h_{i_x}^y - i \lambda_{i_x} \sin(k_z)] & 0 & \\ \delta[h_{i_x}^x + i h_{i_x}^y + i \lambda_{i_x} \sin(k_z)] & \epsilon_k + \delta_{i_x, j_x} [-h_{i_x}^z + \lambda_{i_x} \sin(k_y)] & -\delta \Delta_{i_x} & \\ 0 & -\delta \Delta_{i_x}^* & -\epsilon_k - \delta[h_{i_x}^z + \lambda_{i_x} \sin(k_y)] & -\delta[h_{i_x}^x + i h_{i_x}^y - i \lambda_{i_x} \sin(k_z)] \\ \delta \Delta_{i_x}^* & 0 & -\delta[h_{i_x}^x - i h_{i_x}^y + i \lambda_{i_x} \sin(k_z)] & -\epsilon_k - \delta[h_{i_x}^x + i h_{i_x}^y - i \lambda_{i_x} \sin(k_z)] \end{pmatrix} \quad (10.4)$$

where I defined short-hand notation

$$\begin{aligned} \epsilon_k &\equiv \epsilon_{i_x, j_x, k_y, k_z}, \\ \delta &\equiv \delta_{i_x, j_x}. \end{aligned} \quad (10.5)$$

just to make the matrix fit the page. So H_{k_y, k_z} is a $4N_x \times 4N_x$ matrix. Assume that this matrix has an eigenvalue E_{n, k_y, k_z} with eigenvector

$$\begin{pmatrix} u_{1nk_y k_z} \\ v_{1nk_y k_z} \\ w_{1nk_y k_z} \\ x_{1nk_y k_z} \\ u_{2nk_y k_z} \\ \dots \\ x_{N_x n k_y k_z} \end{pmatrix}. \quad (10.6)$$

Then it follows from Eq. (10.3) that

$$\sum_{j=1}^{N_x} H_{i_j k_y k_z} \begin{pmatrix} u_{jnk_y k_z} \\ v_{jnk_y k_z} \\ w_{jnk_y k_z} \\ x_{jnk_y k_z} \end{pmatrix} = E_{nk_y k_z} \begin{pmatrix} u_{ink_y k_z} \\ v_{ink_y k_z} \\ w_{ink_y k_z} \\ x_{ink_y k_z} \end{pmatrix}. \quad (10.7)$$

Consider the 1st row of this equation, which reads

$$\sum_{j=1}^{N_x} \left[\left(\epsilon_{ij k_y k_z} + \delta_{ij} [h_i^z - \lambda_i \sin(k_y)] \right) u_{jnk_y k_z} + \delta_{ij} [h_i^x - i h_i^y - i \lambda_i \sin(k_z)] v_{jnk_y k_z} + \delta_{ij} \Delta_i x_{jnk_y k_z} \right] = E_{nk_y k_z} u_{ink_y k_z}. \quad (10.8)$$

Consider next the 3rd row which reads:

$$\sum_{j=1}^{N_x} \left[-\delta_{ij} \Delta_i^* v_{jnk_y k_z} - \left(\epsilon_{ij k_y k_z} + \delta_{ij} [h_i^z + \lambda_i \sin(k_y)] \right) w_{jnk_y k_z} - \delta_{ij} [h_i^x + i h_i^y - i \lambda_i \sin(k_z)] x_{jnk_y k_z} \right] = E_{nk_y k_z} w_{ink_y k_z}. \quad (10.9)$$

Now take Eq. (10.9) and:

- Let $k_y, k_z \rightarrow -k_y, -k_z$.
- Complex conjugate everything.
- Multiply both sides with -1 .

This results in

$$\sum_{j=1}^{N_x} \left[\delta_{ij} \Delta_i v_{jn,-k}^* + \left(\epsilon_{ij,-k} + \delta_{ij} [h_i^z - \lambda_i \sin(k_y)] \right) w_{jn,-k}^* + \delta_{ij} [h_i^x - i h_i^y - i \lambda_i \sin(k_z)] x_{jn,-k}^* \right] = -E_{n,-k} w_{in,-k}^*. \quad (10.10)$$

Above, I used the short-hand notation $-k$ for $-k_y, -k_z$. But looking at Eq. (10.10), we see that this is exactly the 1st row of Eq. (10.3) when using an eigenvector

$$\begin{pmatrix} w_{1n,-k}^* \\ x_{1n,-k}^* \\ u_{1n,-k}^* \\ v_{1n,-k}^* \\ \dots \\ v_{N_x n,-k}^* \end{pmatrix} \quad (10.11)$$

and using an eigenvalue $-E_{n,-k}$. This can be verified by comparing the 2nd and 4th row in the manner done above (i.e. by reversing momentum, complex conjugating, and multiplying everything with -1 in the 4th row).

In other words, the above equations show that if E_{nk} is an eigenvalue of $H_k = H_{k_y, k_z}$ with eigenvector given by Eq. (10.6), then it follows that $-E_{n,-k}$ is also an eigenvalue of H_k with eigenvector given by Eq. (10.11).

Therefore, the total $4N_x$ eigenvalues of H_k can be written

$$E_{1,k}, E_{2,k}, \dots, E_{2N_x,k}, -E_{1,-k}, -E_{2,-k}, \dots, -E_{2N_x,-k}. \quad (10.12)$$

Having established this, let us now look at the consequences this has for the diagonalization of the Hamilton-operator. We define a new basis

$$\Gamma_k = \begin{pmatrix} \gamma_{k1} \\ \gamma_{k2} \\ \dots \\ \gamma_{k,4N_x} \end{pmatrix} \quad (10.13)$$

and the diagonalization matrix P_k containing the eigenvectors of H_k as column vectors:

$$P_k = \begin{pmatrix} u_{11k} & u_{12k} & \dots & u_{1,N_x,k} \\ v_{11k} & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ x_{N_x,1,k} & \dots & \dots & \dots \end{pmatrix} \quad (10.14)$$

and the matrix D_k containing the eigenvalues of H_k :

$$D_k = \text{diag}(E_{1k}, E_{2k}, \dots, E_{4N_x,k}). \quad (10.15)$$

We then have

$$H = H_0 + \frac{1}{2} \sum_{nk} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} \quad (10.16)$$

where the relation between the old and new operators is given by

$$\Gamma_k^\dagger = W_k^\dagger P_k \quad (10.17)$$

or equivalently

$$W_k = P_k \Gamma_k. \quad (10.18)$$

From Eq. (10.17), we then have

$$\gamma_{kn}^\dagger = \sum_i (c_{ik\uparrow}^\dagger u_{ink} + c_{ik\downarrow}^\dagger v_{ink} + c_{i,-k,\uparrow} w_{ink} + c_{i,-k,\downarrow} x_{ink}). \quad (10.19)$$

Note that the corresponding equation in Terrade's thesis is incorrect (probably missing complex conjugation on the coefficients in front of the c -operators). Now, we showed above that for H_{-k} , the eigenvalues can be written as $-E_{nk}$ with eigenvectors

$$\begin{pmatrix} w_{1nk}^* \\ x_{1nk}^* \\ u_{1nk}^* \\ v_{1nk}^* \\ \dots \\ v_{N_x,nk}^* \end{pmatrix}. \quad (10.20)$$

Therefore, one may also write that

$$\gamma_{-kn}^\dagger = \sum_i (c_{i,-k,\uparrow}^\dagger w_{ink}^* + c_{i,-k,\downarrow}^\dagger x_{ink}^* + c_{ik\uparrow} u_{ink}^* + c_{ik\downarrow} v_{ink}^*) \quad (10.21)$$

which follows from considering the relation $W_{-k} = P_{-k} \Gamma_{-k}$ when using the eigenvectors in Eq. (10.20) in the diagonalizing matrix P_{-k} . Note that this means that we have written the eigenvalue spectrum of H_{-k} as:

$$-E_{1,k}, -E_{2,k}, \dots, E_{1,-k}, E_{2,-k}, \dots, \quad (10.22)$$

in effect in that order in the diagonal matrix containing the eigenvalues. Comparing Eq. (28.99) and (28.101), it immediately follows that

$$\gamma_{-kn}^\dagger = \gamma_{kn}. \quad (10.23)$$

Importantly, this shows that not all γ_{kn} operators are independent of each other for all k -values. However, we can now utilize Eq. (10.23) to write the Hamilton-operator expressed only with independent operators. As stated earlier, we have

$$H = H_0 + \frac{1}{2} \sum_{nk} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} \quad (10.24)$$

Split the sum into positive and negative k -values *and* the $k = 0$ part. We denote the latter simply by K and will get back to it in detail in the next section. We get

$$H = H_0 + \frac{1}{2} \sum_{n,k>0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + \frac{1}{2} \sum_{n,k<0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + K. \quad (10.25)$$

Now, comparing Eqs. (10.12) and (10.22), we see that the eigenvalues for $k < 0$ should be expressed in terms of the eigenvalues for $k > 0$ by performing the following substitution in the sum over $k < 0$:

$$E_{nk} \rightarrow -E_{n,-k} \quad (10.26)$$

so that we get the energies in the correct order which allows us to use the relation $\gamma_{n,-k}^\dagger = \gamma_{nk}$ derived above. Otherwise, it will not be permitted. Renaming $k \rightarrow -k$ in the summation over negative k -values:

$$H = H_0 + \frac{1}{2} \sum_{n,k>0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} - \frac{1}{2} \sum_{n,k>0} E_{n,k} \gamma_{n,-k}^\dagger \gamma_{n,-k} + K. \quad (10.27)$$

But we derived above that $\gamma_{n,-k}^\dagger = \gamma_{nk}$. Use this on the third term on the rhs to get

$$\begin{aligned} H &= H_0 + \frac{1}{2} \sum_{n,k>0} (E_{nk} \gamma_{nk}^\dagger \gamma_{nk} - E_{nk} \gamma_{nk} \gamma_{nk}^\dagger) + K \\ &= H_0 - \frac{1}{2} \sum_{n,k>0} E_{nk} + \sum_{n,k>0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + K. \end{aligned} \quad (10.28)$$

In this equation, all γ_{nk} operators are independent and we may set $\langle \gamma_{nk}^\dagger \gamma_{nk} \rangle = f(E_{nk})$ for $k > 0$ so that the free energy evaluates to

$$F = H_0 - \frac{1}{2} \sum_{n,k>0} E_{nk} - \frac{1}{\beta} \sum_{n,k>0} \ln(1 + e^{-\beta E_{nk}}) + F_K \quad (10.29)$$

where F_K is the contribution from the $k = 0$ mode, which will be treated below. If you want the answer right away, it is

$$F_K = -\frac{1}{2} \sum_{E_{n,0} \geq 0} E_{n,0} - \frac{1}{\beta} \sum_{E_{n,k=0} \geq 0} \ln(1 + e^{-\beta E_{n,k=0}}) \quad (10.30)$$

where the notation $\sum_{E_{n,0} \geq 0}$ means summation over all positive eigenvalues for $k = 0$ including *half* of the eigenvalues in all pairs of zero-energy eigenvalues, if such zero-eigenvalues exist.

To be very clear, the full Hamilton-operator for a case with periodic boundary conditions in two out of three directions and where both $k_{y,z} = 0$ and $k_{y,z} = -\pi$ are included (the π is included when N is even), we have

$$H = H_0 - \frac{1}{2} \sum'_{n,k_y,k_z} E_{n,k_y,k_z} + \sum'_{n,k_y,k_z} E_{n,k_y,k_z} \gamma_{n,k_y,k_z}^\dagger \gamma_{n,k_y,k_z} \quad (10.31)$$

where

$$\begin{aligned} \sum'_{n,k_y,k_z} &\equiv \sum_{n,k_y,k_z>0} + \sum_{n,k_y>0,k_z=0} + \sum_{k_y=k_z=0,E_{n,0,0}\geq 0} + \sum_{n,k_y>0,k_z=-\pi} \\ &+ \sum_{k_y=-\pi,k_z=0,E_{n,-\pi,0}\geq 0} + \sum_{k_y=0,k_z=-\pi,E_{n,0,-\pi}\geq 0} + \sum_{k_y=-\pi,k_z=-\pi,E_{n,-\pi,-\pi}\geq 0} \end{aligned} \quad (10.32)$$

Special treatment of $k = 0$

The allowed k -values on a lattice with periodic boundary conditions are

$$k = \frac{2\pi n}{Na} \quad (10.33)$$

for a length $L = Na$ in a given direction where n is an integer. If the number of lattice points is even N , one can set

$$k = -\pi, -\pi + 2\pi/N, \dots, 0, 2\pi/N, \dots, \pi - 2\pi/N. \quad (10.34)$$

If N is odd, one can set

$$k = -\pi + \pi/N, -\pi + 3\pi/N, \dots, \pi - \pi/N. \quad (10.35)$$

Only in the N -odd case does each k -value have a $-k$ partner. In the N -even case, both $k = 0$ and $k = \pi$ are missing negative- k partners. Our derivation assumed that each k -value had a negative partner. Then how should we treat *e.g.* the $k = 0$ mode? It can be taken care of as follows.

The Hamilton-operator has the following form after diagonalizing

$$H = H_0 + \frac{1}{2} \sum_{nk} \gamma_{nk}^\dagger \gamma_{nk} E_{nk} \quad (10.36)$$

where the sum over k are over all k -values (including $k = 0$) and the sum over n is over all $4N_x$ eigenvalues. Above, not all γ_{kn} -operators are independent since

$$\gamma_{n,-k}^\dagger = \gamma_{nk}. \quad (10.37)$$

Using the above relation and that the eigenvalues of the matrix H_{-k} are $-E_{nk}$, we get

$$H = H_0 - \frac{1}{2} \sum_{n,k>0} E_{nk} + \sum_{n,k>0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + \frac{1}{2} \sum_n E_{n,0} \gamma_{n,0}^\dagger \gamma_{n,0} \quad (10.38)$$

All the γ -operators in the $\sum_{n,k>0}$ term are now independent and we may use $\langle \gamma_{nk}^\dagger \gamma_{nk} \rangle = f(E_{nk})$.

The last term on the rhs above is the $k = 0$ term. Assuming our Hamilton-matrix is such that $H_k = H_{-k}$ for $k = 0$ [which is indeed the case in the present scenario and it is also the case also in the AFM paper], it is clear from our treatment above that if $E_{n,k=0}$ is an eigenvalue of $H_{k=0}$, then so is also $-E_{n,k=0}$. Assume then that we arrange the eigenvalues for $k = 0$ such that the positive ones are the first $2N_x$ ones whereas the negative ones are the last $2N_x$ ones. If $E = 0$ is an eigenvalue, then there are two such eigenvalues and we include one zero eigenvalue in the first $2N_x$ ones and the second zero eigenvalue in the last $2N_x$ ones. It then follows that we may write for $k = 0$:

$$\gamma_{2N_x+n,k=0}^\dagger = \gamma_{n,k=0}. \quad (10.39)$$

The last term on the rhs in Eq. (10.38) may then be written

$$\begin{aligned} \frac{1}{2} \sum_n E_{n,0} \gamma_{n,0}^\dagger \gamma_{n,0} &= \frac{1}{2} \sum_{E_{n,0} \geq 0} (\gamma_{n,0}^\dagger \gamma_{n,0} E_{n,0} - \gamma_{n,0} \gamma_{n,0}^\dagger E_{n,0}) \\ &= -\frac{1}{2} \sum_{E_{n,0} \geq 0} E_{n,0} + \sum_{E_{n,0} \geq 0} E_{n,0} \gamma_{n,0}^\dagger \gamma_{n,0}, \end{aligned} \quad (10.40)$$

where the notation $\sum_{E_{n,0} \geq 0}$ means summation over all positive eigenvalues for $k = 0$ including *one* of the eigenvalues in a pair of zero-energy eigenvalues, if such zero-eigenvalues exist. Thus, the total Hamilton-operator is then:

$$H = H_0 - \frac{1}{2} \sum_{n,k>0} E_{nk} - \frac{1}{2} \sum_{E_{n,0} \geq 0} E_{n,0} + \sum_{n,k>0} E_{nk} \gamma_{nk}^\dagger \gamma_{nk} + \sum_{E_{n,0} \geq 0} E_{n,0} \gamma_{n,0}^\dagger \gamma_{n,0}, \quad (10.41)$$

where all operators are now independent of each other.

Self-consistency equation

We have

$$\Delta_i = U_i/N \sum_k \langle c_{ik\uparrow} c_{i,-k\downarrow} \rangle. \quad (10.42)$$

Since $W_k = P_k \Gamma_k$, it follows that

$$c_{ik\uparrow} = \sum_n u_{ink} \gamma_{nk}, \quad c_{i,-k\downarrow}^\dagger = \sum_n x_{ink} \gamma_{nk}. \quad (10.43)$$

But we also found that for H_{-k} , the relation between old and new operators was

$$\begin{pmatrix} c_{1,-k\uparrow} \\ c_{1,-k\downarrow}^\dagger \\ c_{1,k\uparrow} \\ c_{1,k\downarrow}^\dagger \\ \dots \\ c_{N_x,k\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} w_{11k}^* & w_{12k}^* & \dots & w_{1N_x k}^* \\ x_{11k}^* & \dots & \dots & \dots \\ u_{11k}^* & \dots & \dots & \dots \\ v_{11k}^* & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ v_{N_x 1k}^* & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} \gamma_{1,-k} \\ \gamma_{2,-k} \\ \dots \\ \gamma_{4N_x,-k} \end{pmatrix} \quad (10.44)$$

so that we also have

$$c_{i,-k\uparrow} = \sum_n w_{ink}^* \gamma_{n,-k}, \quad c_{ik\downarrow}^\dagger = \sum_n v_{ink}^* \gamma_{n,-k}. \quad (10.45)$$

Therefore, we now have

$$\begin{aligned} \Delta_i &= \frac{U_i}{N} \left(\sum_{k>0} \langle c_{ik\uparrow} c_{i,-k\downarrow} \rangle + \sum_{k<0} \langle c_{ik\uparrow} c_{i,-k\downarrow} \rangle + c_{i0\uparrow} c_{i0\downarrow} \right) \\ &= \frac{U_i}{N} \left(\sum_{k>0,n} (u_{ink} x_{ink}^* \langle \gamma_{nk} \gamma_{nk}^\dagger \rangle) + \sum_{k>0} \langle c_{i,-k\uparrow} c_{ik\downarrow} \rangle + \sum_n u_{in0} x_{in0}^* \gamma_{n0} \gamma_{n0}^\dagger \right) \\ &= \frac{U_i}{N} \left(\sum_{k>0,n} (u_{ink} x_{ink}^* \langle \gamma_{nk} \gamma_{nk}^\dagger \rangle) + \sum_{k>0,n} w_{ink}^* v_{ink} \gamma_{n,-k} \gamma_{n,-k}^\dagger + \sum_n u_{in0} x_{in0}^* \gamma_{n0} \gamma_{n0}^\dagger \right). \end{aligned} \quad (10.46)$$

As explained in the above section regarding the $k = 0$ mode, we arrange the eigenvectors in the diagonalizing matrix for the $k = 0$ case so that the first $2N_x$ are positive whereas the last $2N_x$ are negative. We then have that

$$u_{i,2N_x+n,0} = w_{i,n,0}^*, \quad x_{i,2N_x+n,0} = v_{i,n,0}^* \quad (10.47)$$

and $\gamma_{2N_x+n,0} = \gamma_{n,0}^\dagger$, as previously noted. Therefore, we get in total

$$\begin{aligned} \Delta_i &= \frac{U_i}{N} \left[\sum_{k>0,n} \left(u_{ink} x_{ink}^* [1 - f(E_{nk})] + v_{ink} w_{ink}^* f(E_{nk}) \right) + \sum_n u_{in0} x_{in0}^* \gamma_{n0} \gamma_{n0}^\dagger \right] \\ &= \frac{U_i}{N} \left[\sum_{k>0,n} \left([-u_{ink} x_{ink}^* + v_{ink} w_{ink}^*] f(E_{nk}) + u_{ink} x_{ink}^* \right) + \sum_{E_n \geq 0} \left(f(E_{n0}) (v_{in0} w_{in0}^* - u_{in0} x_{in0}^*) + u_{in0} x_{in0}^* \right) \right]. \end{aligned} \quad (10.48)$$

Sum over all positive k vs. sum over all positive eigenvalues

In previous literature, one often performs a summation over all k but only positive eigenvalues E instead. It should be possible to prove that these two methods (summation over all k , but only positive E vs. summation over positive k and all E) are equivalent, but I would argue that the first method (proven above) is computationally more efficient since we only have to consider half the k -values. In contrast, using the method where one performs a summation over all k -values but only the positive E -values, we still need to diagonalize the full matrix and *then* extract only the positive E -values.

10.1.1 Finite size in all directions: no periodic boundary conditions

In this case, there is no k -index to keep track of so the procedure is simpler. Consider the matrix h_{ij} in the Sci Rep, Atousa. Applying the same type of reasoning as we did above with the 1st and 3rd row, we can show in exactly the same way the eigenvalues come in $\pm$ pairs. Thus, the procedure for your case essentially identical to the treatment of the $k = 0$ mode above. For instance, the free energy should then read (please verify this by going through the above steps carefully):

$$F = H_0 - \frac{1}{2} \sum_{E_n \geq 0} E_n - \frac{1}{\beta} \sum_{E_n \geq 0} \ln(1 + e^{-\beta E_n}). \quad (10.49)$$

The gap-equation is also modified in a similar way as above. My guess is that it should look like

$$\Delta_i = U_i \sum_{E_n \geq 0} \left(f(E_n) (v_{in} w_{in}^* - u_{in} x_{in}^*) + u_{in} x_{in}^* \right). \quad (10.50)$$

10.1.2 Allowed k -values using an AFM with 8×1 basis

Hvis vi aksepterer en begrensning $\tilde{N} = dS + dF = \text{partall}$ (burde ikke være et stort tap $\tilde{N}$ droppe oddetall, ingen fysikk endrer seg hvis vi ser på en total lengde $N=30$ istedet for $N=31$), så tror jeg at jeg har funnet ut av k -verdi problematikken.

La oss ta et helt konkret eksempel: $N=8$. Til $\tilde{N}$ begynne med, har vi da $\text{stepk} = 2\pi/8$ slik at tillatte k -verdier er:

$k_{\text{vec}} = -\pi, -\pi + 2\pi/8, -\pi + 4\pi/8, -\pi + 6\pi/8, 0, 2\pi/8, 4\pi/8, 6\pi/8$

π er ikke med siden den er lik $-\pi$. I Lina sitt notat splitter vi denne k_{vec} inn i to biter som har like mange k -verdier hver: $[-\pi/2, \pi/2)$ vs resten. Dermed skal vi ha følgende k -verdier i intervallet $[-\pi/2, \pi/2)$

$-\pi + 4\pi/8, -\pi + 6\pi/8, 0, 2\pi/8$

Her er den første k -verdien $-\pi + 4\pi/8 = -\pi/2$ samt 0 -verdien spesiell, siden de ikke har noen negativ partner. Disse må altså behandles separat slik at man velger ut kun halvparten av

n-verdiene for disse to k-verdiene. Derimot er $-\pi+6\pi/8 = -2\pi/8$ og $2\pi/8$ hverandres negative partner, slik at her kan vi kun beholde $2\pi/8$ og summere over alle n.

På denne måten ender vi opp med eksakt settet som Lina kaller S:

$S = (E_n > 0 \text{ for } k=-\pi/2 \text{ og } 0) + (\text{samtlige } E_n \text{ for } k=2\pi/8 \text{ siden } 2\pi/8 \text{ ligger i intervallet } (0,\pi/2))$

Disse er altså k-verdiene som skal brukes i AFM-koden. Er du enig? I så fall: hvordan ser plottene ut hvis du implementerer dette?

La meg også for ordens skyld også vise eksplisitt et tilfelle hvor verdien $k=-\pi/2$ ikke er med i kvec, som skjer f.eks. ved $N=10$ (fremdeles partall). Da har vi tillatte verdier:

$k_{\text{vec}} = -\pi, -\pi + 2\pi/10, -\pi + 4\pi/10, -\pi + 6\pi/10, -\pi + 8\pi/10, 0, 2\pi/10, 4\pi/10, 6\pi/10, 8\pi/10$. π er ikke med siden den er lik $-\pi$. I Lina sitt notat splitter vi denne kvec inn i to biter som har like mange k-verdier hver: $[-\pi/2, \pi/2)$ vs resten. Dermed skal vi ha følgende k-verdier i intervallet $[-\pi/2, \pi/2)$

$-\pi + 6\pi/10, -\pi + 8\pi/10, 0, 2\pi/10, 4\pi/10$

mens de fem resterende k-verdiene er eliminerte via symmetri-relasjonene (eq 80-83 i notatet). I k-verdiene ovenfor som vi altså beholder, er det kun 0 som er spesiell: samtlige andre har negativ partner. Det er kun 0 som må behandles separat. Altså ender vi opp med settet:

$S = (E_n > 0 \text{ for } k=0) + (\text{samtlige } E_n \text{ for } k=2\pi/10 \text{ og } k=4\pi/10 \text{ siden disse ligger i intervallet } (0,\pi/2))$.

Med andre ord altså koden ta hensyn til om $-\pi/2$ er med eller ikke. For enkelhets skyld foreslår jeg at vi bare velger N slik at (1) $dS + dF = \text{partall}$ og (2) slik at $-\pi/2$ ikke er med i den opprinnelige kvec. Da kan koden skrives slik at bare 0 er spesiell (dvs den første verdien i kvec), mens alle andre verdier har bidrag fra samtlige E_n .

Låser dette k-problemet?

10.2 Introduction to Green functions

We follow here the lines of Bruus and Flensberg.

Green functions are useful tools to characterize spectral properties, correlations between particles, and the distribution of particles in mesoscopic systems. In the wavefunction representation of quantum mechanics, Green functions are useful mathematical objects to use when treating a system perturbatively. Such Green functions are solutions to a Schrödinger-like equation

$$[i\partial_t - H(\mathbf{r})]G(\mathbf{r}, \mathbf{r}', t, t') = \delta(\mathbf{r} - \mathbf{r}')\delta(t - t'). \quad (10.51)$$

The SE itself is as usual

$$[i\partial_t - H(\mathbf{r})]\Psi(\mathbf{r}, t) = 0 \quad (10.52)$$

and is solved by the wavefunction $\Psi(\mathbf{r}, t)$ and the full Hamiltonian consists of a known part H_0 and a perturbation V : $H = H_0 + V$. We will later derive this exact equation for the retarded Green function. The advanced Green function also satisfies the same equation. Note how the step-functions in time used in the definitions of the R and A Green functions are responsible for giving a finite right-hand side (the δ -functions). Without these step-functions, the equation becomes homogeneous (zero right hand-side).

It is straight-forward to verify that the wavefunction of the system can now be expressed in terms of the Green function in two ways:

$$\Psi(\mathbf{r}, t) = \Psi_0(\mathbf{r}, t) + \int \int d\mathbf{r}' dt' G_0(\mathbf{r}, \mathbf{r}', t, t') V(\mathbf{r}') \Psi(\mathbf{r}', t) \quad (10.53)$$

and

$$\Psi(\mathbf{r}, t) = \Psi_0(\mathbf{r}, t) + \int \int d\mathbf{r}' dt' G(\mathbf{r}, \mathbf{r}', t, t') V(\mathbf{r}') \Psi_0(\mathbf{r}', t) \quad (10.54)$$

where Ψ_0 is the wavefunction that solves the SE without the perturbation V . This illustrates the use of the Green function since the solution for Ψ can now be obtained via iteration:

$$\Psi = \Psi_0 + (G_0 + G_0 V G_0 + \dots) V \Psi_0 \quad (10.55)$$

where we suppressed integration variables. The last paranthesis is just the full Green function G itself, which gives us the so-called Dyson equation:

$$G = G_0 + G_0 V G. \quad (10.56)$$

10.2.1 Distinction between the Green function and the propagator K

The Green function is often called a propagator since it propagates the wavefunction from coordinate to another. A common statement in the literature is that the relation

$$\Psi(\mathbf{r}, t) = \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}', t, t') \Psi(\mathbf{r}', t) \text{ (wrong!)} \quad (10.57)$$

can be verified using the SE and the definition of G . This is in fact not accurate: direct insertion reveals that the equations are not consistent with this definition of $\Psi(\mathbf{r}, t)$.

The resolution is that one has to distinguish between the Green function G which satisfies the equation of motion listed in the beginning of this chapter from the propagator $K(\mathbf{r}, \mathbf{r}', t, t')$ which is defined as

$$G(\mathbf{r}, \mathbf{r}', t, t') = \frac{1}{i} \Theta(t - t') K(\mathbf{r}, \mathbf{r}', t, t'). \quad (10.58)$$

The propagator K can be used to relate the wavefunction Ψ at different positions and times according to:

$$\Psi(\mathbf{r}, t) = \int d\mathbf{r}' K(\mathbf{r}, \mathbf{r}', t, t') \Psi(\mathbf{r}', t') \text{ (correct!)} \quad (10.59)$$

so long as one introduces a boundary condition at equal times, namely

$$K(\mathbf{r}, \mathbf{r}', t, t) = \delta(\mathbf{r} - \mathbf{r}'). \quad (10.60)$$

The consistency between the Green function equation of motion, the Schrodinger equation, and Eq. (10.59) can now be verified by direct inspection.

Where does the boundary condition on K come from? It comes from the fact that K is a propagator that connects the wavefunctions at $(\mathbf{r}_1, t_1)$ and $(\mathbf{r}_2, t_2)$. It is clear from eq. (10.59) that at equal times, the propagator should equal $\delta(\mathbf{r} - \mathbf{r}')$ for consistency. Another way to see this is that the propagator can be written as

$$K = \langle \mathbf{r} | \hat{U}(t, t') | \mathbf{r}' \rangle \quad (10.61)$$

where $\hat{U}(t, t') = e^{-i\hat{H}(t-t')/\hbar}$. At equal times, $\hat{U}(t, t) = 1$ so that $K = \delta(\mathbf{r} - \mathbf{r}')$ due to the delta-function normalization of position basis vectors.

The propagator allows us to identify an expansion of the Green function in wavefunction eigenstates. First, we note that we may write

$$\begin{aligned}\Psi(\mathbf{r}_1, t_1) &= \langle \mathbf{r}_1 | \Psi(t_1) \rangle \\ &= \langle \mathbf{r}_1 | e^{-i\hat{H}(\mathbf{r}_1)(t_1-t_2)} \Psi(t_2) \rangle \\ &= \int d\mathbf{r}_2 \langle \mathbf{r}_1 | e^{-i\hat{H}(\mathbf{r}_1)(t_1-t_2)} | \mathbf{r}_2 \rangle \Psi(\mathbf{r}_2, t_2)\end{aligned}\quad (10.62)$$

by using a completeness relation $\int d\mathbf{r}_2 |\mathbf{r}_2\rangle \langle \mathbf{r}_2|$. Comparing this to Eq. (10.59), it is clear that

$$\begin{aligned}K(\mathbf{r}_1, \mathbf{r}_2, t_1, t_2) &= \langle \mathbf{r}_1 | e^{-i\hat{H}(\mathbf{r}_1)(t_1-t_2)} | \mathbf{r}_2 \rangle \\ &= \sum_n \langle \mathbf{r}_1 | n \rangle \langle n | e^{-i\hat{H}(\mathbf{r}_1)(t_1-t_2)} | \mathbf{r}_2 \rangle \\ &= \sum_n \langle \mathbf{r}_1 | n \rangle \langle n | \mathbf{r}_2 \rangle e^{-iE_n(t_1-t_2)} \\ &= \sum_n \Psi_n(\mathbf{r}_1, t_1) \Psi_n^\dagger(\mathbf{r}_2, t_2).\end{aligned}\quad (10.63)$$

Here, $\{|n\rangle\}$ is the complete set of eigenstates of $\hat{H}$. We define $\tilde{\psi}^T(\mathbf{r}_2, t_2) \equiv \psi_n^\dagger(\mathbf{r}_2, t_2)$. Therefore, we have proved the expansion of the retarded Green function in position eigenstates of $\hat{H}$:

$$G^R(\mathbf{r}_1, \mathbf{r}_2, t_1, t_2) = \frac{1}{i} \theta(t_1 - t_2) \sum_n \Psi_n(\mathbf{r}_1, t_1) \tilde{\Psi}_n^T(\mathbf{r}_2, t_2). \quad (10.64)$$

10.3 Matrix Green functions: retarded, advanced, Keldysh, and anomalous

The above consideration can be generalized to many-particle physics and a second quantized description of quantum mechanics. We will now define matrix Green functions which, similarly to the scalar Green function treated above, are solutions of equations of motions with similar structure as the Schrödinger-like equation, justifying calling them Green's functions. Again, computing the Green functions will give us access to various physical quantities and the Green functions themselves can be obtained in a perturbative fashion (like in the section above).

It is natural to first consider normal Green functions G which may be thought of as a type of probability amplitude for propagation of particles along a certain direction of time. The retarded, advanced, time-ordered (casual), and Keldysh Green functions are defined as

$$\begin{aligned}G_{\alpha\beta}^R(\mathbf{r}, \mathbf{r}', t, t') &= -i\theta(t - t') \langle [\psi_\alpha(\mathbf{r}, t), \psi_\beta(\mathbf{r}', t')^\dagger]_+ \rangle, \\ G_{\alpha\beta}^A(\mathbf{r}, \mathbf{r}', t, t') &= i\theta(t' - t) \langle [\psi_\alpha(\mathbf{r}, t), \psi_\beta(\mathbf{r}', t')^\dagger]_+ \rangle, \\ G_{\alpha\beta}^K(\mathbf{r}, \mathbf{r}', t, t') &= -i \langle [\psi_\alpha(\mathbf{r}, t), \psi_\beta(\mathbf{r}', t')^\dagger]_- \rangle, \\ G_{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') &= -iT \langle \psi_\alpha(\mathbf{r}, t) \psi_\beta(\mathbf{r}', t')^\dagger \rangle.\end{aligned}\quad (10.65)$$

where now $\psi(\mathbf{r}, t)$ are second-quantized fermion field *operators* (and not scalar or spinor solutions to the time-dependent SE, as in the previous section). The time-ordering operator has the effect

that it moves the operator with the biggest time to the left, which can be summarized as *later to left*. An accompanying sign change occurs if a field operator is moved in this way. Therefore, one may alternatively write

$$G_{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') = -i\Theta(t - t')\langle\psi_\alpha(\mathbf{r}, t)\psi_\beta(\mathbf{r}', t')^\dagger\rangle + i\Theta(t' - t)\langle\psi_\beta(\mathbf{r}', t')^\dagger\psi_\alpha(\mathbf{r}, t)\rangle. \quad (10.66)$$

At equal times $t = t'$, the step-function is equal to $1/2$ and $\mathcal{T}$ thus acts as a normal-ordering operator in this case. Note that the retarded Green function (and advanced, since the two are closely related) has to satisfy a particular criterion at equal times. This is because the spectral weight A is obtained from the imaginary part of G^R , and the spectral weight has to obey a sum rule. This means that integrating A over all energies has to equal 1. Since $G^R(t, t) = \int dE G^R(E)$ by definition of the Fourier-transform in relative time/energy. Therefore, the imaginary part of $G^R(t, t)$ must equal a specific value, irrespective of which system one considers.

From the above definitions, there follows a general relation between the retarded and advanced Green function in energy-space. Here, energy E is the Fourier-transform of the relative time-coordinate $t - t'$ of the Green function, so that

$$G_{\alpha\beta}^R(\mathbf{r}, \mathbf{r}', E, T) = \int_{-\infty}^{\infty} G_{\alpha\beta}^R(\mathbf{r}, \mathbf{r}', t, t') e^{iE(t-t')} d(t - t'). \quad (10.67)$$

and $T = (t + t')/2$ is the center-of-mass time coordinate. A similar type of transformation can be done for the relative space-coordinate, which then turns into $\mathbf{p}$. Coming back to the relation between G^R and G^A , using that $\langle AB \rangle^* = \langle B^\dagger A^\dagger \rangle$ we get:

$$\begin{aligned} [G_{\alpha\beta}^A(\mathbf{r}, \mathbf{r}', t, t')]^* &= -i\Theta(t' - t)\langle[\psi_\beta(\mathbf{r}', t'), \psi_\alpha^\dagger(\mathbf{r}, t)]_+\rangle \\ &= G_{\beta\alpha}^R(\mathbf{r}', \mathbf{r}, t', t). \end{aligned} \quad (10.68)$$

In other words, complex conjugating G^A gives G^R with all particle indices interchanged. In energy-space, the relation takes the form (omitting center-of-mass time dependence for brevity of notation):

$$\begin{aligned} G_{\alpha\beta}^A(\mathbf{r}, \mathbf{r}', E) &= \left[\int d\tau e^{-iE\tau} G_{\beta\alpha}^R(\mathbf{r}', \mathbf{r}, -\tau) \right]^* \\ &= \left[\int dx e^{iEx} G_{\beta\alpha}^R(\mathbf{r}', \mathbf{r}, x) \right]^* \\ &= [G_{\beta\alpha}^R(\mathbf{r}', \mathbf{r}, E)]^*. \end{aligned} \quad (10.69)$$

where we for brevity introduced $\tau \equiv t - t'$.

Let us now turn to the anomalous Green function F which characterizes pairing correlations in the system, for instance of the superconducting type. In order to discuss the possibility of pairing correlations which are odd under exchange of time coordinates, it is natural to start with the time-ordered Green function F which exists at all times. The reason for why one cannot discuss the symmetry properties of for instance F^R and F^A individually with respect to exchange of time coordinates is that they are only partially defined on the time-axis (due to the Θ -function). Therefore, when the sign of relative time (or energy) changes, one should pass from one to the other. Therefore, we expect that pair correlations which are antisymmetric in time should result in some specific relation between F^R and F^A . We now prove this rigorously.

First of all, we define the anomalous Green functions in the same way as the normal ones:

$$\begin{aligned} F_{\alpha\beta}^R(\mathbf{r}, \mathbf{r}', t, t') &= -i\Theta(t - t')\langle[\psi_\alpha(\mathbf{r}, t), \psi_\beta(\mathbf{r}', t')]_+\rangle, \\ F_{\alpha\beta}^A(\mathbf{r}, \mathbf{r}', t, t') &= i\Theta(t' - t)\langle[\psi_\alpha(\mathbf{r}, t), \psi_\beta(\mathbf{r}', t')]_+\rangle, \\ F_{\alpha\beta}^K(\mathbf{r}, \mathbf{r}', t, t') &= -i\langle[\psi_\alpha(\mathbf{r}, t), \psi_\beta(\mathbf{r}', t')]_-\rangle, \\ F_{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t') &= -iT\langle\psi_\alpha(\mathbf{r}, t)\psi_\beta(\mathbf{r}', t')\rangle. \end{aligned} \quad (10.70)$$

Now, F describes a two-fermion correlation function and the Pauli exclusion principle therefore places restrictions on the symmetry properties of F at equal times $t = t'$. It states that two half-integer spin fermions that are identical cannot simultaneously reside in the same quantum state and that the function characterizing the state of the fermions must be odd under an exchange of the particles at equal times. This means that the anomalous Green function F must always satisfy the following relation:

$$F_{\alpha\beta}(\mathbf{r}, \mathbf{r}', t, t) = -F_{\beta\alpha}(\mathbf{r}', \mathbf{r}, t, t). \quad (10.71)$$

This in fact follows from the very definition of F by writing in the same way as Eq. (10.66). We note in passing that F^R and F^A also satisfy the Pauli principle at equal times, but from the way they are constructed one can easily show that they in fact have to vanish completely at equal times $F^R(t, t) = F^A(t, t) = 0$. Therefore, it is more useful to consider F which does not necessarily have to vanish at equal times. In the energy representation, we have

$$F_{\alpha\beta}(\mathbf{r}, \mathbf{r}', E) = \int d\tau e^{iE\tau} F_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \tau) \quad (10.72)$$

where we suppressed T and used $\tau \equiv t - t'$. It is clear that if F is an antisymmetric function of relative time, meaning that F changes sign under an exchange of time coordinates, then also $F(E) = -F(-E)$ with all other spin and spatial indices left intact. An antisymmetric correlation function in time thus means that $F(E)$ is antisymmetric in E . We can now formulate this as a criterion for F^R and F^A . To do so, we see from the definitions in Eq. (10.70) that (omitting spatial indices for brevity of notation):

$$F_{\alpha\beta}(t, t') = \frac{1}{2}[F_{\alpha\beta}^R(t, t') + F_{\alpha\beta}^A(t, t') + F_{\alpha\beta}^K(t, t')]. \quad (10.73)$$

Fourier-transforming relative time, we get

$$F_{\alpha\beta}(E) = \frac{1}{2}[F_{\alpha\beta}^R(E) + F_{\alpha\beta}^A(E) + F_{\alpha\beta}^K(E)]. \quad (10.74)$$

As discussed in JP Morten thesis' appendix and also proven in Zagorskyn's book (section 3.3.2), one can use the so-called Kubo-Martin-Schwinger boundary condition for *equilibrium and stationary* systems and show that generally

$$F_{\alpha\beta}^K(E) = [F^R(E) - F^A(E)] \tanh(\beta E/2). \quad (10.75)$$

Therefore, we get

$$F_{\alpha\beta}(E) = F_{\alpha\beta}^R(E)[1 + T(E)]/2 + F_{\alpha\beta}^A(E)[1 - T(E)]/2. \quad (10.76)$$

We defined $T(E) \equiv \tanh(\beta E/2)$. An odd-frequency pairing correlation $F_{\alpha\beta}(E) = -F_{\alpha\beta}(-E)$ then dictates that

$$F_{\alpha\beta}^R(E) = -F_{\alpha\beta}^A(-E). \quad (10.77)$$

For even-frequency, one instead has $F_{\alpha\beta}^R(E) = F_{\alpha\beta}^A(-E)$. The classification of an odd-frequency state based on $F(E) = -F(-E)$ holds both in and out of equilibrium, whereas the specific relation between F^R and F^A above assumed equilibrium. However, it is reasonable to expect that the same classification should be possible also out of equilibrium since the retarded and advanced Green functions do not depend on the distribution function in the system and are thus equal both in and out of equilibrium. In fact, we can prove this for the quasiclassical Green function. By performing $\int d\xi_{\mathbf{p}}$ on Eq. (10.74), we get the quasiclassical version

$$f(E) = f^R + f^A + f^K \quad (10.78)$$

where all the f 's are now matrices in spin space and we dropped the overall factor 1/2 for simplicity (the proof does not depend on it). We generally have in quasiclassical theory (due to the normalization condition for the Green function) that:

$$\hat{g}^K = \hat{g}^R \hat{h} - \hat{h} \hat{g}^A \quad (10.79)$$

where the 4×4 matrices are

$$\hat{g}^{R,A} = \begin{pmatrix} g^{R,A} & f^{R,A} \\ -\tilde{f}^{R,A} & -\tilde{g}^{R,A} \end{pmatrix} \quad (10.80)$$

and all the entries are 2×2 matrices in spin space. The distribution function must have the form

$$\hat{h} = \begin{pmatrix} h & 0 \\ 0 & -\tilde{h} \end{pmatrix} \quad (10.81)$$

when it is chosen as diagonal, and since h is real (occupation numbers) we have $\tilde{h}(E) = h(-E)$. We then see that

$$\begin{aligned} f(E) &= f^R + f^A - f^R \tilde{h} - f^A h \\ &= f^R(1 - \tilde{h}) + f^A(1 - h). \end{aligned} \quad (10.82)$$

To satisfy $f(E) = -f(-E)$, we then see that we must have $f^R(E) = -f^A(-E)$, now proven also out of equilibrium.

From the above, it is clear that we can construct explicitly even-frequency and odd-frequency amplitudes from F^R and F^A under general circumstances as follows:

$$\begin{aligned} F_{\text{odd-freq}, \alpha\beta}^R(\mathbf{r}, \mathbf{r}', E) &= \frac{F^R(\mathbf{r}, \mathbf{r}', E) - F^A(\mathbf{r}, \mathbf{r}', -E)}{2}, \\ F_{\text{even-freq}, \alpha\beta}^R(\mathbf{r}, \mathbf{r}', E) &= \frac{F^R(\mathbf{r}, \mathbf{r}', E) + F^A(\mathbf{r}, \mathbf{r}', -E)}{2}. \end{aligned} \quad (10.83)$$

Direct inspection verifies that these Green functions are odd and even under $E \rightarrow (-E)$, corresponding to an exchange of time coordinates. Above, we reinstated the position coordinates for clarity.

10.4 Definition of boson and fermion Green functions

The governing principle used when defining these Green functions is that regardless of whether we have fermions/bosons, we want the relation between Green functions themselves to hold true.

The classic RMP from 1986 by Rammer and Smith covers all of these relations. John Ove also defines the general Green function, both fermionic and bosonic case, in section 2.1 here <https://folk.ntnu.no/johnof/green-2014.pdf> and these definitions are consistent with Rammer and Smith. For instance, looking at Rammer and Smith section II A and B, we should have general relations like

$$\begin{aligned} G^R &= \theta(t_1 - t_{1'}) (G^> - G^<), \\ G^K &= G^> + G^<, \\ G^> &= G^< \text{ at equal times} \end{aligned} \quad (10.84)$$

and so on, irrespective of whether these are fermions or bosons. This necessitates sign difference in *e.g.* the definition of the lesser Green function in eq 2.5 if Rammer and Smith for the boson/fermion case. It also necessitates switching commutators with anticommutators in the boson/fermion case. With respect to the comment above about the definition of the boson/fermion Green functions, one could wonder if a hybrid type of Green function with different boson operators, neither one being $\dagger$, such as $G^< = -i\langle \nu_q(t_1) s_k^-(t_2) \rangle$, as in the Kato *et al.* paper on spin-pumping, should follow the same conventions. However, we are free to define such a composite object and call it a lesser GF. Then, we define a corresponding contour-ordered GF. It is mathematically correct that the contour-ordered GF equals our definition of a lesser GF when choosing the times t_1 and t_2 on the contour appropriately. Then, one proves that the object defined as a lesser Green function is a bullet product between two contour-ordered Green functions. The Langreth rule (rewriting the integral to regular time axis) can now be applied with the standard result, which only depends on which time coordinates we have chosen (and not per se that we named our object a lesser GF).

10.5 Matsubara Green functions: imaginary time

The retarded Green function can be defined in a more general fashion, allowing the operators inside the expectation value to be either bosons or fermions and even describing different types of particles within each species:

$$G_{AB}^R(t, t') = -i\theta(t - t') \langle [A(t), B(t')]_{\pm} \rangle \quad (10.85)$$

where $\pm$ is for fermions/bosons. The operators A and B are single-particle second quantized operators. The Matsubara technique is used to work out the retarded Green function in a convenient way for equilibrium systems. This is accomplished by mapping the Matsubara Green function, where time and frequency arguments are imaginary quantities, to G^R . Treating time as an imaginary quantity turns out to be particularly useful when performing perturbation theory and leading up to Feynman diagrams, as we will discuss later.

As a preliminary to introducing the Matsubara Green function, we start by considering the following correlation function

$$G_{AB}(t, t') = -\langle A(t)B(t') \rangle, \quad (10.86)$$

from which it follows that $G^R = i\theta(t - t')(G_{AB} \mp G_{BA})$. By definition of expectation values, we know that

$$G_{AB}(t, t') = -\frac{1}{Z} \text{Tr}\{e^{-\beta H} A(t)B(t')\}. \quad (10.87)$$

Assume that $H = H_0 + V$ where V is the perturbation. The interaction picture, where part of the time-dependence is placed on the wavefunctions and part on the operators, provides a systematic way of expanding in powers of V . We could utilize this and write

$$G_{AB}(t, t') = -\frac{1}{Z} \text{Tr} \left[e^{-\beta H} \hat{U}(0, t) \hat{A}(t) \hat{U}(t, t') \hat{B}(t') \hat{U}(t', 0) \right] \quad (10.88)$$

where we have defined

$$\begin{aligned} \hat{A}(t) &= e^{iH_0 t} A e^{-iH_0 t}, \\ \hat{U}(t, t_0) &= e^{iH_0 t} e^{-iH(t-t_0)} e^{-iH_0 t_0}, \end{aligned} \quad (10.89)$$

valid for a time-independent H and thus V . If V is time-dependent, we must instead use:

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{i} \right)^n \int_{t_0}^t dt_1 \dots \int_{t_0}^t dt_n \mathcal{T} \left(\hat{V}(t_1) \dots \hat{V}(t_n) \right) = \mathcal{T} \left(e^{-i \int_{t_0}^t dt' \hat{V}(t')} \right). \quad (10.90)$$

The evolution operator $\hat{U}$ above can be expanded in V , but the problem arises for $e^{-\beta H}$ which must also be expanded in V . It becomes a mess, frankly. However, the problem can be solved by using imaginary times instead of real times. Keep in mind that this is merely a mathematical trick without physical content.

10.5.1 Introducing imaginary time

The idea of using imaginary time is not as crazy as one might think. Both the density operator $\rho = e^{-\beta H}/Z$ and the time evolution operator $U(t) = e^{-iHt}$ are exponential functions of the Hamiltonian and satisfy similar differential equations. U satisfies the SE

$$i\partial_t U = HU \quad (10.91)$$

while ρ is the solution to

$$\partial_\beta \rho = -H\rho, \quad (10.92)$$

known as the Bloch equation. We underline again that we here consider now only *time-independent* Hamiltonians in this section. If they are not time-independent, we cannot use ordinary equilibrium statistical mechanics, but must instead use a non-equilibrium formalism.

Now, to treat U and ρ in the same go, the trick is to replace the time argument by an imaginary quantity:

$$t \rightarrow -i\tau. \quad (10.93)$$

Here, τ is real and has dimension time. We will see that in the end, this allows us to treat both U and ρ in a single expansion in powers of V . Moreover, we will see that we can go back to physically real times from the imaginary time function in a well-defined manner.

In the Heisenberg picture, the time-dependence is removed from the wavefunctions and attached to the operators via $e^{iHt} A e^{-iHt}$. By substituting it with τ , we have

$$A(\tau) = e^{\tau H} A e^{-\tau H}. \quad (10.94)$$

In the same way, we can also define the interaction picture operator for imaginary times as

$$\hat{A}(\tau) = e^{\tau H_0} A e^{-\tau H_0}. \quad (10.95)$$

Going back to the object of interest G_{AB} , we can write a product of operators $A(\tau)B(\tau')$ in terms of the corresponding operators in the interaction picture as follows:

$$A(\tau)B(\tau') = \hat{U}(0, \tau) \hat{A}(\tau) \hat{U}(\tau, \tau') \hat{B}(\tau') \hat{U}(\tau', 0), \quad (10.96)$$

since the time-evolution operator $\hat{U}$ in the interaction picture is

$$\hat{U}(\tau, \tau') = e^{\tau H_0} e^{-(\tau - \tau')H} e^{-\tau' H_0} \quad (10.97)$$

after replacing it with τ . It follows that

$$\hat{U}(\tau, \tau'') \hat{U}(\tau'', \tau') = \hat{U}(\tau, \tau'). \quad (10.98)$$

We can obtain an explicit expression for $U(\tau, \tau')$ by differentiating Eq. (10.97) with respect to τ :

$$\partial_\tau \hat{U}(\tau, \tau') = e^{\tau H_0} (H_0 - H) e^{-(\tau - \tau')H} e^{-\tau' H_0} = -\hat{V}(\tau) \hat{U}(\tau, \tau'). \quad (10.99)$$

By integrating this equation and iterating it, carefully keeping the order of the operators involved, we end up with

$$\begin{aligned} \hat{U}(\tau, \tau') &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{\tau'}^{\tau} \dots \int_{\tau'}^{\tau} \mathcal{T}(\hat{V}(\tau_1) \dots \hat{V}(\tau_n)) \\ &= \mathcal{T} \exp \left(- \int_{\tau'}^{\tau} d\tau_1 \hat{V}(\tau_1) \right). \end{aligned} \quad (10.100)$$

The time-ordering operator $\mathcal{T}$ is defined as usual: $\mathcal{T}A(\tau)B(\tau') = A(\tau)B(\tau')$ for $\tau > \tau'$ and $\mp B(\tau')A(\tau)$ for $\tau' > \tau$ with $\mp$ for fermions/bosons.

We now proceed to show that the density operator naturally can be treated within the imaginary time formalism. We see that

$$e^{-\beta H} = e^{-\beta H_0} \hat{U}(\beta, 0) = e^{-\beta H_0} \mathcal{T} e^{-\int_0^\beta d\tau_1 \hat{V}(\tau_1)}. \quad (10.101)$$

If we now consider the *time-ordered* expectation value of the operators AB ,

$$\langle \mathcal{T}A(\tau)B(\tau') \rangle = \frac{1}{Z} \text{Tr}[e^{-\beta H} \mathcal{T}A(\tau)B(\tau')], \quad (10.102)$$

we use Eqs. (10.96) and (10.101) and obtain

$$\langle \mathcal{T}A(\tau)B(\tau') \rangle = \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} \hat{U}(\beta, 0) \mathcal{T} \{ \hat{U}(0, \tau) \hat{A}(\tau) \hat{U}(\tau, \tau') \hat{B}(\tau') \hat{U}(\tau', 0) \} \right]. \quad (10.103)$$

We can write this more compactly as

$$\langle \mathcal{T}A(\tau)B(0) \rangle = \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} \mathcal{T} \hat{U}(\beta, 0) \hat{A}(\tau) \hat{B}(0) \right] = \frac{\langle \mathcal{T} \hat{U}(\beta, 0) \hat{A}(\tau) \hat{B}(0) \rangle_0}{\langle \hat{U}(\beta, 0) \rangle_0}. \quad (10.104)$$

We have used that $Z = \text{Tr}[e^{-\beta H}] = \text{Tr}[e^{-\beta H_0} \hat{U}(\beta, 0)]$ and where the averages $\langle \dots \rangle_0$ depending on $e^{-\beta H_0}$ appear after normalizing with $1/Z_0 = 1/\text{Tr}[e^{-\beta H_0}]$. Moreover, we have used that we can set $\tau' = 0$ without loss of generality because, as we will prove in the next subsection, $\langle \mathcal{T}A(\tau)B(\tau') \rangle$ only depends on the relative time coordinate $\tau - \tau'$.

The proof of Eq. (10.104) is outlined below and relies on a property which we prove in the next subsection: the range of τ is $-\beta < \tau < \beta$. We thus start with

$$\begin{aligned}\langle \mathcal{T}A(\tau)B(0) \rangle &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} \hat{U}(\beta, 0) \mathcal{T} \{ \hat{U}(0, \tau) \hat{A}(\tau) \hat{U}(\tau, 0) \hat{B}(0) \hat{U}(0, 0) \} \right] \\ &= \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} \mathcal{T} \{ \hat{U}(\beta, \tau) \hat{A}(\tau) \hat{U}(\tau, 0) \hat{B}(0) \} \right],\end{aligned}\quad (10.105)$$

where we used that (i) β is always greater than τ , so that we could move the time-evolution operator inside the time-ordering bracket, (ii) $\hat{U}(\beta, 0)\hat{U}(0, \tau) = \hat{U}(\beta, \tau)$, and (iii) $\hat{U}(0, 0) = 1$. We now notice that it is allowed to commute $\hat{U}$ and $\hat{A}$ inside the time-ordering product in general if $\hat{A}$ is a bosonic operator and also if $\hat{A}$ is fermionic so long as H only contains terms with an *even* number of fermion operators (such as $A^\dagger A$ or $A^\dagger A^\dagger A A$). This follows for fermions since an even number of permutations does not produce a minus sign after the time-ordering operator has acted. We then end up with

$$\langle \mathcal{T}A(\tau)B(0) \rangle = \frac{1}{Z} \text{Tr} \left[e^{-\beta H_0} \mathcal{T} \{ \hat{U}(\beta, 0) \hat{A}(\tau) \hat{B}(0) \} \right], \quad (10.106)$$

which completes the proof. In the case where H contains an odd number of fermion operators (such as a Tomonaga-Luttinger liquid after introducing quasiparticle fermion operators), it is not immediately clear that one can commute $\hat{U}$ and the operators A and B , but this is a rather special case.

Let us also briefly remind ourselves of the meaning of Tr in the computation of expectation values. It has the meaning of a summation over all possible quantum states that the system can have *and, equivalently*, the actual trace operation for a matrix. Which operation that should be used depends on whether we are using a matrix representation for the operators inside the $\text{Tr}\{\dots\}$ expression. This equivalence is proven as follows:

$$\begin{aligned}\langle A \rangle &= \text{Tr} \{ e^{-\beta H} A \} \\ &= \sum_{\alpha} \langle \alpha | e^{-\beta H} A | \alpha \rangle \quad (\text{sum over all possible states } \{|\alpha\rangle\}) \\ &= \sum_{\alpha\alpha'} \langle \alpha | e^{-\beta H} | \alpha' \rangle \langle \alpha' | A | \alpha \rangle \\ &= \sum_{\alpha\alpha'} (e^{-\beta H})_{\alpha\alpha'} A_{\alpha'\alpha} \quad (\text{these are now matrix elements}) \\ &= \text{Tr} \{ e^{-\beta H} A \}.\end{aligned}\quad (10.107)$$

The final expression involving Tr is independent on which basis we actually use: if $|\alpha\rangle$ are the eigenstates of the Hamiltonian, as above, then we have $(e^{-\beta H})_{\alpha\alpha'} = e^{-\beta E_{\alpha}} \delta_{\alpha\alpha'}$.

The merit of Eq. (10.104) is that the correlation function now has a single $\hat{U}$ operator that can be expanded in the potential V in a much simpler way than the original complicated expression. We should note that the final correlation function Eq. (10.104) does have an extra time ordering operator compared to the one we started with, but even so it is clear that the imaginary time treatment allows for a great simplification.

To see why this is useful in practice in order to compute physical quantities, we need to relate this correlation function written in imaginary time to correlation function with real time arguments. This is our next task.

We note in closing this subsection that what we done compared to the usual real-time evolution in terms of the operators $e^{\pm iHt}$ is to have set $it = \tau$. Since we have stated that τ is real, this

corresponds to t being imaginary: hence the name "imaginary-time formalism". Note that τ being real, means that $e^{\pm H\tau}$ is not unitary! This has the important implication that

$$A^\dagger(\tau) \neq [A(\tau)]^\dagger \quad (10.108)$$

unlike the case for unitary real-time evolution.

10.5.2 Matsubara Green function

The Matsubara Green function is defined as

$$G_{AB}(\tau, \tau') \equiv -\langle \mathcal{T} A(\tau) B(\tau') \rangle, \quad (10.109)$$

where $\mathcal{T}$ is the time-ordering operator in imaginary time τ :

$$\mathcal{T} A(\tau) B(\tau') = \theta(\tau - \tau') A(\tau) B(\tau') \mp \theta(\tau' - \tau) B(\tau') A(\tau) \quad (10.110)$$

for fermions and bosons. Now, three useful properties follow directly from the definition of the Matsubara Green function.

- Firstly, G_{AB} is a function of the time difference only:

$$G_{AB}(\tau, \tau') = G_{AB}(\tau - \tau'). \quad (10.111)$$

This follows from the cyclic properties of the trace. If one considers $\tau > \tau'$, one obtains

$$\begin{aligned} G_{AB}(\tau, \tau') &= -\frac{1}{Z} \text{Tr} \{ e^{-\beta H} e^{\tau H} A e^{-\tau H} e^{\tau' H} B e^{-\tau' H} \} \\ &= -\frac{1}{Z} \text{Tr} \{ e^{-\beta H} e^{-\tau' H} e^{\tau H} A e^{-\tau H} e^{\tau' H} B \} \\ &= G_{AB}(\tau - \tau'). \end{aligned} \quad (10.112)$$

The proof is similar for $\tau' > \tau$. The same property holds for the real-time retarded Green function, which also only depends on the relative time for time-independent Hamiltonians.

- Secondly, convergence for $G_{AB}(\tau, \tau')$ is only guaranteed if

$$-\beta < \tau - \tau' < \beta. \quad (10.113)$$

This is clearly seen using the Lehmann representation with the eigenstates $\{|n\rangle\}$ of the Hamiltonian. Let us again assume $\tau > \tau'$ for concreteness (just so we don't have to drag along the time-ordering operator):

$$\begin{aligned} G_{AB}(\tau - \tau') &= -\frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | A(\tau) B(\tau') | n \rangle \\ &= -\frac{1}{Z} \sum_{nm} e^{-\beta E_n} e^{(E_n - E_m)(\tau - \tau')} \langle n | A | m \rangle \langle m | B | n \rangle \\ &= -\frac{1}{Z} \sum_{nm} e^{[(\tau - \tau') - \beta] E_n} e^{-E_m(\tau - \tau')} \langle n | A | m \rangle \langle m | B | n \rangle, \end{aligned} \quad (10.114)$$

since $A(\tau) = e^{H\tau} A e^{-H\tau}$. Due to the factor $e^{[(\tau - \tau') - \beta] E_n}$, we can only have convergence if $(\tau - \tau') < \beta$. While E_n can be negative, it cannot take arbitrarily large negative values: it has to be bounded from below, otherwise one would be able to extract infinite amounts of energy by de-exciting the particle which is non-physical. On the other hand, it does not have to be bounded from above. Therefore, convergence requires that $(\tau - \tau') - \beta < 0$. The inequality $-\beta < (\tau - \tau')$ follows when considering the Lehmann representation in the case $\tau' > \tau$.

- Thirdly, we have the periodicity (anti-periodicity for fermions):

$$G_{AB}(\tau) = \mp G_{AB}(\tau + \beta) \text{ for } \tau < 0 \quad (10.115)$$

Here, we set $\tau' = 0$ without loss of generality. This again follows from the cyclic properties of the trace by starting with $G_{AB}(\tau + \beta) = (-1/Z) \text{Tr}\{e^{-\beta H} e^{(\tau+\beta)H} A e^{-(\tau+\beta)H} B\}$. For positive τ , we have

$$G_{AB}(\tau) = \mp G_{AB}(\tau - \beta) \text{ for } \tau > 0 \quad (10.116)$$

As before, upper sign is for fermions, lower for bosons. We see that for any sign of τ , G_{AB} is periodic with an interval 2β . Therefore, we only need to consider the interval $-\beta < \tau < \beta$ anyway.

Because of its periodicity, we can expand G_{AB} in a Fourier-series in this interval:

$$G_{AB}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\pi n\tau/\beta} G_{AB}(n) \quad (10.117)$$

where the coefficients are given by

$$G_{AB}(n) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{i\pi n\tau/\beta} G_{AB}(\tau). \quad (10.118)$$

Due to the antiperiodicity relation derived above, the coefficients can be further simplified to

$$G_{AB}(n) = \int_0^{\beta} d\tau e^{i\pi n\tau/\beta} G_{AB}(\tau), \quad (10.119)$$

where n is even for bosons and n is odd for fermions. We will use the following notation from now on for the Fourier-transform of the Matsubara Green function:

$$G_{AB}(i\omega_n) = \int_0^{\beta} d\tau e^{i\omega_n\tau} G_{AB}(\tau) \quad (10.120)$$

where $\omega_n = (2n+1)\pi/\beta$ for fermions and $\omega_n = 2\pi n/\beta$ for bosons, where n is an integer. Note how information about temperature enters through β .

10.5.3 Connection between Matsubara and retarded Green functions

Having introduced the technical aspects of the Matsubara Green function, we shall now motivate why it has been introduced at all. We will show that there exists a function $G_{AB}(z)$, where z is a complex variable, that is analytic everywhere except on the real axis, that is equal to the Matsubara Green function $G_{AB}(i\omega_n)$ on the imaginary axis while it is equal to $G_{AB}^R(\omega)$ for z infinitesimally above the real axis.

This means that once we have one of the two, the other one follows by analytic continuation. In the cases where it is easier to compute the Matsubara function $G_{AB}(i\omega_n)$, this is a powerful method for finding the corresponding retarded function. We will prove that the appropriate analytic continuation is

$$i\omega_n \rightarrow \omega + i0^+. \quad (10.121)$$

In contrast to the real-time retarded Green function, Matsubara merges time and temperature into a single variable. The perturbation series is then carried out for this imaginary time parameter. Moreover, you can use Wick's theorem on the Matsubara Green function since it is time-ordered whereas you cannot on the real-time retarded Green function since it is not time-ordered. This shows why it is useful to master the imaginary time formalism and Matsubara Green function.

We prove the relation between G_{AB} and G_{AB}^R using the Lehmann representation. The single-particle Matsubara Green function for a fermion c is defined as

$$G(\tau, \tau') = -\langle \mathcal{T} c(\tau) c^\dagger(\tau') \rangle, \quad (10.122)$$

but we will prove the analytic continuation for the more general definition with arbitrary operators A and B .

Retarded Green function.

Using the fundamental definition of the retarded Green function in the time-domain, we have

$$G_{AB}^R(t - t') = -i\theta(t - t') \frac{1}{Z} \sum_{nm} (e^{-\beta E_n} + e^{-\beta E_m}) e^{i(E_n - E_m)(t - t')} \langle m|A|n \rangle \langle m|B^\dagger|n \rangle. \quad (10.123)$$

Fourier-transforming, we get (letting $t - t' \equiv t$):

$$\begin{aligned} G_{AB}^R(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G^R(t) \\ &= -\frac{i}{Z} \sum_{nm} (e^{-\beta E_n} + e^{-\beta E_m}) |\langle m|c^\dagger|n \rangle|^2 \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_n - E_m)t}. \end{aligned} \quad (10.124)$$

We now use that

$$\begin{aligned} \theta(t) &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\tilde{\omega} \frac{e^{-i\tilde{\omega}t}}{\tilde{\omega} + i0^+} \\ \delta(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{ixt} \end{aligned} \quad (10.125)$$

which when inserted gives the result

$$G_{AB}^R(\omega) = \frac{1}{Z} \sum_{nm} \frac{\langle m|A|n \rangle \langle m|B^\dagger|n \rangle}{\omega + E_n - E_m + i0^+} (e^{-\beta E_n} + e^{-\beta E_m}). \quad (10.126)$$

Matsubara Green function.

We now compute $G_{AB}(i\omega)$ by considering $G_{AB}(\tau)$ for $\tau > 0$. We only need to consider $\tau > 0$ to find $G_{AB}(i\omega)$, as is clear from Eq. (??). Thus,

$$\begin{aligned} G_{AB}(\tau > 0) &= -\langle A(\tau)A(0) \rangle \\ &= -\frac{1}{Z} \sum_{nm} e^{-\beta E_n} e^{(E_n - E_m)\tau} \langle m|A|n \rangle \langle m|B^\dagger|n \rangle \end{aligned} \quad (10.127)$$

via the same Lehmann representation procedure that we used for G_{AB}^R . It follows then from Eq. (10.120) that

$$\begin{aligned} G(i\omega_k) &= -\frac{1}{Z} \sum_{nm} e^{-\beta E_m} \langle m|A|n \rangle \langle m|B^\dagger|n \rangle \int_0^\beta d\tau e^{(i\omega_k + E_n - E_m)\tau} \\ &= \frac{1}{Z} \frac{\langle m|A|n \rangle \langle m|B^\dagger|n \rangle}{i\omega_k + E_n - E_m} (e^{-\beta E_n} + e^{-\beta E_m}), \end{aligned} \quad (10.128)$$

where we used that $e^{i\omega_k\beta} = -1$. Comparing Eqs. (10.126) and (10.128), we see that the retarded and Matsubara Green functions are indeed related via the analytic continuation Eq. (10.121). We underline that this way of performing the analytic continuation from Matsubara to retarded GF requires that the Matsubara $G_{AB}(z)$ is indeed analytic in the entire upper half-plane. This is the case for free fermion-like Matsubara Green functions, but may not always be the case for an arbitrary Matsubara GF.

Finally, we note that the concept "analytical continuation" in mathematics is really defined as an *extension* of the domain in which a function is analytical. In the present case when going from the Matsubara G^M to the retarded G^R Green function, we are strictly speaking not extending the domain in which the function (Matsubara GF) is analytical: we are changing the domain in which the function is analytical. To see this, note that $G^M(z)$ is analytical for all z except on the real line. The function $G^R(z)$, on the other hand, is analytical for all z on the real line and in the upper half-plane. So we are extending the domain of analyticity to include the real axis, but G^R is not analytical everywhere in the lower half-plane. Therefore, if we only consider the upper half plane, then $i\omega_n \rightarrow \omega + i\delta$ may be called an analytical continuation (since then the domain is extended to include the real line), but not if we consider the entire complex plane.

10.5.4 Computing the Matsubara Green function for non-interacting fermions

Will add here.

10.6 Retarded/Advanced Green function and justification for adding infinitesimal imaginary part to energy

In this section, we prove for a general Hamiltonian why it is necessary to perform $E \rightarrow E \pm i0^+$ for the retarded/advanced Green functions. We start with considering the definition of the retarded Green function:

$$G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) = -i\theta(t_1 - t_2) \langle \{\psi(\mathbf{r}_1, t_1), \psi^\dagger(\mathbf{r}_2, t_2)\} \rangle \quad (10.129)$$

obeys the following equation of motion

$$\begin{aligned} i\hbar\partial_{t_1} G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) &= \hbar\delta(t_1 - t_2)\delta(\mathbf{r}_1 - \mathbf{r}_2) - i\theta(t_1 - t_2) \langle \{i\hbar\partial_{t_1} \psi(\mathbf{r}_1, t_1), \psi^\dagger(\mathbf{r}_2, t_2)\} \rangle \\ &= \hbar\delta(t_1 - t_2)\delta(\mathbf{r}_1 - \mathbf{r}_2) + \hat{H}(\mathbf{r}_1)G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2). \end{aligned} \quad (10.130)$$

This can be seen from the time evolution of the field operators

$$i\hbar\partial_t \psi(\mathbf{r}, t) = [\psi(\mathbf{r}, t), \hat{H}(\mathbf{r})]. \quad (10.131)$$

For a stationary problem, we can Fourier-transform the relative coordinate $t_1 - t_2$ and one obtains

$$[E + i\delta - \hat{H}(\mathbf{r}_1)]G^R(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (10.132)$$

The reason for the appearance of the infinitesimal quantity $\delta \rightarrow 0$ is to ensure the proper boundary condition for the retarded Green function at very large relative times t . To see, this consider the Fourier-transform from $t \equiv t_1 - t_2$ to E in more detail. The equation of motion for $G^R(t)$ has the form:

$$[i\hbar\partial_{t_1} - \hat{H}(\mathbf{r}_1)]G^R(\mathbf{r}_1, \mathbf{r}_2, t) = \hbar\delta(t)\delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (10.133)$$

We now Fourier-transform to energy-space by $\int_{-\infty}^{\infty} dt e^{iEt}$. Assume for simplicity that there is no center-of-mass dependence on $(t_1 + t_2)/2$. In that case $\partial_{t_1} = \partial_t$, and we get

$$\int dt e^{iEt} i \partial_t G^R(\mathbf{r}_1, \mathbf{r}_2, t) - \hat{H}(\mathbf{r}_1) G^R(\mathbf{r}_1, \mathbf{r}_2, E) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (10.134)$$

We can treat the first term via a partial integration:

$$\int_{-\infty}^{\infty} dt e^{iEt} i \partial_t G^R(\mathbf{r}_1, \mathbf{r}_2, t) = -E e^{iEt} G^R(\mathbf{r}_1, \mathbf{r}_2, t) \Big|_{-\infty}^{\infty} + E \int_{-\infty}^{\infty} dt e^{iEt} G^R(\mathbf{r}_1, \mathbf{r}_2, t). \quad (10.135)$$

From the definition of G^R , it is clear that $G^R(t \rightarrow -\infty) = 0$ due to the step-function in relative time. But the $t \rightarrow \infty$ part of the surface term in the partial integration is less clear. It is not obvious that it can be disregarded. However, we can ensure that it is disregarded if we let $E \rightarrow E + i\delta$ where $\delta \rightarrow 0^+$ is an infinitesimal quantity. In that case, we get a factor $e^{-\delta t}$ in the surface term which ensures that the surface term vanishes also for $t \rightarrow \infty$.

Adding the infinitesimal imaginary part the energy is in fact equivalent to multiplying $G(\mathbf{r}_1, \mathbf{r}_2, t)$ with a factor $e^{-\delta t}$, which thus ensures that the object $G'(\mathbf{r}_1, \mathbf{r}_2, t) = \lim_{\delta \rightarrow 0^+} G(\mathbf{r}_1, \mathbf{r}_2, t) e^{-\delta t}$ has the correct asymptotic behavior for large t . Physically, it is reasonable that the Green function should go to zero as the relative time approaches infinity in light of its interpretation as a propagator. The remaining term in the above partial integration now takes the form:

$$(E + i\delta) \int_{-\infty}^{\infty} dt e^{iEt} e^{-\delta t} G^R(\mathbf{r}_1, \mathbf{r}_2, t) = (E + i\delta) G'^R(\mathbf{r}_1, \mathbf{r}_2, E) \quad (10.136)$$

where now $G'(E)$ is the Fourier-transform of $G'(t)$. The same also goes for the Fourier-transform we did of the term $\hat{H}(\mathbf{r}_1) G^R(t)$, so ultimately we find the equation:

$$[E + i\delta - \hat{H}(\mathbf{r}_1)] G'^R(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (10.137)$$

This is the same as the announced result Eq. (28.26), only that we have been more accurate and used G' (which is guaranteed the correct asymptotic behavior for $t \rightarrow \infty$) rather than G . In the following, we simply omit the prime on the Green function.

The main point is then that by letting $E \rightarrow \lim_{\delta \rightarrow 0^+} E + i\delta$, we get an equation of motion for a retarded Green function which satisfies the correct physical boundary condition. We also note that the advanced Green function satisfies an identical equation of motion as Eq. (28.26), but from its definition it follows that it is zero for $t > 0$. Therefore, one has to let $E \rightarrow E - i\delta$ to ensure that the surface term vanishes and that the Green function goes to zero at $t \rightarrow -\infty$. This justification for letting $E \rightarrow E \pm i\delta$ is completely general and irrespective of the exact form of $\hat{H}(\mathbf{r}_1)$. In effect, it does not assume for instance a simple free-electron gas.

10.7 McMillan-method for constructing Green function in heterostructures

McMillan developed a method to compute the Green function in ballistic heterostructures, including superconductors, based on incoming and outgoing scattering states in the system [57]. Details of

this procedure and how to choose the various wavefunctions that enter the Green function are given in the master thesis of Lina Johnsen and, to some extent, the Furusaki-Tsukada paper [58]. Here, we comment on some finer points in the derivation which are, unfortunately, not treated carefully and correctly in most of the literature.

10.7.1 Why can the Green function be decomposed into a product solution in frequency space?

The real-space equations of motion for the Green function

$$\begin{aligned} [E + i\delta - H(\mathbf{r}_1)]G(\mathbf{r}_1, \mathbf{r}_2, E) &= \delta(\mathbf{r}_1 - \mathbf{r}_2), \\ G(\mathbf{r}_1, \mathbf{r}_2, E)[E + i\delta - [H(\mathbf{r}_2)]^\dagger] &= \delta(\mathbf{r}_1 - \mathbf{r}_2). \end{aligned} \quad (10.138)$$

The sign of δ should be the same in both equations. After Fourier-transforming the equation of motion for the retarded Green function to energy-space (over relative coordinate) and to momentum-space for translationally invariant coordinates (typically the y -axis), one has the following equations of motion for the transformed Green function:

$$\begin{aligned} [E + i\delta - H(x_1, p_y)]G(x_1, x_2, p_y, E) &= \delta(x_1 - x_2), \\ G(x_1, x_2, p_y, E)[E + i\delta - [H(x_2, p_y)]^\dagger] &= \delta(x_1 - x_2). \end{aligned} \quad (10.139)$$

Here, we emphasize that † means the matrix operations of complex conjugation and transpose it does *not mean* hermitian conjugate in the operator sense. In performing the Fourier-transformation over $\mathbf{r}$, we had to discard a surface term of the type

$$ip_y e^{ip_y y} G(y) \Big|_{y \rightarrow -\infty}^{y \rightarrow \infty} \quad (10.140)$$

This is justified if G vanishes in these limits which has to be verified in the end for the final result. For free electrons, this is the case for both 2D and 3D (have not checked 1D yet). For instance, in the 3D case, we have $G \propto e^{ik|\mathbf{r}|}/|\mathbf{r}|$.

McMillan now states that the solution to this equation can be written as

$$G(x_1, x_2, p_y, E) = \psi(x_1, p_y, E) \tilde{\psi}^T(x_2, p_y, E) \quad (10.141)$$

where the wavefunctions ψ and $\tilde{\psi}$ satisfy:

$$\begin{aligned} [E + i\delta - H(x_1, p_y)]\psi(x_1, p_y, E) &= 0, \\ \tilde{\psi}^T(x_2, p_y, E)[E + i\delta - [H(x_2, p_y)]^\dagger] &= 0. \end{aligned} \quad (10.142)$$

where H in the second equation acts toward left. At $x_1 = x_2$, the δ -function in the equation of motion for the Green function is obtained by imposing a boundary condition on the G stating that its derivative has to have a jump of $2m$ at $x_1 = x_2$.

Here, a key point regarding the effect of † on H must be emphasized. Since $H(x_1)$ contains $-i\partial_{x_1}$, we see that $H^\dagger(-i\partial_{x_1}) = H(i\partial_{x_1})$. We do not have $H = H^\dagger$ due to the meaning of † in the present context.

We see that ψ and $\tilde{\psi}$ are eigenfunctions of Hamilton-operators with the same sign of the p_y -coordinate. Moreover, they are both in general superpositions since a given energy E can have different modes propagating in different directions. The McMillan-method provides a way to set up these superpositions in a way which covers all possible ways that a particle can propagate between $\mathbf{r}_1$ and $\mathbf{r}_2$ at a given energy E and momentum p_y , as is explained in detail in L. G. Johnsen's thesis.

10.7.2 Diverging wavefunction for incoming subgap quasiparticles

A problem seems to arise for incoming quasiparticles from a superconductor when the energy is subgap, $E < \Delta$. Consider a superconductor located at $x < 0$. An incoming e-like quasiparticle then has a factor $e^{iq_e x}$ where $q_e = \sqrt{2m(\mu + \sqrt{E^2 - \Delta^2})}$. For subgap energies, q_e is complex and gives a factor $e^{-\Omega x}$ where $\Omega \propto \sqrt{\Delta^2 - E^2} > 0$. Since x is negative, this factor blows up deep inside the superconductor at $x \rightarrow -\infty$. In effect, the wavefunction ψ diverges deep inside the superconductor. Is this physical and can this give a physically correct behavior for the resulting Green function?

The answer is actually yes to both questions. First of all, a subgap quasiparticle can only be incoming toward the superconducting interface if its amplitude is infinitely large deep inside the superconductor. This is because it is not a stable excitation and thus decays on order of the coherence length scale. Secondly, the fact that the amplitude grows as one moves deep inside the superconductor is not necessarily a problem. It turns out that the Green function itself does *not* diverge deep inside the superconductor (see [58]) even if ψ does. This is because the Green function measures correlations between particles and not just how large the amplitude of a specific particle is at a given point.

A similar conundrum arises when considering a ferromagnet for $x < 0$ and an incoming particle when the exchange field h is much larger than the chemical potential μ . In that case, the wavevector also becomes imaginary since $k = \sqrt{2m(\mu + E - h)} \simeq i\sqrt{2mh}$ for $h \gg \mu$. An incoming particle with such a wavevector then also diverges deep inside the ferromagnet, but if we compute the Green function in an FN bilayer one finds that it still does not diverge. The explanation is the same.

10.7.3 Consistency check: free electron in N

For consistency, we would expect to get the standard result

$$G(E, \mathbf{p}) = \frac{1}{E + i\delta - \xi_{\mathbf{p}}} \quad (10.143)$$

for a free electron in a normal metal when using the McMillan approach. We start with writing

$$G(x_1, x_2, p_y, E) = \psi(x_1, p_y, E) \tilde{\psi}(x_2, p_y, E) \quad (10.144)$$

where we have shown that the wavefunctions must satisfy

$$\begin{aligned} H(x_1, p_y) \psi(x_1, p_y) &= E \psi(x_1, p_y), \\ H^*(x_2, p_y) \tilde{\psi}(x_2, p_y) &= E \tilde{\psi}(x_2, p_y). \end{aligned} \quad (10.145)$$

Based on the procedure for how to choose ψ and $\tilde{\psi}$, for a bulk normal metal we should have

$$\psi(x_1) = e^{ik_x x_1}, \quad \tilde{\psi}(x_2) = e^{-ik_x x_2} \quad (10.146)$$

where $k_x = \sqrt{k_F^2 - p_y^2}$ and $k_F = \sqrt{2m\mu}$. We now have for $x_1 > x_2$

$$G_+ = G(x_1, x_2, p_y, E) = \alpha e^{ik_x(x_1 - x_2)} \quad (10.147)$$

while for $x_2 > x_1$

$$G_- = G(x_1, x_2, p_y, E) = \beta e^{-ik_x(x_1 - x_2)} \quad (10.148)$$

The boundary conditions at $x_1 = x_2$ are:

$$\begin{aligned} G_+ &= G_-, \\ \partial_{x_1} G_+ - \partial_{x_1} G_- &= 2m. \end{aligned} \quad (10.149)$$

The first gives $\alpha = \beta$. The second gives

$$ik_x(\alpha + \alpha) = 2m \quad (10.150)$$

so that $\alpha = -im/k_x$. Thus, the Green function is:

$$G(x_1, x_2, p_y, E) = G(x, p_y, E) = -\frac{im}{k_x} e^{ik_x|x_1 - x_2|}. \quad (10.151)$$

This gives us, with $x \equiv x_1 - x_2$ as the Green function only depends on the relative x -coordinate as is reasonable for a bulk normal metal. One may verify by direct insertion that the above Green function satisfies the equation of motion

$$[E + i\delta - H(x_1, p_y)]G(x_1, x_2, p_y, E) = \delta(x_1 - x_2) \quad (10.152)$$

at all points, including $x_1 - x_2 = 0$. We can now find the momentum-space Green function:

$$G(\mathbf{p}, E) = \int_{-\infty}^{\infty} dx G(x, p_y, E) e^{-ip_x x}. \quad (10.153)$$

We get:

$$G(\mathbf{p}, E) = -\frac{im}{k_x} \int_{-\infty}^{\infty} dx e^{ik_x|x| - ip_x x}. \quad (10.154)$$

Evaluation of this integral gives exactly the desired result when taking into account the $i\delta$ that exists in k_x .

It is also worth commenting on consistency between the McMillan-method in real space and a different way of obtaining $G(x_1, x_2, E)$. We know now the result from the McMillan-method. One can also show (see L. G. Johnsen's thesis) that generally

$$G(x_1, x_2, t_1, t_2) = i\theta(t_1 - t_2) \sum_n \psi_n(x_1, t_1) [\psi_n^*(x_2, t_2)]^T. \quad (10.155)$$

Here, $\psi_n(x_1, t_1) = \psi_n(x_1) e^{-iE_n t_1}$ where $\psi_n(x_1)$ are position eigenfunctions of the Hamiltonian $\hat{H}(x_1)$. We dropped the y -index since it is not important for the present discussion. Considering now free electrons, ψ is a scalar and we get

$$G(x_1, x_2, t_1, t_2) = i\theta(t) \sum_n \psi_n(x_1) \psi_n^*(x_2) e^{-iE_n t}. \quad (10.156)$$

We can now Fourier-transform $\int e^{i\omega t}$ and get:

$$G(x_1, x_2, \omega) = i \sum_n \psi_n(x_1) \psi_n^*(x_2) \int dt \theta(t) e^{i(\omega - E_n)t}. \quad (10.157)$$

We perform a partial integration, where the surface term is zero when we let $\omega \rightarrow \omega + i\delta$ as before, and get

$$G(x_1, x_2, \omega) = i \sum_n \frac{\psi_n(x_1) \psi_n^*(x_2)}{\omega + i\delta - E_n}. \quad (10.158)$$

This is consistent with the McMillan-result, as seen when performing the summation over n and taking into account that $E_n = k_x^2/2m - \mu$ and that $\psi(x) = e^{ik_x x}$ for free electrons in 1D. If one includes the y -dependence in the form of $e^{ik_y y}$, the summation $\sum_n$ becomes a summation over both n_x and n_y quantum numbers determining k_x and k_y , so that one ends up with:

$$G(x_1, x_2, p_y, \omega) = i \sum_{n_x, n_y} \frac{e^{ik_{x,n_x}(x_1-x_2)}}{\omega + i\delta - E_{n_x, n_y}} \delta(p_y - k_{y, n_y}). \quad (10.159)$$

Performing the summation over n_y effectively replaces k_y with p_y everywhere. Then, we are left with

$$G(x_1, x_2, p_y, \omega) = i \sum_{n_x} \frac{e^{ik_{x,n_x}(x_1-x_2)}}{\omega + i\delta - E_{n_x}(p_y)}. \quad (10.160)$$

Actually, the summation over n_x should be an integration over k_x since it is a continuous variable, so $\sum_{n_x} \rightarrow \frac{1}{2\pi} \int dk_x$. The resulting integral can be evaluated via contour-integration with an upper or lower half-circle in the complex plane:

$$\oint dk_x = \int_{-\infty}^{\infty} dk_x + \int_{\Gamma} dk_x \quad (10.161)$$

where the choice of contour is dictated by the requirement that the Γ arc part of the integral has to vanish. The result is again identical to McMillan.

10.8 Non-equilibrium Green functions

Real-time correlation functions, also known as Green functions, give physical information about a system. This is true both for systems in and out of equilibrium. Thus, it is of interest to compute 1-particle time-ordered Green functions such as

$$\begin{aligned} G(\mathbf{x}, t, \mathbf{x}', t') &= -i \langle T \{ \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \} \rangle \\ &= -i \text{Tr}[\rho T \{ \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \}] \end{aligned} \quad (10.162)$$

where the time-dependence of the field operators are given in the Heisenberg picture and ρ is an arbitrary non-equilibrium density matrix for a time-dependent Hamiltonian $\mathcal{H}(t)$. To accomplish this goal, we will introduce the Keldysh contour and contour-ordered Green functions which can be treated in perturbation theory. As a side note, we remark that such a perturbation expansion is different than the quasiclassical treatment of Green functions used when deriving the Usadel equation, since there we derive an equation of motion for the full Green function without expanding the Green function itself. But let us first briefly recap the limiting case of equilibrium.

10.8.1 Equilibrium many-body theory

Consider for simplicity the case of zero temperature. The density matrix is simply

$$\rho = |\Omega\rangle\langle\Omega|, \quad (10.163)$$

where $|\Omega\rangle$ is the exact ground-state of an interacting, but time-dependent Hamiltonian H . Thus, we have

$$H = H_0 + H_{\text{int}} \quad (10.164)$$

which is time-independent and H_{int} describes interaction between the particles. If there was a time-dependent perturbation $V(t)$ driving the system out of equilibrium, the full Hamiltonian would be

$$\mathcal{H}(t) = H + V(t). \quad (10.165)$$

Since we first consider equilibrium, set $V(t) = 0$. The time-ordered Green function

$$G = -i\langle\Omega|T\{\psi(\mathbf{x}, t)\psi^\dagger(\mathbf{x}', t')\}|\Omega\rangle \quad (10.166)$$

can now be evaluated using conventional Feynman-Dyson perturbation theory. The trick here is to express the correlator in terms of interaction picture operators and the interacting vacuum with the free vacuum $|0\rangle$, as we will elaborate on.

Recall that in the interaction picture, part of the time-dependence is transferred to the operators and part is transferred to the state itself. Let t_0 be a reference time so that $\psi(\mathbf{x}, t_0)$ is the operator in the Schrödinger picture while

$$\psi(\mathbf{x}, t) = e^{iH(t-t_0)}\psi(\mathbf{x}, t_0)e^{-iH(t-t_0)} \quad (10.167)$$

is the operator in the Heisenberg picture. The interaction picture operators are given by

$$\psi_I(\mathbf{x}, t) = e^{iH_0(t-t_0)}\psi(\mathbf{x}, t_0)e^{-iH_0(t-t_0)} \quad (10.168)$$

and thus the Heisenberg picture operators $\psi(\mathbf{x}, t)$ and the interaction picture operators $\psi_I(\mathbf{x}, t)$ relate as

$$\psi(\mathbf{x}, t) = U^\dagger(t, t_0)\psi_I(\mathbf{x}, t)U(t, t_0) \quad (10.169)$$

where

$$U(t, t_0) = e^{iH_0(t-t_0)}e^{-iH(t-t_0)} \quad (10.170)$$

is a time-evolution operator. Note that since H and H_0 do not necessarily commute, U is not simply $e^{-iH_{\text{int}}(t-t_0)}$. The idea is now to replace the Heisenberg operators in Eq. (10.166) with interaction picture operators and also establish a relation between the vacuum $|\Omega\rangle$ of the interacting theory H and the vacuum $|0\rangle$ of the free theory H_0 . A motivation for replacing Heisenberg with interaction picture operators can be seen *e.g.* in ϕ^4 scalar interacting theory, where it can be shown that the interaction picture fields $\phi_I(\mathbf{x}, t)$ satisfy the free K-G equation and thus enjoy a free mode expansion which is simple and convenient to work with.

To proceed, consider the time evolution operator in more detail. Simply inserting its definition, it is easy to verify that it satisfies

$$i\partial_t U(t, t_0) = H_I(t)U(t, t_0) \quad (10.171)$$

where now $H_I(t)$ is the interacting part of the Hamiltonian *in the interaction picture*, i.e.

$$H_I(t) = e^{iH_0(t-t_0)} H_{\text{int}} e^{-iH_0(t-t_0)}. \quad (10.172)$$

To find an explicit expression for U , we rewrite Eq. (10.171) as an integral equation

$$U(t, t_0) = \frac{1}{i} \int_{t_0}^t H_I(t') U(t', t_0) dt' + U(t_0, t_0). \quad (10.173)$$

This equation is solved via iteration, by starting with the initial guess $U^{(0)}(t, t_0) = 1$ and then obtaining

$$U^{(1)}(t, t_0) = 1 + \frac{1}{i} \int_{t_0}^t dt_1 H_I(t_1) U^{(0)}(t_1, t_0), \quad (10.174)$$

and so on [we used that $U(t_0, t_0) = 1$]. The exact solution is then given by the n -th iteration for $n \rightarrow \infty$, which gives us

$$U(t, t_0) = 1 + \sum_{n=1}^{\infty} \left(\frac{1}{i}\right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} \dots \int_{t_0}^{t_{n-1}} dt_n H_I(t_1) H_I(t_2) \dots H_I(t_n). \quad (10.175)$$

Note how the $H_I(t_i)$'s in the integrand are time-ordered. Because of this, we can write the solution in a more compact way. Consider *e.g.* the second term and observe that

$$\int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 H_I(t_1) H_I(t_2) = \frac{1}{2} \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 T\{H_I(t_1) H_I(t_2)\}. \quad (10.176)$$

This can be seen as follows. Consider the right-hand side of the above equation, which is:

$$\frac{1}{2} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 H_I(t_1) H_I(t_2) + \frac{1}{2} \int_{t_0}^t dt_1 \int_{t_1}^t dt_2 H_I(t_2) H_I(t_1), \quad (10.177)$$

where the first term is obtained for the $t_1 > t_2$ part of the integral whereas the second term is obtained for the $t_2 > t_1$ part. The point is now that these two terms are in fact identical, which proves that Eq. (10.176) holds. The fact that the two terms are identical can be seen by considering a similar argument as in the QM2 exercise 4 solution for a double integral: just rename $t_2 \leftrightarrow t_1$ and look at the integration area.

With this reasoning applied to all other terms as well, the time-evolution operator thus takes the form

$$\begin{aligned} U(t, t_0) &= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n T\{H_I(t_1) \dots H_I(t_n)\} \\ &= T\{e^{-i \int_{t_0}^t dt' H_I(t')}\}. \end{aligned} \quad (10.178)$$

The time-evolution operator is thus verified to have the following properties

- $U^\dagger(t_1, t_2) = U^{-1}(t_1, t_2) = U(t_2, t_1)$.
- $U(t_1, t_2)U(t_2, t_3) = U(t_1, t_3)$ for $t_1 \geq t_2 \geq t_3$.

Now we know exactly how to relate the Heisenberg fields to the interaction picture fields. It remains to establish a relation between the free vacuum $|0\rangle$ and the interacting vacuum $|\Omega\rangle$. Doing so will allow us to compute the real-time Green function in the interacting case via correlators evaluated in the non-interacting, free case.

Let $|n\rangle$ be an eigenstate of the full Hamiltonian, so that

$$H|n\rangle = E_n|n\rangle \quad (10.179)$$

and $H = H_0 + H_{\text{int}}$ as stated previously. We then have for the free vacuum that:

$$\begin{aligned} e^{-iHT}|0\rangle &= e^{-iHT} \sum_n |n\rangle \langle n|0\rangle \\ &= e^{-iE_\Omega T} |\Omega\rangle \langle \Omega|0\rangle + \sum_{|n\rangle \neq |\Omega\rangle} e^{-iE_n T} |n\rangle \langle n|0\rangle \end{aligned} \quad (10.180)$$

where the T is now a time, and not the time-ordering operator. Since Ω is the vacuum, by definition we must have $E_n > E_\Omega$ for all n . Taking the limit $T \rightarrow \infty(1-i\epsilon)$ where ϵ is an infinitesimal, positive quantity, only the vacuum state will survive in the above equation:

$$\lim_{T \rightarrow \infty(1-i\epsilon)} e^{-iHT}|0\rangle = \lim_{T \rightarrow \infty(1-i\epsilon)} e^{-iE_\Omega T} |\Omega\rangle \langle \Omega|0\rangle. \quad (10.181)$$

We can thus solve this for the interacting ground-state, and thus obtain

$$|\Omega\rangle = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{e^{-iHT}|0\rangle}{e^{-iE_\Omega T} \langle \Omega|0\rangle}. \quad (10.182)$$

We are thus assuming that $\langle \Omega|0\rangle \neq 0$. We can bring this to a form involving the time-evolution operator by shifting $T \rightarrow T + t_0 = t_0 - (-T)$ for an arbitrary time constant t_0 and then writing for $e^{-iH(t+t_0)}|0\rangle$:

$$e^{-iH(t_0-(-T))} e^{-iH_0(-T-t_0)}|0\rangle = U(t_0, -T)|0\rangle, \quad (10.183)$$

since $|0\rangle = e^{-iH_0(-T-t_0)}|0\rangle$ if we assume that the energy reference level has been set so that $H_0|0\rangle = 0$. With such a reference level, we have $E_\Omega \neq 0$ since the two vacua are different. We thus get:

$$|\Omega\rangle = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{U(t_0, -T)|0\rangle}{e^{-iE_\Omega[t_0-(-T)]} \langle \Omega|0\rangle}. \quad (10.184)$$

In a similar manner, starting from $\lim_{T \rightarrow \infty(1-i\epsilon)} \langle 0|e^{-iHT}$ gives

$$\langle \Omega| = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0|U(T, t_0)}{e^{-iE_\Omega(T-t_0)} \langle 0|\Omega\rangle}. \quad (10.185)$$

We can now finally compute the real-time Green function $G = -i\langle \Omega|T\{\psi(\mathbf{x}, t)\psi^\dagger(\mathbf{x}', t')\}|\Omega\rangle$. Suppose first that $t \geq t_0 \geq t'$. Keep in mind that t_0 was an arbitrary time constant we chose, so we can

always choose it to satisfy the above inequality. We then get

$$\begin{aligned}
\langle \Omega | \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') | \Omega \rangle &= \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{1}{e^{-iE_\Omega(T-t_0)} \langle 0 | \Omega \rangle} \overbrace{\langle 0 | U(T, t_0) U(t, t_0)^\dagger \psi_I(\mathbf{x}, t) U(t, t_0) \psi(\mathbf{x}, t)^{\psi(\mathbf{x}, t)} } \\
&\times \overbrace{U(t', t_0)^\dagger \psi_I^\dagger(\mathbf{x}', t') U(t', t_0) U(t_0, -T) | 0 \rangle}^{\psi^\dagger(\mathbf{x}', t')} \times \frac{1}{e^{-iE_\Omega[t_0 - (-T)]} \langle \Omega | 0 \rangle} \\
&= \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{1}{|\langle 0 | \Omega \rangle|^2 e^{-i2E_\Omega T}} \times \langle 0 | U(T, x_0) \psi_I(\mathbf{x}, t) U(t, t') \psi_I^\dagger(\mathbf{x}', t') U(t', -T) | 0 \rangle.
\end{aligned} \tag{10.186}$$

Note that we could use the contraction $U(t, t_0)U(t_0, t') = U(t, t')$ due to the assumed time-ordering. The constant prefactor can be expressed differently by noting that

$$\langle \Omega | \Omega \rangle = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{1}{|\langle 0 | \Omega \rangle|^2 e^{-i2E_\Omega T}} \times \langle 0 | U(T, t_0) U(t_0, -T) | 0 \rangle. \tag{10.187}$$

Thus, under the assumption that $t \geq t'$, we have arrived at

$$\frac{\langle \Omega | \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') | \Omega \rangle}{\langle \Omega | \Omega \rangle} = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0 | U(T, t) \psi_I(\mathbf{x}, t) U(t, t') \psi_I^\dagger(\mathbf{x}', t') U(t', -T) | 0 \rangle}{\langle 0 | U(T, -T) | 0 \rangle}. \tag{10.188}$$

The nominator can be written

$$\langle 0 | T \{ \psi_I(\mathbf{x}, t) \psi_I^\dagger(\mathbf{x}', t') U(T, t) U(t, t') U(t', -T) | 0 \rangle \tag{10.189}$$

where the time-ordering operator takes care of the correct order. A small note regarding the fields ψ is in order here. If they are bosonic, there is no extra sign when the time-ordering operator exchanges bosonic fields and the above equation holds. If they are fermionic, it also holds if one assumes that H only contains terms which are even in the number of fermion fields (as is usually the case).

Now, we could repeat the same derivation for $t \leq t'$ and arrive at the same result. Therefore, we have in general the following expression which is suitable for a perturbation expansion:

$$\frac{\langle \Omega | T \{ \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \} | \Omega \rangle}{\langle \Omega | \Omega \rangle} = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0 | T \{ \psi_I(\mathbf{x}, t) \psi_I^\dagger(\mathbf{x}', t') e^{-i \int_{-T}^T H_I(t) dt} | 0 \rangle}{\langle 0 | T e^{-i \int_{-T}^T dt H_I(t)} | 0 \rangle}. \tag{10.190}$$

Note that we omitted the time-ordering operator coming from $U(T, -T)$ since it is redundant due to the already-present time-ordering operator in the expression. The above formula can also be generalized to higher n -point correlators. For instance, in scalar field theory one has:

$$\frac{\langle \Omega | T \{ \prod_i \phi(x_i) \} | \Omega \rangle}{\langle \Omega | \Omega \rangle} = \lim_{T \rightarrow \infty(1-i\epsilon)} \frac{\langle 0 | T \{ \phi_I(x_i) e^{-i \int_{-T}^T H_I(t) dt} | 0 \rangle}{\langle 0 | T e^{-i \int_{-T}^T dt H_I(t)} | 0 \rangle}. \tag{10.191}$$

We finally note that by assuming that the interacting vacuum state is normalized:

$$\langle \Omega | \Omega \rangle = 1, \tag{10.192}$$

one obtains the standard formula found in the literature. We underline that the field operators on the left-hand side (in the original expression for the correlator) are in the Heisenberg picture,

whereas the field operators and $H_I(t)$ on the right-hand side are in the interaction picture.

The time evolution operator that we defined, $U(\infty, -\infty) = T\{e^{-i\int_{-\infty}^{\infty} H_I(t)dt}\}$, is also referred to as the S -matrix in the literature and written

$$S(\infty, -\infty) = T\{e^{-i\int_{-\infty}^{\infty} H_I(t)dt}\} \quad (10.193)$$

Expanding the S -matrix in a power series and using Wick's theorem generates Feynman diagrams, and the disconnected diagrams cancel against the phase-factor in the denominator of Eq. (10.190). The denominator is indeed essentially a phase-factor since in equilibrium, the states at minus and positive infinite times should be physically equivalent and can at most differ by a phase-factor.

In the finite temperature case, we have to use a thermal density matrix

$$\rho = \frac{e^{-\beta H}}{Z} \quad (10.194)$$

where $Z = \text{Tr}\{e^{-\beta H}\}$ is the partition function. In this case, one can use the Matsubara formalism to set up a perturbation theory in imaginary time (including temperature as an imaginary time) and then again using Wick's theorem for each term in the perturbation expansion since each such term will be an average over a non-interacting density matrix $\rho_0 = e^{-\beta H_0}/Z_0$.

10.8.2 Non-equilibrium case

We now turn our attention to the non-equilibrium case where the Hamiltonian contains a time-dependent perturbation $V(t)$. The interaction picture will now be defined using V as the perturbation rather than H_{int} (as in the previous section). In the non-equilibrium case, temperature is not well-defined. Thus, we cannot use the Matsubara technique which consists of a simultaneous expansion of the density matrix and the time-evolution operators allowed by the similar functional form of these two operators at finite temperature. Moreover, we cannot simply state that the density matrix is a simple projection down on to the ground state as in the $T = 0$ limit. Therefore, we have to consider a different approach.

We start by considering zero temperature and a generic density matrix operator

$$\rho = \sum_{\phi} p_{\phi} |\phi\rangle\langle\phi| \quad (10.195)$$

where $|\phi\rangle$ is an arbitrary, complete set of quantum states (in the Heisenberg picture). Recall that in the Heisenberg picture, the density matrix is time-independent: $\rho = \text{constant}$. This can be seen by first considering the density matrix in the Schrödinger picture, where the time evolution of states is given by $|\phi_S(t)\rangle = e^{-iHt}|\phi(0)\rangle$, giving

$$\begin{aligned} \rho_S(t) &= \sum_{\phi} p_{\phi} |\phi_S(t)\rangle\langle\phi_S(t)| \\ &= \sum_{\phi} p_{\phi} e^{-iHt} |\phi(0)\rangle\langle\phi(0)| e^{iHt} \\ &= e^{-iHt} \rho(0) e^{iHt}. \end{aligned} \quad (10.196)$$

Thus, it is clear that in the Heisenberg picture we have $\rho = e^{iHt} \rho_S(t) e^{-iHt} = \rho(0)$. It is convenient to study the Green function for one state at the time, namely the expectation value

$$G_{\phi}(\mathbf{x}, t, \mathbf{x}', t') = -i\langle\phi|T\{\psi(\mathbf{x}, t)\psi^{\dagger}(\mathbf{x}', t')\}|\phi\rangle. \quad (10.197)$$

Note that the full Green function is

$$\begin{aligned}
G(\mathbf{x}, t, \mathbf{x}', t') &= -i\langle T\{\psi(\mathbf{x}, t)\psi^\dagger(\mathbf{x}', t')\} \rangle \\
&= \text{Tr}[\rho T\{\psi(\mathbf{x}, t)\psi^\dagger(\mathbf{x}', t')\}] \\
&= \sum_{n, \phi} p_\phi \langle n | \phi \rangle \langle \phi | T\{\psi(\mathbf{x}, t)\psi^\dagger(\mathbf{x}', t')\} | n \rangle \\
&= \sum_{\phi} p_\phi \langle \phi | T\{\psi(\mathbf{x}, t)\psi^\dagger(\mathbf{x}', t')\} | \phi \rangle \\
&= \sum_{\phi} p_\phi G_\phi.
\end{aligned} \tag{10.198}$$

We are now considering a non-equilibrium case, and thus use the full Hamiltonian

$$\mathcal{H}(t) = H + V(t) \tag{10.199}$$

where H is the unperturbed equilibrium Hamiltonian that may include an interaction term H_{int} . All time-dependence lies in $V(t)$. The field operator in the interaction picture (using V as our interaction term in this non-equilibrium case) is now

$$\psi_I(\mathbf{x}, t) = e^{iHt} \psi(\mathbf{x}) e^{-iHt}, \tag{10.200}$$

where we set the reference time to zero to keep the notation as light as possible, $t_0 = 0$. Thus, in the Heisenberg picture we obtain

$$\psi(\mathbf{x}, t) = U^\dagger(t) \psi_I(\mathbf{x}, t) U(t) = S(0, t) \psi_I(\mathbf{x}, t) S(t, 0), \tag{10.201}$$

where $S(t, 0) = e^{iHt} U(t)$ with

$$U(t) = T\{e^{-i\int_0^t dt_1 \mathcal{H}(t_1)}\}. \tag{10.202}$$

Note how the time evolution operator $U(t)$ is not simply e^{-iHt} since $\mathcal{H}$ is now time-dependent. Generally, we have the S -matrix expression

$$S(t, t') = e^{iHt} U(t, t') e^{-iHt'} = T\{e^{-i\int_{t'}^t dt_1 V_I(t_1)}\}, \tag{10.203}$$

where $V_I(t) = e^{iHt} V(t) e^{-iHt}$ is the non-equilibrium perturbation in the interaction picture. Substituting these relations into our above expression for G_ϕ yields

$$G_\phi(\mathbf{x}, t, \mathbf{x}', t') = -i\langle \phi | T\{S(0, t) \psi_I(\mathbf{x}, t) S(t, 0) S(0, t') \psi_I^\dagger(\mathbf{x}', t') S(t', 0) | \phi \rangle. \tag{10.204}$$

The interaction picture state is given in the standard way by

$$|\phi_I(t)\rangle = S(t, 0) |\phi(0)\rangle = S(t, 0) |\phi_I(0)\rangle \tag{10.205}$$

where in the last step we used that all pictures coincide at $t = 0$ (since we chose $t_0 = 0$ as our reference time). Using that $[S(t, 0)]^{-1} = S(0, t)$, we get that

$$|\phi\rangle = S(0, \pm\infty) |\phi_I(\pm\infty)\rangle. \tag{10.206}$$

Combining all these results, we obtain

$$G_\phi = -i\langle \phi_I(\infty) | S(\infty, 0) T\{S(0, t) \psi_I(\mathbf{x}, t) S(t, t') \psi_I^\dagger(\mathbf{x}', t') S(t', 0)\} S(0, -\infty) | \phi_I(-\infty) \rangle. \tag{10.207}$$

Now, in exactly the same way as we did in the equilibrium case, we can consider the two cases $t \geq 0 \geq t'$ and $t \leq 0 \leq t'$ and show that because $S(\infty, -\infty)$ is itself a time-ordered product, we can in both cases write:

$$G_\phi(\mathbf{x}, t, \mathbf{x}', t') = \langle \phi_I(\infty) | T \{ S(\infty, -\infty) \psi_I(\mathbf{x}, t) \psi_I^\dagger(\mathbf{x}', t') \} | \phi_I(-\infty) \rangle \quad (10.208)$$

Note that although it might seem restrictive to have $t \geq 0 \geq t'$ rather than just $t \geq t'$, this occurs just because we chose the reference point to be zero. Had we chosen any other reference point t_0 , we would have had the criterion $t \geq 0 \geq t'$. Since we can choose t_0 as we like and there is *no dependence* on t_0 in the final expression Eq. (10.208), the result we derived when choosing $t_0 = 0$ has no loss of generality.

So far, everything we have done is correct in a general non-equilibrium setting. We should thus be able to recover the conventional Feynman expression Eq. (10.190) if we take the equilibrium limit. However, note that in going to equilibrium where $V = 0$, we would still have to account for the fact that we have defined $\psi_I(\mathbf{x}, t)$ differently in the present case (using the full H) than in the equilibrium case (where we only used H_0) in order to get exactly the same expression.

There is a key point which is worth discussing when taking the equilibrium limit. To obtain Eq. (10.190), we would have to use the following crucial fact: $|\phi_I(\infty)\rangle$ and $|\phi_I(-\infty)\rangle$ differ only by a phase factor. This is not true out of equilibrium for the following reason. We take the equilibrium limit of our non-equilibrium considerations by considering an adiabatically varying perturbation $V(t) = e^{-\epsilon|t|}V_0$ where ϵ is a positive infinitesimal. We assume $V(t)$ is so slowly varying that we can use the adiabatic theorem and the system thus remains in equilibrium at all times. Let our $|\phi\rangle$ used in G_ϕ above be the ground state of the full Hamiltonian $\mathcal{H}$ denoted $|\Omega\rangle$, meaning that it is also the ground-state of H in the limit $t \rightarrow \pm\infty$, and assume that this is a non-degenerate state. Since the time evolution is assumed adiabatic, we can use the adiabatic theorem to say that

$$|\phi_I(\pm\infty)\rangle = \lim_{\epsilon \rightarrow 0} S_\epsilon(\pm\infty, 0) |\Omega\rangle \quad (10.209)$$

is also an eigenstate of H . Since we assumed that $|\Omega\rangle$ was non-degenerate, these two states can differ at most by a phase factor

$$|\phi_I(\infty)\rangle = e^{iL} |\phi_I(-\infty)\rangle \quad (10.210)$$

Clearly,

$$e^{iL} = \langle \phi_I(-\infty) | S(\infty, -\infty) | \phi_I(-\infty) \rangle \quad (10.211)$$

by assuming a normalized $|\Omega\rangle$ as before, and so the extra phase-factor in the nominator of Eq. (10.208) that comes from replacing $|\phi_I(\infty)\rangle$ with $|\phi_I(-\infty)\rangle$ is cancelled by dividing on Eq. (10.211). This gives exactly Eq. (10.190) when we assume a normalized interacting vacuum, since it follows from Eq. (10.209) that $\langle \Omega | \Omega \rangle = \langle \phi_I(-\infty) | \phi_I(-\infty) \rangle$.

As mentioned, the ground-state at asymptotic positive and negative times are not just related by a phase-factor in the general time-dependent, non-equilibrium case since the Hamiltonian $\mathcal{H}(t)$ is then not necessarily adiabatic. Even if the Hamiltonian $\mathcal{H}$ should be time-independent, but we still have an arbitrary density matrix due to the presence of a constant V - the important case of a nonequilibrium steady state - we still cannot use the adiabatic theorem. The reason is that generic quantum states $|\phi\rangle$ are not necessarily eigenstates of $\mathcal{H}$ and the adiabatic theorem only applies to

eigenstates of $\mathcal{H}$. In other words, while we can consider one specific state $|\phi\rangle$ which is the ground-state of $\mathcal{H}$, an arbitrary density matrix which describes the full Green function G will contain many other states and the initial and final values for all the other states are not just distinguished by a phase-factor.

Thus, out of equilibrium the initial and final states are not simply related. This is clear physically since when a system is driven out of equilibrium, the asymptotic future can be different from its initial preparation in the remote past. To approach such problems, we will look at various non-equilibrium contours to avoid any reference to the state in the asymptotic future and instead base the perturbation expansion solely on $|\phi_I(\infty)\rangle$, the initially prepared state.

10.8.3 The Schwinger-Keldysh contour

The framework we are to present was originally developed by Schwinger, Craig, and Mills and popularized by Keldysh. In order to avoid having to say something about the unwanted asymptotic future state $|\phi_I(\infty)\rangle$, we use the S -matrix to rewind the time back to the asymptotic past via

$$|\phi_I(\infty)\rangle = S(\infty, -\infty)|\phi_I(-\infty)\rangle. \quad (10.212)$$

Our equation derived for G_ϕ in the previous section then takes the form

$$iG_\phi(\mathbf{x}, t, \mathbf{x}', t') = \langle \phi_I(-\infty) | S(-\infty, \infty) T\{S(\infty, -\infty) \psi_I(\mathbf{x}, t) \psi_I^\dagger(\mathbf{x}', t')\} | \phi_I(-\infty) \rangle. \quad (10.213)$$

Note that we cannot now merge $S(-\infty, \infty)$ with $S(\infty, -\infty)$ since there is a time-ordering operator between them. However, we can get around this problem by introducing a two-branch contour C and order operators along this contour according to a contour-ordering operator T_c . This contour is shown in the figure below and is known as the *Schwinger-Keldysh contour*. It consists of two oriented branches $C = C_+ \cup C_-$ with the forward branch C_+ extending from $-\infty$ to ∞ and the backward branch C_- extending from ∞ to $-\infty$.

We now let the time variables t and t' exist on this contour. Thus, a value t can exist on both the upper and lower contour. We define the fundamental object of non-equilibrium many-body theory, namely the contour-ordered Green function:

$$\begin{aligned} G_{T_c}(\mathbf{x}, t, \mathbf{x}', t') &= -i \langle T_c \{ \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \} \rangle \\ &= \text{Tr}[\rho T_c \{ \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \}]. \end{aligned} \quad (10.214)$$

Here, ρ is the density matrix in the Heisenberg picture. We know this since any expectation value of a quantity A must have the same value in any picture. So *e.g.* in the Schrödinger picture, we have

$$\langle A \rangle = \text{Tr}\{\rho_S(t) A_S\} = \text{Tr}\{\rho_H A_H(t)\}. \quad (10.215)$$

The derivation is quite technical but follows a similar structure as in the equilibrium case: see section 1.2 and 1.3 in <http://www.physics.arizona.edu/~stafford/Courses/560A/nonequilibrium.pdf>. The point is the following. Neglect the interactions H_{int} so that we only have a free Hamiltonian plus the time-dependent perturbation $V(t)$. In the end, one arrives at an expression

$$G_{T_c}(\mathbf{x}, t, \mathbf{x}', t') = -i \langle T_c \{ S_c \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \} \rangle \quad (10.216)$$

where the expectation value is to be taken using a density matrix ρ determined by the free Hamiltonian, $\rho = e^{-\beta H_0} / \text{Tr}\{e^{-\beta H_0}\}$. Moreover, we defined

$$S_c = T_c e^{-i \oint_C d\tau V_I(\tau)} \quad (10.217)$$

where the integral is to be taken along the Keldysh contour and V_I is the perturbation in the interaction picture, i.e. $V_I(t) = e^{iH_0 t} V(t) e^{-iH_0 t}$. In the zero-temperature case, the above becomes

$$G_{T_c}(\mathbf{x}, t, \mathbf{x}', t') = -i \langle 0 | T_c \{ S_c \psi(\mathbf{x}, t) \psi^\dagger(\mathbf{x}', t') \} | 0 \rangle. \quad (10.218)$$

Now one can do a perturbation expansion of the exponential in S_c and compute the contour-ordered Green function. But the goal was to obtain the time-ordered Green function, so how is this related to the contour-ordered Green function? This is via Langreth's theorem, which we consider next.

10.8.4 Langreth's theorem

10.9 Non-equilibrium Green function technique on lattice

da har jeg fått klarhet i de to spørsmålene vi snakket om.

Fortegn til t_s . Karl har brukt eq 2, med $-t_s$, men han har også brukt en negativ verdi for t_s , dvs. $t_s = -1$. Derfor er det konsistent med at du får samme resultat som han når du bruker $+t_s$ i eq 2 med $t_s > 0$. Vi kan i prinsippet bruke hvilke fortegn vi vil for hoppeelementene, både i normal-regionen og i leads. I artikkelen har vi altså valgt fortegnene til hoppingen slik at dispersjonsrelasjonen er $+2|t|\cos(k)$ i både leads og reservoir.

Hvor inngår EF. Alle likningene i artikkelen med $f(E - eV)$, $\Sigma_l(E - eV)$, et.c. samt de som står i appendix er korrekte slik de står. Den eneste plassen Fermi energien E_F inngår er i Fermi-Dirac. Med andre ord, vi har at

$$f(E - eV) = 1/[1 + \exp(\beta(E - E_F - eV))] \quad (10.219)$$

og det er ingen E_F i verken Hamiltonian for sentralregionen eller leads. Det som menes med "Here, $f(E)$ is the Fermi-Dirac et.c." i teksten er altså at det ligger en E_F innbakt i definisjonen av $f(E)$, som vist ovenfor."

Når det gjelder det som står om μ_L, R i figure captions, så er μ_L, R bare short-hand notation for det som skal trekkes fra energien i Fermi-Dirac. Med andre ord, vi kan skrive

$$f(E - eV_L) = 1/[1 + \exp(\beta(E - \mu_L))] \quad (10.220)$$

hvor altså $\mu_L = E_F + eV_L$.

Si ifra hvis noe er uklart eller fremdeles ikke gir mening.

Chapter 11

Phase transitions and path integral formalism

11.1 Types of transitions

11.2 Landau free energy

11.2.1 Lifshitz invariant

A Lifshitz invariant is a term which does not respect spatial inversion symmetry in the free energy, for instance a first order derivative. Such terms can be present in noncentrosymmetric superconducting systems when spin-orbit coupling is present.

11.3 Mermin-Wagner theorem

Mermin-Wagner theorem: at a finite temperature $T \neq 0$, a continuous symmetry cannot be spontaneously broken in a system that has dimension $d \leq 2$ with isotropic and sufficiently short-range interactions.

Put into more informal terms, this essentially means that thermal fluctuations become highly relevant in $d \leq 2$ and that they cause long-range fluctuations with so little energy cost that any ordered state (such as a ferromagnetic or superconducting state) becomes impossible to realize. At best, we can achieve a quasi-long-range order characterized by an algebraic decay (inverse power law of position). We will comment below in particular on the importance of the criteria such as "isotropic" and "sufficiently short-range".

We underline that the theorem does *not apply* to discrete symmetries such as the 1D or 2D Ising model. Let us illustrate the consequences of the theorem for a magnetic state and also see how the word "isotropic" is of key importance. In fact, by introducing a magnetic anisotropy in the system, a long-range magnetic order can be restored. This can be understood intuitively by the fact that the anisotropy creates an energy gap for the magnons and thus prevents them from being easy to excite at low temperatures.

Let us consider a temperature-dependent magnetization $M(T)$ where

$$M(T) = M(T = 0) - \Delta M(T) \tag{11.1}$$

where $\Delta M(T)$ is the reduction of the magnetization due to thermally excited spin-waves. To compute this quantity, we integrate over the density of states $N(E)$ for the magnons and multiply with their probability to be thermally occupied. The latter is governed by Bose-Einstein statistics, and we find

$$\Delta M(T) \sim \int_0^\infty \frac{N(E)}{e^{E/k_B T} - 1} dE \quad (11.2)$$

The crucial observation here is that the DOS depends on the dimensionality d . Let us assume that the excitations are described by a dispersion

$$E \sim k^n \quad (11.3)$$

and an infinitesimal volume element dV_k in d -dimensional momentum space then has the k -dependence:

$$dV_k \sim k^{d-1} dk. \quad (11.4)$$

The dispersion relation provides us with

$$\frac{dk}{dE} \sim E^{-1} E^{1/n}. \quad (11.5)$$

Therefore, we can express the volume element in k -space as

$$k^{d-1} dk = E^{(d-n)/n} dE = N(E) dE \quad (11.6)$$

where we defined the DOS:

$$N(E) \sim E^{(d-n)/n}. \quad (11.7)$$

It is important how the DOS behaves in different dimensions. For instance, in two dimensions $d = 2$ the spin-wave DOS in a ferromagnet ($n = 2$) is

$$N(E) = \text{constant}. \quad (11.8)$$

Plugging this into our expression for the change in magnetization induced by the spin-waves, we obtain:

$$\begin{aligned} \Delta M(T) &\sim \int_0^\infty \frac{\text{constant}}{e^{E/k_B T} - 1} dE \\ &\sim T \int_0^\infty \frac{1}{e^x - 1} dx. \end{aligned} \quad (11.9)$$

For small x , the integrand goes like $1/x$ and the integral thus diverges logarithmically. In effect, $\Delta M(T)$ diverges for any finite temperature T . This means that there can be no magnetic order at $T > 0$.

11.3.1 Role of anisotropy

If there is an easy axis (anisotropy) in the system, the dispersion acquires a different form. For instance, in a magnetic system with an easy axis anisotropy we have a spin-wave dispersion

$$E = A + Dk^2 \quad (11.10)$$

where A is a constant that determines the spin-wave gap (the minimum energy required to excite a spin-wave). Therefore, the previous integral Eq. (11.9) no longer has $E = 0$ as its lower limit, but instead $E = A$. As a result, the lower boundary ensures that the integral does not diverge and magnetic order is thus stabilized as a direct result of anisotropy.

11.3.2 Role of interaction range

Sticking with magnetic systems as a concrete example, let us assume longer-range interactions (such as dipolar interactions), which changes the dispersion to $E \sim \sqrt{k}$ for small k . In this case, $N(E) \sim E^3$ so that the integral

$$\Delta M(T) \sim \int_0^\infty \frac{E^3}{e^{E/k_B T} - 1} dE \quad (11.11)$$

does not diverge at its lower boundary. Therefore, magnetic order is again stabilized in this model by making the interactions be sufficiently long-ranged.

11.3.3 Role of dimensionality

To see how going to higher dimensions that d stabilizes long-range order, let us set $d = 2 + \epsilon$ where ϵ is a continuous parameter (for the sake of argument). Considering again a conventional dispersion $E \sim k^2$, we get

$$N(E) \sim E^{\epsilon/2} \quad (11.12)$$

which in turn leads to

$$\Delta M(T) \sim T \int_0^\infty \frac{dx}{x^{1-(\epsilon/2)} + \dots} \quad (11.13)$$

which does not diverge so long as $\epsilon > 0$. A slight deviation from true two-dimensionality again stabilises the order.

11.3.4 Real-world application

Although all the conditions for when Mermin-Wagner applies are difficult to strictly fulfil in a realistic system, the theorem nevertheless gives a qualitative explanation for why the ordering temperature T_c is usually reduced for thinner films: the role of thermal fluctuations becomes more important.

11.3.5 Mermin-Wagner for a superconductor

A key point shown above was that a gap in the excitation spectrum stabilized magnetic order. But we have to be careful here: it is the gap in the excitation spectrum of the *Goldstone modes* associated with spontaneous breaking of the continuous symmetry which is important. In the magnetic case, these Goldstone modes are the magnons. A magnetic anisotropy introduces a gap in their spectrum. Consider now a superconductor instead. We know that the quasiparticle excitations are gapped by $|\Delta|$. Yet this does not stabilize superconducting order in low dimensions at $T \neq 0$. The point here is that the quasiparticle excitations are *not* the Goldstone modes in the superconducting state. Instead, the Goldstone modes are excitations in the phase θ of the order parameter $\Delta = |\Delta|e^{i\theta}$, i.e. phase-fluctuations. These are massless and thus destabilize superconducting order in $d = 2$ for the same reason that ungapped magnons destabilize magnetic order: they cost no energy to excite at finite temperature.

However, it is possible to gap the Goldstone modes in a superconductor as well, for instance by taking into account the role of long-ranged Coulomb repulsion. In this case, a similar situation arises as when we gap magnons by an anisotropy: superconductivity becomes stabilized at $T \neq 0$ in $d = 2$.

11.4 Functional field integral formalism

We here summarize some key concepts for the functional field integral formalism (also referred to as path integral formalism) applied to non-relativistic condensed matter systems at finite temperature. This is a powerful methodology which allows you to study the effect of fluctuation corrections to mean-field theory and to compute correlators at finite temperatures using functional field integrals. In terms of a potential course, a rough sketch for the outline of topics could be as follows.

- Introductory concepts:

- Second quantization for fermions and bosons
- Grassmann numbers: algebra and integration/differentiation
- Coherent states
- Multidimensional Gaussian integrals

- Functional integral formulation of many-body physics

- Non-relativistic quantum mechanical path integral
- Partition function and statistical mechanics
- Functional integral using coherent states as basis
- Application: free electron gas & Matsubara sums
- Application: free boson gas & Matsubara sums

- Green functions

- Green functions at finite temperatures
- Green functions out of equilibrium

- Hubbard-Stratonovich decoupling

- Handling interaction terms in the Hamiltonian
- Application: BCS-theory
- Free energy and self-consistent equations
- About fluctuations
- Hubbard-model with $U \rightarrow \infty$:

- Spontaneously broken continuous symmetries and Goldstone modes

- Transverse and longitudinal fluctuations

- Magnetic impurities in metals: Anderson- and Kondo-models

- Anderson-model
- Kondo-model

- Heavy fermion systems - Interacting 1D systems: Luttinger liquid - Landau-theory for phase transitions and Ginzburg-Landau expansion

11.4.1 How to perform a Hubbard-Stratonovich decoupling

Thus, the general prescription for how to perform a Hubbard-Stratonovich decoupling and bosonize a fermionic interacting problem is:

1. Write down the partition function

$$Z = \int D\psi^\dagger D\psi e^{S_0 + S_I} \quad (11.14)$$

2. Assume that H_I , contained in S_I , has normal-ordered interaction terms of the type $V\psi^\dagger\psi^\dagger\psi\psi$. We are not writing out summation over indices explicitly here and V is scalar here (the treatment can be generalized to a matrix).
3. Introduce $J = \psi\psi$ so that $e^{S_I} = e^{VJ^\dagger J}$.
4. Use that $e^{VJ^\dagger J} = \int Da^\dagger Dae^{-\frac{1}{V}a^\dagger a + J^\dagger a + Ja^\dagger}$ where a is a bosonic field.
5. Collect all terms that are bilinear in ψ in a spinor Ψ so that

$$Z = \int D\psi^\dagger D\psi Da^\dagger Dae^{-\frac{1}{V}a^\dagger a + \Psi^\dagger G^{-1}\Psi}. \quad (11.15)$$

6. Finally, integrate out the fermionic degrees of freedom and obtain the exact result (after which a mean-field treatment can be invoked):

$$Z = \int Da^\dagger Dae^{-\frac{1}{V}a^\dagger a + \text{Tr} \ln(G^{-1})}. \quad (11.16)$$

11.4.2 Equivalence between mean-field approximation and saddle-point approximation

For an interacting quantum system, the Hubbard-Stratonovich transformation and mean-field approximation are methods often used to decouple interaction terms in the Hamiltonian.

In the first method, auxiliary fields are introduced via an integral identity, and then approximated by their saddle-point values. In the second method, operators are directly replaced by their mean values. In both methods, order parameters can then be solved self-consistently to yield the decoupled Hamiltonian. We will show below that these methods are fully equivalent.

First, note that the saddle-point approximation is also called the method of steepest descent. It is a method used to approximate the value of an integral of the type

$$I = \int_a^b dx e^{-Nf(x)} \quad (11.17)$$

in the limit $N \rightarrow \infty$. Due to the rapid exponential decay of the integrand, the integral will be dominated by the minimum of the function f in the interval. One shows that by Taylor-expanding $f(x)$ around x_0 , one obtains (see <https://www.lpthe.jussieu.fr/~leticia/teaching/icfp2023/MathSupport.pdf>)

$$I \simeq e^{-Nf(x_0)} [Nf''(x_0)]^{-1/2} \int_{y_a}^{y_b} dy e^{-\frac{1}{2}(y-y_0)^2}. \quad (11.18)$$

Here, x_0 is the minimum which ensures that $f''(x_0) \geq 0$. The Gaussian integral is an error function and one can find its numerical value in a table. This is the saddle point method. An even simpler approximation is just to replace f with $f(x_0)$ in the integral.

Let us now show the equivalency between the methods. Consider a action containing interactions of the form

$$Z = \int \mathcal{D}\phi e^{-S_0[\phi] + \frac{\lambda}{2} f[\phi] f[\phi]}. \quad (11.19)$$

Here, $f[\phi]$ is a functional of ϕ , describing the interactions in the system that we are interested in, and $S_0[\phi]$ is the action we perturb around. This is typically a free theory. The interaction term can also be generalized to $f[\phi^*, \phi]g[\phi^*, \phi]$, as relevant for *e.g.* superconductivity ($c^\dagger c^\dagger c c$), and also adding indices. Generalizing the procedure below shows that the proof still holds.

Mean field theory

The essential assumption is that

$$f[\phi] = M + (f[\phi] - M) \equiv M + \delta M \quad (11.20)$$

where δM is assumed to be small. This gives us the action coming from a mean-field approximation of the operators in the Hamiltonian that produces the action in the first place. Keeping first-order terms in δM gives

$$f[\phi] f[\phi] \simeq 2M f[\phi] - M^2. \quad (11.21)$$

Plug it back into the partition function to obtain

$$Z_{\text{mf}}[M] = e^{-\lambda M^2/2} \int \mathcal{D}\phi e^{-S_0[\phi] + \lambda M f[\phi]}. \quad (11.22)$$

The self-consistency relation is that

$$M = \langle f[\phi] \rangle_{\text{mf}} = \frac{1}{\lambda} \partial_M \ln \left(e^{\lambda M^2/2} Z_{\text{mf}}[M] \right) \quad (11.23)$$

since the derivative brings down a $f[\phi]$ inside the integral. Note that the latter is equivalent to

$$\partial_M \ln Z_{\text{mf}}[M] = 0 \quad (11.24)$$

which means that the mean-field approximation extremizes the free energy $F = -(1/\beta) \ln(Z)$.

H-S transformation and saddle-point approximation The essential identity for this transformation is

$$e^{\frac{\lambda}{2} f[\phi] f[\phi]} = \int \mathcal{D}\phi e^{-\frac{\lambda M^2}{2} + \lambda M f[\phi]}. \quad (11.25)$$

Plugging this into the original partition function provides

$$Z = \int \mathcal{D}M e^{-\lambda M^2/2} \int \mathcal{D}\phi e^{-S_0[\phi] + \lambda M f[\phi]} = \int \mathcal{D}M e^{-S_{\text{HS}}[M]} \quad (11.26)$$

where the Hubbard-Stratonovich action is:

$$S_{\text{HS}}[M] = \frac{\lambda M^2}{2} - \ln \left(\int \mathcal{D}\phi e^{-S_0[\phi] + \lambda M f[\phi]} \right). \quad (11.27)$$

Connection between mean-field and Hubbard-Stratonovich From the reasoning above, we can directly see that

$$S_{\text{HS}}[M] = -\ln Z_{\text{mf}}[M]. \quad (11.28)$$

Equivalently, we can write

$$Z = \int \mathcal{D}M Z_{\text{mf}}[M]. \quad (11.29)$$

The saddle-point approximation is now

$$Z \simeq e^{-S_{\text{HS}}[M_0]} = Z_{\text{mf}}[M_0] \text{ with } S'_{\text{HS}}[M_0] = 0. \quad (11.30)$$

The latter condition comes from the fact that M_0 is supposed to minimize the action S_{HS} . As usual, any constant prefactors coming from the functional integral are not written out, since they cancel when computing any physical observable.

Note how the Hubbard-Stratonovich action being extremal is exactly equivalent to the extremality of the mean-field free energy, in effect $M_0 = M$.

Beyond mean field theory

Finally, we note that although they are equivalent, the Hubbard-Stratonovich transformation is more systematic, as it might be easier to figure out how to go beyond mean-field. By doing the saddle-point approximation more accurately, keeping second order terms in the Taylor-expansion as shown initially in this section, we find a better approximation

$$Z \simeq \frac{Z_{\text{mf}}[M_0]}{\sqrt{S''_{\text{HS}}[M_0]}}. \quad (11.31)$$

This should be possible to use in order to test how reliable/stable the mean field approximation is.

11.4.3 Derivation of Ginzburg-Landau free energy for a superconductor

In physics, a partition function describes the statistical properties of a system in thermodynamic equilibrium. Partition functions are functions of the thermodynamic state variables, such as the temperature and volume.

The starting point is to consider the quantum mechanical expression for the partition function Z in the grand canonical ensemble:

$$Z = \text{Tr}\{e^{-\beta \hat{H}}\} \quad (11.32)$$

where $\hat{H}$ includes the chemical potential via a term $-\mu \hat{N}$. Consider a non-relativistic single particle. Using a position eigenvector basis to evaluate the trace and inserting a number of completeness

relations with different imaginary time labels τ , we arrive at

$$\begin{aligned} Z &= \text{Tr}\{e^{-\beta\hat{H}}\} \\ &= \int dx \langle x | e^{-\beta H} | x \rangle \\ &= \int dx \int_{x(0)}^{x(\beta)} \mathcal{D}[x(\tau)] e^{-\frac{1}{\hbar} \int_0^\beta d\tau H[x(\tau)]}. \end{aligned} \quad (11.33)$$

Here, the start and endpoints are equal which follows from the path integral calculation of the matrix element $\langle x | e^{-\beta H} | x \rangle$. Z ends up being an imaginary-time path integral. Note that we can drop $\int dx$ above if we by $\int \mathcal{D}[x(\tau)]$ implicitly mean integration over all possible paths $x(\tau)$ between all periodic start/endpoints $x(0) = x(\beta)$, as opposed to one particular start/endpoint.

Now, we want to use a different basis than the position eigenstates $\{|x\rangle\}$ to write Z for a many-particle system. We will use coherent boson/fermion states instead, because it is impractical to use position eigenstates for identical particles due to all the (-1) factors appearing due to permutations of fermions.

First, we note that by using standard Gaussian integration formulas for complex number and Grassmann-numbers can be used to derive that

$$\prod_k \int d\xi_k^* d\xi_k e^{-\zeta_i^* A_{ij} \zeta_j + \zeta_i J_i^* + \zeta_i^* J_i} = e^{J_i^* (A^{-1})_{ij} J_j} e^{\mp \text{Tr} \ln A} \quad (11.34)$$

where $\mp$ is for bosons/fermions. Here, A is a matrix while $\{J_i, J_i^*\}$ are a set of complex numbers for bosons or Grassmann-numbers for fermions. We will find use for this formula later.

Next, the trace of an operator $\hat{A}$ can be computed by inserting a completeness relation for coherent states as follows. A coherent bosonic state $|\phi\rangle$ satisfies $a_\lambda |\phi\rangle = \phi_\lambda |\phi\rangle$ where ϕ_λ is the eigenvalue and a_λ is a destruction operator whereas

$$|\phi\rangle = \exp\left[\sum_\lambda \phi_\lambda a_\lambda^\dagger\right] |0\rangle. \quad (11.35)$$

For a fermionic coherent state, due to the different properties of Grassmann numbers, one instead has $c_\lambda |\psi\rangle = \zeta_\lambda |\psi\rangle$ where

$$|\psi\rangle = \exp\left[-\sum_\lambda \zeta_\lambda c_\lambda^\dagger\right] |0\rangle. \quad (11.36)$$

For both fermions and bosons, however, the same completeness relation is fulfilled:

$$\int \int \prod_\lambda d\zeta_\lambda^* d\zeta_\lambda \exp\left[-\sum_\lambda \zeta_\lambda^* \zeta_\lambda\right] |\psi\rangle \langle \psi| = 1. \quad (11.37)$$

One then derives that the trace of an operator is

$$\begin{aligned} \text{Tr}\{A\} &= \sum_n \langle n | A | n \rangle \\ &= \int \int \prod_k d\zeta_k^* d\zeta_k e^{-\sum_\lambda \zeta_\lambda^* \zeta_\lambda} \langle s\psi | A | \psi \rangle \end{aligned} \quad (11.38)$$

where $s = \pm 1$ for bosons/fermions.

We can now compute the partition function Z by performing the trace over $e^{-\beta H}$ with a coherent state basis. Let us use the boson notation from now on, so that fields are denoted ϕ and eigenvalues ϕ_λ , but the calculation is still valid for both fermions and bosons. From the above, we have

$$Z = \int \prod_{\lambda} d\phi_{\lambda}^* d\phi_{\lambda} e^{-\sum_{\lambda} \phi_{\lambda}^* \phi_{\lambda}} \langle s\phi | e^{-\beta H} | \phi \rangle. \quad (11.39)$$

Note that we have put all numerical multiplicative constants, such as 2π , into the common prefactor in front of the integral to keep the notation light since this prefactor cancels anyway when computing observables (expectation values).

Consider then a second quantized Hamiltonian (for instance a lattice Hamiltonian) $H = H(a_{\lambda}^{\dagger}, a_{\lambda})$, which consequently produces the eigenvalues ϕ_{λ} of the coherent states in the matrix element: $\langle \phi | H(a_{\lambda}^{\dagger}, a_{\lambda}) | \phi \rangle = H(\phi_{\lambda}^{\dagger}, \phi_{\lambda})$. The expression for the partition function can then be manipulated, by inserting a bunch of completeness relations, going from a discrete index k to a continuous index τ for these relations:

$$Z = \int \prod_{\lambda} d\phi_{\lambda}^*(\tau) d\phi_{\lambda}(\tau) e^{-\sum_{\lambda} \int_0^{\beta} [\phi_{\lambda}^*(\tau) \partial \phi_{\lambda}(\tau) / \partial \tau + H\{\phi_{\lambda}^*(\tau) \phi_{\lambda}(\tau)\}]}. \quad (11.40)$$

The integration is now over all fields $\phi_{\lambda}(\tau)$ for all λ and τ .

Chapter 12

Superconductivity

12.1 A brief history of the key developments of the theory of superconductivity

Ginzburg-Landau theory can be derived from a microscopic model, namely BCS. This is done by using the path integral formalism to integrate out the fermions, and then expand the Landau free energy in the order parameter field and its derivatives.

12.2 London model

12.2.1 Meissner effect

The Meissner effect, combined with a phenomenon known as quantum locking, enables stable superconducting levitation. This can be understood as follows. Consider first two ordinary magnets with their S poles facing each other. They will repel. However, if one attempts to make one levitate above the other, additional mechanical stabilization sideways is needed. Otherwise, one magnet will not be able to levitate in a stable manner above the other.

In contrast, if one replaces one of the magnets with a superconductor, the magnetic levitation is stable even without any mechanical support sideways. First, let us understand why the superconductor levitates. The Meissner effect ensures that the superconductor creates a magnetic moment $\boldsymbol{\mu}$ that points in the opposite direction of the magnetization $\boldsymbol{M}$ of the magnet lying under it. This is due to the shielding currents which create an opposing magnetic moment to the external field $\boldsymbol{B}$ created by $\boldsymbol{M}$. Now, there are two forces acting on the superconductor. One is gravity, pointing downwards. The other is the magnetic force between the magnetic and the superconductor, which is given $\boldsymbol{F} = -\nabla U$ where $U = -\boldsymbol{\mu} \cdot \boldsymbol{B}$ is the potential energy of the superconductor in the magnetic field $\boldsymbol{B}$. Since $\boldsymbol{\mu}$ and $\boldsymbol{B}$ are oppositely oriented, the potential energy is minimized by placing them as far apart as possible. The gradient of $\boldsymbol{\mu} \cdot \boldsymbol{B}$ points upwards since this scalar product becomes less negative the further separated they are. Therefore, the superconductor will hover over the magnet at a point where the magnetic force counters the gravitational force in magnitude.

What about quantum locking? This is the reason why the superconductor can levitate in a stable manner above the magnet, unlike another magnet. The flux lines coming from the underlying magnet penetrate the superconductor if it is type II or a very thin type I superconductor. The precise region where these flux lines penetrate is typically governed by the presence of defects or impurities in the superconductor, which pins the flux lines to that specific place. If one attempts to push the levitating superconductor sideways, perturbing it, this pinning of the flux lines will push it

back to where it was. Therefore, the superconductor floats above the magnet in the same position.

12.2.2 Phase coherence

12.3 Fundamental theorems regarding superconductivity: Anderson and Kohn-Luttinger

Anderson's theorem: ...

Another key theorem dates back to unconventional pairing studied by Kohn and Luttinger in 1965, who studied models of itinerant electrons that had bare short-range repulsive interactions.:

Kohn-Luttinger theorem: assuming that a Fermi-surface exists in the system, one can always find a temperature T where the system will become superconducting with pairing in a sufficiently high angular momentum channel l regardless of what the original interaction between the fermions is.

In effect, even a system with electrons repelling each other via the Coulomb-interaction, superconductivity will ultimately appear in a higher angular momentum channel (certainly not s -wave) if one just makes the temperature T low enough. The higher the angular momentum of the Cooper pairing providing the superconducting instability is, the lower T_c will be. One can say that BCS phonon-mediated s -wave superconductivity uses retardation in time to avoid the Coulomb-interaction, whereas the Kohn-Luttinger mechanism described here uses higher angular momentum channels to avoid the Coulomb-interaction.

Let us look at this in more detail. Consider a set of fermions interacting via a weak repulsive potential, so that we may use perturbation theory. This can be described *e.g.* via the Hubbard-model:

$$H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (12.1)$$

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. Here, $U > 0$ is repulsive. It can be taken as a model representation of the screened Coulomb interaction which is indeed highly local if one assumes that the charge density is high which leads to a very small screening length.

If you try to do mean-field theory in the usual way, one quickly realizes that conventional spin-singlet on-site pairing with amplitude $\langle c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger \rangle$ is not impossible: the only solution is that the expectation value is zero.

What Kohn and Luttinger realized, was that when we try to pair electrons using bare Coulomb repulsion, there may be several other electrons in between the two electrons that we are trying to pair. These electrons can be *polarized*, in the same way that happens when you put a static charge in a metal: due to the sharp Fermi surface, it polarizes the electron gas around it and creates an oscillating electronic charge density (Friedel oscillations). The appearance of oscillations can be understood from the fact that we describe electrons as waves quantum mechanically, so the interference between many such electron waves in the total distribution of electrons at different distances from the inserted static charge interfere destructively at some points (lowering the density) and constructively at other points (increasing the density).

The Friedel oscillations take place not only in quasi-1D (with periodic boundary conditions along y and finite size along x so that there are many different waves corresponding to different k_y) and higher dimensions, but also in pure 1D. We can still describe plane-wave like solutions in an 1D chain which thus have a quantum wavevector, and interference can then take place between different waves corresponds to energy states filled up to the Fermi level. In other words, all the standing waves from different wave vectors up to the Fermi edge add up. Since they oscillate in phase close to the barrier they interfere constructively, but the farther away from the barrier the more the standing waves dephase leading to destructive interference. We note in passing that it essentially the same physics, but generalized to include the spin-degree of freedom, which is reasonable for the oscillations in the RKKY interaction between magnetic impurities or magnetic layers.

Let us now connect this reasoning to the Cooper pairing problem via Coulomb repulsion. An electron moving through a metal will polarize the electrons around it (note the difference from distorting the ion lattice, as in BCS-theory) and create a similar effect as the static charge described above. Therefore, a second electron could come along and sense these potential oscillations. Indeed, the second electron could even lower its energy sufficiently to create a bound-state with the first electron *if* it was in an orbit relative the first electron (i.e. characterized by a relative angular momentum quantum number l) which preferentially sampled the attractive part of the potential. This is impossible to achieve in an s -wave state, but it could happen in a higher angular momentum channel such as p -wave or d -wave.

In other words, if the second electron moves relative the first one in a way that it spends most of its time in the regions where the Coulomb interaction is reduced (low density) while it avoids regions where the Coulomb interaction is strong (high density), it can mostly avoid the harmful effect of the Coulomb repulsion and still be attracted to the original electron. This then requires that there is a relative motion between the two electrons, *e.g.* characterized by a p -wave orbital.

The effective $e-e$ interaction thus acquires the same oscillatory behavior as the potential of a static charge. Kohn and Luttinger considered this effective interaction up to second order in U within the framework of the Hubbard-model and found a critical temperature in channel l :

$$T_c^l \simeq E_F e^{-2.5l^4}, l \gg 1. \quad (12.2)$$

Clearly, T_c^l drops very fast with increasing l .

12.4 Attractive interaction: r -space vs. k -space

In BCS-theory, the picture usually presented is that two electrons moving in opposite directions effectively interact in an attractive manner via a distortion of the lattice. Formally, this can be described by a phonon-mediated interaction. Although this interaction $\tilde{V}(\mathbf{q}, \omega)$ is only attractive in a certain regime, one approximates it with a constant attractive interaction so long as the energy transfer ω is smaller than the Debye energy ω_D and so long as the momentum transfer $\mathbf{q}$ causes the scattered electrons to lie within the shell $E_F \pm \omega_D$ ($\omega_D \ll E_F$). A constant interaction (albeit in a limited part of momentum-space) certainly qualifies as a long-range interaction, as opposed to a contact-interaction which is only finite at a specific point in the relevant space. Therefore, it follows that the corresponding real-space interaction between the electrons in BCS-theory should essentially be a contact-interaction. Let $\mathbf{r}$ be the relative coordinate between the electrons and $\mathbf{q}$

its Fourier-transform. We then have:

$$V(\mathbf{r}) = \int \tilde{V}(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}} d\mathbf{q} \quad (12.3)$$

so that if $\tilde{V}(\mathbf{q}) = V_0$ one obtains $V(\mathbf{r}) = V_0\delta(\mathbf{r})$, i.e. a contact-interaction. This is consistent with the picture of two electrons passing by each other, because even though they avoid each other in time, they do not avoid each other in space (the attractive interaction is caused by them passing through the same region).

12.5 Expanding order parameter in lattice harmonics

Consider a 2D square lattice. The pairing interaction $V(\mathbf{r}_i - \mathbf{r}_j)$ between electrons on sites $\mathbf{r}_i$ and $\mathbf{r}_j$ has to respect the lattice symmetry. Considering both on-site and n.n. interactions, we may write

$$V(\mathbf{r}_i, \mathbf{r}_j) = U\delta_{\mathbf{r}_i, \mathbf{r}_j} + V[\delta_{\mathbf{r}_i, \mathbf{r}_j + \hat{x}} + \delta_{\mathbf{r}_i, \mathbf{r}_j - \hat{x}} + \delta_{\mathbf{r}_i, \mathbf{r}_j + \hat{y}} + \delta_{\mathbf{r}_i, \mathbf{r}_j - \hat{y}}]. \quad (12.4)$$

Fourier-transforming this to momentum-space according to [which can be seen to be the correct formula when going from real-space attractive H to momentum-space attractive H]:

$$V(\mathbf{k}, \mathbf{k}') = \sum_{ij} V(\mathbf{r}_i, \mathbf{r}_j) e^{i(\mathbf{k} - \mathbf{k}')(\mathbf{r}_j - \mathbf{r}_i)} \quad (12.5)$$

gives

$$V(\mathbf{k}, \mathbf{k}') = U + V(\cos k_x \cos k'_x + \cos k_y \cos k'_y + \sin k_x \sin k'_x + \sin k_y \sin k'_y). \quad (12.6)$$

This allows us to express $V(\mathbf{k}, \mathbf{k}')$ as

$$V(\mathbf{k}, \mathbf{k}') = \sum_i \lambda_i g_i(\mathbf{k}) g_i(\mathbf{k}') \quad (12.7)$$

where

$$\lambda_1 = 4\pi^2 U, \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = 2\pi^2 J \quad (12.8)$$

and

$$\begin{aligned} g_1(\mathbf{k}) &= \frac{1}{2\pi}, \\ g_2(\mathbf{k}) &= \frac{1}{2\pi} [\cos k_x + \cos k_y], \\ g_3(\mathbf{k}) &= \frac{1}{2\pi} [\cos k_x - \cos k_y], \\ g_4(\mathbf{k}) &= \frac{1}{2\pi} [\sin k_x + \sin k_y], \\ g_5(\mathbf{k}) &= \frac{1}{2\pi} [\sin k_x - \sin k_y]. \end{aligned} \quad (12.9)$$

This means that the gap can now be written as

$$\Delta_{\mathbf{k}} = \sum_i \lambda_i \Delta_i g_i(\mathbf{k}), \quad (12.10)$$

where we defined

$$\Delta_i = \sum_{\mathbf{k}'} \lambda_i g_i(\mathbf{k}') \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}. \quad (12.11)$$

The problem is g_4 and g_5 . At first glance, Eq. (12.10) suggests that a gap $\Delta_{\mathbf{k}} \propto g_4(\mathbf{k})$ should be allowed, namely by choosing $\Delta_{i=4} \neq 0$ and all other $\Delta_i = 0$. But in such a case, the absolute value of such a gap (which enters the fermion excitation energies) is

$$|\Delta_{\mathbf{k}}| \propto |\sin k_x + \sin k_y| \quad (12.12)$$

and does not respect the symmetries of the square lattice, since it is not invariant under *e.g.* $k_y \rightarrow -k_y$. This seems physically incorrect.

Note that the question is not whether a state $\Delta_{\mathbf{k}} \propto g_4(\mathbf{k})$ can be obtained as the ground-state or not (minimizing the free energy), but just whether such a solution is in principle allowed (for instance as a local minimum in the free energy).

Let us then investigate if a solution where $\Delta_{i=4} \neq 0$ while $\Delta_{1,2,3,5} = 0$ is consistent with Eq. (12.10) and Eq. (12.11). If $\Delta_{i=4}$ is the only non-zero coefficient, then we know that

$$\Delta_{\mathbf{k}} \propto \sin k_x + \sin k_y. \quad (12.13)$$

We now plug this into the expression for each of the coefficients $\Delta_{1,2,3}$, in which case it follows that all of these will be zero since the quantity we are performing a summation over is odd-in- $\mathbf{k}$. For instance, consider the Δ_2 coefficient:

$$\Delta_2 \propto \sum_{\mathbf{k}'} \lambda_2 \frac{1}{2\pi} [\cos k'_x + \cos k'_y] \frac{\sin k'_x + \sin k'_y}{2\sqrt{\varepsilon_{\mathbf{k}}'^2 + \Delta_{i=4}^2} |\sin k'_x + \sin k'_y|^2}. \quad (12.14)$$

The normal-state dispersion $\varepsilon_{\mathbf{k}}'$ has to satisfy the same symmetries as the lattice itself, and thus fulfils $\varepsilon_{\mathbf{k}'} = \varepsilon_{-\mathbf{k}'}$. It then follows that the quantity we are performing a summation over is odd-in- $\mathbf{k}'$ and the summation equals zero.

However, Δ_5 cannot be made zero. Specifically:

$$\Delta_5 \propto \sum_{\mathbf{k}'} \lambda_5 \frac{1}{2\pi} [\sin k'_x - \sin k'_y] \frac{\sin k'_x + \sin k'_y}{2\sqrt{\varepsilon_{\mathbf{k}}'^2 + \Delta_{i=4}^2} |\sin k'_x + \sin k'_y|^2}. \quad (12.15)$$

The quantity we are performing a summation over is even-in- $\mathbf{k}'$ and the result is finite.

The solution to the problem is thus that although we can expand the gap $\Delta_{\mathbf{k}}$ in harmonic functions that include $\sin k_x + \sin k_y$ and $\sin k_x - \sin k_y$, the allowed solution for the gap $\Delta_{\mathbf{k}}$ can never be $\sin k_x + \sin k_y$ or $\sin k_x - \sin k_y$ alone: if one is finite, the other one exists as well.

It is also worth noting that one can choose $g_4(\mathbf{k}) = \sin k_x$ and $g_5(\mathbf{k}) = \sin k_y$ instead of the $g_{4,5}$ choices we made above. In that case, a similar analysis shows that it is possible to get a pure g_4 or pure g_5 solution. An important take-away message is thus that the magnitude of the SC gap also has to satisfy the lattice symmetries in order to be physically acceptable.

12.6 Self-consistency equation

We can obtain a self-consistency equation for the gap Δ in two ways in BCS theory:

- We can use the definition $\Delta = U\langle c_{i\uparrow}c_{i\downarrow} \rangle$.
- We can derive the free energy and then demand that $\partial F/\partial \Delta = 0$.

Both results give identical results. At first glance, it is not so clear why this occurs. The first method utilizes the canonical transformation to quasiparticle operators, whereas the second utilizes that and in addition places the extra demand that the free energy should have stationary (minimum) point. In other words, why does the first method automatically give the optimal value for Δ ?

The answer can be found by looking at the path integral formulation of the superconducting Hamiltonian after performing a Hubbard-Stratonovich decoupling so that we have a bilinear fermion model coupled to a fluctuating complex fields Δ . Note that this is still exact since we have not performed a mean-field approximation. The path integral takes the form

$$Z = \int \mathcal{D}[\bar{\Delta}, \Delta] e^{-S[\bar{\Delta}, \Delta]} \quad (12.16)$$

where the action is

$$S[\bar{\Delta}, \Delta] = V \int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g} + \sum_{\mathbf{k}} \text{Tr} \ln[\partial_\tau + H(\mathbf{k})] \quad (12.17)$$

with $H(\mathbf{k})$ being the BCS Hamiltonian. Now, the path integral Z can only be evaluated for a static configuration of the complex field Δ . But in BCS theory, it is precisely this configuration which gives the physical state of the system. To see this, note that S is extensive in the volume V . This means that if we are able to find a static configuration of $\Delta = \Delta_0$ which minimizes S , so that $S = VS_0$ and $\delta S/\delta \Delta = 0$, then any fluctuations $\delta \Delta$ around this configuration can be shown to lead to a variance of the expectation value of the complex field Δ which scales like $1/V$ (the reason being precisely that S is extensive in V , meaning that the exponent in the path integral is proportional to V). In effect, the expectation value of Δ in the thermodynamic limit $V \rightarrow \infty$ becomes Δ_0 since fluctuations can then be ignored.

As a result, the mean-field approximation to the path integral is essentially exact for the BCS model. This finally explains why the very definition of the mean-field ansatz alone gives the optimal value of Δ in the BCS model where higher-order fluctuations are discarded: the mean-field ansatz is a self-consistently defined, static value for Δ which must be the minimum when fluctuations are discarded (as they are in the thermodynamic limit in the path integral formalism).

12.7 Unconventional superconductivity

12.7.1 Avoiding Coulomb interaction in time or space: *s*-wave vs. *p*-wave/*d*-wave

We thus reiterate that the electrons avoid Coulomb repulsion in time for conventional *s*-wave pairing (attraction in the $l = 0$ channel) and can thus be modelled using onsite pairing. On the other hand, for unconventional pairing in a higher- l channel (such as *p*-wave), the electrons avoid

Coulomb interaction in space by letting the order parameter have nodes and thus avoiding overlap between the electron wavefunctions in certain regions of their relative position (which after Fourier-transformation is momentum). The unconventional scenario is thus particularly relevant when strong onsite Coulomb repulsion exists which prevents any form for s -wave pairing. By pairing in a higher- l channel instead, the electrons can lower their energy and still avoid (partially) the Coulomb interaction.

12.7.2 Behavior of unconventional order parameters near interfaces/edges

In the chiral p -wave case, consider an edge to vacuum with interface normal $\mathbf{n} = \mathbf{x}$. It is known that such an interface is pair-breaking to the p_x wave component and that zero-energy states are formed. Interestingly, this leads to an enhancement of the p_y -wave order parameter near the edge because *more electrons are now available* due to the broken p_x -wave Cooper pairs.

12.7.3 Noncentrosymmetric superconductors

The normal-state Hamiltonian contains both kinetic energy and the antisymmetric spin-orbit coupling

$$H_N = \sum_{\mathbf{k}} \phi_{\mathbf{k}}^\dagger \begin{pmatrix} \epsilon_{\mathbf{k}} & \lambda(k_x - ik_y) \\ \lambda(k_x + ik_y) & \epsilon \end{pmatrix} \phi_{\mathbf{k}}. \quad (12.18)$$

Time-reversal T acting on the original fermion operators is derived (see earlier in these notes) to be

$$T(z c_{\mathbf{k}\sigma}) = -\sigma z^* c_{-\mathbf{k}, -\sigma} \quad (12.19)$$

where z is any complex scalar. The above normal-state Hamiltonian may be diagonalized to yield the relation

$$\psi_{\mathbf{k}} = P^\dagger \phi_{\mathbf{k}} \quad (12.20)$$

where $\psi_{\mathbf{k}}$ contains the new, diagonalized fermion operators while P is the diagonalization matrix containing the eigenvectors of H_N :

$$\phi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \end{pmatrix}, \quad \psi_{\mathbf{k}} = \begin{pmatrix} \gamma_{\mathbf{k}+} \\ \gamma_{\mathbf{k}-} \end{pmatrix}, \quad P^\dagger = \begin{pmatrix} 1 & e^{-i\phi} \\ -e^{i\phi} & 1 \end{pmatrix}. \quad (12.21)$$

Here, $e^{i\phi} = e^{i\phi(\mathbf{k})} = -e^{i\phi(-\mathbf{k})}$ since we defined

$$e^{i\phi(\mathbf{k})} \equiv \frac{k_x + ik_y}{k_x^2 + k_y^2}. \quad (12.22)$$

Assuming that the eigenenergies of H_N , that read $E_{\mathbf{k}\pm} = \epsilon_{\mathbf{k}} \pm \lambda|\mathbf{k}|$, are sufficiently well split by a large SOC parameter λ , we can consider only intraband pairing in the $+$ and $-$ bands individually. This means that a reasonable ansatz for the superconducting Hamiltonian is

$$H_S = \sum_{\mathbf{k}\mathbf{k}'\lambda} V_{\lambda,\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k}\lambda}^\dagger \gamma_{-\mathbf{k}\lambda}^\dagger \gamma_{-\mathbf{k}'\lambda} \gamma_{\mathbf{k}'\lambda} (?). \quad (12.23)$$

But there is a subtle point here. Such a pairing interaction does not correspond to the typical scenario of pairing between time-reversed states. This is because the time-reversal operation acting on the diagonalized states $\gamma_{\mathbf{k}\pm}$ gives rise to an extra phase-factor which affects the form of H_S .

To see this, consider the following superconducting H instead which explicitly considers pairing between time-reversed states:

$$H_S = \sum_{\mathbf{k}\mathbf{k}'\lambda} V_{\lambda,\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k}\lambda}^\dagger T\{\gamma_{\mathbf{k}\lambda}^\dagger\} \gamma_{-\mathbf{k}'\lambda} T\{\gamma_{-\mathbf{k}'\lambda}\}. \quad (12.24)$$

Since

$$\begin{aligned} T\{\gamma_{\mathbf{k}\lambda}^\dagger\} &= e^{-\lambda i\phi(\mathbf{k})} \gamma_{-\mathbf{k}\lambda}^\dagger, \\ T\{\gamma_{\mathbf{k}\lambda}\} &= e^{\lambda i\phi(\mathbf{k})} \gamma_{-\mathbf{k}\lambda}, \end{aligned} \quad (12.25)$$

we obtain

$$H_S = \sum_{\mathbf{k}\mathbf{k}'\lambda} V_{\lambda,\mathbf{k},\mathbf{k}'} e^{-i\lambda\phi(\mathbf{k})} e^{i\lambda\phi(\mathbf{k}')} \gamma_{\mathbf{k}\lambda}^\dagger \gamma_{-\mathbf{k}\lambda}^\dagger \gamma_{-\mathbf{k}'\lambda} \gamma_{\mathbf{k}'\lambda}. \quad (12.26)$$

The above transformation properties of the γ -operators under time-reversal follow by writing them out in terms of the original fermion operators and then using Eq. (12.19). Defining

$$\tilde{V}_{\lambda,\mathbf{k},\mathbf{k}'} = V_{\lambda,\mathbf{k},\mathbf{k}'} t(\mathbf{k}) t^*(\mathbf{k}'), \quad t(\mathbf{k}) = e^{-i\lambda\phi(\mathbf{k})}, \quad (12.27)$$

we may then write

$$H_S = \sum_{\mathbf{k}\mathbf{k}'\lambda} \tilde{V}_{\lambda,\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k}\lambda}^\dagger \gamma_{-\mathbf{k}\lambda}^\dagger \gamma_{-\mathbf{k}'\lambda} \gamma_{\mathbf{k}'\lambda}. \quad (12.28)$$

The important point to note here is that the pairing potential $\tilde{V}$ is odd in both $\mathbf{k}$ and $\mathbf{k}'$ while V is even in both $\mathbf{k}$ and $\mathbf{k}'$ since the phase-factor $t(\mathbf{k})$ is odd in $\mathbf{k}$. This follows from the anti-commutation relation satisfied by the γ -operators. The pairing potential between the time-reversed fermion states $V(\mathbf{k}, \mathbf{k}')$ is also invariant under the point group symmetry operations g of the lattice: $V_{\lambda,g^{-1}\mathbf{k},g^{-1}\mathbf{k}'} = V_{\lambda,\mathbf{k},\mathbf{k}'}$. This has to be the case for a time-reversal symmetric Hamiltonian since applying time-reversal should yield the same Hamiltonian, while the Hamiltonian simultaneously should be invariant under the symmetry operations of the point-group $\mathcal{G}$ of the lattice. This is seen mathematically by considering the transformation properties of the γ -operators under a point group symmetry operation, as shown in Curnoe *et al.* PRB 2004.

The momentum dependence of the pairing potential V must reflect the underlying lattice symmetry and can therefore be represented using the basis functions of the irreducible representations of $\mathcal{G}$. For more details on this, see the later chapter on group theory applied to lattices. The even basis functions $\eta(\mathbf{k})$ must be used due to the required even-symmetry in $\mathbf{k}$ of V . Thus, we may write

$$V_{\lambda,\mathbf{k},\mathbf{k}'} = - \sum_a V_\lambda^a \sum_{i=1}^{d_A} \eta_{a,i}(\mathbf{k}) \eta_{a,i}^*(\mathbf{k}'). \quad (12.29)$$

Here, $\eta_{a,i}(\mathbf{k})$ are even basis function where a labels the irreducible representation (which has dimensionality d_a) of $\mathcal{G}$ which correspond to pairing channels of different symmetry. The irreducible representation that is realized physically is the one giving the maximum critical temperature.

After performing a mean-field approximation on the above Hamiltonian, one finds that the pairing is a mixture of singlet and triplet pairing in the original fermion basis.

12.8 The superconducting coherence length and magnetic penetration depth

12.8.1 Coherence length

The length scale ξ is known as the superconducting coherence length and is a measure of how far fluctuations in the superconducting order parameter will spread. Alternatively, it can be thought of as the size of the Cooper pair (we show why mathematically shortly). In the ballistic limit, BCS-theory provides the following expression:

$$\xi = \frac{\hbar v_F}{\pi \Delta}. \quad (12.30)$$

It is worth commenting that some authors omit the factor π , since the dimension is still correct. We see that as $T \rightarrow T_c$, $\xi \rightarrow \infty$ meaning that fluctuations in the order parameter field propagate an infinite distance. This is the hallmark of a critical point (second order phase transition).

The way to derive the above result in BCS theory is to compute the extent of the pair correlations in the superconducting state. In effect, one may consider the anomalous correlator

$$\Delta(x - y) = \langle c_{\uparrow}(x) c_{\downarrow}(y) \rangle \quad (12.31)$$

in real space where c are the original fermion operators in real space as obtained by Fourier-transforming the momentum space ones (c_k). Using the BCS ground-state, one finds that $\Delta(x - y)$ decays with $|x - y|$ over a length scale $\xi = \hbar v_F / \Delta$. One computes this by noting that different wavevectors k are decoupled in the BCS ground-state and using that only the vicinity of the Fermi surface will contribute to this anomalous correlator, where the electron spectrum may be linearized.

The question about which order parameter to use for a superconducting system merits some examination. A problem with the usual order parameter $\Delta_i = U \langle c_{i\uparrow} c_{i\downarrow} \rangle$ is that for any system with a fixed number of electrons, this will clearly be zero. Instead, one may consider a different order parameter which can be finite even in a system with a fixed number of electrons while at the same time catching the possibility of long-range order. Such an order parameter can be written

$$\Delta_{ij}^{\text{long-range}} = \langle b_i^{\dagger} b_j \rangle, \quad b_j = c_{j\uparrow} c_{j\downarrow}. \quad (12.32)$$

In effect, $\Delta_{ij}^{\text{long-range}}$ measures the correlation between pairs of electrons at different sites. If this order parameter remains finite as $i - j \rightarrow \infty$, we have long-range order in the system. As one approaches T_c , fluctuations in the system (meaning that the phase of the pairs of electrons at sites i and j is randomized) should cause $\Delta_{ij}^{\text{long-range}} \rightarrow 0$. In other words, the 2-point correlator for two particular electrons vanishes over the coherence length, but a material can still have coherence over macroscopic length scales due to the 4-point correlator being finite (the coherence between pairs of electrons).

Strictly speaking, the size of a Cooper pair need not be equal to the length scale over which fluctuations take place (which are equal for a BCS s -wave superconductor). In unconventional superconductors, like high- T_c d -wave ones, pairs can exist that are incoherent. Then, fluctuations in the phase spread over the entire system but individual Cooper pairs still exist (although these are phase-incoherent with other pairs).

Anisotropic order parameter For an anisotropic and possibly sign-changing order parameter like d -wave or p -wave, the question is which expression one should use for the gap in the denominator

of ξ . This issue was addressed in <https://arxiv.org/pdf/cond-mat/0109486> who computed the correlation function

$$\langle \delta|\Delta_q| \delta|\Delta_{-q}| \rangle \quad (12.33)$$

where $\delta|\Delta_q|$ are the fluctuations of the order parameter magnitude for Cooper pairs with center-of-mass momentum q . In effect, we have $|\Delta_q| = \Delta_0 + \delta|\Delta_q|$ where $\Delta_0 = \Delta(\mathbf{k})$ is the saddle-point value of the order parameter (which may in general be momentum-dependent, like in the d -wave case). They found that the above correlation function, which expresses over which distance fluctuations in the magnitude of the order parameter are correlated, decays over a distance

$$\xi = \frac{\hbar v_F}{\pi \langle |\Delta_0| \rangle} \quad (12.34)$$

where v_F is the Fermi velocity (averaged value over the Fermi surface). In this way, it is the average value of the magnitude of the order parameter which enters, so this is a finite value even for nodal order parameters. Different gap symmetries then only introduce a numerical prefactor in the expression for the coherence length, since the average value is less than the maximum amplitude of the gap.

The above value for ξ is then also the spatial cutoff which determines the coarse-graining that permits a phase-fluctuation-only theory. In other words, if one considers a theory where the physics at length scales below ξ is neglected, only phase-fluctuations are relevant to include in the action S .

It worth noting that the interpretation of "healing" length of the superconducting order parameter near an interface before it recovers to its bulk value is consistent with the above calculation of the coherence length. Namely, the interface induces a change $\delta|\Delta|$ in the magnitude of the order parameter, and this change affects the order parameter over a distance ξ .

The presence of an interface, which breaks translational symmetry, may affect the above formula since momentum is not a good quantum number in the direction perpendicular to the interface. Therefore, one may for instance find in a lattice tight-binding model with a vacuum interface at $x = 0$ that the healing length for a p_y -wave and p_x -wave order parameter may be different, since the averaging procedure may effectively differ in the x and y direction.

Derivation based on uncertainty principle in quantum mechanics

The length scale associated with the gap can also be argued for in the following manner. According to the uncertainty principle of quantum mechanics, as we have derived carefully in a previous section, Δt in the equation

$$\Delta E \Delta t \geq \hbar/2 \quad (12.35)$$

is the time required for the expectation value of a physical quantity A to change by an amount equal to its standard deviation ΔA and ΔE is the standard deviation of the Hamiltonian H . With this in mind, we can state that the time required for the electrons in the Cooper pair to lose their binding energy Δ_0 should exceed $\tau_p \sim \hbar/\Delta_0$.

Let us examine this a bit more closely. In writing this, we have assumed that $\Delta E = \Delta_0$. Why is this the case? Consider the pairing problem of two electrons in a Fermi sea that have an attractive interaction in a thin shell (determined by ω_D) around the Fermi level. One finds that the electrons in a Cooper pair lower their energy by an amount equal to the binding energy 2Δ . Now,

the two-electron wavefunction describing this bound pair of electrons cannot have sharply defined momentum, because then it would be completely delocalized. In turn, this would give an infinite coherence length since the spatial size of the Cooper pair would be infinite. Note that we have to distinguish between the BCS total state for a superconductor $|\psi\rangle$ and the two-electron wavefunction in the Cooper problem $\psi(\mathbf{r}_1, \mathbf{r}_2)$. Let us do the math for the Cooper problem wavefunction to see how this gives rise to a finite size ξ of the Cooper pair.

Cooper started by considering a wavefunction

$$\psi(r_1, r_2) = \sum_{kq} u_k(q) e^{ikr_1} e^{-i(k+q)r_2} \chi_{\text{spin}} \quad (12.36)$$

where χ_{spin} is the singlet spin part of the wavefunction and we have omitted the vector notation for the momenta for brevity. In effect, we have written the two-electron wavefunction in a general form by using a plane-wave basis for the electrons. This is exact for independent electrons that do not interact. We assume that the wavefunction has zero center of mass momentum so that $u_k(q) = u_k \delta_{q,0}$ since there exists arguments for why this should maximize the phase space to make Cooper pairs. Omitting the spin part, we have

$$\psi(r_1, r_2) = \sum_k u_k e^{iik(r_1 - r_2)}. \quad (12.37)$$

This is an even function in k so that there is an amplitude for the two electrons to live on top of each other at $r_1 = r_2$. This implies that the spin part must be singlet.

We now want to use this wavefunction as an ansatz for solving the SE with a Hamiltonian that includes a weak interaction between the electrons:

$$H = -\nabla_1^2/2m - \nabla_2^2/2m + V(r_1 - r_2). \quad (12.38)$$

Inserted into $H\psi = E\psi$ and Fourier-transforming the equation with respect to $r = r_1 - r_2$, we get

$$(E - 2\epsilon_k)u_k = \sum_{k'} V_{kk'} u_{k'} \quad (12.39)$$

We now want to find the eigenvalue E of this bound state. To simplify the calculations, we assume that $V_{kk'} = -V$ for $0 < \xi_k, \xi_{k'} < \omega_D$ where $\xi_k = \epsilon_k - E_F$ and $V_{kk'} = 0$ otherwise. This is motivated by the fact that the entire Fermi sea should be non-interacting and is filled up to E_F at $T = 0$. Thus, only states k that satisfy $E_F < \epsilon_k < E_F + \omega_D$ can interact with each other. The bound-state equation then takes the form

$$u_k = \frac{V \sum_{k'}' u_{k'}}{2\epsilon_k - E} \quad (12.40)$$

where the $'$ superscript indicates the restricted range of values for the summation over k' . Summing over k , we get

$$\begin{aligned} \frac{1}{V} &= \sum_k' \frac{1}{2\epsilon_k - E} \\ &= \frac{1}{2} N_0 \int_{E_F}^{E_F + \omega_D} d\epsilon \frac{1}{2\epsilon - E} \\ &= \frac{1}{2} N_0 \ln \left[\frac{2E_F + 2\omega_D - E}{2E_F - E} \right]. \end{aligned} \quad (12.41)$$

Since we have assumed a weak interaction, any bound-state should be able to exist just barely below the Fermi level, so $2E_F - E$ can be treated as a small positive quantity and is negligible compared to $2\omega_D$. This gives

$$\Delta = 2E_F - E \simeq 2\omega_D e^{-2/N_0 V}. \quad (12.42)$$

The quantity Δ is the binding energy of the electrons which thus form a bound state with energy slightly below $2E_F$. Note that by restricting the k -sum, we only considered electrons that without interaction would have had an energy of at least $2E_F$.

Interlude: importance of the existence of a Fermi sea in the Cooper problem

When obtaining the effective $e - e$ attractive interaction via phonons using the Schrieffer-Wolff transformation, the potential $V(\mathbf{q})$ depends only on the momentum-transfer caused by the phonons. There is no information contained in this potential about the scattering only affecting electrons near the Fermi level. As one makes the constant-potential approximation inside the Debye frequency, one arrives at the BCS Hamiltonian with an effective interaction $V_{\mathbf{k}\mathbf{k}'}$. However, in this Hamiltonian one states that the potential only exists when both $\mathbf{k}$ and $\mathbf{k}'$ individually correspond to electron states close to the Fermi level. This seems to be in contrast to the original interaction which only depends on one momentum $\mathbf{q}$.

The reason is that when approximating $V(\mathbf{q})$, a series of assumptions come into play. One is the assumption about opposite momentum pairing, which makes the phase-space for attractive interaction much larger than the phase-space when the momenta are not opposite (this becomes more important the more narrow the thin shell around the Fermi sea is). Another is the assumption about opposite spins of the scattered electrons, since this allows the electrons to get close in real space without worrying about the Pauli principle. But a third assumption is that the potential is only active for momenta transfer for electrons that are close to the Fermi level. The motivation for this assumption is as follows.

In the Cooper problem, it is shown that an infinitesimal attractive interaction between two electrons added to an already filled Fermi sea gives rise to a bound state which has an energy lower than twice the Fermi energy. This implies that the very concept of a Fermi sea does not work when such an attractive interaction exists, since all electron states below the Fermi level are supposed to already be full.

But we could ask: couldn't we consider an attractive between two electrons deep inside the Fermi sea and arrive at the same bound-state, thus indicating that all electrons in the entire Fermi sea could participate in the superconducting condensate? This problem is analyzed in detail in chapter 2 here https://materias.df.uba.ar/sa2020c2/files/2012/07/Lecture-BCS_Fernandes.pdf, but the essence can be captured by considering section 3.4.1 in the Sudbo-book. The analysis is general up to eq 3.31 in the sense that it is valid for any value of E_F . However, assume now for sake of argument that E_F is absent, so that we consider free electrons without any background Fermi sea. Then, we can no longer transition from eq 3.31 to 3.32 by assuming that the DOS at the Fermi level is approximately constant in the thin shell of thickness ω_D : the DOS goes like $\sqrt{E}$ and will not be constant for low energies. Instead, taking into account the $\sqrt{E}$ factor in the integrand, one arrives at a qualitatively different result compared to the case where $E_F \gg \omega_D$: a bound-state does not form for an arbitrary small interaction V . Instead, it has to be larger than some critical value.

In other words: the smaller we make the Fermi energy, gradually removing the Fermi sea, the harder it will be for the potential to create a bound state that destabilizes the Fermi-sea, which is the precursor to the superconducting state.

This is precisely the justification for saying that $V(\mathbf{q})$ not only depends on the momentum-transfer $\mathbf{q}$, but that this transfer also has to be between electron states close to the Fermi level.

How is this then useful to estimate the coherence length? Well, the two-electron wavefunction for the Cooper pair is a sum over k -states, i.e. it has to have a spread in its momentum expectation value. As seen from the integrand $(2\epsilon_k - E)^{-1} = (2\xi_k + \Delta)^{-1}$ above, this is peaked at the Fermi level $\xi_k = 0$ and has an energy spread of Δ for the states involved in the pairing. More specifically, when $\xi_k = \Delta$, the integrand has dropped in value to 1/10 of its value at $\xi_k = 0$. So the k -states between $\xi_k = 0$ and $\xi_k = \Delta$ are the main contributors to the integral and the associated energy spread of the electrons is thus Δ . A more detailed derivation is given in Ref.[62] where the same result is found.

Now, we have finally justified why $\Delta E \sim \Delta$ for the two-electron Cooper wavefunction: it is a sum over k -states and thus does not have a sharply defined momentum. Therefore, the lifetime of this state is given by $\tau_p \sim \hbar/\Delta$ where we used the notation $\tau_p = \Delta t$.

If an electron moves ballistically during a time interval τ_p , the distance it covers is $\tau_p v_F$. This distance determines the size of the Cooper pair and gives the coherence length

$$\xi \sim \hbar v_F / \Delta. \quad (12.43)$$

If the superconductor is made of objects of size ξ , its properties cannot change on a scale much smaller than ξ . This places a limitation on phase gradients in the superconductor, and hence the magnitude of the supercurrent, of the form $(\nabla\phi)_{\max} \sim 1/\xi$. This can in turn be used to estimate the critical field H_c by using the quantum mechanical expression for the current $\mathbf{j} = -e^2 n_s / mc (\mathbf{A} - \hbar \nabla\phi / 2e)$ and the London expression for the maximal supercurrent expressed in terms of the magnetic field.

Alternatively, we could identify from the above treatment the spread in momentum values Δk for the Cooper pair wavefunction and then use the position-momentum uncertainty relation $\Delta r \sim \hbar / \Delta k$ to estimate the spread Δr in position for the electrons in the pair. The latter would be an estimate of the size of the pair. To do so, we saw that momentum states in the range

$$k_F < k < k_F + \delta k \quad (12.44)$$

were the most important in determining the bound-state energy where

$$(k_F + \delta k)^2 / 2m - E_F = \Delta \quad (12.45)$$

This gives

$$k_F \delta k / m = \Delta \rightarrow \delta k = \Delta / v_F. \quad (12.46)$$

Thus, we find

$$\delta r \sim \hbar v_F / \Delta. \quad (12.47)$$

SC	T_c (K)	ξ (nm)	λ (nm)	GL $\kappa = \lambda/\xi$	B_c and B_{c2} (T)
Al	1.2	1600	16	0.01	0.01
Pb	7.2	83	37	0.445	0.08
In	3.14	70	40	0.57	0.03
Sn	3.72	230	14	0.06	0.03
Nb	9.3	38	39	1.026	0.82
NbTi	10	4	240	60	15
Nb ₃ Sn	18.3	3	65	21.7	30
MgB ₂	39	6	140	23.3	74
YBCO	92	1.5	150	100	100
Bi ₂ Sr ₂ Cu ₂ O _{8+δ}	85	1.5	200	117.6	120

In the dirty limit, the superconducting coherence length is reduced and takes a different form than the BCS-result ξ_{BCS} . It is obtained via

$$\begin{aligned}
 \xi &= \sqrt{l_{\text{mfp}} \xi_{\text{BCS}}} \\
 &= \sqrt{v_F \tau \hbar v_F / \pi \Delta} \\
 &= \sqrt{\frac{v_F^2 \tau}{\pi} \frac{\hbar}{\Delta}} \\
 &\simeq \sqrt{\frac{\hbar D}{\Delta}}.
 \end{aligned} \tag{12.48}$$

Above, we used the definition of the diffusion coefficient due to elastic impurity scattering in the self-consistent Born approximation: $D \equiv \frac{1}{3} v_F^2 \tau$ (assuming movement in three spatial dimensions). We underline that the above calculation just shows what happens for two electrons that interact attractively in an otherwise non-interacting Fermi sea. To find the true superconducting ground state for the entire system (all electrons) when taking into account that other electrons can also form pairs, we have to consider the BCS ansatz for the state vector $|\psi\rangle$. This is done later in these notes.

12.8.2 Penetration depth

12.8.3 Typical values

Pure elements are typically type I. All parameter values denote the BCS value and are modified in the dirty limit by the mean free path (see later section below). It should be noted that the coherence length in Al is much less than 1.6 μm in thin films, order hundreds of nm.

12.9 Type I vs. Type II: electromagnetic response of superconductors

When a superconducting sample is exposed to an external magnetic field, there is a competition between two phenomena which ultimately determine whether the superconductor is in a Meissner state, with screening currents blocking the magnetic field, or if vortices appear. The free energy F_S of a superconductor that completely expels all magnetic flux must be $F_S(H) = F_S(0) + \mu_0 H^2/2$. It has increased its energy since it has to shield the field H , and the energy increase must be equal to the missing energy density of the field. In practice, this energy increase must be the kinetic energy

of the circulating shielding supercurrent that cancels the field H . Imagine that we have a material with temperature right above T_c , so that $T = T_c + \delta T$. Applying a magnetic field, it will penetrate the material. Imagine we lower the temperature infinitesimally to $T = T_c - \delta T$. The material is now a superconductor and expels the magnetic field. But energy must be conserved, and thus the missing energy that came from the field inside the superconductor must be provided from something else, namely the kinetic energy of the shielding supercurrent. Now, if the superconductor chooses to let the field penetrate a distance λ , its free energy is reduced since it doesn't have to put up shielding supercurrents inside the region λ . This is known as a negative surface energy. At the same time, there is an increase in the free energy from the loss of superconductivity over a region ξ : with no Cooper pairs to put up shielding supercurrents, the condensation energy is also smaller. These effects compete, and the net surface energy σ can be shown to go like (using some approximations):

$$\sigma \propto \frac{1}{2} \mu_0 H^2 (\xi^2 - \lambda^2). \quad (12.49)$$

As seen, if $\xi \gg \lambda$ it is clear that the energy cost of having this type of normal-superconducting surface is positive and the superconductor wants to minimize the number of such surfaces. This corresponds to the Meissner state. But if $\lambda \gg \xi$, there is an energy gain and the superconductor wants to maximize the number of such normal-superconductor surfaces. This is done via vortices, which each have precisely this kind of transitions between normal and superconducting regions, and the superconductor creates as many of these vortices as possible by minimizing the flux in these vortices down to the quantum limit of one flux quantum. Put differently, subdivision of the superconductor into an alternating sequence of thin normal and superconducting slices is energetically favourable if the London penetration depth exceeds the coherence length.

In an extreme type II superconductor, the above explanation means that there is a small distance ξ from the interface in which superconducting order recovers whereas there is a large distance λ over which shielding supercurrents build up to screen the field. As a consequence, there has to be a interval $\xi < x < \lambda$ in which Cooper pairs coexist with a largely unscreened magnetic field. How can this be? This can be understood by noting that the penetration depth λ depends inversely on the density of Cooper pairs. Thus, a large λ means that the Cooper pair density n_S is low so that even if the Cooper pairs in the interval $\xi < x < \lambda$ set up screening currents, they are too weak to shield the field since the current density is weak due to the small n_S . In other words, as soon as Cooper pairs exist (a distance ξ from the interface), they will try to screen the field, but if their density n_S is low the penetration depth λ can still be large and the effect of the screening currents in a layer of thickness $< \lambda$ is weak.

Coherence length and penetration depth in the dirty limit

The temperature dependence of both the coherence length and the penetration depth is $1/\sqrt{1 - T/T_c}$. In other words, both diverge as $T \rightarrow T_c$. Although their temperature-dependence is similar, their dependence on the mean free path $l_{\text{mfp}} = v_F \tau$ in the system is *not*. We remind the reader that a clean sample has $l_{\text{mfp}} \gg \xi_0$ whereas a dirty sample has $l_{\text{mfp}} \ll \xi_0$. Here, ξ_0 and λ_0 is the coherence length and (London) penetration depth in the clean limit.

In the dirty limit $l_{\text{mfp}} \ll \xi_0$, we have

$$\begin{aligned} \xi &\propto \sqrt{\xi_0 l_{\text{mfp}}}, \\ \lambda &\propto \lambda_0 \sqrt{\frac{\xi_0}{l_{\text{mfp}}}}. \end{aligned} \quad (12.50)$$

We see that ξ becomes smaller in the dirty limit, whereas λ becomes bigger. This could explain why a type II response $\lambda/\xi \gg 1$ is found in the Usadel-framework which is in the dirty limit.

We note that the London model discussed earlier assumes a local connection between the supercurrent and magnetic field. However, this cannot hold in a situation where $\xi \gg \lambda$ (type I), since the supercurrent is then carried by Cooper pairs with extent ξ much larger than the characteristic scale of magnetic field variation λ . In the clean limit, one must therefore instead use the Pippard model for non-local electrodynamics of superconductors. Then, the supercurrent becomes related to the average of the magnetic field in a region of size ξ . In dirty materials where the coherence length is reduced and the penetration depth increases, however, the local electrodynamics picture holds.

To understand physically how the coherence length changes when the mean free path decreases, consider that the scattering time between two impurity collisions is $\tau_s = l_{\text{mfp}}/v_F \equiv l/v_F$. If $\tau_s < \tau_p$ (the characteristic time of interaction in a Cooper pair), we should consider the electron motion to be diffusive with a diffusion coefficient $D \sim v_F^2 \tau_s$. The coherence length in such a scenario is then determined by the distance the electron diffuses during the time τ_p

$$\xi_{\text{dirty}} = \sqrt{D\tau_p} = \sqrt{v_F l \hbar / \Delta_0} = \sqrt{\xi_0 l}. \quad (12.51)$$

Dirty materials are usually in the London regime.

12.9.1 Maxwell's equations and boundary conditions in a superconductor

It is instructive to solve Maxwell's equation in a superconductor exposed to an external magnetic field to show how the field is screened. It turns out that there are some subtleties regarding the boundary conditions that deserve exposition. Below, we consider two models: one simple which is analytically solvable and one more realistic which relies on numerics.

Simple analytical model

One of Maxwell's equations reads

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} \quad (12.52)$$

where we have assumed that there is no time-dependent electric field. Here, $\mathbf{J}$ is the total current density and $\mathbf{B}$ is the magnetic field. Generally, we have

$$\mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M}) \quad (12.53)$$

where the magnetization is associated with bound currents and the $\mathbf{H}$ -field with free (conduction currents). Bound currents generate a polarization in response to *e.g.* an external field. We thus have

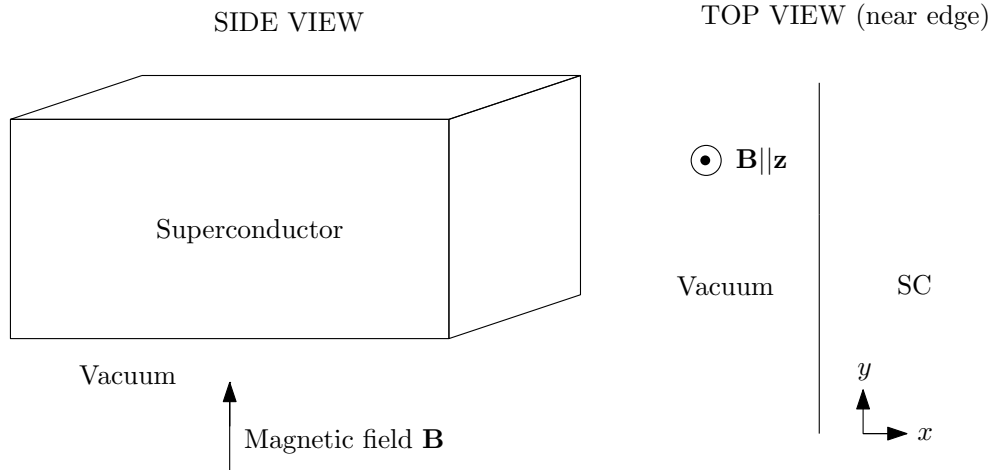
$$\mathbf{J} = \mathbf{J}_{\text{bound}} + \mathbf{J}_{\text{free}} \quad (12.54)$$

where

$$\nabla \times \mathbf{M} = \mathbf{J}_{\text{bound}}. \quad (12.55)$$

The boundary conditions for electromagnetic fields dictate that

$$\mathbf{n} \cdot (\mathbf{B}_1 - \mathbf{B}_2) = 0 \quad (12.56)$$



on side 1 and 2 of an interface with normal $\mathbf{n}$. This follows due to the absence of magnetic charges, $\nabla \cdot \mathbf{B} = 0$. Moreover, in the absence of free currents, one also has continuity of a tangential component of the $\mathbf{H}$ -field:

$$\mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = 0. \quad (12.57)$$

We are now ready to look at a superconductor interfaced to vacuum with an external magnetic field. We consider the situation shown in the figure above.

First, let us assume that there are no free currents in the problem. In effect, we will treat the shielding supercurrent as a bound current providing a magnetization. Thus, let us for simplicity write drop the subscript on $\mathbf{J}_{\text{bound}}$. It is now convenient to make some choices for the particular gauge considered in the problem. It can be shown from G-L theory that the supercurrent is given by

$$\mathbf{J} = -\frac{\mathbf{A}}{\mu_0 \lambda^2} \quad (12.58)$$

where λ is the penetration depth, if one uses a gauge where the superconducting order parameter is real. Since no current can flow into vacuum, we need to use a gauge where $\mathbf{A}$ satisfies $\mathbf{n} \cdot \mathbf{A} = 0$ in order to be consistent with Eq. (12.58). Since $\nabla \cdot \mathbf{J} = 0$ due to current conservation, we must also have a gauge where $\nabla \cdot \mathbf{A} = 0$.

Thus, we have the following quantities in the superconducting region:

$$\mathbf{B} = (0, 0, B), \quad \mathbf{M} = (0, 0, M), \quad \mathbf{A} = (0, A(x), 0) \quad (12.59)$$

when we consider an edge located at $x = 0$, so that the current runs along the y -axis. In general, the current will circulate in the superconducting film as a response to the external field. We want to determine which effect the current has on the field inside the superconductor. The external field is written $\mathbf{B}_{\text{ext}} = (0, 0, B_0)$.

Consider first the Maxwell equation, which in our gauge-choice takes the form

$$\nabla^2 \mathbf{A} = \mathbf{A} / \lambda^2. \quad (12.60)$$

The general solution reads

$$A(x) = ae^{x/\lambda} + be^{-x/\lambda}. \quad (12.61)$$

We consider here a semi-infinite superconducting region as one moves away from the interface, so the exponentially growing solution is not physical, as it would give a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ that exponentially grows as one moves away from the interface. We thus have

$$A(x) = be^{-x/\lambda} \quad (12.62)$$

where b is a constant to be determined from the boundary conditions. The boundary condition $\mathbf{H}_1 = \mathbf{H}_2$ at $x = 0$ (we only have a tangential component of $\mathbf{H}$ and can thus drop the $\mathbf{n} \times$ operation) gives us

$$\mathbf{B}_{\text{ext}}|_{x=0} = \nabla \times \mathbf{A}|_{x=0} - \mu_0 \mathbf{M}|_{x=0} \quad (12.63)$$

after multiplying with μ_0 . This gives

$$\partial_x A|_{x=0} = B_0 + \mu_0 M|_{x=0}. \quad (12.64)$$

We thus need to know what the magnetization is. We can obtain the magnetization from the relation $\nabla \times \mathbf{M} = \mathbf{J}$ which gives

$$J_x = \partial_y M, \quad J_y = -\partial_x M. \quad (12.65)$$

The first equation tells us that $M = M(x)$ since $J_x = 0$. Integrating the second equation gives

$$M = \int dx \frac{A}{\mu_0 \lambda^2} = -\frac{b}{\mu_0 \lambda} e^{-x/\lambda} + c_0 \quad (12.66)$$

where c_0 is a constant and we used Eq. (12.62). Inserting this general expression for magnetization into the boundary condition Eq. (12.64) and *assuming* that $M(x=0) = 0$ produces

$$-\frac{b}{\lambda} = B_0. \quad (12.67)$$

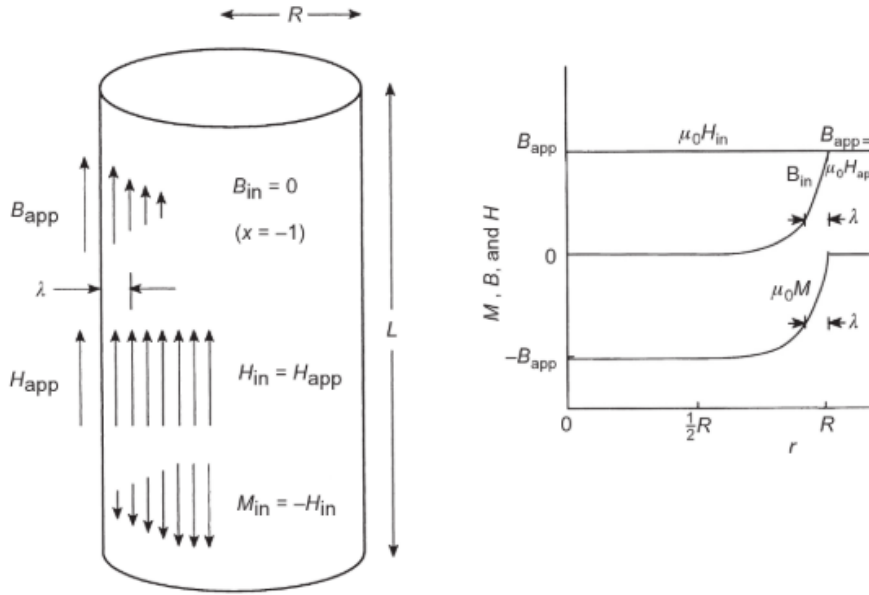
With our assumption of zero magnetization at the interface, it then also follows that $c_0 = -B_0/\mu_0$. The physical motivation behind this assumption is that the magnetization induced by the shielding current in the superconductor needs to gradually build up to an appreciable value as one moves into the bulk in order to create a magnetization that is strong enough to cancel the external field. Since we also have $\mathbf{H}_1 = \mathbf{H}_2$, this means that B is continuous at the interface. The magnetic field inside the superconductor can now be determined by taking the curl of Eq. (12.62):

$$B = B_0 e^{-x/\lambda}. \quad (12.68)$$

This is the Meissner screening of the field due to the superconducting correlations. We see that $B(x \rightarrow \infty) = 0$ and the current density $J_y(x \rightarrow \infty) = 0$. At the same time, we see that $M(x \rightarrow \infty) = -B_0/\mu_0$ since the general expression for M according to our above solution is:

$$M(x) = \frac{B_0}{\mu_0} (e^{-x/\lambda} - 1) \quad (12.69)$$

We summarize our findings in the figure above, taken from "Superconductivity" by C. Poole *et al.*. The picture is then that the $\mathbf{B}$ field is screened and goes to zero. The $\mathbf{H}$ -field remains constant



throughout the system whereas the magnetization is zero at the interface, and then builds up gradually as to cancel the constant $\mathbf{H}$ -field and give $\mathbf{B} = 0$ in the bulk of the superconductor.

What about a scenario where the magnetic field is normal to the superconducting surface? Consider a superconducting slab (bulk) where a magnetic field is applied pointing toward the slab, say z -direction. At the sides of the slab, the field is parallel to the surface, precisely as the scenario we considered above. We saw that shielding currents were generated, cancelling the total magnetic field (pointing in the z -direction) inside the superconductor. If we then move toward the lower surface of the slab, where the field was perpendicular to that surface, it means that $B_z = 0$ there. But $\nabla \cdot \mathbf{B}$, universally valid, means that B_z is continuous across the superconducting interface. This holds since $\partial_z B_z = 0$, so that $B_{z,out} = B_{z,in}$. This analysis holds far away from the corners of the superconductors where the field can only depend on the z -coordinate. Therefore, the field lines bend where the magnetic field hits the superconductor, so that they run parallel to the surfaces of the superconducting slab everywhere.

The analysis becomes more complicated close to corners and when taking into account finite size effects, but for a bulk superconductor the main conclusion holds that the magnetic field is absent deep inside the superconductor. For finite size superconductors, the effect of the demagnetization field will also modify the field right outside of the superconductor. The demagnetization field $\mathbf{H}_d$ is the contribution to the total $\mathbf{H}$ -field created by the magnetization $\mathbf{M}$ within the superconductor due to shielding supercurrents.

Apparent paradox and resolution

How can the magnetization in the bulk of the superconductor, far away from the interface where no screening currents exist, be finite? Consider the cylinder geometry shown in the picture. We can disregard demagnetization effects (the modification of the field right outside the superconductor) for a long cylinder when an external magnetic field is applied along its axis, so that the magnetic field right outside the superconducting surface is exactly equal to the applied field far away from it.

Demagnetization can, however, not be neglected for arbitrary geometries, such as a superconducting plane in a perpendicular field. "Plane" here means that the aspect ratio is such that the height divided on length is a small number: it matters not what the height is in absolute values. Only the aspect ratio is important with regard to demagnetization effects. We will comment more on the effect of demagnetization after resolving the paradox.

Regarding the cylindrical geometry, we know for instance from Biot-Savart's law that the magnetic field at the center of a circular wire carrying current scales like $1/R$ where R is the radius of the circular wire. It should go to zero as $R \rightarrow \infty$. More specifically, the value of the magnetic field at the center axis of a circular wire carrying current at a height z is:

$$B = \frac{\mu_0 I R^2}{2(R^2 + z^2)^{3/2}}. \quad (12.70)$$

At $z = 0$, we get the aforementioned $1/R$ dependence.

It thus seems like the magnetic field produced by the shielding currents should go to zero at the center of the cylinder if $R \rightarrow \infty$, and thus the magnetization there should be zero, in contrast to what we found above. The resolution to this paradox is that in order to neglect demagnetization effects like we have done, we need to have a long cylinder geometry. In effect, an aspect ratio $h/R \gg 1$ where h is the height of the cylinder. Thus, if we let $R \rightarrow \infty$, we also have to let $h \rightarrow \infty$. Dividing the cylinder into thin cylindrical slices with height dz , these each carry a current $\tilde{J}dz$ where $\tilde{J}$ is the effective total shielding current circulating the cylinder per unit height.

The contribution from one such slice is then, according to Eq. (12.70), dB where

$$dB = \frac{\mu_0 \tilde{J} dz R^2}{2(R^2 + z^2)^{3/2}}. \quad (12.71)$$

To find the magnetic field produced by the shielding currents at a center point in the cylinder, we thus have to integrate and find the total contribution from the entire cylinder:

$$B = \int_{-h}^h \frac{\mu_0 \tilde{J} dz R^2}{2(R^2 + z^2)^{3/2}}. \quad (12.72)$$

The result is finite even when $R \rightarrow \infty$ so long as $h \gg R$. Therefore, although each slice gives zero contribution in the limit $R \rightarrow \infty$, the total cylinder gives a net magnetization in the center despite its infinite radius so long as we maintain the aspect ratio. This resolves the paradox.

It is useful to contrast this situation with an infinite superconducting plane subject to a perpendicular magnetic field. First, we remind ourselves that the demagnetization field $\mathbf{H}_d$ is the contribution to the total $\mathbf{H}$ -field created by the magnetization $\mathbf{M}$ within the material. It exists both inside the material and outside of it. The part which is outside of the material is often referred to as the stray field. The term demagnetizing field reflects the tendency of this field to reduce the total magnetic moment of the material.

It is difficult to compute the demagnetization field for arbitrarily shaped materials, even when the magnetization is uniform. However, for objects such as spheres, flat plates, and long rods/cylinders, $\mathbf{H}_d$ is linearly related to $\mathbf{M}$ by a constant n . This constant is known as the demagnetizing factor. For our long cylinder placed in a uniform magnetic field along the axis, the demagnetization factor

n is close to zero, which is why we can neglect the demagnetization field. On the other hand, for a flat plate (the "plane" referred to above) n is close to 1.

The total $\mathbf{H}$ -field inside the superconductor will thus be the sum of the external $\mathbf{H}$ -field and the demagnetization field created by the magnetization itself. We may thus write that

$$\mathbf{H} = \mathbf{H}_{\text{ext}} + \mathbf{H}_{\text{demag}}. \quad (12.73)$$

Now, the demagnetization field inside the material can for ellipsoidal bodies be written as

$$\mathbf{H}_{\text{demag}} = -n\mathbf{M} \quad (12.74)$$

where n is the demagnetization factor. Since we know that $\mathbf{H} = -\mathbf{M}$ deep inside the superconductor, we have that deep inside the superconductor

$$\mathbf{H} = \frac{1}{1-n} \mathbf{H}_{\text{ext}}. \quad (12.75)$$

In other words, the field deep inside the superconductor can reach the critical strength $\mathbf{H}_c$ *before* the external field reaches $\mathbf{H}_c$. This becomes especially clear in the infinite plane geometry where $n \rightarrow 1$. We see that an infinitesimal externally applied field H_{ext} is enough to create a huge $\mathbf{H}$ -field inside the superconductor, which should thus destroy superconductivity.

Does that mean that thin films can never be superconducting due to demagnetization effects? No. In fact, if we accepted that the $\mathbf{H}$ -field inside the superconductor would exceed the critical superconducting field even for an infinitesimal value of $\mathbf{H}_{\text{ext}}$, then superconductivity would be lost so that $\mathbf{M} \rightarrow 0$ and $\mathbf{H}_{\text{demag}} \rightarrow 0$. But then we would have an infinitesimal field inside the material, which should not prevent the material from being superconducting.

The compromise found by the superconductor is that some parts go normal and some parts stay superconducting. This is called an intermediate state. For a type I superconductor, the normal parts are just normal laminae which enter the superconductor and divide superconducting regions. For a type II superconductor, we get vortices. This happens immediately for an infinite plane in a perpendicular field, whereas it is in general happens for an applied external field satisfying

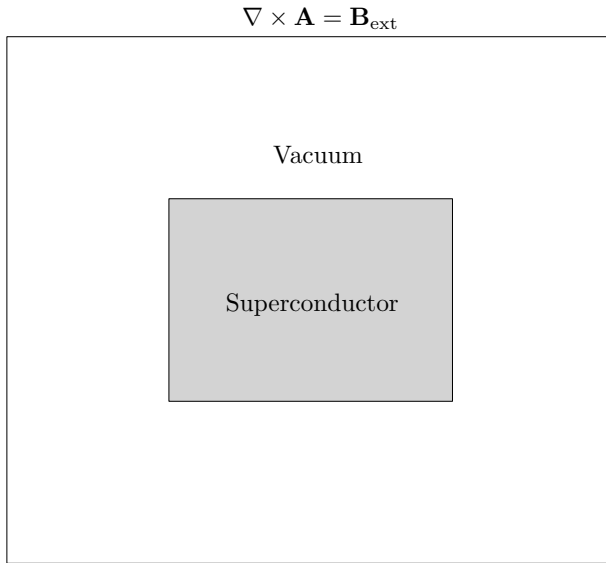
$$\frac{1}{1-n} H_c < H_{\text{ext}} < H_c. \quad (12.76)$$

Due to the demagnetization field, the field lines at the surface of a superconductor also change, depending on its shape. Since the magnetic field is "pushed" out of the superconductor, the magnetic field lines bundle together and increase at the edges of the superconductor.

More realistic numerical model

Note that by not solving Maxwell in the vacuum region, but instead fixing the field to be B_0 , we are not accounting for the demagnetization field produced by the superconductor which modifies the magnetic field both inside and outside of it. This approach is then not suitable if one is interested in determining how the field outside the superconductor changes. On the other hand, the approach is suitable if one is only interested in the screening properties inside the superconductor itself.

An approach which is more realistic and which will take into account the modification of the field outside of the superconductor, such as demagnetization effects, is the one shown in the figure below.



Here, we draw a vacuum-box outside of the superconductor and make it big enough so that we can set the boundary condition $\mathbf{B} = \mathbf{B}_{\text{ext}}$ at its boundary. Then, we may solve Maxwell everywhere else inside the vacuum box and only need to enforce $\mathbf{A} \cdot \mathbf{n}$ at either the vacuum or superconductor boundary, in order to make the $\mathbf{A}$ -potential unique ($\nabla \cdot \mathbf{A} = 0$ is not sufficient to fix the gauge). Also, if the current is obtained *e.g.* quasiclassically, one has to use appropriate boundary conditions for the current so that nothing flows into vacuum.

12.9.2 Divergent magnetization current $\nabla \times \mathbf{M} = \mathbf{J}_{\text{bound}}$ at edge?

Consider a uniform magnetized object such that the magnetization drops to zero as one moves outside the material. Does this mean that $\nabla \times \mathbf{M}$ in the Maxwell equation diverges due to the step-function behavior of $\mathbf{M}$? Write more ...

12.9.3 Suppressed Meissner effect in thin films

A special case is worth mentioning. Imagine that there is no Meissner effect and that the field can just penetrate the superconductor, while still having superconductivity. This can be realized in a thin-film superconductor with an in-plane magnetic field. The easiest way to understand this is to note that a magnetic field changes over a length scale λ , the penetration depth, inside a superconductor. If one then has a thin superconducting film of thickness d , consider that the appropriate boundary conditions at the edges of the film is that the tangential component of the $\mathbf{H}$ -field must be continuous (i.e. the $\mathbf{H}$ -field inside the superconductor has to equal the applied field outside of it). Therefore, if $d \ll \lambda$, the field does not have room to change inside the superconductor and hence the field must be constant throughout the SC region and equal to the applied field. Therefore, the orbital (Meissner) effect has been strongly reduced.

Formally, we can prove the absence of screening currents from the London equations. We assume again that $M = 0$ right at the interface, so that the total magnetic field B gradually decays as one moves into the superconductor. Let the interfaces be located at $x = -d/2$ and $d/2$. Solving for B

with the same boundary condition on both sides yields the solution

$$B(z) = \frac{B_0 \cosh(z/\lambda)}{\cosh(d/2\lambda)}. \quad (12.77)$$

When d/λ , the denominator is $\simeq 1$ and the nominator is $\simeq 1$ regardless of z -value. Hence, $B \simeq B_0$ inside the entire superconductor. There is no screening. The shielding current $J \propto \partial_z B(z)$ becomes proportional to $\tanh(d/2\lambda)$ at the two interfaces, and hence also vanishes in the limit $d/\lambda \ll 1$.

As we will see below, the thin-film superconductor with in-plane magnetic field produces a homogeneous spin-splitting due to the Zeeman-effect of the unscreened magnetic field and absent screening currents. There is another scenario where a homogeneous spin-splitting arises in the superconductor, but where the screening currents are absent due to a lack of magnetic field all together in the superconductor. This occurs in a thin-film ferromagnetic insulator/superconductor bilayer where the surface dimensions of the film far exceed the thickness of the film. To see this, the key is to note that for a thin-film where the aspect ratio of thickness and surface area becomes very small, the demagnetization field from the magnetic film vanishes. A 2D ferromagnet polarized in-plane has no stray field, because the magnetic poles are infinitely separated ¹.

On this account, the H -field is zero at both the superconducting interfaces. Since $M = 0$ at the superconducting edges, the boundary conditions are $B = 0$ and the only solution of $\nabla^2 B = (1/\lambda^2)B$ inside the superconductor is $B = 0$ inside the superconductor. Hence, no screening currents.

Interlude: magnetic dipole on top of a superconducting surface

An apparent problem arises if we consider a magnetic adatom on the surface of a thin superconducting film. Intuitively, we might expect that there should be no screening currents here either, since we know that for an entire ferromagnetic film on top of a superconductor, there are no screening currents. The components of the dipole-field parallel to the superconducting film should not be screened since the physical situation is the same as in the Meservey-Tedrow case (thin-film superconductor with in-plane field). The component of the dipole-field normal to the superconducting plane is also not screened so long that the film is sufficiently thin. This is because the effective penetration depth for a thin superconducting film $d \ll \lambda$ is the Pearl length $\lambda_{\text{eff}} = \lambda^2/d$. So long that the width W of the superconductor is smaller than λ_{eff} , this means that an applied magnetic field perpendicularly to the film will penetrate the superconductor uniformly: see <https://arxiv.org/abs/1008.2231>, <https://arxiv.org/pdf/cond-mat/0001035>, and Phys. Rev. Research 6, 023190 (2024).

So let us apply the same type of calculation as we did for the bulk and thin-film case to see what happens with screening currents for a dipole in a superconductor. This is in fact the case treated by all people looking at magnetic adatom chains on superconductors in the context of Majoranas.

¹The stray field is defined as the external magnetic field produced by a magnetic material. The stray field of an infinitely thin magnetic layer is zero outside the layer because there are no magnetic charges to produce a field. This holds both for the in-plane and out-of-plane configuration. The H -field produced inside the thin magnetic layer is very different in the two cases, however. For an in-plane magnetization, the poles at the surfaces are so widely separated that the produced H -field is completely negligible. For an out-of-plane magnetization, the two poles at the surfaces are close and produce an exactly cancelling field $H = -M$ so that $B = 0$ inside the ferromagnet. See fig. 2.1. in <https://epub.uni-regensburg.de/10440/1/diss-main.pdf>.

However, all of them neglect the screening current induced by the magnetic dipole.

To check if this is warranted, the relevant boundary conditions are as usual $H_{\text{in}} = H_{\text{out}}$ for the parallel components. Consider a point right below the dipole so that we only need to consider the parallel component. Then $B = B_0$ inside the SC at this point. At the other interface, we can set $H = 0$ as boundary condition since the dipole-field is reduced quickly (like $1/r^3$) as one moves away from it. Even if we include a finite value, much smaller than B_0 at the other interface, the problem we are about to show remains. Doing the calculation yields

$$B = \frac{B_0 \sinh[z + d/2]/\lambda}{\sinh(d/\lambda)} \quad (12.78)$$

for the magnetic field inside the SC. The screening current, being the derivative of B , at the dipole surface $z = d/2$ then becomes:

$$J(z = d/2) = \frac{B_0}{\mu_0 \lambda} \frac{1}{\tanh(d/\lambda)}. \quad (12.79)$$

This diverges when $d/\lambda \rightarrow 0$. In other words, the thinner the superconductor, the stronger the screening currents!

This seems completely opposite to what we would have expected for the thin-film superconductor in the presence of an in-plane magnetic field and in contact with a thin FI: in both the latter cases, there is no screening at all. How can a single magnetic dipole induce infinite screening currents?

The resolution must be that we have erroneously replaced $\nabla^2 B$ with $\partial_z^2 B$ in the equation determining the magnetic field inside the superconductor. This is allowed in the two cases mentioned above, since there is no variation in the xy -plane, but in the dipole case this does not hold. Taking into account the variation of the B -field in full 3D-space should alter the calculation so that there is no divergence. *End interlude.*

In the extreme thin-film limit where d is just a few monolayers, the superconductor can undergo a Kosterlitz-Berezinskii transition. Such a thin film is not required to observe the absence of a Meissner effect, however. It is also worthwhile to mention that for thin type II superconductors, the Abrikosov vortices that appear for a perpendicular magnetic field turn into Pearl vortices. Such vortices have a size (flux radius) of $2\lambda^2/d$ instead of λ and are otherwise similar to Abrikosov vortex except for their magnetic field profile which, due to the dominant air-metal interface, diverges as $1/r$ at short distances from the center. Abrikosov's vortices, instead, have very short range interaction and diverge as $\log(1/r)$ near the center.

Recall first that at zero temperature the superconductor has zero spin susceptibility since all electrons are paired. Now, consider first the non-superconducting state. If the free energy without a magnetic field is F_N , then applying a field lowers the free energy to F due to the finite spin susceptibility of the normal metal (since it has a non-zero density of states at the Fermi level):

$$F = F_N - \frac{1}{2} \chi_p \mu_0 H^2 \quad (12.80)$$

where $\chi_p = 2\mu_0 \mu_B^2 N_0$ is the paramagnetic susceptibility and N_0 is the normal-state Fermi level DOS per spin. The reduction in energy is due to the Zeeman-effect of the field coupling to the electron

spins.

A superconductor at $T = 0$ has free energy

$$F = F_S \quad (12.81)$$

without any Meissner effect since the superconductor has zero spin susceptibility at zero temperature. We neglected the field energy density $\propto H^2$ since it is the same in both cases. At the critical field $H = H_c$, the free energies of the normal state and the superconducting state (both with magnetic field) must be the same as the superconducting state is no longer favored. Now, BCS theory tells us that the free energy density between a normal metal and a superconductor *without field* goes like $F_N - F_S = -\frac{1}{2}N_0\Delta_0^2$ where N_0 is the DOS. At the phase transition, we thus have:

$$F_N - \frac{1}{2}\chi_p\mu_0H^2 = F_S \quad (12.82)$$

which gives us the critical field

$$H_c = \Delta_0/\sqrt{\mu_0\chi_p}. \quad (12.83)$$

This can be rewritten as

$$\mu_B B_c = \Delta_0/\sqrt{2} \quad (12.84)$$

where $B_c = \mu_0 H_c$ and is the Clogston-Chandrasekhar limiting field.

12.10 Ways to destroy superconductivity: critical field and critical current

Beyond a critical field H_{c2} and critical current I_c applied to the superconductor, superconductivity breaks down completely. The common reason for this is that the kinetic energy of the Cooper pairs exceeds their binding energy, and thus favors energetically that the system reverts to the normal state. In the case of an applied magnetic field, the Cooper pairs indeed gain kinetic energy because of the Meissner screening currents that flow at the surface (within a distance λ) of the superconductor. When the kinetic energy is high enough (due to the increasingly larger current required to screen a growing field), it is simply more favorable to not screen the field anymore and the system reverts to being normal.

In the case of a critical current, there are some nuances that are worth bringing forth. If we apply the reasoning above and say that superconductivity breaks down when $E_{\text{kin-pair}} > 2\Delta$, we still know that a current should flow even in the normal resistive state. The charge carriers are now single electrons, but they also have a kinetic energy *and* a potential energy due to the existence of a voltage drop (finite electric field) in the conductor: E_{single} . Therefore, a more precise statement regarding the critical depairing current is that it is the current where

$$E_{\text{kin-pair}} > 2\Delta + 2E_{\text{single}}. \quad (12.85)$$

It is clear that the kinetic energy of the electrons after the phase transition has to be smaller than the kinetic energy before the transition. This can be understood by noting that as the current increases toward its critical value, fewer and fewer superconducting electrons (Cooper pairs) become

available since the order parameter Δ decreases toward zero. Therefore, to carry the current, their momentum has to become large in order to compensate for their fewer numbers. Right after the transition, all electrons near the Fermi level become available to carry current, and therefore do not need to carry as much momentum each as the very few Cooper pairs right before the transition: hence, their kinetic energy is lower.

Finally, we should also point that the above estimate is approximative and neglects an important qualitative issue. Namely, the energy gap E_g is not necessarily the same as the superconducting order parameter Δ . We know that the energy of quasiparticle excitations in the superconductor is

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} \quad (12.86)$$

where $\xi_{\mathbf{k}} = k^2/2m - \mu$ and thus a minimum energy $E_g = \Delta$ is required to excite a particle from the condensate at rest. If the condensate is moving, we can perform a Doppler shift on the momentum of the second quantized operators in the original Hamiltonian used to derive this expression: $\mathbf{k} \rightarrow \mathbf{k} - m\mathbf{v}_s$ where $\mathbf{v}_s$ is the superfluid velocity. As a consequence, the excitation energy now becomes [?]

$$E_{\mathbf{k}} = \sqrt{\tilde{\xi}_{\mathbf{k}}^2 + \Delta^2} - \hbar\mathbf{k} \cdot \mathbf{v}_s \quad (12.87)$$

where $\tilde{\xi}_{\mathbf{k}} = \xi_{\mathbf{k}} + \frac{1}{2}m\mathbf{v}_s^2$. This means that the kinetic energy of the quasiparticles $\xi_{\mathbf{k}}$ now effectively also includes the contribution from the fact that the whole condensate is moving with a superfluid velocity ($m\mathbf{v}_s^2/2$). Alternatively, one can think of this as a shift in the chemical potential for the Cooper pairs. In addition, the energy quasiparticle energy E has received a Doppler-shift $\hbar\mathbf{k} \cdot \mathbf{v}_s$. The latter term means that the minimum energy required to excite a particle is not Δ anymore, but $\Delta - \hbar\mathbf{k} \cdot \mathbf{v}_s$. Therefore, the energy gap in the current-carrying state of the superconductor diminishes linearly with the superfluid velocity.

However, superconductivity is not destroyed when $E_g = 0$. There are in fact two critical velocities: the Landau critical velocity v_L (where $E_g \rightarrow 0$) and the critical superfluid velocity v_c where superconductivity is destroyed ($\Delta \rightarrow 0$). The order parameter Δ still remains up to v_c . This can be understood as follows. When the *Landau critical velocity* v_L is reached, we have

$$v_L \hbar k_F = \Delta. \quad (12.88)$$

Here, we assumed that the shift of the effective chemical potential is negligible (i.e. $\mu \gg \frac{1}{2}m\mathbf{v}_s^2$) so that the minimum energy gap occurs at $k = k_F$. However, as this value is reached, only an infinitesimal part of the electrons in the system have no energy gap to the excitation band: namely, the part of the electrons which have a momentum that have $\mathbf{k} \parallel \mathbf{v}_s$. For instance, at the Landau critical velocity the energy gap is *doubled* for electrons with $\mathbf{k} \parallel -\mathbf{v}_s$. Unlike a BEC, one cannot put an arbitrary number of electrons into the same quantum state. Therefore, it is not enough that only a small part of momentum space allows for zero energy gap: this is not sufficient in order for the supercurrent to transfer all of its momentum into normal single-particle excitations. As a result, superconductivity (characterized by Δ) survives for higher velocities than v_L , namely up to $v_c > v_L$. At v_c , a sufficient portion of electron momenta directions have zero energy gap and the condensate has been depleted since there is now enough phase space available for normal single-particle excitations to carry the current.

The dimensionality is thus important here in light of the phase-space argument. In a quasi-1D superconductor (hypothetically at least), v_c would coincide with v_L because the Fermi surface only consists of two points (instead of a sphere as in 3D). Thus, there is no extra room for phase-space growth after one has reached a superfluid velocity $v_s = v_L$ and Δ has to collapse immediately.

The above discussion illustrates an important difference between superconductors and Bose superfluids, namely what happens when the critical velocity v_c is reached. For the Bose case, the superfluidity is lost when $v = v_c$ whereas *gapless* superconductivity may persist up to a higher critical velocity $v_{c,2} > v_c$ in a superconductor. The reason for this is that even if elementary excitations may be created at arbitrarily small energies in the superconductor when $v = v_c$, these excitations are fermions. In three dimensions, the energy gap separating the condensate and the excitations has only vanished on an infinitesimal portion of the Fermi sphere when $v = v_c$ whereas a finite phase space is required to excite an appreciable number of fermions. The quasiparticle generation then continues to grow in rate after $v > v_c$ until the *superconducting order parameter* has vanished as well. In the regime $v_c < v < v_{c,2}$, part of the Fermi surface is not gapped but there still exists a superconducting order parameter. This should be contrasted with the behavior of the bosonic excitations in a Bose superfluid, which do not require the same finite phase space due to the absence of Pauli exclusion. Note that this reasoning is only valid in higher dimensions than one: for the one-dimensional case, the superconducting order parameter drops to zero at $v = v_c$ since there is no room for phase space growth (the entire Fermi "surface", consisting of two points $\pm k_F$, is non-gapped).

The above scenario is an example of gapless superconductivity where the energy gap may vanish at parts of the Fermi surface whereas the order parameter is still non-zero due to the fact that there is not enough phase space available to excite a sufficient amount of the condensate into quasiparticle states.

12.10.1 Temperature-dependence of the gap

In a ferromagnet, more magnons (quasiparticles) are thermally excited as temperature increases. Since magnons reduce the magnetization, increasing temperature ultimately causes the spontaneous magnetization to be zero. In this way, we can understand why the magnetization is reduced as temperature increases.

But what about the superconducting order parameter $\Delta(T)$? The point is now that if a Cooper pair is broken up into two thermally excited quasiparticle (which is possible at finite temperatures), some states in $\mathbf{k}$ -space are now *blocked* by excited quasiparticles. Thus, there is less phase space available for Cooper pairs to reside in and Δ is reduced. Mathematically, this can be seen from the selfconsistency equation:

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle c_{\mathbf{k}'\uparrow} c_{-\mathbf{k}'\downarrow} \rangle, \quad (12.89)$$

where $V_{\mathbf{k}\mathbf{k}'}$ is the attractive interaction that only exists for pairs of momenta $\mathbf{k}, \mathbf{k}'$ that fall inside a thin shell centered around the Fermi momentum. When states at some values of $\mathbf{k}'$ in this sum are occupied by quasiparticles, the corresponding expectation value $\langle c_{\mathbf{k}'\uparrow} c_{-\mathbf{k}'\downarrow} \rangle$ is reduced and thus Δ shrinks. Since $E_0 \propto \Delta^2$, the condensation energy E_0 resulting from the existence of Cooper pairs is also reduced because fewer pairs exist.

12.11 Broadening of the superconducting transition

Experimentally, one observes that the superconducting transition broadens when (1) T_c becomes smaller, (2) when the magnetic field increases or (3) for inhomogeneous, polycrystalline samples. Here, we give an explanation for these observations. By superconducting transition we mean the drop in ρ as a function of temperature.

12.11.1 Why SC transition typically broadens for a lower T_c

When T_c becomes lower, the gap becomes smaller and thus the superconducting coherence length increases. Let L be the thickness of the superconductor. This means that the ratio L/ξ decreases as the thickness of the MNN layer becomes larger. In effect, the dimensionality of the superconductor becomes effectively more 2D-like. Theory shows that fluctuations in the superconducting order parameter become more prominent the more 2D-like the superconductor becomes. This means as one approaches T_c , some parts of the sample start becoming superconducting before others, which widens the transition as a whole.

There are many ways to suppress T_c , including in proximity structures such as S/N or S/F. Increasing the thickness of the non-superconducting layer causes a lower T_c and should therefore make the transition broader.

12.11.2 Why SC transition broadens in inhomogeneous, polycrystalline samples

When you have multiple grains, the mean free path is going to vary across the sample spatially. This changes the local superconducting order parameter and thus the coherence length. In turn, this causes local variations in when a grain becomes superconducting. A larger distribution of T_c thus causes a wider transition. Same thing goes when applying field, where one also observes that the transition broadens. Different grains have different crystallographic orientations, and both the (1) mean free path dependence on H_{c2} (through the coherence length) and the (2) crystallographic orientations of the grains which couples to anisotropies in the critical field (IP vs OOP) makes different grains transition at different temperatures.

12.12 Vortices and gauge-invariant phase difference

Superconductors (type II ones, to be more specific) display flux quantization. What this means is that the superconductor lets through some magnetic flux in the form of vortices, rather than maintaining the Meissner state all the way up to the critical field (as type I superconductors do). This magnetic flux has to be quantized, as we now demonstrate.

12.12.1 Flux quantization

Imagine that some region of a superconductor has magnetic flux penetrating it. We know that the superconducting condensate is described by an order parameter $\psi = |\psi|e^{i\phi}$. Walking around any closed contour that encapsulates this region of magnetic flux has to bring us back to the starting point. Mathematically, the line integral of the gradient $\nabla\phi$ around this contour has to give the result $2\pi n$. Physically, this is reasonable since the order parameter has to be single valued at any

point, so that $\int_1^2 d\mathbf{l} \cdot \nabla\phi = \phi_2 - \phi_1$ regardless of which path one takes. Thus, we have

$$\oint d\mathbf{l} \cdot \nabla\phi = 2\pi n, \quad (12.90)$$

so that the order parameter ψ has the same value at the start and end point (these points are the same point for a closed contour). Now, we should actually take into account the presence of a magnetic vector potential $\mathbf{A}$ into this argument since we assume that the region under consideration has magnetic flux penetrating it. The key here is that $\mathbf{A}$ is coupled to the superconducting phase ϕ . This occurs via the requirement of local gauge-invariance: by demanding that the U(1) symmetry of the superconducting state is local rather than global (since the phase should not affect the physics, regardless of whether we choose a constant value or a different value at different points in space), we generate a coupling between the order parameter field ψ and $\mathbf{A}$. In order to keep the free energy F for a field of charge q invariant under a change of superconducting phase $\phi \rightarrow \phi' = \phi + \frac{q}{\hbar}\lambda(\mathbf{r})$, we must simultaneously transform the vector potential $\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla\lambda(\mathbf{r})$. Thus, the locally *gauge-invariant* gradient of the superconducting phase has to be written $\nabla\phi - \frac{q}{\hbar}\mathbf{A}$. We see that this object is invariant under a gauge-transformation, since:

$$\begin{aligned} \nabla\phi' - \frac{q}{\hbar}\mathbf{A}' &= \nabla\phi + \frac{q}{\hbar}\nabla\lambda - \frac{q}{\hbar}(\mathbf{A} + \nabla\lambda) \\ &= \nabla\phi - \frac{q}{\hbar}\mathbf{A}. \end{aligned} \quad (12.91)$$

For a superconductor, we know that $q = -2e$. A gradient in the gauge-invariant order parameter produces a supercurrent response, as can be seen *e.g.* from the Ginzburg-Landau equations. Imagine then that we have some vortex in a bulk superconductor. Let us choose an integration path around the vortex which is sufficiently large that the shielding supercurrent is zero: the path passes through the bulk region of the superconductor where no magnetic field exists. We thus get:

$$\oint d\mathbf{l} \cdot (\nabla\phi - \frac{q}{\hbar}\mathbf{A}) = 0. \quad (12.92)$$

Since the order parameter has to be single-valued, we use Eq. (12.90) and get:

$$\frac{2\pi}{\Phi_0} \oint d\mathbf{l} \cdot \mathbf{A} = 2\pi n. \quad (12.93)$$

Using Stokes theorem, this can be rewritten as

$$\int \int_S d\mathbf{S} \cdot (\nabla \times \mathbf{A}) = n\Phi_0 \quad (12.94)$$

which is equivalent to

$$\Phi = n\Phi_0, \quad (12.95)$$

since $\nabla \times \mathbf{A} = \mathbf{B}$ and Φ is the magnetic flux through the surface S enclosed by the contour. The flux is thus *quantized* in units of Φ_0 , the superconducting flux quantum. The superconducting phase ϕ must thus be a discontinuous function in the presence of vortices: winding the phase around the vortex will advance it with $2\pi n$. If it was continuous, the fundamental theorem of calculus would guarantee us that $n = 0$. Note that even if we increase the surface S enclosed by the contour, the flux will not increase since $\mathbf{B} = 0$ in the bulk of the superconductor.

Proof for necessity of discontinuity of the phase. Let us show this in more detail. The phase of the superconducting order parameter Ψ may be written as

$$\phi = \arctan\left(\frac{\text{Im}\Psi}{\text{Re}\Psi}\right). \quad (12.96)$$

The winding number is obtained as the change in ϕ after having traversed along a closed path, so that

$$\oint_C \nabla\phi = 2\pi n, \quad (12.97)$$

where n is the winding number of the path C . We see that θ is bounded with a range of $[-\pi/2, \pi/2]$, but it is discontinuous wherever $\text{Re}\Psi = 0$. To see why a non-trivial winding number $n \neq 0$ requires discontinuities, we observe the following. For any bounded function $f(x)$ containing discontinuities at discrete locations x_i , $i = 1, 2, 3, \dots$, the integral of its derivative is obtained as

$$\begin{aligned} \int_a^b \frac{df}{dx} dx &= \lim_{\epsilon \rightarrow 0} \int_a^{x_1-\epsilon} \frac{df}{dx} dx + \sum_{i=1}^{n-1} \int_{x_i+\epsilon}^{x_{i+1}-\epsilon} \frac{df}{dx} dx + \int_{x_n+\epsilon}^b \frac{df}{dx} dx \\ &= f(b) - f(a) + \lim_{\epsilon \rightarrow 0} \sum_{i=1}^n [f(x_i - \epsilon) - f(x_i + \epsilon)]. \end{aligned} \quad (12.98)$$

where we used the fundamental theorem of calculus in the last equality. The limit $\epsilon \rightarrow 0$ is well-defined since f is bounded. For a closed path, $f(a) = f(b)$, and we see that the integral becomes the sum of the value of the discontinuities encountered along the path. Thus, for a winding number $n = 1$, two discontinuities of value π must be traversed around any closed loop, implying a topological charge of 1.

We end by noting that in the context of Josephson junctions, we know that the gauge-invariant superconducting phase ϕ_{GI} must be

$$\phi_{\text{GI}} = \phi + \frac{2e}{\hbar} \int \mathbf{A} \cdot d\mathbf{l} \quad (12.99)$$

according to our above expression for the gauge-invariant superconducting phase gradient

$$\nabla\phi_{\text{GI}} = \nabla\phi + \frac{2e}{\hbar} \mathbf{A}. \quad (12.100)$$

Therefore, it is clear that the gauge-invariant superconducting phase difference between any two points in a Josephson junction is:

$$\phi_{\text{GI}}(2) - \phi_{\text{GI}}(1) = \phi(2) - \phi(1) + \frac{2e}{\hbar} \int_1^2 \mathbf{A} \cdot d\mathbf{l} \quad (12.101)$$

where the integration path is taken from point 1 to 2 across the Josephson junction. In this way, one can obtain for instance the modification of Andreev bound-state energy for a given trajectory between two points on the left (1) and right (2) superconductor (which reads $E = \Delta_0 \cos(\Delta\phi/2)$) in a transparent SNS junction with length $L \ll \xi$) in the presence of a vector potential by simply replacing $\Delta\phi \rightarrow \Delta\phi + \frac{2e}{\hbar} \int_1^2 \mathbf{A} \cdot d\mathbf{l}$. It should be emphasized that this only accounts for the vector potential effect on the phase-difference and not the Lorentz-force alteration of the trajectories of the electrons and holes in the system. The latter can be neglected if the field B is small enough that the curvature radius of the resulting cyclotron orbits is much smaller than the length L of the junction.

12.12.2 Screening currents and vortices due to Lorentz-force?

What is the source of screening currents and vortices in a superconductor? Can one say that they arise due to the Lorentz-force acting on the Cooper pairs?

Screening currents and diamagnetism

It is useful to initiate this discussion by recalling the Bohr-van Leeuwen theorem which has as a consequence that classical physics gives zero magnetism due to orbital currents (including no diamagnetism). In other words, inclusion of the $\mathbf{A}$ -field via minimal coupling produces zero net diamagnetic response in any classical system in equilibrium. We recall also that the $\mathbf{A}$ -field enters via minimal coupling in order to produce the correct Lorentz-force in a Lagrangian formalism.

If one instead considers a quantum mechanical model with a Hamilton-operator for a 3D electron gas, one obtains a net magnetic response when a $\mathbf{A}$ -field is present (due to *e.g.* an external magnetic field). This is so-called Landau diamagnetism. In short, one computes the magnetization of the system via $M \propto \partial F / \partial B$ where F is the free energy obtained from the eigenvalues of the system. One may then compute *e.g.* the susceptibility $\chi = dM/dB$ and finds a diamagnetic response of the Landau levels.

In this sense, one could say something along the lines of that a quantum mechanical treatment of the Lorentz-force produces diamagnetism. However, this would be a heuristic statement.

Now, let us turn to the superconducting case. Is it correct to say that it is the Lorentz-force which is the source of the diamagnetic response (screening currents) set up by the superconductor? First, we should note that the diamagnetic response of a 3D free electron gas and a superconductor is qualitatively different. In the free electron gas case, a constant magnetization is generated, oppositely directed to the external magnetic field. This results in a net, lower magnetic field inside the material compared to outside. In the superconducting case, the magnetic field decays inside the material and reaches zero after the penetration depth.

The point is that this behavior cannot be attributed solely to the appearance of $\mathbf{A}$ as a minimal coupling in the Hamiltonian or Lagrangian. Additionally, one needs a charged condensate described by a complex order parameter field $\psi = |\psi|e^{i\theta}$. When a non-zero vacuum expectation value exists for such a field (like in a superconductor) and this field spontaneously breaks U(1) symmetry, the Higgs-mechanism shows that the gauge-field $\mathbf{A}$ acquires a mass. This can be shown either in a gauge-invariant way or by selecting a specific gauge where the vector potential becomes massive [55]. The fact that the gauge-field acquires mass already implies that the electromagnetic interactions have become short-ranged inside the superconductor, since interactions mediated by massive gauge bosons have a finite range. However, it is also possible to see explicitly that a screening current arises by deriving the Euler-Lagrange equations from a Lagrangian which has both the order parameter field which spontaneously breaks U(1) symmetry and the gauge-field $\mathbf{A}$ [55].

So it becomes too simplistic to say that the Lorentz-force is the reason for screening currents in a superconductor: the screening currents and massive photon arises because of how a superconductor responds to an electromagnetic field, and this requires both a charged condensate described by an order parameter that spontaneously breaks U(1) symmetry as well as the Higgs-mechanism, which describes the interplay between this spontaneously broken symmetry and the gauge-field $\mathbf{A}$.

Does the photon become massive because of the screening currents or do the screening currents arise because the photon is massive in a superconductor? This chicken-egg complication is spurious, because both happen at the same time. This can be illustrated by an analogy. Consider a dielectric material and apply an external $\mathbf{E}$ -field. The dipoles in the material are reoriented so that the net electric field inside the material becomes reduced compared to outside of the material. What happens first - the reorientation of the dipoles or the modification of the $\mathbf{E}$ -field inside the material? Both happen at the same time, just like the screening currents and modification of the $\mathbf{B}$ -field inside a superconductor occur simultaneously - one does not occur before the other.

Vortices

What about vortices - is the Lorentz force responsible for them? So far, we have seen that it is the interplay between a spontaneously broken $U(1)$ symmetry for a charged order parameter field and the presence of a gauge-field $\mathbf{A}$ coupled to this order parameter field which results in screening currents and massive photons, precisely via the Higgs mechanism. The vortices come into the pictures because of the requirement that the order parameter has to be single-valued. Due to the phase-factor $e^{i\theta}$ in the order parameter ψ , single-valuedness for ψ allows phase windings of integer numbers of 2π in θ . From the gauge-invariant expression for supercurrent $\mathbf{J} \propto \hbar \nabla \theta + 2e\mathbf{A}$, one can then show that if magnetic flux exists in a superconductor, it has to be quantized.

It is again too simplistic to say that the vortices arise as a result of the Lorentz-force in the form of the minimal coupling to $\mathbf{A}$, because such a statement misses out on essential ingredients such as the requirement of single-valuedness of the order parameter and the fact that the order parameter describes a macroscopically phase-coherent condensate.

Whether or not vortices appear when a magnetic field is applied, can be discussed from the perspective of energetics as done *e.g.* in the SudbÅy textbook. In short, depending on whether $\lambda < \xi$ or vice versa, it becomes favorable for the superconductor to maximize the number of normal-superconductor interfaces which leads to vortex formation. But the fact that vortices can exist, requires more than just saying that the Lorentz-force is acting on Cooper pairs: the phase-coherence and single-valuedness of the order parameter is pivotal in this regard.

12.12.3 Sending a supercurrent

<https://physics.umd.edu/courses/Phys798S/AnlageSpring16/Lecture>

12.12.4 Proximity-induced vortices in SNS systems

Let us comment on how this is related to proximity-induced vortices, that were discussed in Ref. [?]. The authors showed that for wide junctions $W \gg L$, applying a magnetic flux to a SNS Josephson junction would produce an array of vortices in the center of the junction. How are these vortices related to type II superconductor vortices? First of all, they were not standard Josephson vortices because they had a normal core: the pair correlation function vanishes at their center. Moreover, the phase exhibited a 2π winding upon traversing a vortex and they were accompanied by a circulating current. The only property of an Abrikosov vortex that they did not possess was flux quantization. To see why this is the case, consider that the prediction of these proximity-induced vortices was obtained under the assumption that $\mathbf{A}$ was fully screened in the superconductors whereas the external field $\mathbf{B}$ was constant throughout the normal metal. In effect, the influence of screening currents on $\mathbf{B}$ in the N region was neglected by assuming that their magnitude was sufficiently small. This

is equivalent to stating that the Josephson penetration depth λ_J was much larger than the N size: $\lambda_J \gg W, L$.

A useful analogy here is that the situation is effectively as if we were inside a vortex line (i.e. inside a radius r smaller than the penetration depth λ) where the field can penetrate more or less homogeneously: an integration contour chosen inside the vortex line will give more and more flux the larger the contour is until it engulfs the entire vortex. The same occurs for the proximity-induced vortices of a 2D SNS junction with dimensions smaller than the relevant penetration depth for this system, namely λ_J . In this case, we can approximate the field as penetrating homogeneously even if there will be a small correction from circulating currents. There is thus no flux-quantization since we're inside a flux line.

From the equation for the supercurrent $\mathbf{J} \propto \hbar \nabla \phi - 2e \mathbf{A}$, integration along a closed contour enclosing one proximity-induced vortex (where the phase winding is 2π) will give

$$\oint \mathbf{J} \cdot d\mathbf{l} \propto \Phi - \Phi_0. \quad (12.102)$$

Since the magnetic field penetrates homogeneously, Φ depends on the precise contour and thus there must be a contribution from the integral over the current as well in order to satisfy the equation. The current changes its circulation pattern depending on how far away from the vortex center one is [?]. Close to it, it circulates in a way that creates a field along $\mathbf{B}$. This is where the pair correlation is close to zero. As one moves away from the vortex, superconducting correlations are restored and a screening current sets in and circulates in the opposite direction.

Note that there is no contradiction between taking into account the contribution from the supercurrent in the above equation and at the same time saying that we neglect the screening effect of the supercurrent on the magnetic field. The latter is an approximation stemming from the fact that we're considering a junction much smaller than λ_J . Ideally, we should solve Usadel and Maxwell self-consistently. Doing so, we would find a small correction to the homogeneous nature of the external flux through the N part due to the screening currents. However, we would still need to take into account the screening current in the above equation in order to satisfy it since Φ would not differ much at all from a homogeneously penetrating field. A self-consistent treatment would then just give a minor correction to the screening current pattern.

Summarizing, if one uses an approach where the screening effect of the induced supercurrent is neglected, one finds proximity-induced vortices which have all the properties of Abrikosov vortices except flux quantization. It is as if one is looking at the inside of a vortex line (i.e. within a radius of the penetration depth) where the magnetic field exists more or less homogeneously. Thus, the flux increases the larger area one considers as long as one stays inside the core.

Treatment in quasiclassical 2D geometry

We here mention some aspects of the linearized treatment of a 2D SNS junction and a 2D S-halfmetal-S junction for energies near $E = 0$ which must be handled with care.

In the SNS case, a linearized solution can be found in the wide-junction limit. The main assumption here is that the solution varies much slower in the y -direction than the x -direction. From the obtained solution for the anomalous Green function f (see *e.g.* Cuevas and Bergeret, JLTP 2008), one sees that at $E = 0$ this assumption is violated in $f \propto e^{-2\pi i x y n / W}$ since it then varies equally fast in the x and y -directions. Therefore, it strictly speaking cannot be used exactly at $E = 0$.

The same problem occurs in the linearized wide-junction limit solution in the S-halfmetal-S case. However, an additional problem arises in the linearized boundary conditions. The main term kept on the right hand side of the equation of $\partial_x f_{\uparrow} = \dots$ is proportional to $c_{\text{BCS}} s_{\text{BCS}}$ and thus vanishes at $E = 0$ since $c_{\text{BCS}} = 0$ for that energy. This means that all other higher-order terms in $f_{\uparrow}$ that are discarded on the right-hand side cannot be neglected at $E = 0$ since the main term vanishes. The solution obtained for $f_{\uparrow}$ thus cannot strictly speaking be used for $E = 0$, but it can still predict the vortex positions since $f_{\uparrow}$ vanishes for *all energies* at those points.

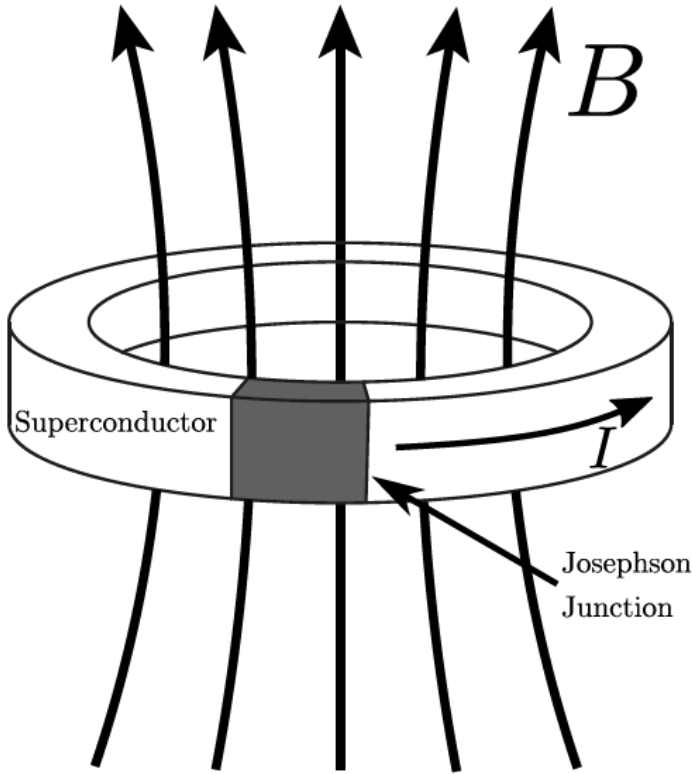
It is also interesting to note that without a magnetic field in a S/halfmetal heterostructure, one finds that $f_{\uparrow}(E = 0) \neq 0$ so that the DOS $N(0) > 1$ as triplets always enhance the DOS at $E = 0$. With the magnetic field present, however, Eirik Fyhn's numerical investigations seem to imply that the field destroys the triplets (or at least strongly suppresses them) at $E = 0$ so that $N(0) = 1$. There exists no simple way to analytically prove this though, since the linearized solution for $f_{\uparrow}$ is not valid at $E = 0$ as explained above. For vortices appearing in a half-metal, one finds $N(0) = 1$ at the vortex-cores whereas the DOS surrounding the vortices can be either positive or negative for very small E , but not exactly $E = 0$. In the case $E = 0$, we have $N(0) = 1$ also away from the vortex cores.

12.13 Controlling the superconducting phase difference and measuring the current-phase relation

When a phase difference exists between the order parameters of two superconductors, a supercurrent flows across the junction in response. This can be understood from the Ginzburg-Landau equation relating the supercurrent $\mathbf{J}$, a gradient in the phase $\nabla\phi$, and the gauge field $\mathbf{A}$: the presence of $\nabla\phi$ implies $\mathbf{J} \neq 0$. So how can one establish a phase difference between two superconductors? One way is to simply current-bias the system, i.e. to send a current through a Josephson junction. To accommodate the supercurrent, the superconducting phase $\phi = \phi(x)$ has to wind in the superconductors and through any material separating the superconductors (which also have an effective order parameter in the presence of a proximity effect), and this means that a phase difference occurs between the superconductors. For a constant supercurrent, $\mathbf{J} \propto \hbar \nabla\phi$ implies that ϕ winds linearly with position x .

A different way to tune the phase difference, which is more convenient in order to probe the full range of possible phase differences $[0, 2\pi]$, is to pass a magnetic flux through a superconducting loop when the loop is interrupted by a Josephson junction. When a flux is applied to the loop, screening currents are generated which oppose the external flux.

Consider first the case without any Josephson junction, i.e. a pure superconducting loop. Imagine that the loop is thick enough so that the supercurrent response to the externally applied flux in the bulk of the superconductor vanishes. This is because the screening currents in a superconductor only exist within a region of thickness λ in the vicinity of the surface. Integrating now the Ginzburg-Landau equation $\mathbf{J} \propto \hbar \nabla\phi + 2e\mathbf{A}$ around the loop with $\mathbf{J} = 0$ and using that the superconducting order parameter must be single-valued in the same point (so that the phase difference across the loop must be $2\pi n$), one obtains that the flux Φ through the loop must be quantized in elementary flux quanta Φ_0 , i.e. $\Phi = n\Phi_0$. The shielding supercurrent plotted versus the applied field $\mu_0 \mathbf{H}$ will thus increase up until $\mathbf{H}$ is strong enough to send a flux quantum Φ_0 through the loop. The supercurrent should then drop to zero, and then start to increase again until the field reaches $2\Phi_0$



so that the net flux through the loop only passes in units of Φ_0 .

We showed above that the relation

$$\int \mathbf{A} \cdot d\mathbf{l} = \frac{\Phi_0}{2\pi} \int \nabla\phi \cdot d\mathbf{l} \quad (12.103)$$

holds in any region where $\mathbf{J} = 0$. Now consider the case where we interrupt the superconducting loop with a Josephson junction, i.e put a normal metal in it, see figure below. Since $\mathbf{B} = \nabla \times \mathbf{A}$, the line integral of $\mathbf{A}$ around the ring must equal the enclosed flux

$$\oint \mathbf{A} \cdot d\mathbf{l} = \Phi. \quad (12.104)$$

The entire integral around the ring is decomposed into the part inside the superconductor and the part across the weak link (normal metal):

$$\oint = \int_{\text{SC}} + \int_{\text{link}}. \quad (12.105)$$

The phase ϕ of the superconducting order parameter has to be single valued, as before, so that

$$\oint \nabla\phi \cdot d\mathbf{l} = 2\pi n. \quad (12.106)$$

This can be rewritten as

$$\int_{\text{SC}} \nabla \phi \cdot d\mathbf{l} = 2\pi n - \int_{\text{link}} \nabla \phi \cdot d\mathbf{l}. \quad (12.107)$$

From Eq. (12.104), defining $e^* = -2|e|$ as the Cooper pair charge, we now have

$$\begin{aligned} \frac{e^*}{\hbar} \Phi &= \frac{e^*}{\hbar} \oint \mathbf{A} \cdot d\mathbf{l} \\ &= \frac{e^*}{\hbar} \int_{\text{link}} \mathbf{A} \cdot d\mathbf{l} + \frac{e^*}{\hbar} \int_{\text{SC}} \mathbf{A} \cdot d\mathbf{l} \\ &= \frac{e^*}{\hbar} \int_{\text{link}} \mathbf{A} \cdot d\mathbf{l} + \int_{\text{SC}} \nabla \phi \cdot d\mathbf{l} \\ &= \frac{e^*}{\hbar} \int_{\text{link}} \mathbf{A} \cdot d\mathbf{l} - \int_{\text{link}} \nabla \phi \cdot d\mathbf{l} + 2\pi n \\ &= -\gamma + 2\pi n. \end{aligned} \quad (12.108)$$

Here, $\gamma = \nabla \phi - \frac{e^*}{\hbar} \mathbf{A}$ is the previously introduced gauge-invariant superconducting phase difference. It follows then that this phase-difference is determined by the flux:

$$\gamma = -\frac{e^*}{\hbar} \Phi + 2\pi n \quad (12.109)$$

and the $2\pi n$ can be discarded since all physical properties of the system are 2π -periodic. We see that the phase of a Josephson junction in a superconducting ring is tunable by applying a magnetic flux. If we choose the gauge $\mathbf{A}$ so that it has zero component along the Josephson junction, the phase difference is simply $\nabla \phi$ across the junction.

12.14 Electrostatic potentials and time-dependent phases in superconductors

Local gauge-invariance demands that the following transformations leave the equation of motions of a system invariant for a superconductor where the order parameter has charge $q = -2e$:

$$\begin{aligned} \psi_\sigma &\rightarrow \psi'_\sigma = \psi_\sigma e^{-i\chi/2}, \\ \phi &\rightarrow \phi' = \phi + \chi, \\ U &\rightarrow U' = U + \dot{\chi}/2, \\ \mathbf{A} &\rightarrow \mathbf{A}' = \mathbf{A} - \nabla \chi/2. \end{aligned} \quad (12.110)$$

Here, ϕ is the phase of the superconducting order parameter $\Delta = |\Delta|e^{i\theta}$, U is the electrostatic potential, $\mathbf{A}$ is the magnetic vector potential. We've here omitted some natural constants since they are not important for the main point we want to make in this section. If we consider only the second-quantized Hamilton-operator expressed in terms of field operators $\{\psi_\sigma, \psi_\sigma^\dagger\}$, this is also invariant for a time-independent χ . There is, however, no requirement that the quantum mechanical Hamilton-operator need be invariant under a gauge-transformation: just look at the Schrödinger equation which is not invariant unless you also transform the wavefunction.

We previously showed that the gauge-invariant superconducting phase gradient had to include a contribution from the vector potential: $\nabla \phi_{\text{GI}} = \nabla \phi + 2\mathbf{A}$. Now, we want to consider what happens

when an electrostatic potential is present instead of the magnetic vector potential gauge field. In other words, imagine that we have two bulk superconductors with constant phases ϕ_1 and ϕ_2 . A voltage U is applied between them. The general expression for the gauge-invariant superconducting phase gradient $\nabla\phi_{\text{GI}}$, which includes the contribution from the electrostatic potential U , has to read:

$$\nabla\phi_{\text{GI}} = \nabla\phi + 2 \int d\tau \nabla U(\mathbf{r}, \tau). \quad (12.111)$$

One can verify by the transformation rules above that if this equation holds, then making a gauge transformation with $\chi = \chi(\mathbf{r}, t)$ leads to the same equation expressed in terms of the new gauge fields:

$$\nabla\phi_{\text{GI}} = \nabla\phi' + 2 \int d\tau \nabla U'(\mathbf{r}, \tau). \quad (12.112)$$

From this, we can prove the AC Josephson effect: namely that a voltage applied across a Josephson junction results in a gauge-invariant time-dependent superconducting phase difference. By integrating the above equation from point 1 inside the left superconductor to point 2 inside the right superconductor:

$$\Delta\phi_{\text{GI}} \equiv \phi_{\text{GI}}(2) - \phi_{\text{GI}}(1) = \phi_2 - \phi_1 + \int d\tau \Delta U(\tau). \quad (12.113)$$

where $\Delta U(t') = U_2(t') - U_1(t')$. If a constant voltage difference is applied across the junction, $\Delta U(t') = U_0$, it is clear that $\Delta\phi_{\text{GI}} = \Delta\phi_0 + 2U_0 t$ where $\Delta\phi_0 = \phi_2 - \phi_1$ and the gauge-invariant phase difference which drives the supercurrent oscillates with time. We also see that

$$\frac{\partial \Delta\phi_{\text{GI}}}{\partial t} = \Delta U(t). \quad (12.114)$$

Does this mean that if a constant electrostatic potential exists in a superconductor, the phase gradient must be time-dependent? No. Imagine we just have one superconductor and let 1 and 2 be two points inside this superconductor. Now, $\Delta U = 0$ since $U = \text{constant}$. Therefore, the phase-difference $\Delta\phi_{\text{GI}} = \Delta\phi_0$ between these points is time-independent.

For a bulk superconductor with a finite electrostatic potential (but zero electric field and zero current), we know that we can set $U = \text{constant}$ which then according to Eq. (12.114) means we can set the intrinsic phase ϕ of the superconducting order parameter as a constant (for instance zero) since $\Delta U(t) = 0$.

The gauge-transformation arguments above help us understand the S -matrix transformation where $S = e^{-ieVt\hat{\rho}_3}$ in the PRB by Cuevas *et al.* treating the AC Josephson effect in SNS structures with the Usadel equation. Let the right superconductor be at zero voltage and have zero superconducting phase $\phi = 0$. If a voltage-difference (keep in mind that the measurable voltage-difference is $\int \mathbf{E} \cdot d\mathbf{l}$ which is expressed via the gauge-invariant electric field) exists across the junction, it means that this has to be reflected both in the distribution function and the phase of the left superconductor. The phase is affected since we know that the gauge-invariant superconducting phase is time-dependent in the presence of a voltage difference. Therefore, the left superconductor should have a Green function matrix with both shift in the energy argument of the real part of the Green function (which expresses the DOS) and the distribution functions as well as an effective time-dependent phase of

the superconducting order parameter.

Now, the actual form of the Green function is determined by the equation of motion for it which is derived from the Hamiltonian $\hat{H}$. For a bulk BCS superconductor we have:

$$\left[i \frac{\partial}{\partial t_1} \hat{\rho}_3 - \hat{H}(1) \right] \check{G}(1, 2) = \delta(1 - 2) \hat{1}. \quad (12.115)$$

The $\hat{1}$ is understood to be repeated along the diagonal of $\check{G}$. Here, $\hat{H}(1) = -(\nabla_1^2/2m)\hat{1} - \mu\hat{1} + \hat{\Delta}$ where

$$\hat{\Delta} = \begin{pmatrix} 0 & 0 & 0 & \Delta \\ 0 & 0 & -\Delta & 0 \\ 0 & \Delta^* & 0 & 0 \\ -\Delta^* & 0 & 0 & 0 \end{pmatrix} \quad (12.116)$$

We know that the solution for $\check{G}(1, 2)$ is the BCS bulk Green function.

But let us instead now say that we are interested in finding what the Green function matrix looks like if we put an electrostatic potential eV on the superconductor. If the solution for the Green function has a time-independent phase when $eV = 0$, we should now expect to find a time-dependent superconducting phase in the Green function describing this superconductor at $eV \neq 0$. To investigate this, let us define the transformation:

$$\psi'_\sigma = \psi_\sigma e^{-ieVt}. \quad (12.117)$$

One can then verify simply from the definition of the Green function matrix $\check{G}$ that

$$\check{G}(t_1, t_2) = e^{-ieVt_1\hat{\rho}_3} \check{G}'(t_1, t_2) e^{+ieVt_2\hat{\rho}_3} \quad (12.118)$$

where $\check{G}$ is defined with expectation values of ψ_σ whereas $\check{G}'$ is defined with expectation values of ψ'_σ . The superconducting order parameter is now expressed as

$$\hat{\Delta} = \begin{pmatrix} 0 & 0 & 0 & \langle \psi_\uparrow \psi_\downarrow \rangle \\ 0 & 0 & \langle \psi_\downarrow \psi_\uparrow \rangle & 0 \\ 0 & \langle \psi_\uparrow^\dagger \psi_\downarrow^\dagger \rangle & 0 & 0 \\ \langle \psi_\downarrow^\dagger \psi_\uparrow^\dagger \rangle & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & \Delta' e^{2ieVt} \\ 0 & 0 & -\Delta' e^{2ieVt} & 0 \\ 0 & (\Delta')^* e^{-2ieVt} & 0 & 0 \\ -(\Delta')^* e^{-2ieVt} & 0 & 0 & 0 \end{pmatrix} \quad (12.119)$$

where we defined $\Delta' \equiv \langle \psi'_\uparrow \psi'_\downarrow \rangle$. A key observation here is that we can write:

$$\hat{\Delta} = e^{-ieVt_1\hat{\rho}_3} \hat{\Delta}' e^{ieVt_1\hat{\rho}_3} \quad (12.120)$$

where we defined

$$\hat{\Delta}' = \begin{pmatrix} 0 & 0 & 0 & \Delta' \\ 0 & 0 & -\Delta' & 0 \\ 0 & (\Delta')^* & 0 & 0 \\ -(\Delta')^* & 0 & 0 & 0 \end{pmatrix} \quad (12.121)$$

This follows since $\hat{\Delta}$ has the same type of structure as the Green function matrix itself in terms of expectation values of fermion operators. We can then express Eq. (12.115) in terms of the primed superconducting order parameter and Green function as follows:

$$\left[i \frac{\partial}{\partial t_1} \hat{\rho}_3 + \nabla_1^2 / 2m + \mu - e^{-ieVt_1\hat{\rho}_3} \hat{\Delta}' e^{ieVt_1\hat{\rho}_3} \right] e^{-ieVt_1\hat{\rho}_3} \check{G}'(t_1, t_2) e^{+ieVt_2\hat{\rho}_3} = \delta(1-2) \hat{1}, \quad (12.122)$$

Now, the time derivation operator on the left side acts on $e^{-ieVt_1\hat{\rho}_3}$ as well as on $\check{G}'$ and thus produces:

$$e^{-ieVt_1\hat{\rho}_3} \left[i \frac{\partial}{\partial t_1} \hat{\rho}_3 + \nabla_1^2 / 2m + eV + \mu - \hat{\Delta}' \right] \check{G}'(t_1, t_2) e^{+ieVt_2\hat{\rho}_3} = \delta(1-2) \hat{1}, \quad (12.123)$$

where we've used that $e^{-ieVt_1\hat{\rho}_3}$ commutes with $\hat{\rho}_3$. We move the exponentials over to the right hand side to produce:

$$\left[i \frac{\partial}{\partial t_1} \hat{\rho}_3 + \nabla_1^2 / 2m + eV + \mu - \hat{\Delta}' \right] \check{G}'(t_1, t_2) = \delta(1-2) e^{ieVt_1\hat{\rho}_3} e^{-ieVt_2\hat{\rho}_3}. \quad (12.124)$$

But since $e^{ieVt_1\hat{\rho}_3} e^{-ieVt_2\hat{\rho}_3} = 1$ if $t_1 = t_2$, we can omit this factor due to the $\delta(1-2)$ -function. In effect, we end up with

$$\left[i \frac{\partial}{\partial t_1} \hat{\rho}_3 + \nabla_1^2 / 2m + eV + \mu - \hat{\Delta}' \right] \check{G}'(t_1, t_2) = \delta(1-2). \quad (12.125)$$

This is exactly the same equation of motion as for the BCS superconductor (as seen by simply omitting the ' notation) except for a voltage shift eV . In effect, the Green function $\check{G}'$ for a superconductor with a voltage shift is obtained by the matrix multiplication Eq. (12.118) from the Green function $\check{G}$ of a BCS superconductor without any voltage shift. The transformation Eq. (12.118) effectively introduces a shift both in the distribution functions, the real part of the normal Green function component, and also multiplies the anomalous part with $e^{\pm ieVT}$ where T is the center-of-mass time-coordinate [36]. Specifically, a straightforward calculation upon introducing the Wigner representation and Fourier transforming gives the following retarded part of the Green function:

$$\hat{G}'(T, E) = \begin{pmatrix} \underline{g}_{\text{BCS}}^{\text{R}}(E - eV) & e^{-ieVT} \underline{f}_{\text{BCS}}(E) \\ e^{ieVT} \underline{f}_{\text{BCS}}(E) & -\underline{g}_{\text{BCS}}^{\text{R}}(E + eV) \end{pmatrix} \quad (12.126)$$

and the distribution function matrix

$$\hat{h}' = \begin{pmatrix} \tanh[\beta(E - eV/2)/2] \hat{1} & \hat{0} \\ \hat{0} & \tanh[\beta(E + eV/2)] \hat{1} \end{pmatrix}. \quad (12.127)$$

Screening of electric fields in superconductors

Magnetostatic fields are screened over penetration depth λ in superconductors due to Meissner effect. But what about electrostatic fields? An electric field is screened over the Thomas-Fermi length in a normal metal, which is extremely short (order Angstrom) since the charge carrier density is high enough to recombine efficiently. Same is true in metallic superconductors: a longitudinal electrostatic field applied to a superconductor should be screened over Thomas-Fermi [see Phys. Rev. B 65, 144511 (2002) and <https://iopscience.iop.org/article/10.1088/1674-1056/27/5/057401/pdf>]. There is some controversy to this in light of the recent gate-voltage experiments done on supercurrents by Giazotto *et al.*, but several experiments trying to reproduce their results have failed, which seems to confirm that it is the Thomas-Fermi length which is the relevant one. Note that when a current is injected into a superconductor via an electric field in an adjacent normal metal, the electric field can penetrate a very long distance due to charge imbalance.

12.15 Triplet Cooper pairs

The two electrons of the Cooper pair need not necessarily form a singlet pair, they can also pair in a triplet state. This is consistent with the Pauli principle. The triplet states are $(\uparrow\downarrow + \downarrow\uparrow)/\sqrt{2}$, $\uparrow\uparrow$, $\downarrow\downarrow$ and all have $S = 1$. Their respective quantum numbers for the spin projection along the quantization axis are $S_z = 0, S_z = +1, S_z = -1$. Recall that the quantization axis is defined as the axis for which the basis states one uses are eigenstates of the corresponding component of the spin-operator.

A common misconception is that the $\sigma\sigma$ triplet states have parallel spins. Actually, only their component along the quantization axis (usually taken as z) is the same: the two spins of the electrons form an angle between each other in plane perpendicular to the quantization axis. In contrast, the spins of the electrons in the Cooper pair are completely antiparallel in the singlet state.

To see this, we can compute the expectation value of the dot product between the two spins $\mathbf{S}_1$ and $\mathbf{S}_2$ of the electrons. We set $\hbar = 1$ for brevity of notation. We know that $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ and $S = 1$ for a triplet state, $S = 0$ for a singlet state, while $S_1 = S_2 = \frac{1}{2}$. The expectation value $\langle \mathbf{S}^2 \rangle = S(S+1)$. Since

$$\mathbf{S}^2 = \mathbf{S}_1^2 + \mathbf{S}_2^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 \quad (12.128)$$

we can write:

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \langle (\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2)/2 \rangle. \quad (12.129)$$

For the singlet state, we thus obtain

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 0 - 3/4 = -3/4. \quad (12.130)$$

It is clear that $\mathbf{S}_1 \parallel -\mathbf{S}_2$. For the triplet state, we instead obtain

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = (2 - 3/4 - 3/4)/2 = 1/4. \quad (12.131)$$

This corresponds to an angle ϕ between the spins determined by $3/4 \cos \phi = 1/4$ so that $\phi \simeq 70.5^\circ$.

12.15.1 Spin and angular momentum properties of triplet Cooper pairs

These properties are conveniently described using the $\mathbf{d}_{\mathbf{k}}$ -vector formalism that is described in detail in Leggett RMP 1975 and also with some details and worked examples in Maeno RMP 2003.

The spin expectation value of a superconducting state described by a $\mathbf{d}_{\mathbf{k}}$ -vector is given by:

$$\langle \mathbf{S}_{\mathbf{k}} \rangle = i\mathbf{d}_{\mathbf{k}} \times \mathbf{d}_{\mathbf{k}}^* \quad (12.132)$$

whereas the relative angular momentum of the electrons in the Cooper pair is given by eq. 7.48 in Leggett RMP 1975 (it is also derived there):

$$\langle \mathbf{L} \rangle \propto -i\hbar \sum_j \int \frac{d\Omega_{\mathbf{k}}}{4\pi} (\mathbf{d}_{\mathbf{k}})_j^* (\mathbf{k} \times \nabla_{\mathbf{k}}) (\mathbf{d}_{\mathbf{k}})_j \quad (12.133)$$

where $(\mathbf{d}_{\mathbf{k}})_j$ is the j 'th component of the $\mathbf{d}_{\mathbf{k}}$ vector:

$$\mathbf{d}_{\mathbf{k}} = \left(\frac{\Delta_{\downarrow} - \Delta_{\uparrow}}{2}, \frac{-i(\Delta_{\downarrow} + \Delta_{\uparrow})}{2}, \Delta_z \right) \quad (12.134)$$

with $\Delta_z = \frac{1}{2}(\Delta_{\uparrow\downarrow} + \Delta_{\downarrow\uparrow})$.

12.16 Cooper pairs and quasiparticles

There are several good textbooks (Abrikosov or Tinkham) which treat the Cooper pair instability in detail, and we will therefore not cover it here. We just caution that the treatment of the BCS theory varies surprisingly much both in quality and with regard to which conclusions that one arrives at as one considers different textbooks or lecture notes. It is thus important to not oversimplify the problem and make too general statements.

12.16.1 Binding energy of Cooper pair

The essence of the Cooper pair instability is that if one considers a normal-state Fermi sea which is completely filled at $T = 0$, and then add two extra electrons right above E_F which interact attractively, they form a bound state which has a net energy that is lower than $2E_F$. The binding energy may be written as 2Δ , as we will later connect it to the superconducting energy gap Δ separating the condensate from single-particle excitations.

12.16.2 All excitations cost energy, including holes

Keep in mind that both electron excitations and hole excitations in the normal-state cost energy. Creating a hole (i.e. removing an electron) from a state $k < k_F$ (below the Fermi energy) costs energy! How can this be? First, consider an electron excitation ...

We can also formalize this argument mathematically by defining an operator d_k which has the following properties: $d_k = c_k^\dagger$ if $k > k_F$ while $d_k = c_k$ if $k < k_F$. In this way, d_k represents an excitation operator because regardless of what k is, it creates an excitation: either an electron above k_F or a hole below k_F . Now, the total energy of the normal-state is

$$H = \sum_k (\varepsilon_k - \mu) c_k^\dagger c_k \quad (12.135)$$

We can rewrite this in terms of the d_k operator as follows: ...

$$\begin{aligned} H &= \dots \\ &= \dots + \sum_k |\varepsilon_k - \mu| d_k^\dagger d_k. \end{aligned} \quad (12.136)$$

This expression makes it clear that whether we create an electron or hole excitation, there is a positive energy cost associated with it, namely $|\varepsilon_k - \mu|$.

Turning our attention to the superconducting state, we know that a standard diagonalization of the BCS Hamiltonian in the mean-field approximation provides the energy eigenvalues (let $\xi_k \equiv \varepsilon_k - \mu$)

$$E_k = \sqrt{\xi_k^2 + \Delta^2} > 0. \quad (12.137)$$

As in the normal-state, excitations cost energy. The single-particle excitations are separated from the condensate of Cooper pairs by a gap Δ . It is conceptually important to realize that it thus costs an energy Δ to add a single, unpaired quasiparticle to the superconductor - in contrast, breaking

up an existing Cooper pair costs an energy 2Δ because both electrons of the Cooper pair must be excited to quasiparticle states. The binding energy is thus 2Δ whereas the single-particle energy gap is Δ .

12.16.3 Deriving the density of states for electrons in a superconductor

We can also make a statement about what the density of states for single-electron excitations is in the superconducting state. The number of available single-particle states in $\mathbf{k}$ -space cannot change even after the superconducting phase transition - they are just shifted to different energies. One way to understand this heuristically is to conduct a thought-experiment where all the Cooper pair electrons are excited into single-particle states. Since the number of electrons in a material doesn't change upon a phase-transition, it means that the same number of states must be available before and after the transition to fit the electrons into. We have

$$\int N(\xi_k) d\xi_k = \int N_S(E) dE \rightarrow N_S(E) = N(\xi_k) \frac{d\xi_k}{dE} \quad (12.138)$$

One thus arrives at

$$N_S(E) = \frac{E}{\sqrt{E^2 - \Delta^2}}. \quad (12.139)$$

We emphasize at this point that this derivation does not say something about *which single-particle states* that are actually occupied in the normal and superconducting states. In the normal state, all states up to E_F are filled before the transition. At $T = 0$, in the superconducting state, there are no single-particle excitations and only Cooper pairs exist. Therefore, the above argument just provides us a mean to calculate the available density of states, but that does not mean that single-electrons reside in them at a given temperature (and as we have just argued, none do at $T = 0$).

12.16.4 Where do the Cooper pairs live?

We established in the section above that there is an excitation gap Δ from the condensate up to the lowest-lying available single-particle state. It is tempting to state that this means that the Cooper pairs thus live at the normal-state Fermi energy E_F , since the excitation spectrum then reduces to the correct result in the limit $\Delta \rightarrow 0$. However, this seems at odds with the idea that electrons interacting attractively should reduce their energy compared to the normal-state Fermi level, thus causing the instability of the Fermi sea. Therefore, it seems more likely that the energy where the Cooper pairs reside should be somewhere below E_F , and that this energy gradually moves toward E_F as Δ is reduced with temperature.

For a bulk superconductor, it is not important exactly where the Cooper pairs reside: the only that that matters is that there is a single-particle excitation gap Δ and a binding energy 2Δ required to break a Cooper pair. For book-keeping purposes, one might then well say that the condensate resides at E_F . However, the issue becomes relevant again when considering heterostructures, such as an NS bilayer. Giaever showed in his Nobel-prized awarded and pioneering experimental work that tunneling only takes place when the applied voltage exceeds Δ . This clearly proves that the *condensate has to reside at the Fermi level of the N side* which is calibrated during the transient tunneling taking place when equilibrium is established between the two materials. This explains why the Cooper pairs are pictured at the normal-state Fermi level in the BTK treatment.

12.16.5 Excitation picture and semiconductor picture of a superconductor

When considering plots of the density of states in a superconductor, one typically presents a curve that is symmetric around $E = 0$. Are there available states below the condensate for negative energies $E < 0$? Are all these single-particle states (which are a mix of electron- and hole-states) then filled at $T = 0$? See also chapter 6 in [69] for a detailed description.

The answer is that it depends on which picture, out of several equivalent ones, that we use: the excitation picture or the semiconductor picture of a superconductor. Consider for simplicity $T = 0$. In the excitation picture, we know that the BCS ground state is described by that no excitations with positive energy $E > 0$ exist. However, we could rewrite the BCS Hamiltonian from

$$H = \text{constant} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \gamma_{\mathbf{k}\sigma}^{\dagger} \gamma_{\mathbf{k}\sigma} \quad (12.140)$$

where $E_{\mathbf{k}} > 0$ is the excitation energy and

$$\gamma_{\mathbf{k}\sigma}^{\dagger} = u_{\mathbf{k}}^* c_{\mathbf{k}\sigma}^{\dagger} - \sigma v_{\mathbf{k}}^* e^{-i\phi} c_{-\mathbf{k},-\sigma}, \quad (12.141)$$

to a form

$$H = \text{new constant} + \sum_{\mathbf{k}} (E_{\mathbf{k}} \gamma_{\mathbf{k},+}^{\dagger} \gamma_{\mathbf{k},+} - E_{\mathbf{k}} \eta_{\mathbf{k},+}^{\dagger} \eta_{\mathbf{k},+}) \quad (12.142)$$

where $\eta_{\mathbf{k},+} \equiv \gamma_{\mathbf{k},\downarrow}^{\dagger}$. This is similar to how we could rewrite a free electron gas Hamiltonian to an electron part and a hole part by defining a hole operator $h \equiv c^{\dagger}$ for one of the spin species. In effect, we have above traded the spin degree of freedom for an electron/hole degree of freedom.

The BCS ground-state is of course exactly the same, but its definition is no longer that there are no quasiparticles (which is *different* from no *excitations*). Instead, in the new form of the Hamiltonian operator, it is clear that all states created by $\eta_{\mathbf{k},+}^{\dagger}$ are filled at $T = 0$. In effect, there is a band of negative energies filled in the BCS ground-state. The quasiparticles in this band are part electrons, part holes.

The latter is the so-called semiconductor model of a superconductor where we have a mirrored band structure around the normal-state Fermi level. In this case, it is clear that we have an electron density of states for $E < 0$. In the excitation picture, only the excitation density of states is available. Again, this is similar to how we can rewrite the Hamiltonian $H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$ for a free electron gas, where $\epsilon_{\mathbf{k}}$ can be both positive and negative, to be expressed solely in terms of *excitations*. The filled electrons below the Fermi level are still there in the excitation picture, but are expressed in terms of hole excitations instead. Note that in both pictures, there is a constant term in the Hamiltonian describing the condensation energy, but this constant energy is different in the two pictures.

Tunneling in the two pictures

The physical picture for tunneling between a superconductor and a normal metal is as follows in the semiconductor picture in the tunneling limit (disregarding Andreev reflection here, but this can be incorporated using the BTK formalism). We have filled negative energy states $E < 0$, and empty positive energy states $E > 0$. Tunneling occurs when $eV > \Delta$ or $eV < -\Delta$. In the case where $eV > \Delta$, electrons can tunnel between available states in the N part and the allowed

single-particle band in the superconductor. Note that the charge carried by the electron added to the superconductor from the normal metal (as a linear combination of quasiparticles, which are the long-lived excitations in a superconductor) at $eV > \Delta$ enters as a charge imbalance which relaxes to charge carried by a supercurrent (Cooper pairs) over a distance of the charge relaxation length (see discussion Tinkham, 2nd edition, section 11.5).

For $eV < -\Delta$, a filled quasiparticle from the $E < 0$ band in the superconductor instead can tunnel over to an available state in the normal metal. So the current changes sign compared to $eV > \Delta$. The lost quasiparticle again is manifested in the superconductor in the form of charge imbalance which relaxes to charge carried by a supercurrent. Thus, if we send in a current from the superconductor toward a normal metal, the supercurrent should be converted to a charge imbalance near the interface and causes tunneling as a single-particle from the $E < 0$ band over to the normal metal. Note how the semiconductor band structure and density of states smoothly joins up with the normal-state band structure and density of states when $\Delta \rightarrow 0$. Note how the condensate of Cooper pairs does not have to be involved in the description of tunneling in the semiconductor picture, at least prior to the charge imbalance decay.

Instead, in the *excitation picture*, particle transitions under transport are not purely horizontal in the energy band diagram. It is nevertheless a physically equivalent way of describing transport between a superconductor and another material. For $eV < -\Delta$, what happens in the excitation picture is that a Cooper pair breaks up so that one electron tunnels into the normal metal at an energy $E = eV$ (below $-\Delta$) whereas the other electron in the Cooper pair enters an excited state in the superconductor at $E = -eV$ (above Δ). The transitions are thus not horizontal in the band diagram. In this way, energy is still conserved since the Cooper pair starts out with $E = 0$. The incoming supercurrent from the S side carries a charge $-2e$ and only $-e$ is transferred. The excited electron remaining on the S side accounts for the missing current, because this excitation will ultimately be converted back into a supercurrent flowing back into the superconductor. This happens because of charge imbalance decay and gives rise to a supercurrent carried by half a Cooper pair, so that there is a net supercurrent carrying charge $-e$ moving toward the interface. The point is now that this is formally equivalent to describing tunneling from a single-particle density of states at $E < -\Delta$, at least as far as the charge transport across the interface is concerned, as is the case in the semiconductor picture. For instance, the quasiparticle tunneling from the $E < 0$ band into the normal metal in the semiconductor picture, thus leaving an empty state in the $E < 0$ band, corresponds precisely to an excitation in the $E > 0$ band in the excitation picture. Note how the condensate of Cooper pairs has to be involved to describe tunneling in the excitation picture for voltages less than $-\Delta$, even prior to considering charge imbalance decay.

The above explanation in the *excitation picture* also holds in the event of a spin-split superconductor where spin- $\uparrow$ particles are shifted with energy $-\hbar$ and spin- $\downarrow$ particles are shifted with energy $+\hbar$. In this case, tunneling should set in already at $eV = -\Delta + \hbar$. What happens physically is that the spin- $\downarrow$ electron in the Cooper pair tunnels into N at $E = -\Delta + \hbar$ whereas the spin- $\uparrow$ electron becomes an excited state in S at the allowed band $E = \Delta - \hbar$. In this way, energy is again conserved and the process is equivalent to the semiconductor model with a valence band for spin- $\downarrow$ commencing at $E = -\Delta + \hbar$ (consistent with the fact that it is a spin- $\downarrow$ electron which tunnels into N).

Mathematically, the excitation picture tunneling can be described in terms of modified quasiparticle operators in the superconductor which take into account creation and destruction of Cooper pairs.

Whereas the $\gamma_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ operators above correspond to the usual fractional charge quasiparticle operators in a superconductor, one may instead define modified operators according to

$$c_{\mathbf{k}\sigma} = u_{\mathbf{k}}^* \tilde{\gamma}_{\mathbf{k}\sigma}^\dagger + v_{\mathbf{k}} S^\dagger \tilde{\gamma}_{-\mathbf{k}, -\sigma}. \quad (12.143)$$

Here, c is the usual electron annihilation operator whereas $S, S^\dagger$ annihilate/create a Cooper pair. In this way, one sees that the $\tilde{\gamma}$ operators annihilate *electrons* rather than fractional charge quasiparticles in the superconductor. This is true since creating a Cooper pair and removing an electron is the same as creating an electron. A standard tunnel Hamiltonian

$$H_T = \sum_{\mathbf{k}\sigma} T d_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \text{h.c.} \quad (12.144)$$

(assuming momentum conserving tunneling for simplicity) where d is the electron on the N side and c is the electron on the S side, can then be written as four different processes [see Jochum *et al.*, J. Appl. Phys. **83**, 3217 (1998)] involving creation/destruction of Cooper pairs and modified quasiparticle operators on the superconducting side corresponding exactly to the physical explanation given above.

Are there electron states at negative energy in a superconductor?

Yes, if one uses a model with a cutoff on the attractive interaction: electron states outside the thin-shell of attractive interaction do not participate in Cooper pairing and thus remain as filled states below the normal-state Fermi level. This is more clearly visualized in the semiconductor picture, just like the presence of filled electron states is more clearly visualized when using the quasiparticle picture rather than excitation picture (electrons and holes) for a normal metal.

12.16.6 A superconductor is not a Fermi liquid

It is important to realize that a superconductor is not a Fermi liquid in the usual sense (although its normal-state can be). One way to see this is that since quasiparticles in a Fermi liquid must be perturbatively connected to the non-interacting electrons, the superconducting state does not fit the bill since the superconducting state cannot be obtained via perturbation theory (singular perturbation). Moreover, a superconductor does not have a well-defined Fermi surface with a sharp drop of the single-particle occupancy at $T = 0$: there is no quasiparticle residue Z_k in the Green function for the electrons in the superconducting state, which mathematically proves that the superconducting state is not a Fermi liquid.

A free-electron Green function can be written as

$$G_0(\mathbf{k}, \omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} \quad (12.145)$$

where ω is the frequency (electron energy) and $\delta_{\mathbf{k}}$ is an infinitesimal number the inverse lifetime of the quasiparticle. In a Fermi liquid, where the electrons have been 'dressed' by interactions described by the one-particle irreducible self-energy $\Sigma_{\mathbf{k}}$, the electron Green function takes the form

$$G(\mathbf{k}, \omega) = \frac{Z_{\mathbf{k}}}{\omega - \tilde{\varepsilon}_{\mathbf{k}} + i\tau_{\mathbf{k}}}. \quad (12.146)$$

Here, the effect of the self-energy is twofold. On the one hand, it renormalizes the normal-state dispersion according to the self-consistency equation

$$\tilde{\varepsilon}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} + \text{Re}\{\Sigma(\mathbf{k}, \tilde{\varepsilon}_{\mathbf{k}})\}, \quad (12.147)$$

and it also renormalizes the lifetime so that

$$1/\tau_{\mathbf{k}} = \text{Im}\{\Sigma(\mathbf{k}, \tilde{\varepsilon}_{\mathbf{k}})\}. \quad (12.148)$$

Can we write the Green function for the original electron excitations in the same way as Eq. (12.146) in the superconducting state? It is well-known that in the superconducting state, one finds

$$G(\mathbf{k}, \omega) \propto \frac{\omega + \varepsilon_{\mathbf{k}}}{\omega^2 - \varepsilon_{\mathbf{k}}^2 - \Delta^2}, \quad (12.149)$$

clearly showing that there is no resemblance left between the original excitations and the electrons in the superconducting state.

We thus reiterate that quasiparticles in a superconductor are not quasiparticles in the sense of Landau Fermi liquid theory, since the superconducting ground state does not connect adiabatically to the Fermi sea state.

12.16.7 Why are quasiparticles in superconductors partially electrons and holes?

In a superconductor, a Cooper pair consists of two bound electrons. Breaking up a Cooper pair gives an excited state in the system, but shouldn't the excitation then be an electron? Instead, we know that the quasiparticles in superconductors are partially electrons and holes. Taking into account our above discussion of the normal metal case as a preliminary, this can now be understood after realizing one extra piece of information. Namely, there is no Fermi surface in the superconducting state. BCS theory shows that the probability that the pair of states $(k, -k)$ are occupied by a Cooper pair is $v_k^2 = \frac{1}{2}(1 - \xi_k/E_k)$ where $\xi_k = k^2/2m - \mu$ where μ is the *normal-state* Fermi level and $E_k = \sqrt{\xi_k^2 + \Delta^2}$. For instance, at $k = k_F$ we have a 50% chance of $(k, -k)$ being occupied by a Cooper pair. Therefore, unlike the normal metal case, in a superconductor some states $k < k_F$ *remain empty* even in the $T = 0$ ground-state. This means that it is possible to create an electron-like excitation in the superconductor even at $k < k_F$ at $T = 0$, unlike the normal metal case.

We are now interested in saying something about the nature of the elementary excitation above the superconducting ground-state: creating a quasiparticle by breaking a Cooper pair such that one of the electrons are missing. A Cooper pair has two electrons at k and $-k$, respectively. Consider the superconducting ground-state. We now want to consider an excitation consisting of the state k being occupied while $-k$ is empty, corresponding to an incomplete Cooper pair. Strictly speaking, to break the pair we have to excite both electrons in the pair to quasiparticles since there are no single-electron states available at the Fermi level. However, to understand why the excitation of these electrons in the pair are part electron, part hole, it is sufficient to consider just the excitation of one such electron to begin with.

The key to understanding why this excitation is partly electron and partly hole is that this scenario can be achieved in *two ways*. First, consider the case where we add an extra electron to the superconductor in an empty state k while the state $-k$ remains empty. We know from the discussion above that we can do this both for $k < k_F$ and $k > k_F$. Adding an electron in this way clearly corresponds to an electron-like excitation.

But we can achieve k being occupied and $-k$ being empty in a different way. Consider again the superconducting ground-state and now remove an electron from the $-k$ state of a Cooper pair, such

that an uncoupled electron remains at state k . We know that removing an electron from $-k$ will correspond to a hole excitation with momentum k . Note that this hole can again have both $k < k_F$ or $k > k_F$ since there is no Fermi surface in the superconducting state.

We have now accomplished the following. The excitation of the superconducting state corresponding to an incomplete Cooper pair (occupied k , empty $-k$) can be achieved by creating an electron excitation *or* a hole excitation. Therefore, it makes sense that the excitation in total acts partly as electron and partly as a hole. The weight of the electron- and hole-like character is determined by how the precise value of k , since this dictates the value of the coherence factors u_k and v_k that map the original electrons and holes ($c^\dagger$ and c) to the quasiparticles ($\gamma^\dagger$ and γ) in the superconducting state.

12.16.8 Are all electrons in a superconductor part of Cooper pairs at zero temperature?

The answer is no. A passage from the textbook by Rose-Innes, given below, gives a good qualitative explanation. To understand the passage, recall that in the Cooper pair problem of two attractively interacting electrons with $\mathbf{k} > \mathbf{k}_F$, the kinetic energy is raised compared to the normal-state ground state since we have added electrons above the Fermi level, but this kinetic energy gain is outweighed by the gain in potential energy from their interaction. This suggests that the Fermi level might self-destruct as a pair of electrons at (or slightly above) the Fermi level would pair up, thus reducing the Fermi level.

'One might at first think that there is no limit to the number of electrons which may be raised from $\mathbf{k} < \mathbf{k}_F$ to form Cooper pairs with a resultant lowering of the total energy, so that we should end up with all the electrons having $\mathbf{k} > \mathbf{k}_F$. This, however, is clearly absurd, and the reason why is not hard to find. In order that a pair of electrons may be scattered from $(\mathbf{k}_i \uparrow, -\mathbf{k}_i \downarrow)$ to $(\mathbf{k}_j \uparrow, -\mathbf{k}_j \downarrow)$ the states $(\mathbf{k}_i \uparrow, -\mathbf{k}_i \downarrow)$ must first be occupied and the states $(\mathbf{k}_j \uparrow, -\mathbf{k}_j \downarrow)$ must be empty. As more and more electrons form Cooper pairs with $\mathbf{k} > \mathbf{k}_F$ the chance of finding the states $(\mathbf{k}_j \uparrow, -\mathbf{k}_j \downarrow)$ empty becomes progressively smaller and smaller, so the number of scattering processes which may take place is reduced, with a consequent decrease in the magnitude of the negative potential energy. Eventually a condition is reached in which the lowering of the potential energy is insufficient to outweigh the increase in the kinetic energy, and it is no longer possible to lower the total energy of the electrons by forming Cooper pairs. There will be an optimum arrangement which gives the lowest overall energy, and this arrangement can be described by specifying the probability $v_{\mathbf{k}}^2$ of the pair state $(\mathbf{k}_i \uparrow, -\mathbf{k}_i \downarrow)$ being occupied in the wavefunction ψ_{BCS} .'

In fact, at zero temperature not all of the electrons in the BCS ground state (GS) form Cooper pairs. This can be seen in the BCS model from the fact that the attractive interaction only exists within a thin-shell of the normal-state Fermi level, so that $\Delta_{\mathbf{k}} = 0$ far away from $\mathbf{k} = \mathbf{k}_F$. One way to think about this is that deep inside the Fermi surface, there is no available states for scattering events, including the phonon-mediated ones, and thus there is no effective attraction to form the Cooper pairs. For the same reason, the single electrons occupying states deep inside the Fermi surface do not carry any resistive current, since an electric field cannot displace them to higher energy levels: the Pauli-principle prevents them from moving.

The fact that all electrons in a superconductor at $T = 0$ are not in Cooper pairs can also be seen from the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in the postulated BCS GS given in the original post. When $\mathbf{k}$ is

far below the Fermi surface, then $|\xi_{\mathbf{k}}| \gg \Delta$ with $\xi_{\mathbf{k}} < 0$. In this case, $u_{\mathbf{k}} \rightarrow 0$ and $v_{\mathbf{k}} \rightarrow 1$. This means that the states far below the Fermi surface are almost fully occupied by electrons created by $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$. These electrons are created in pairs, but the key point is that *they are not Cooper pairs*. We emphasized this in a previous section as well. Namely, the pair creation operator does not tell us anything regarding whether the pair is a Cooper or just a normal pair. Only when it is close to the Fermi surface, and thus possible to have phonon-mediated scattering (modelled in BCS theory by saying that $\xi_{\mathbf{k}}$ has to lie within a thin shell around the normal-state Fermi level), may we interpret $v_{\mathbf{k}}^2$ as the Cooper pair probability.

In summary, the BCS GS looks like the following: deep down inside the Fermi surface, it consists of normal electrons despite the fact that $v_{\mathbf{k}}^2 = 1$. Close to the Fermi surface, it is a superposition of an empty state, with probability amplitude $u_{\mathbf{k}}^2$, and occupied Cooper pairs at $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$, with amplitude $v_{\mathbf{k}}^2$, as expressed by $|\psi_{\text{BCS}}\rangle$. The fact that not all electrons are in Cooper pairs in the ground-state is still consistent with the BCS wavefunction since there are no *excitations* in the system (filled single-electron states for momenta well below the Fermi level are not excitations).

12.17 BCS wavefunction and uncertainty in N and ϕ

12.17.1 BCS wavefunction as quasiparticle vacuum

The groundstate of a superconductor is a state where only Cooper pairs exist and no quasiparticles. We can construct such a state $|\Phi_{\text{BCS}}\rangle$ by noting that when any quasiparticle operator $\gamma_{\mathbf{k}\sigma}$ acts on it, it should produce zero since no quasiparticles are available to annihilate. This is ensured if we choose

$$|\psi_{\text{BCS}}\rangle \propto \prod_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma} |0\rangle \quad (12.150)$$

as the BCS groundstate where $|0\rangle$ denotes bare vacuum (a state which is annihilated by any $c_{\mathbf{k}\sigma}$ operator). We see that $\gamma_{\mathbf{k}\sigma} |\psi_{\text{BCS}}\rangle = 0$ is satisfied for any $(\mathbf{k}, \sigma)$ since $\gamma_{\mathbf{k}\sigma}^2 = 0$.

Having established the BCS groundstate is an important step since it allows us to evaluate expectation values for any combination of γ and $\gamma^\dagger$ operators (or even c and $c^\dagger$ operators by using the transformation between them), which can be of relevance with regard to *e.g.* evaluation of Green functions.

Let us derive $|\psi_{\text{BCS}}\rangle$ in detail by using that the quasiparticle fermion operators that diagonalize the Hamiltonian are expressed via the normal electrons as

$$\gamma_{\mathbf{k}\sigma}^\dagger = u_{\mathbf{k}}^* c_{\mathbf{k}\sigma}^\dagger - \sigma v_{\mathbf{k}}^* e^{-i\phi} c_{-\mathbf{k}, -\sigma}. \quad (12.151)$$

For simplicity, let us begin with a wavefunction containing just two factors from Eq. (12.150). For instance, we see that

$$\gamma_{\mathbf{k}\uparrow} \gamma_{-\mathbf{k}\downarrow} |0\rangle = v_{\mathbf{k}} e^{i\phi} (u_{\mathbf{k}} + v_{\mathbf{k}} e^{i\phi} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle. \quad (12.152)$$

Now, taking the product over all $\mathbf{k}$ -values, which are both positive and negative, on both sides of this equation, we obtain

$$\prod_{\mathbf{k}} (\gamma_{\mathbf{k}\uparrow} \gamma_{-\mathbf{k}\downarrow} |0\rangle) = \prod_{\mathbf{k}} v_{\mathbf{k}} \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} e^{i\phi} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle \propto \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} e^{i\phi} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle \quad (12.153)$$

This verifies Eq. (12.150). To make the wavefunction normalized, one can verify that omitting the proportionality constant $\prod_{\mathbf{k}} v_{\mathbf{k}}$ achieves this goal. We thus arrive at the normalized ground-state wavefunction which BCS used:

$$|\psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} e^{i\phi} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}) |0\rangle = (u_{\mathbf{k}_1} + v_{\mathbf{k}_1} e^{i\phi} c_{\mathbf{k}_1\uparrow}^{\dagger} c_{-\mathbf{k}_1\downarrow}^{\dagger}) (u_{\mathbf{k}_2} + v_{\mathbf{k}_2} e^{i\phi} c_{\mathbf{k}_2\uparrow}^{\dagger} c_{-\mathbf{k}_2\downarrow}^{\dagger}) \dots |0\rangle. \quad (12.154)$$

where ϕ is the phase of the superconducting mean-field order parameter $\Delta = |\Delta|e^{i\phi}$. This form shows that the probability of the states $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ being occupied by a Cooper pair is $|v_{\mathbf{k}}|^2$ whereas the probability that it is empty is $|u_{\mathbf{k}}|^2$. This is consistent with the fact that $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$. Strictly speaking, since the gap $\Delta_{\mathbf{k}}$ vanishes when outside the thin-shell given by the Debye frequency, we should remove the phase $e^{i\phi}$ for such $\mathbf{k}$ -vectors while $v_{\mathbf{k}} \rightarrow 1$ now means that the electron pair states are occupied, but as single-particles and not as part of a Cooper pair.

We can make a connection between the BCS ground-state wavefunction $|\psi_N\rangle$ and a general N -electron wavefunction expressed in terms of momentum eigenfunctions and with Cooper pairing built in. Such a wavefunction will in its general form look like:

$$|\psi_N\rangle = \sum g(\mathbf{k}_i, \dots, \mathbf{k}_l) c_{\mathbf{k}_i\uparrow}^{\dagger} c_{-\mathbf{k}_i\downarrow}^{\dagger} \dots c_{\mathbf{k}_l\uparrow}^{\dagger} c_{-\mathbf{k}_l\downarrow}^{\dagger} |0\rangle. \quad (12.155)$$

Here, $\mathbf{k}_i$ and $\mathbf{k}_l$ denote the first and last of the $\mathbf{k}$ -values in the band which are occupied by Cooper pairs in a given term of the sum. The sum itself goes over all possible combinations of $N/2$ momenta $\{\mathbf{k}_i, \dots, \mathbf{k}_l\}$ that are part of the $M > N/2$ total available $\mathbf{k}$ -values. There are $N/2$ momenta involved since for N particles there are $N/2$ Cooper pairs. The factor g specifies the weight with which the product of this set of $N/2$ pairs of creation operators appear. The maximum total number of electrons is $2M$ since there are M possible $\mathbf{k}$ -values and a spin degeneracy of 2.

The connection is now it is seen from the expressions for $|\psi_{\text{BCS}}\rangle$ and $|\psi_N\rangle$ that $|\psi_{\text{BCS}}\rangle$ can be expanded precisely in terms of these fixed- N particle wavefunctions as

$$|\psi_{\text{BCS}}\rangle = \sum_N \lambda_N |\psi_N\rangle \quad (12.156)$$

where each $|\psi_N\rangle$ then contains $N/2$ Cooper pairs (the precise form of λ_N is not important here). If all $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are finite, there is a finite probability of the BCS wavefunction containing any number of pairs ranging from 0 to M , i.e. N ranging from 0 to $2M$. Clearly, $|\psi_{\text{BCS}}\rangle$ is not an eigenstate of the number operator $\hat{N}$. Instead, the BCS wavefunction is then a superposition of states with different numbers of Cooper pairs. However, the expectation value for the number operator is sharply peaked around the value

$$\langle \hat{N} \rangle = \langle \psi_{\text{BCS}} | \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} | \psi_{\text{BCS}} \rangle = \sum_{\mathbf{k}} 2|v_{\mathbf{k}}|^2. \quad (12.157)$$

A proof is found in the book by Tinkham on pages 50 and 51, but the above expression makes sense in light of the interpretation of $|v_{\mathbf{k}}|^2$ as the probability of the pair state $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ being occupied by a Cooper pair. As will be discussed in the next section, we have to be careful with this statement when taking the normal-state limit $\Delta \rightarrow 0$.

The ground-state energy of the BCS wavefunction can also be computed (see pages 54-57 Tinkham), and one obtains

$$\langle \psi_{\text{BCS}} | H | \psi_{\text{BCS}} \rangle = \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - \frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}} \right) - \frac{\Delta^2}{V} \quad (12.158)$$

where V is the attractive interaction and we used

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} (\Delta c_{\mathbf{k}\sigma}^\dagger c_{-\mathbf{k},-\sigma}^\dagger + \text{h.c.}) \quad (12.159)$$

and $\xi_{\mathbf{k}} = \mathbf{k}^2/2m - \mu$.

12.17.2 Obtaining the normal-state limit from the BCS wavefunction

Some care has to be exercised when taking the $\Delta \rightarrow 0$ limit for the BCS wavefunction and its ground-state energy. First of all, we see that in the limit $\Delta \rightarrow 0$, we get:

$$u_{\mathbf{k}} = \begin{cases} 1 & \text{if } \xi_{\mathbf{k}} > 0 \\ 0 & \text{if } \xi_{\mathbf{k}} < 0 \end{cases}, \quad (12.160)$$

where the sign of $\xi_{\mathbf{k}}$ is determined by whether $\mathbf{k} < \mathbf{k}_F$ or $\mathbf{k} > \mathbf{k}_F$, while:

$$v_{\mathbf{k}} = \begin{cases} 0 & \text{if } \xi_{\mathbf{k}} > 0 \\ 1 & \text{if } \xi_{\mathbf{k}} < 0 \end{cases}. \quad (12.161)$$

We emphasize here that $v_{\mathbf{k}}$ does therefore not go to zero in the normal-state limit $\Delta \rightarrow 0$, as it is defined here. This is in contrast to the BTK coherence factors u and v which are defined as $u^2 = \sqrt{(1 + \sqrt{E^2 - \Delta^2}/E)}/2$ and $v^2 = \sqrt{(1 - \sqrt{E^2 - \Delta^2}/E)}/2$ under the assumption that $E \geq 0$. For these factors, we indeed have $u = 1$ and $v = 0$ for $\Delta \rightarrow 0$, but then again these are defined differently than our quantities $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ above.

The above definition of $v_{\mathbf{k}} \neq 0$ for all $\mathbf{k}$ when $\Delta \rightarrow 0$ makes sense in light of the fact that we should be able to describe hole-excitations even in the normal state of the system. The diagonalized quasiparticle operators $\gamma_{\mathbf{k}\sigma}$ are seen from Eq. (12.151) to satisfy

$$\gamma_{\mathbf{k}\sigma} = \begin{cases} c_{\mathbf{k}\sigma} & \text{if } \xi_{\mathbf{k}} > 0 \\ c_{-\mathbf{k},-\sigma}^\dagger & \text{if } \xi_{\mathbf{k}} < 0 \end{cases}. \quad (12.162)$$

when $\Delta \rightarrow 0$. Hence, the Bogoliubov quasiparticles are in the normal-state electrons for energies $\xi_{\mathbf{k}} > 0$ whereas they are holes for $\xi_{\mathbf{k}} < 0$. Their dispersion is $E_{\mathbf{k}} = |\xi_{\mathbf{k}}|$ since in the superconducting state $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$ is chosen as the positive root. Excitation energies are always positive. So the $\Delta \rightarrow 0$ limit is consistent with the normal-state properties in terms of the excitations of the system.

But now what about the interpretation from the previous section of $v_{\mathbf{k}}^2$ as the probability of a Cooper pair occupation? We note that the BCS wavefunction $|\psi_{\text{BCS}}\rangle$ in the limit $\Delta \rightarrow 0$ reduces to (according to the behavior of u and v):

$$\lim_{\Delta \rightarrow 0} |\psi_{\text{BCS}}\rangle = \prod_{\mathbf{k} > \mathbf{k}_F} |0\rangle \prod_{\mathbf{k} < \mathbf{k}_F} (c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle. \quad (12.163)$$

This makes sense: there are no excitations above the Fermi level at $T = 0$ in a normal metal, and all states are filled below the Fermi surface. These filled states are not, of course, Cooper pairs if $\Delta \rightarrow 0$, but they are nevertheless filled single-particle states.

We also obtain a physically reasonable expression for the ground-state energy of the system in the limit of $\Delta \rightarrow 0$:

$$\lim_{\Delta \rightarrow 0} \langle \psi_{\text{BCS}} | H | \psi_{\text{BCS}} \rangle = \sum_{\mathbf{k} < \mathbf{k}_F} 2\xi_{\mathbf{k}} \quad (12.164)$$

since the terms in the ground-state energy for $\mathbf{k} > \mathbf{k}_F$ give zero contribution due to $E_{\mathbf{k}} = \xi_{\mathbf{k}}$ for such momenta. Thus, the ground-state energy of the normal metal at $T = 0$ is simply the sum over all filled states below the Fermi surface times two due to spin degeneracy.

Summarizing, $v_{\mathbf{k}} \rightarrow 0$ does not go to zero for all momenta in the $\Delta \rightarrow 0$ limit. However, this is consistent since the $v_{\mathbf{k}} \neq 0$ factor correctly describes hole excitations for $\mathbf{k} < \mathbf{k}_F$ in that case. Moreover, the interpretation of $v_{\mathbf{k}}^2$ given previously holds in the superconducting case, but should be modified to the following to be valid in general: $v_{\mathbf{k}}^2$ is the probability that a pair of electron states ($\mathbf{k} \uparrow, -\mathbf{k} \downarrow$) is occupied. In the superconducting state, this is a Cooper pair *if* $\mathbf{k}$ is such that it lies within the thin shell where the attractive interaction exists ($|\xi_{\mathbf{k}}| < \omega_D$). For other $\mathbf{k}$ in the superconducting state, *e.g.* deep below the Fermi level, we have $v_{\mathbf{k}}^2 = 1$ as it just describes a pair of single, uncorrelated electrons. In the normal-state of the system, we always have $v_{\mathbf{k}}^2 = 1$ for $\mathbf{k} < \mathbf{k}_F$ as all single-particle states are filled, although they are not Cooper pairs.

12.17.3 Uncertainty relation for number of pairs and superconducting phase

A useful connection between the number of electrons N and the superconducting phase ϕ is established by noting that we can project out the contribution from the state $|\psi_N\rangle$ to the total BCS groundstate in Eq. (12.156) by a method invented by P. W. Anderson. First, note that the multiplication over $\mathbf{k}$ in Eq. (12.155) produces a large number of terms which can be grouped as a sum according to Eq. (12.156). The terms corresponding to $N/2$ Cooper pairs, and thus together comprising the $|\psi_N\rangle$ contribution to the sum, are identified by the fact that they have a common phase factor $e^{iN\phi/2}$. We mention that N must be an even number since only pairs are included in the wavefunction. This $|\psi_N\rangle$ can then be projected out by multiplying the BCS ground state by $e^{-iN\phi/2}$ and then integrating over the phase ϕ from 0 to 2π . This procedure will give zero as result except for those terms which have $N/2$ factors of $e^{i\phi}$, corresponding to the creation of $N/2$ pairs. In effect,

$$|\psi_N\rangle = \int_0^{2\pi} \pi_0 d\phi e^{-iN\phi/2} \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} e^{i\phi} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle. \quad (12.165)$$

In effect, by integrating over ϕ so that the superconducting phase is completely uncertain we enforce a precise specification of the number of particles N . Put in other words, a state with a fixed number of Cooper pairs has a contribution from BCS wavefunctions with all possible superconducting phases. On the other hand, for a fixed ϕ we have seen above that the uncertainty ΔN must be large since the BCS wavefunction is a superposition of a large number of states with different amounts of Cooper pairs. This implies that there exists an uncertainty relation between N and ϕ of the form

$$\Delta N \Delta \phi \geq \text{constant}. \quad (12.166)$$

This serves as motivation for treating N and ϕ as canonical variables, although we do not pretend as if we have shown this fact rigorously.

12.17.4 Does BCS theory predict supercurrent and Meissner response?

The BCS theory does a beautiful job in explaining the concept of Cooper pairs and the prediction of an order parameter Δ giving rise to an energy gap $|\Delta|$ in the excitation spectrum and a superconducting phase ϕ which is shared by all Cooper pair-states. However, the BCS wavefunction describes its ground-state and does not immediately explain why the Cooper pairs are capable of carrying a resistanceless current or the Meissner effect in a superconductor, the latter being the most fundamental feature of superconductivity.

However, the BCS theory (developed in 1957) establishes the microscopic origin of the U(1) order parameter field ψ used in the phenomenological Ginzburg-Landau theory (developed in 1950), and the *latter* does explain why a supercurrent can exist. That is, an electric current flowing without any applied voltage and thus without energy loss. In fact, quite generally we have that when a material can be described by a macroscopic order parameter field $\psi = |\psi|e^{i\phi}$ which spontaneously breaks a global U(1) symmetry in a gauge theory, a supercurrent is possible. We proceed to show this.

The free energy of a conventional superconductor can be written in a gauge-invariant way as

$$F[\psi, \mathbf{A}] = \int d\mathbf{r} \left[\alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m} \left| \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right) \psi \right|^2 + \frac{B^2}{2\mu_0} \right] \quad (12.167)$$

Here, $q = -2e$ is the charge of the Cooper pairs in the case where condensate under consideration is a superconductor. The free energy is a functional of the field $\psi = |\psi|e^{i\theta}$ describing the charged condensate and the vector potential $\mathbf{A}$ which gives the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. Note how we have used the minimal coupling in the derivative to make the free energy gauge invariant under a simultaneous gauge-transformation in θ and $\mathbf{A}$. The last term is the energy density of the magnetic field. The free energy above may be written

$$\begin{aligned} F &= \int d\mathbf{r} \left[\alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m} \left(\frac{\hbar}{i} \nabla \psi \right)^* \cdot \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right) \psi + \frac{1}{2m} \left(-q\mathbf{A}\psi \right)^* \cdot \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right) \psi + \frac{B^2}{2\mu_0} \right] \\ &= \int d\mathbf{r} \left[\alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m} \psi^* \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right)^2 \psi + \frac{B^2}{2\mu_0} \right]. \end{aligned} \quad (12.168)$$

Note that we are using the vacuum magnetic permeability μ_0 in the expression for the energy density of $\mathbf{B}$. This might seem strange given that magnetic fields are completely shielded from superconductors, so that the magnetic permeability μ inside a superconducting material is in fact zero. This should give an infinitely high energy cost associated with a magnetic field, i.e. by using $B^2/2\mu$. The reason for why we are using μ_0 above is that the screening of the magnetic field $\mathbf{B}$ inside the superconductor only occurs when the effect of the condensate is taken into account: namely, that it produces screening currents. So in an effective model for the magnetic field alone (without ψ) where the superconductivity is implicitly taken into account, we should have used μ instead of μ_0 in the energy density. Instead, the material itself we are considering may well have μ_0 as its normal-state magnetic permeability and only when solving the Ginzburg-Landau equations (to be derived below) for the spatial dependence of ψ and $\mathbf{A}$, we obtain the screening effect that $\mathbf{B} \rightarrow 0$ inside the superconductor.

We can now derive the two GL equations by minimizing the above free energy with respect to ψ and $\mathbf{A}$. For the former, we get (strictly speaking minimizing wrt. ψ^*):

$$\frac{\delta F}{\delta \psi} = 0 \rightarrow \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right) \psi = 0 \quad (12.169)$$

Minimizing with respect to $\mathbf{A}$, i.e. setting the functional derivative $\delta F/\delta \mathbf{A}$ equal zero. One way to do this is to write $\mathbf{A}(\mathbf{r}) = \mathbf{A}_0(\mathbf{r}) + \mathbf{a}(\mathbf{r})$ to get:

$$F[\psi, \mathbf{A}_0] + \int d\mathbf{r} \left(\left[-\frac{q}{2m} \left(\left[\frac{\hbar}{i} \nabla \psi \right]^* \psi + \psi^* \frac{\hbar}{i} \nabla \psi \right) \cdot \mathbf{a} + \frac{q^2}{m} |\psi|^2 \mathbf{A}_0 \cdot \mathbf{a} + \frac{1}{\mu_0} (\nabla \times \mathbf{B}_0) \cdot \mathbf{a} \right] + \mathcal{O}(\mathbf{a}^2) \right). \quad (12.170)$$

To get this, we used that

$$(\nabla \times \mathbf{A}_0) \cdot (\nabla \times \mathbf{a}) = \mathbf{a} \cdot (\nabla \times \nabla \times \mathbf{A}_0) - \nabla \cdot [(\nabla \times \mathbf{A}_0) \times \mathbf{a}]. \quad (12.171)$$

and set $\mathbf{B}_0 = \nabla \times \mathbf{A}_0$. At the stationary value of F with respect to a variation in the vector potential, the coefficient in front of $\mathbf{a}$ must vanish. Dropping the subscript on $\mathbf{A}_0$, we thus end up with

$$-\frac{iq\hbar}{2m} (\nabla \psi^* \psi - \psi^* \nabla \psi) + \frac{q^2}{m} |\psi|^2 \mathbf{A} + \frac{1}{\mu_0} \nabla \times \mathbf{B} = 0. \quad (12.172)$$

Using Maxwell's equation in the absence of time-dependent electric fields, $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$, we get

$$\mathbf{J} = \frac{iq\hbar}{2m} (\nabla \psi^* \psi - \psi^* \nabla \psi) - \frac{q^2}{m} |\psi|^2 \mathbf{A} \quad (12.173)$$

This shows that a phase-gradient, causing $\nabla \psi \neq 0$, in the order parameter drives the supercurrent.

We see that when a material can be described by a macroscopic order parameter field $\psi = |\psi|e^{i\phi}$ which spontaneously breaks U(1) symmetry, a supercurrent is made possible. This is not the case for an ordinary metal, which cannot be described by a macroscopic wavefunction. While Cooper pair states all have the same quantum mechanical phase ϕ (as evident from the BCS wavefunction), all electron states in a metal do not have the same quantum mechanical phase (as evident by inspecting Bloch wavefunctions).

The Ginzburg-Landau theory was introduced as a phenomenological theory, but it was later shown that it can be derived as a limiting case of Gor'kov theory (which is a microscopic theory).

As for the Meissner effect, it would take ideas developed in the early 1960s by Anderson and Higgs to put this on a firmer basis than the phenomenological theory developed by London and Pippard in the 1930s. More precisely, the Meissner effect also originates from the existence of a charged condensate described by a macroscopic order parameter field ψ which spontaneously breaks U(1) symmetry. The Meissner effect can be shown by considering spontaneous symmetry breaking in a field theory with a gauge field via the Higgs mechanism. Alternatively, one can also microscopically derive the Meissner effect using *e.g.* quasiclassical theory where the inclusion of a magnetic field leads to a supercurrent response $\mathbf{j} \propto \mathbf{A}$ that exists only so long as $\Delta \neq 0$.

12.18 Pairing mechanism for conventional superconductors: phonon exchange

The accepted model for electron attraction in conventional superconductors is through phonon exchange. However, there appears to be a problem with energy conservation related to electron scattering mediated by phonons. Consider two electrons with $+k$ and $-k$ scattering into two

electrons with $+k'$ and $-k'$. The Feynman diagram for this process can be drawn and conservation of 4-momentum at each vertex gives the equations:

$$k - q = k' \text{ and } -k + q = -k'. \quad (12.174)$$

in addition to

$$E(k) = E(k - q) + \omega \text{ and } E(-k) + \omega = E(-k + q). \quad (12.175)$$

The phonon carries momentum q and energy ω whereas the electrons were assumed to have an energy dispersion $E(k)$. The problem here is that if the dispersion relation is symmetric, as is the case *e.g.* for the usual $E(k) = k^2/2m$, the only way to satisfy the above equations is to set $\omega = 0$. This means that there is no energy-transfer between the electrons.

This has catastrophic consequences since the phonon interaction is dwarfed by the Coulomb interaction at $\omega = 0$ and has no way of overcoming it. In other words, if we do a canonical transformation on a Hamiltonian where there is an electron-phonon interaction of the type $\sum_k c_{k+q}^\dagger c_k a_q$, we end up with an effective interaction between the electrons of the type:

$$V_{kk'} = \frac{\omega_q}{[(E_k - E_{k'})^2 - \omega_q^2]} \quad (12.176)$$

where ω_q is the dispersion of the phonon. Here, there is no restriction imposed from the calculation that E_k must equal $E_{k'}$, i.e. energy conservation. However, if we demand it, then only $\omega = E_k - E_{k'} = 0$ is allowed and it seems hopeless to get electron attraction.

On the other hand, if instead of a canonical transformation we use a two-electron perturbation theory approach, energy conservation is enforced. Careful consideration shows that even though we demand energy conservation, $\omega = 0$ is not necessarily required. The reason is as follows. The retarded Green function for a free electron is

$$G^R(\omega, k) = \frac{1}{\omega - E_k + i\delta}. \quad (12.177)$$

It clearly has a pole when $\omega = E_k$. However, $\omega \neq E_k$ is not forbidden: there is still spectral weight of the electron at such frequencies, especially when the inverse lifetime δ grows. Therefore, the inaccuracy in the treatment using the canonical transformation is that we assume that the electron frequency in the Green function must equal its dispersion relation whereas it does not *have to*. This is accounted for when one does the two-electron perturbation theory approach and the ω -dependence of $V_{kk'}$ comes out even when energy conservation is required.

The two approaches give the same result if one turns a blind eye for a moment and simply replaces $E_k - E_{k'}$ with ω in the canonical transformation approach, permitting ω to be non-zero. In other words, the canonical transformation method gives the same result as many-body perturbation theory in the end, but there is an intermediate step which is not entirely accurate.

12.19 Tunneling: single-particle, Josephson effect, and Fraunhofer pattern

12.19.1 Single-particle tunneling

It is important to note that $N_S/N_0 = |\varepsilon|/\sqrt{\varepsilon^2 - \Delta^2}$ is the electronic density of states: it is obtained *e.g.* from the real part of the quasiclassical Green's function $g_{\uparrow, \uparrow}$ which is computed from

the expectation value of the original electron operators in the superconducting state. One might then wonder how charge can be conserved for single-particle tunneling from a normal metal into a superconductor. Take an electron incoming from the N side, which has charge $-|e|$. This can tunnel into the superconductor if its energy exceeds the superconducting gap, since the DOS is finite there. However, if quasiparticles in superconductors carry fractional charge, how can electric charge be conserved? Is it correct to think of an electron tunneling from N and becoming one quasiparticle in S? The answer is no. The point is that when the electron tunnels into the superconductor, it should be thought of as a superposition of quasiparticles: one electron-like and one hole-like. This can be seen *e.g.* from the fact BdG transformation between electron and quasiparticle operators:

$$c_{\mathbf{k},\sigma}^\dagger = u_{\mathbf{k},\sigma} \gamma_{\mathbf{k},\sigma}^\dagger + v_{\mathbf{k},\sigma} \gamma_{-\mathbf{k},-\sigma}. \quad (12.178)$$

So creating an electron is the same as creating a superposition of an ELQ and a HLQ. The total charge is then conserved. Now, each quasiparticle in the superconductor carries by *itself* a fractional charge (but always spin 1/2) and so can give rise to very large spin lifetimes since their group velocities are also slowed down substantially near the gap edge $\varepsilon \rightarrow \Delta$.

Let us now consider some aspects of single-particle tunneling in N/S systems. The general tunneling formula is:

$$I = I_0 \int_{-\infty}^{\infty} N_L(\varepsilon) N_R(\varepsilon) [f_L(\varepsilon) - f_R(\varepsilon)]. \quad (12.179)$$

Consider now an NIS junction and apply a voltage $+eV$ (raising the entire energy band) on the N side. We get:

$$I = I_0 \int_{-\infty}^{\infty} N_N(\varepsilon - eV) N_S(\varepsilon) [f(\varepsilon - eV) - f(\varepsilon)] \quad (12.180)$$

We have subtract eV from ε on the N side since the new Fermi energy now is at $\varepsilon = eV$, i.e. when the argument of the DOS and f is zero on the N side. Consider the $T \rightarrow 0$ limit for analytical progress. We then have $f(\varepsilon) = \Theta(-\varepsilon)$ (step function). It follows that $dI/d(eV) = N_N(0)N_S(eV)$, by assuming that N_N is energy-independent near the Fermi level. If we apply the voltage $-eV$ on the S side, one can show by starting from the general formula that we get the same current as applying $+eV$ on the N side by making the substitution $\varepsilon' = \varepsilon + eV$. This automatically means that the conductance will also be the same, but let us prove this explicitly. The point is that we want to show that it would be false to assert that in the present case, we should get $dI/d(eV) = N_S(0)N_N(eV)$ in analogy to the first case considered. If that were the case, it looks like the conductance would always be zero. Instead, let us show the correct procedure. We have that:

$$\frac{dI}{d(eV)} = \int_{-\infty}^{\infty} d\varepsilon N_N \left[\frac{dN_S(\varepsilon + eV)}{d(eV)} \cdot [f(\varepsilon) - f(\varepsilon + eV)] + N_S(\varepsilon + eV) \delta(-\varepsilon - eV) \right] \quad (12.181)$$

since the derivative of a step function is a delta function. We obtain further (writing $N_N \equiv N_N(0)$)

for brevity):

$$\begin{aligned}
\frac{dI}{d(eV)} &= N_N \int_{-eV}^0 \frac{dN_S(\varepsilon + eV)}{d(eV)} d\varepsilon + N_N N_S(0) \\
&= N_N \int_{-eV}^0 \left[\frac{1}{\sqrt{(\varepsilon + eV)^2 - \Delta^2}} - \frac{(\varepsilon + eV)^2}{[(\varepsilon + eV)^2 - \Delta^2]^{3/2}} \right] d\varepsilon + N_N N_S(0) \\
&= N_N [\ln(2\sqrt{(\varepsilon + eV)^2 - \Delta^2} + eV + \varepsilon)]|_{-eV}^0 \\
&\quad - N_N [\ln(2\sqrt{(\varepsilon + eV)^2 - \Delta^2} + eV + \varepsilon) - \frac{eV + \varepsilon}{\sqrt{(\varepsilon + eV)^2 - \Delta^2}}]|_{-eV}^0 + N_N N_S(0) \\
&= N_N N_S(0) + \frac{eV + \varepsilon}{\sqrt{(\varepsilon + eV)^2 - \Delta^2}}|_{-eV}^0 = N_N N_S(eV). \tag{12.182}
\end{aligned}$$

Finally, we could even consider a scenario where N and S change place so that we have an S/N junction. Now apply $+eV$ to the S side and use the general formula. One then finds, after substituting $\varepsilon' = \varepsilon - eV$, that the current $I(eV)$ in the present case is equal to the current in the N/S case when $+eV$ is applied to the N side but with the replacement $eV \rightarrow (-eV)$. This is physically reasonable, since all that matters is the voltage difference: not where it is applied (as long as we disregard asymmetries around the Fermi level for the DOS).

12.19.2 Josephson tunneling and derivation of expression for thermodynamic current

Non-strict derivation

The Josephson effect describes the supercurrent flow between two superconductors separated by a non-superconducting material when there exists a phase difference $\delta\phi$ between the superconductors. It is an equilibrium property in the sense that no voltage or temperature difference is required, which means that it is possible to describe it quantitatively using the free energy of the system. The fact that the Cooper pair number N operator and the phase ϕ of the superconducting order parameter are canonically conjugate variables plays an important role with respect to the Josephson effect. To see this, recall that for canonically conjugate variables the following equation is satisfied (analogously to Hamilton's equations in classical mechanics):

$$i\hbar\dot{N} = i\frac{\partial H}{\partial\phi}, \tag{12.183}$$

where H is the Hamiltonian of the system. The supercurrent across the junction, naming the superconductors 1 and 2, must be given by the time-derivative of the difference between the Cooper pair number operators (if a net current flows, we must have $\dot{N}_1 = -\dot{N}_2$ due to current conservation):

$$I_{sc} = \langle I \rangle = -2|e|\langle \dot{N}_1 \rangle. \tag{12.184}$$

Using the canonical relations, we can rewrite this as

$$I_{sc} = -\frac{2|e|}{\hbar} \langle \partial_{\phi_1} H \rangle. \tag{12.185}$$

But physically, the Hamiltonian can only depend on the phase difference $\Delta\phi = \phi_1 - \phi_2$, since each phase individually does not matter. Therefore, the phases can only enter in the combination $\phi_1 - \phi_2$,

meaning that $\partial_{\phi_1} = \partial_{\Delta\phi}$. We then obtain:

$$I_{\text{sc}} = -\frac{2|e|}{\hbar} \langle \partial_{\Delta\phi} H \rangle. \quad (12.186)$$

To link this to the free energy, we start by reminding ourselves that

$$F = U - TS = -\frac{1}{\beta} \ln Z, \quad (12.187)$$

where the partition function is given by

$$Z = \text{Tr}\{e^{-\beta H}\} = \sum_p e^{-\beta E_p} \quad (12.188)$$

The trace is taken over a complete set of states, meaning in practice evaluating the Hamiltonian in all states where 0 or 1 fermions sit in each allowed mode. Now, the expectatoin value of an operator A is in general

$$\langle A \rangle = \frac{1}{Z} \text{Tr}\{A e^{-\beta H}\}. \quad (12.189)$$

Therefore, the derivative of the free energy with respect to a variable x that the Hamiltonian depends on (such as phase difference) becomes:

$$\frac{\partial F}{\partial x} = -\frac{1}{\beta Z} \frac{\partial Z}{\partial x} = \frac{1}{Z} \text{Tr}\left\{ \frac{\partial H}{\partial x} e^{-\beta H} \right\} = \left\langle \frac{\partial H}{\partial x} \right\rangle. \quad (12.190)$$

Thus, we finally see that:

$$I_{\text{sc}} = -\frac{2|e|}{\hbar} \frac{\partial F}{\partial \Delta\phi}. \quad (12.191)$$

Since N and ϕ are canonical variables, it is natural to associate an uncertainty relation $\Delta N \Delta\phi \geq \hbar/2$ with them. A strict proof of this relation is however not trivial, especially since the phase is 2π -periodic and thus one could argue that $\Delta\phi$ is infinite.

Strict derivation

The above formula is related to an expression one often sees in the literature, namely

$$\mathbf{J} = -\frac{\delta F}{\delta \mathbf{A}} \quad (12.192)$$

where $F = F[\mathbf{A}]$ is in general a function of the vector potential $\mathbf{A}$. Since the gauge-invariant phase gradient is $\nabla\phi - 2e\mathbf{A}$, we see that differentiating with respect to a phase difference is essentially the same as differentiating with respect to a vector potential. Let us now give a rigorous derivation of this equation, which holds in a stationary situation.

At a fixed temperature, i.e. in equilibrium, the work done on a system is equal to the change in the Helmholtz free energy. Magnetic fields do no work, but electric fields do. The energy change δF in the system due to the presence of currents and electric fields over an infinitesimal time dt is:

$$\delta F = \delta W = dt \int \mathbf{J} \cdot \mathbf{E} d\mathbf{r}. \quad (12.193)$$

This can be derived using that the work done by an electric field is the work performed on charged particles moving through the field. In turn, this is the charge multiplied with the potential difference it moves through: $W = q\Delta V$. Thus, $W = q \int \mathbf{E} \cdot d\mathbf{l}$. Differentiating wrt. time and generalizing the above formula to a current density flowing through space, rather than just a single charge moving through a line, gives the above equation.

For a stationary system, Ampere-Maxwell's law states $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$, so that

$$\delta F = \delta W = \frac{1}{\mu_0} dt \int (\nabla \times \mathbf{B}) \cdot \mathbf{E} d\mathbf{r}. \quad (12.194)$$

Set $\mu_0 = 1$ for now and we will reinstate it later. Using a vector identity for such a triple product, we get

$$\delta F = -dt \int \nabla \cdot (\mathbf{E} \times \mathbf{B}) d\mathbf{r} + dt \int \mathbf{B} \cdot (\nabla \times \mathbf{E}) d\mathbf{r}. \quad (12.195)$$

Using the divergence theorem on the first term allows us to rewrite it as an integral over an infinite surface S . Since fields should vanish at an infinite distance from their sources, we have

$$\int \nabla \cdot (\mathbf{E} \times \mathbf{B}) d\mathbf{r} = \oint (\mathbf{E} \times \mathbf{B}) \cdot \hat{\mathbf{n}} dS = 0. \quad (12.196)$$

Using now Faraday's law for the second term gives

$$\begin{aligned} \delta F &= -dt \int \mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} d\mathbf{r} \\ &= - \int \mathbf{B} \cdot \delta \mathbf{B} d\mathbf{r} \\ &= - \int \mathbf{B} \cdot \delta (\nabla \times \mathbf{A}) d\mathbf{r} \\ &= - \int \mathbf{B} \cdot (\nabla \times \delta \mathbf{A}) d\mathbf{r}. \end{aligned} \quad (12.197)$$

Using the triple vector product identity again, we rewrite this as

$$\delta F = - \int (\nabla \times \mathbf{B}) \cdot \delta \mathbf{A} d\mathbf{r}. \quad (12.198)$$

Reinstating now μ_0 , we see that this is precisely

$$\delta F = - \int \mathbf{J} \cdot \delta \mathbf{A} d\mathbf{r}, \quad (12.199)$$

so that using the definition of a functional derivative

$$\delta F = \int \frac{\delta F}{\delta \mathbf{A}} \delta \mathbf{A} d\mathbf{r} \quad (12.200)$$

gives the final result

$$\mathbf{J} = - \frac{\delta F}{\delta \mathbf{A}}. \quad (12.201)$$

To connect this with the typical formula used in the superconducting case, $\frac{\delta F}{\delta \Delta \phi}$ where $\Delta \phi$ is the phase-difference, the point is to note that due to gauge-invariance it must always be the combination $\Delta \phi - \mathbf{A}$ that appears in any dependence that an observable quantity has on these quantities. Therefore, differentiating with respect to $\mathbf{A}$ is (up to a sign and some prefactor) the same as differentiating with respect to $\Delta \phi$.

Finally, we discuss some aspects of the AC Josephson effect and its inverse. The AC Josephson effect occurs when a DC voltage is applied to the junction. The acceleration of the charge carriers, due to the AC nature of the current, leads to microwave radiation being generated. First, keep in mind that the gauge-invariant superconducting phase difference $\nabla \phi$ which drives a supercurrent is given by

$$\nabla \phi = \nabla \phi_0 + \frac{2e}{\hbar} \mathbf{A}. \quad (12.202)$$

Here, ϕ_0 is the phase of the superconducting order parameter. If you integrate this across a junction, the component of $\mathbf{A}$ that is perpendicular to the junction gives a net contribution:

$$\phi_L - \phi_R = (\phi_{L,0} - \phi_{R,0}) - \frac{2\pi}{\Phi_0} \int_R^L A_z dz. \quad (12.203)$$

Since $\mathbf{B} = \nabla \times \mathbf{A}$, we see that a flux penetrating the junction (flux direction perpendicular to the current flow) will affect the gauge-invariant superconducting phase difference. But what about an electric field? We know that an electric field can be written as $\mathbf{E} = -\partial_t \mathbf{A}$ in a gauge where the electric scalar potential is zero. Thus, if there exists an electric field *that points in the same direction as the current, i.e. the junction*, then we have

$$\partial_t(\phi_L - \phi_R) = -2\pi\Phi_0^{-1} \int \partial_t A_z dz = 2\pi\Phi_0^{-1} \int E_z dz = 2\pi\Phi_0^{-1} V \quad (12.204)$$

so that

$$\frac{\partial \Delta \phi}{\partial t} = \frac{2e}{\hbar} V \quad (12.205)$$

which is the well-known Josephson phase relation. This brings us to the inverse AC Josephson effect. By irradiating the Josephson junction with microwaves in such a way that the AC electric field is applied along the junction direction, this induces an AC voltage $V(t)$ which in turn modifies the superconducting phase difference. If one applies, in addition to these microwaves, a constant DC voltage across the junction (V_0), then Shapiro steps appear in the $I - V$ curve whenever $V_0 \propto \omega$ where ω is the microwave frequency. This is manifested as a step in the $I - V$ diagram where a DC Josephson effect occurs at these special points.

12.19.3 Fraunhofer pattern and gauge-choice

Consider an SNS junction. The response of the supercurrent to an externally applied magnetic field may be quantum mechanically computed using for instance the BdG framework by setting up wavefunctions, matching them at interfaces via proper boundary conditions (continuity of wavefunction and conservation of particle flux via the velocity operator), and then identifying the energies E that give a non-trivial value for the coefficients of the wavefunctions). The question is now how one can take into account the vector potential $\mathbf{A}$ which exists due to the external field $\mathbf{B} = \nabla \times \mathbf{A} \neq 0$.

The common approximation to make (which still captures the Fraunhofer response in the appropriate limit of a wide and thin separating interlayer) is that the superconductors fully screen the field and that the penetration depth $\lambda \rightarrow 0$, so that the superconductors can be treated as bulk ones. It might thus be tempting to simply take $\mathbf{A} = 0$ inside the superconductors and select a gauge $\mathbf{A}$ inside the normal metal which provides the desired magnetic field profile, usually taken as $\mathbf{B} = B_0 \mathbf{z}$. However, as we will now show one has to be careful with the gauge choice.

We consider first an SN junction with the interface. Let's say that the x -axis is along the junction direction so that y is transverse to it. The interface is at $x = 0$. One possible gauge choice is then $\mathbf{A} = [-B_0 y \theta(x), 0, 0]$. Note that even though this gauge couples to $\hat{p}_x$, it is still Hermitian since the Hamiltonian $H = (\mathbf{p} - q\mathbf{A})^2/2m = (\mathbf{p}^2 + q^2 \mathbf{A}^2 - q\mathbf{p}\mathbf{A} - q\mathbf{A}\mathbf{p})/2m$ is automatically symmetrized. Then, $\mathbf{A} = 0$ in the superconductor and there is also no screening current flowing along the interface since $\mathbf{J} = \nabla\phi - \text{constant} \times \mathbf{A}$.

It should be noted that with the above gauge, the velocity operator does acquire a contribution from the vector potential. This means that the boundary condition is altered from the usual continuity of derivative. This can also be seen by integrating the BdG equation over a small interval centered at the interface. More precisely, one should obtain an additional contribution of the type $B_0 y \psi$ in the boundary condition that usually is associated with continuity of $d\psi/dx = \psi'$. This seemingly makes the boundary condition y -dependent, but the point is that with this gauge choice ψ acquires an additional phase factor $e^{iB_0 xy}$ when solving the SE which thus produces $B_0 y$ when differentiated with respect to x . The scattering coefficients for the different parts of the wavefunction can then be obtained as usual.

Now, we could also have taken $\mathbf{A} = [0, B_0 x \theta(x), 0]$. In this case, we get

$$\mathbf{B} = B_0 \theta(x) \mathbf{z} + B_0 x \delta(x) \mathbf{z}. \quad (12.206)$$

However, the second term is zero since $x\delta(x) = 0$. Both gauge choices work well.

If we now turn to the SNS case, we must be careful when introducing the second superconductor on the right side (say $x = L$). We could now choose

$$\mathbf{A} = -B_0 y [\theta(x) - \theta(x - L)] \mathbf{x} \quad (12.207)$$

which gives $\mathbf{A} = 0$ in the superconductors and $\mathbf{B} = B_0 \mathbf{z}$ in the normal metal. The wavefunctions in the superconductors can then be taken as bulk (but $\mathbf{A}$ enters the boundary condition as mentioned above). However, let's say that we now want to choose the other gauge, namely:

$$\mathbf{A} = B_0 [x\theta(x) - (x - L)\theta(x - L)] \mathbf{y}. \quad (12.208)$$

This also gives $\mathbf{B} = B_0 \mathbf{z}$ in the normal metal while it gives $\mathbf{B} = 0$ in the left superconductor. Also, there is no problem at the interfaces since $x\delta(x) = 0$ and $(x - L)\delta(x - L) = 0$. However, in the *right* superconductor located at $x > L$ we get that

$$\mathbf{A} = B_0 L \mathbf{y}. \quad (12.209)$$

A constant vector potential must therefore exist there. Although this does not give any magnetic field, it does induce a screening current in the $\mathbf{y}$ direction. The only way to counter this, to ensure that $\mathbf{J} = 0$, is to make the superconducting phase y -dependent so that $\nabla\phi - \text{constant} \times \mathbf{A} = 0$, i.e.

$$\phi \propto y.$$

Summarizing, in the SNS case we can either (1) choose a gauge which allows us to use bulk superconducting wavefunctions, but where $\mathbf{A}$ enters the boundary condition, or (2) choose a gauge which allows us to use the bulk superconducting wavefunction in one of the superconductors while the superconducting phase becomes y -dependent in the other (however, $\mathbf{A}$ does not enter the boundary conditions now).

12.19.4 Choice of $\mathbf{A}$ in N affects choice of phase difference in S

It is clear that to obtain the same physics when $\mathbf{A}$ is altered in a specific region of space, such as in the N or S region of a Josephson junction, the phase of a superconducting order parameter in the same region must also be changed correspondingly according to the transformations we have highlighted previously.

However, what is perhaps less intuitive is that the choice of $\mathbf{A}$ in the N region of an SNS junction dictates which phase we have to choose in the S regions *even if $\mathbf{A}$ is kept equal zero* there. First of all, in order to change the SC phase without changing the physics in the S regions on their own, the change in phase must be constant so that $\phi \rightarrow \phi + C$ while $\mathbf{A} \rightarrow \mathbf{A} + \nabla C = \mathbf{A}$. Secondly, the reason for why we have to change the SC phases when $\mathbf{A}$ in the N region changes is the following: the gauge-invariant phase difference, which drives supercurrent through the system, changes otherwise.

We know that the gauge-invariant phase difference is $\Delta\phi_{\text{GI}} = \Delta\phi - \int \mathbf{A} \cdot d\mathbf{l}$. Let us consider a gauge $\mathbf{A} = -By\hat{x}$ (dropping here the step-functions which make $\mathbf{A}$ zero in the S regions) and zero phase difference across the junction, $\Delta\phi = 0$. This corresponds to a specific physical situation: a specific magnetic field and a specific current pattern. Now, we add a constant C to the gauge: $\mathbf{A} = (-By + C)\hat{x}$. We have not changed the magnetic field in N, but we have changed the current. This can be seen from the fact that $\Delta\phi_{\text{GI}}$ has changed from $\Delta\phi_{\text{GI}} = -ByL$ to $\Delta\phi_{\text{GI}} = -ByL + CL$. Therefore, to compensate this change, we have to choose a different $\Delta\phi = -CL$ in order to regain the same physical situation. This shows how the phase difference depends on the choice of $\mathbf{A}$ in the N region.

12.19.5 Choice of coordinate system affects choice of $\mathbf{A}$ and $\Delta\phi$ to preserve the physics

We also have to be careful with the choice of coordinate system, for instance if the N region extends from $y = 0$ to $y = W$ or from $y = -W/2$ to $y = W/2$. If we used the gauge $\mathbf{A} = -By\hat{x}$ in the first case, then we have to change the gauge to $\mathbf{A} = -B(y + W/2)\hat{x}$ in the second case due to the fact that the two coordinates are related via $y' + W/2 = y$. In fact, if we change coordinate system and keep the gauge $\mathbf{A} = -By\hat{x}$, we have effectively added a constant to $\mathbf{A}$ and as we saw in the preceding section adding a constant to $\mathbf{A}$ requires a change in the superconducting phase difference to obtain the same physics.

12.19.6 Typical parameter values for critical currents in bulk superconductors and Josephson junctions

The first thing to note is that the critical current in a bulk superconductor is much larger than the critical current of a Josephson junction. Moreover, what is often cited is critical current densities.

SC or JJ	Critical current density (A/m ²)	Reference
Al	$10^7 - 10^8$	
Pb	10^8	
Nb	$10^8 - 10^9$	
NbN	10^{10}	
MgB ₂	10^{10}	
YBCO	10^{11}	
Nb/Al-AlN/Nb	$10^4 - 10^6$	[70]
Al/AlO _x /Al	$10^4 - 10^6$	
YBCO JJ break junction/bi-crystal	$10^6 - 10^7$	[71]
Nb/PdNi/Nb	10^8	[72]

Typical cross-sectional areas for JJs range from a few μm^2 to much smaller dimensions like $0.1\mu\text{m} \times 0.1\mu\text{m}$ in modern superconducting qubits, attainable via lithography. The table below shows some characteristic values for the critical current density for bulk superconductors and examples of critical current densities for a few selected JJs.

It is worth to note that since supercurrents only flow at the surface of superconductors (within a layer of order magnetic penetration depth) due to the Meissner effect. So when citing critical current densities, these implicitly assume uniformly distributed supercurrent across the cross-section, which is only approximately true if the dimensions of the cross-section are smaller than the penetration depth. The numbers below are also ballpark: they depend on details of the sample like granularity, mean free path, length of the junction in the JJ case, and so forth. The cited numbers should be regarded as close to upper limits.

12.20 Bogoliubov-de Gennes equations and Andreev approximation

12.20.1 Redundancy in the diagonalization of a superconducting Hamiltonian and the BdG equations

A problem seemingly arises when defining the original fermion operators $c_{k,\sigma}$ in terms of the diagonalizing fermion operators α_{nk} to obtain the BdG equations. We here skip the lattice index i since it is not important for this argument. The problem is that if one defines the new basis containing $\{\alpha_{nk}\}$ according to (as D. Terrade and we do in our papers):

$$\begin{aligned}
 (1) c_{k,\uparrow} &= \sum_n u_{nk} \alpha_{nk}, \\
 (2) c_{k,\downarrow} &= \sum_n v_{nk} \alpha_{nk}, \\
 (3) c_{-k,\uparrow}^\dagger &= \sum_n x_{nk} \alpha_{nk}, \\
 (4) c_{-k,\downarrow}^\dagger &= \sum_n w_{nk} \alpha_{nk},
 \end{aligned}
 \tag{12.210}$$

it looks like eqs. (2) and (4) are inconsistent since they give:

$$\sum_n v_{nk} \alpha_{nk} = \sum_n w_{n,-k}^* \alpha_{n,-k}^\dagger. \quad (12.211)$$

However, these equations are in fact consistent if internal relations exist between the α_{nk} operators in just the same manner as internal relations exist among the c -operators in our original basis. For instance, we know that both $c_{k,\uparrow}$ and $c_{-k,\uparrow}^\dagger$ are part of the basis for the original fermions - therefore, these operators are related via inversion of k and the dagger operation. It is therefore natural that similar relations exist among the α -operators, since they are linear combinations of the original ones [for instance if one inverts the relations (1)-(4)].

Specifically, we see that Eq. (12.211) is satisfied if for instance:

$$\alpha_{n,-k}^\dagger = \alpha_{N-n,k} \quad (12.212)$$

and

$$x_{n,-k}^* = v_{N-n,k} \quad (12.213)$$

where N is the number of n -values that we sum over. If this is correct, we can just as well use (1) and (2) to compute the correlation function $\langle c_{k,up} c_{-k,down} \rangle$ instead of (1) and (4), since the expectation value $\sum_{n,n'} \langle \alpha_{nk} \alpha_{n',-k} \rangle$ that arises when we use (1) and (2) will be finite for $n' = N - n$ due to the relation $\alpha_{n,-k}^\dagger = \alpha_{N-n,k}$.

In this way, everything should be consistent. We would have seen the abovementioned relations between the new operators more easily if we had written them in a similar way as the original ones, i.e. something like $[\alpha_{1,k}, \alpha_{2,k}, \alpha_{1,-k}^\dagger, \alpha_{2,-k}^\dagger, \dots]$, but it is not strictly necessary. We have just given $\alpha_{1,-k}^\dagger$ the name $\alpha_{3,k}$, but this is just notation. It is nevertheless important to keep in mind that there exists internal relations between the new fermions operators $\{\alpha_{nk}\}$ just as there exists such relations between the original fermions $\{c_{k\sigma}\}$ used in the original basis. This is important in order to preserve the number of degrees of freedom in the system so that only the independent operators satisfy $\langle \alpha_{nk}^\dagger \alpha_{nk} \rangle = f(E_{nk})$. This is explained in detail in a previous chapter (BdG diagonalization on a lattice).

12.20.2 Note on relation for the coherence factors u and v in BdG equations

The field operators $\Psi_\sigma(\mathbf{r})$ are defined in terms of the operators $\gamma_{n,\sigma}$ in equations 2.18-2.21 in Kopnin's notes. The point is now that it is also possible to define the quasiparticle operators $\gamma_{n,\sigma}$ (which diagonalize the Hamiltonian) in terms of $\Psi_\sigma(\mathbf{r})$, in effect the *inverse transformation*.

It is straightforward to verify that the inverse transformation becomes

$$\begin{aligned} \gamma_{n,\uparrow} &= \int d\mathbf{r} [u_n^*(\mathbf{r}) \Psi_\uparrow(\mathbf{r}) + v_n^*(\mathbf{r}) \Psi_\downarrow^\dagger(\mathbf{r})], \\ \gamma_{n,\downarrow}^\dagger &= \int d\mathbf{r} [u_n(\mathbf{r}) \Psi_\downarrow^\dagger(\mathbf{r}) - v_n(\mathbf{r}) \Psi_\uparrow(\mathbf{r})]. \end{aligned} \quad (12.214)$$

and *e.g.* $\gamma_{n,\uparrow}^\dagger$ is obtained by taking the hermitian conjugate of the upper line in the above equation. One way to verify that this is the correct inverse transformation is to insert these transformations

into the commutation rules 2.22 for the Ψ -operators and using equations 2.24 and 2.25.

Now, the troublesome equation to prove was 2.38, as far as I understood. But using the above inverse transformations, we can now prove 2.38 by using the last line in 2.23:

$$\{\gamma_{n,\alpha}^\dagger, \gamma_{m,\beta}\} = \delta_{\alpha\beta} \delta_{mn}. \quad (12.215)$$

Let $\alpha = \beta = \uparrow$. We then have δ_{mn} on the right hand side of the equation, which is precisely the right hand side of equation 2.38. It then remains to show that the left-hand side of Eq. (28.214) is identical to the left hand side of equation 2.38 in Kopnin's notes.

This is accomplished by inserting the inverse transformations Eq. (12.214) into the left hand side of Eq. (28.214) and using the commutation rules for the Ψ -fields in equation 2.22 (which we know are true since they are fermion field operators). Inserting the inverse transformations first, Eq. (28.214) becomes:

$$\begin{aligned} \int d\mathbf{r} \int d\mathbf{r}' & \left[u_n(\mathbf{r}) u_m^*(\mathbf{r}') \{ \Psi_\uparrow^\dagger(\mathbf{r}), \Psi_\uparrow(\mathbf{r}') \} + v_n(\mathbf{r}) v_m^*(\mathbf{r}') \{ \Psi_\downarrow(\mathbf{r}), \Psi_\downarrow^\dagger(\mathbf{r}') \} \right. \\ & \left. + u_n(\mathbf{r}) v_m^*(\mathbf{r}') \{ \Psi_\uparrow^\dagger(\mathbf{r}), \Psi_\downarrow^\dagger(\mathbf{r}') \} + v_n(\mathbf{r}) u_m^*(\mathbf{r}') \{ \Psi_\downarrow(\mathbf{r}), \Psi_\uparrow(\mathbf{r}') \} \right] = \delta_{mn} \end{aligned} \quad (12.216)$$

The first two anticommutators are equal to $\delta(\mathbf{r}-\mathbf{r}')$ while the two last are identically zero. Therefore, we end up with

$$\int d\mathbf{r} \left[u_n(\mathbf{r}) u_m^*(\mathbf{r}) + v_n(\mathbf{r}) v_m^*(\mathbf{r}) \right] = \delta_{mn} \quad (12.217)$$

which concludes the proof.

12.20.3 BdG equations for unconventional superconductors: differential operators and symmetrization

Unconventional superconductors, such as d -wave and p -wave, can be written in $\mathbf{k}$ -space in a translationally invariant system as

$$H = \frac{1}{2} \int \frac{d\mathbf{k}}{(2\pi)^2} \psi^\dagger(\mathbf{k}) \mathcal{H}(\mathbf{k}) \psi(\mathbf{k}) \quad (12.218)$$

where we considered 2D for simplicity. The matrix $\mathcal{H}(\mathbf{k})$ contains the gap which for a p -wave chiral superconductor has the form $\Delta(\mathbf{k}) = i\Delta_0 e^{i\phi} (k_x + ik_y)/k_F$. For a d -wave, one has a $\mathbf{k}$ -dependence like $k_x k_y$ or $k_x^2 - k_y^2$.

What does the corresponding real-space Hamiltonian look like? In other words, starting from a generic form

$$H = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) [-\hbar^2 \nabla^2 / 2m - \mu] \psi(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \psi^\dagger(\mathbf{r}) D(\mathbf{r}, \mathbf{r}') \psi^\dagger(\mathbf{r}') + \text{h.c.} \quad (12.219)$$

what does $D(\mathbf{r}, \mathbf{r}')$ have to be to produce the $\mathbf{k}$ -space Hamiltonian? By using that

$$\psi(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{r}), \quad \psi(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^2} e^{i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{k}), \quad (12.220)$$

one verifies that

$$D(\mathbf{r}, \mathbf{r}') = \Delta\left(\frac{\mathbf{r} + \mathbf{r}'}{2}\right)(\partial_{x'} + i\partial_{y'})\delta(\mathbf{r} - \mathbf{r}'). \quad (12.221)$$

In the special case of a spatially homogeneous order parameter, by using that

$$\int dx f(x) \partial_{x'} \delta(x - x') = \frac{df(x')}{dx'} \quad (12.222)$$

one verifies that the Hamiltonian reduces to

$$H = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) [-\hbar^2 \nabla^2 / 2m - \mu] \psi(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} \frac{\Delta_0 e^{i\phi}}{2} \psi^\dagger(\mathbf{r}) (\partial_x + i\partial_y) \psi^\dagger(\mathbf{r}) + \text{h.c.} \quad (12.223)$$

A similar approach can be used in the d -wave case. We also underline that, as shown in the thesis by Henrik Roising on topological superconductivity in chapter 5, that the corresponding BdG equations obtained when diagonalizing the above Hamiltonian automatically will contain an anticommutator that symmetrizes the superconducting term. For instance, one finds

$$[H, \psi(\mathbf{r})] = \left(\frac{\hbar^2}{2m} \nabla^2 + \mu \right) \psi(\mathbf{r}) - \frac{1}{2} \{ \Delta(\mathbf{r}), \partial_{z^*} \} \psi^\dagger(\mathbf{r}) \quad (12.224)$$

where $z = x + iy$. Such an anticommutator ensures hermiticity of the effective BdG Hamiltonian, and needs to be present as soon as you have any quantity which does not commute with derivative operators (such as different masses in a heterostructure or spin-orbit coupling terms).

12.20.4 Andreev approximation with gauge field

The Andreev approximation (also known as WKB or semiclassical approximation) means that the electronic wavelength $1/k_F$ is the shortest lengthscale in the problem. This is known as the Fermi wavelength $\lambda_F = 1/k_F$. This is equivalent to stating that the Fermi energy E_F is the largest energy scale in the system.

Let's now have a look at equations 3.1-3.5 in Kopnin's notes. It is instructive to first consider the case without magnetic field, so let's set $\mathbf{A} = 0$. Inserting 3.1 into 3.2 gives something like (I'm not considering the prefactors β , $\hbar$ et.c. carefully now, but that doesn't make any difference for the argument I'm about to make):

$$(\mathbf{k}_F \cdot \nabla)U + \nabla^2 U + \Delta V = \epsilon U \quad (12.225)$$

We can rewrite this as

$$(\mathbf{k}_F + \nabla) \cdot \nabla U + \Delta V = \epsilon U. \quad (12.226)$$

The point is now that if k_F^{-1} is the shortest lengthscale in the problem, whichever inverse length scale L that is associated with the effect of a gradient operator $\nabla \sim 1/L$ has to satisfy $k_F^{-1} \ll L$. Therefore, we can neglect ∇ compared to $\mathbf{k}_F$ and we obtain the Andreev equation:

$$\mathbf{k}_F \cdot \nabla U + \Delta V = \epsilon U. \quad (12.227)$$

We see that our approximation effectively amounts to neglecting second derivatives in U . So far, so good.

Let us now introduce a gauge field $\mathbf{A} \neq 0$. If we repeat the calculation and again neglect $\nabla^2 U$, there are additional terms compared to equation 3.4 in Kopnin which (as we saw during our meeting) do not seem to vanish. However, the reason for this is that the quasiclassical approximation (meaning that $\lambda_F = k_F^{-1}$ is the shortest lengthscale) means that *additional terms* than $\nabla^2 U$ alone have to be neglected. Let us now prove this.

If we start from equation 3.2 and insert 3.1, we now obtain (without discarding any terms and after cancelling the common prefactor $e^{\beta k r}$ for all terms) something like:

$$\mathbf{k}_F \cdot (\nabla - i\mathbf{A})U + (\nabla - i\mathbf{A})^2 U + \Delta V = \epsilon U \quad (12.228)$$

But we can rewrite this as:

$$(\mathbf{k}_F + \nabla - i\mathbf{A}) \cdot (\nabla - i\mathbf{A})U + \Delta V = \epsilon U \quad (12.229)$$

The point is then that just as our quasiclassical approximation meant that $\mathbf{k}_F \gg \nabla$, it must also mean that $\mathbf{k}_F \gg \mathbf{A}$. Put differently, the Fermi wavelength λ_F has to be much smaller than the lengthscale associated with the magnetic vector potential $\mathbf{A}$ in order for our quasiclassical approximation to be satisfied. Therefore, we are allowed to write $(\mathbf{k}_F + \nabla - i\mathbf{A}) \simeq \mathbf{k}_F$ and then we reproduce the equation by Kopnin.

12.21 Energy of Josephson junction with resistive current and anomalous phase: supercurrent-induced magnetization dynamics

12.21.1 Energy stored in Josephson junction upon establishing a constant current

An important realization concerning the free energy of a static Josephson junction is that the energy has come from the source that is used to establish the current (or phase difference) in the first place. First, it is useful to recall how Ohmic dissipation arises in a normal conductor. When charges move across a resistor, they lose a potential energy qV where V is the voltage drop across the resistor. This energy loss physically comes from interactions between the electrons and the conducting material, such as phonon scattering. The power dissipated in the resistor is the energy dissipated per time, so $P = \Delta q V / \Delta t = IV$.

Now, let the initial value of the phase difference ϕ be zero at zero junction current. As we are increasing the current, according to the current-phase relation also the phase difference ϕ has to change. Furthermore, according to the voltage-phase relation a changing phase difference corresponds to a finite junction voltage. That is, on increasing the current the external source has to supply energy.

Now, the supercurrent flows without resistance, so there is no Ohmic dissipation. But we have still moved charges from high potential energy to low potential energy, so the energy of the charges have changed. But unlike the resistive conductor case, the energy has not dissipated, it has been converted into kinetic energy of the Cooper pairs which are carrying a supercurrent. This amount of kinetic energy can be computed in the same way as the dissipated energy of the Ohmic conductor above: namely $I_S V$ is the power at which the energy of the JJ increases.

In order to calculate the energy stored in the Josephson junction we have to integrate the power

from time $t = 0$ when we start the current increase to time $t = t_0$ when we are stopping the increase:

$$E_J = \int_0^{t_0} I_S V dt. \quad (12.230)$$

Here, V is the voltage applied during the current increase from zero at $t = 0$ to the final value I at $t = t_0$. Using the current-phase and voltage-phase relation, we get straightforwardly

$$E_J = \frac{\Phi_0 I_c}{2\pi} (1 - \cos \phi) \quad (12.231)$$

where $\phi = \phi(t_0)$.

12.21.2 Current bias

Consider first the case without any anomalous phase ϕ_0 . For a current bias I , the current in a Josephson junction may in general consist of a supercurrent and resistive contribution:

$$I = I_c \sin \phi + I_N, \quad I_N = \frac{V}{R} \quad (12.232)$$

where V is the voltage difference between the superconductors. It is related to the gauge-invariant superconducting phase difference ϕ as

$$V = \frac{\dot{\phi}}{2} \quad (12.233)$$

The Joule heating $I_N V$ corresponds to the power dissipated by the resistor in the system. But there is an additional source of energy loss, namely the Gilbert damping. The Gilbert damping represents a loss of energy from the macroscopic dynamics of the local magnetization to microscopic thermal motion. A range of mechanisms might be involved, but eventually the energy is lost to phonons, magnons and thermal excitation of conduction electrons. The Gilbert damping term can be formally introduced by from the LLG equation without α by letting $\mathbf{B}_{\text{eff}} \rightarrow \mathbf{B}_{\text{eff}} + \mathbf{B}_{\text{dis}}$ where $\mathbf{B}_{\text{dis}}$ is an additional damping field that depends on $\partial_t \mathbf{m}$. The field is obtained similarly to how viscous forces in classical mechanics are obtained, namely by differentiating a Rayleigh dissipation function $\mathcal{R}$:

$$\mathcal{R} = \frac{1}{2} \alpha (\partial_t \mathbf{m})^2 \quad (12.234)$$

as follows:

$$\mathbf{B}_{\text{dis}} = -\frac{\delta \mathcal{R}}{\delta (\partial_t \mathbf{m})}. \quad (12.235)$$

This gives $\mathbf{B}_{\text{dis}} = -\alpha \partial_t \mathbf{m}$ and produces the usual Gilbert damping term.

To see how the Gilbert damping is related to energy loss, consider the LLG equation

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \left(-\frac{\delta F}{\delta \mathbf{m}} \right) + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t}. \quad (12.236)$$

The effective field is

$$\mathbf{B}_{\text{eff}} \equiv -\frac{\delta F}{\delta \mathbf{m}}. \quad (12.237)$$

By using that

$$\partial_{\mathbf{m}} F \cdot \partial_t \mathbf{m} = \partial_{\mathbf{m}} F \cdot (\gamma \mathbf{m} \times \partial_{\mathbf{m}} F + \alpha \mathbf{m} \times \partial_t \mathbf{m}) = \alpha \partial_{\mathbf{m}} F \cdot (\mathbf{m} \times \partial_t \mathbf{m}) \quad (12.238)$$

and using the cyclic property of the vector triple product, we can write the above as

$$\begin{aligned} \frac{\partial F}{\partial \mathbf{m}} \cdot \frac{\partial \mathbf{m}}{\partial t} &= -(\alpha/\gamma) \partial_t \mathbf{m} \cdot (\gamma \mathbf{m} \times \partial_{\mathbf{m}} F) = -(\alpha/\gamma) \partial_t \mathbf{m} \cdot (\partial_t \mathbf{m} - \alpha \mathbf{m} \times \partial_t \mathbf{m}) \\ &= -\frac{\alpha}{\gamma} \left(\frac{\partial \mathbf{m}}{\partial t} \right)^2. \end{aligned} \quad (12.239)$$

Now, the total time derivative of the free energy will be the power dissipated in the system. For a free energy F that depends in general on both superconducting phase difference ϕ and magnetization $\mathbf{m}$, $F = F(\phi, \mathbf{m})$, we have

$$\frac{dF}{dt} = \frac{dF(\phi, \mathbf{m})}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial \phi} \frac{\partial \phi}{\partial t} + \frac{\partial F}{\partial \mathbf{m}} \frac{\partial \mathbf{m}}{\partial t}. \quad (12.240)$$

Thus, we see that the last term is given by Eq. (12.239), which we actually recognize as a Rayleigh dissipation function for the magnetization given in Eq. (12.239). Therefore, Eq. (12.239) gives the energy loss rate due to magnetization dynamics in the system.

Assume that there is no explicit time-dependence in the free energy. Then, the remaining term has to be the Joule heating power of the system, since the Joule heating and energy loss due to magnetization dynamics are the two sources of dissipation in the system. Note that this could be different in the case of a constant *voltage* bias, since then the current may be oscillating due to the AC Josephson effect, so that radiation is an extra channel of energy dissipation. Therefore, we have

$$-I_N V = \frac{\dot{\phi}}{2} [I - I_c \sin(\phi)] = \frac{\partial F}{\partial \phi} \frac{\partial \phi}{\partial t}. \quad (12.241)$$

This can be rewritten as

$$-[I - I_c \sin(\phi)]/2 = \frac{\partial F}{\partial \phi} \quad (12.242)$$

which we can solve for the free energy F . We obtain

$$F = f(\mathbf{m}) + \text{constant} - (I\phi + I_c \cos \phi)/2 \quad (12.243)$$

where f is a function that depends on $\mathbf{m}$. This can include for instance anisotropy energies such as $f(\mathbf{m}) = K m_z^2$. Eq. (12.243) is the final result for the free energy of the system. Keep in mind that dissipation through Gilbert-damping is obtained only by combining dF/dt of Eq. (12.243) with the LLG-equation.

Moreover, note that we have used the symbol F for the free energy above, but it should be emphasized that the relevant free energy to use is the Gibbs free energy in the case of a fixed current bias (current as independent variable) while it is the Helmholtz free energy in the case of a fixed phase difference (phase as independent variable). The effective field in the LLG equation is then computed as the functional derivative of the appropriate free energy. Therefore, for magnetization dynamics induced by a phase-biased Josephson junction, it is appropriate to use the Helmholtz free energy which does not include the $-I\phi$ term. See <https://goldbart.gatech.edu/PostScript/TALKS/>

2004_11_oxford/SC-nanoscale-050217.pdf and <https://arxiv.org/pdf/cond-mat/0507315.pdf>, including reference [22] in the latter.

This resolves the seeming ambiguity in Eq. (12.243) that appears when considering a fixed phase difference ϕ , which gives rise to a fixed supercurrent and zero resistive current, since the supercurrent is then *not* just the derivative of the free energy with respect to phase difference. In other words, minimizing the Helmholtz free energy wrt. ϕ gives zero supercurrent (applicable when the system has a fixed applied phase) since the derivative of that free energy equals the supercurrent. But minimizing the Gibbs free energy wrt. ϕ gives a finite supercurrent (applicable when the system has a fixed total current) since the derivative of that free energy is not equal to the supercurrent. The Gibbs free energy thus includes the contribution to the free energy from the *current source itself*. The fact that Eq. (12.243) does not hold for the case of a fixed phase difference ϕ can be seen mathematically by noting that we derived it by cancelling $\partial\phi/\partial t$ on both sides of an equation when deriving it, which is not allowed when that term is zero.

The fact that Eq. (12.243) is physically reasonable can be seen by looking the equation resulting from its minimization with respect to the phase difference at a fixed current bias I . Setting $\partial_\phi F = 0$ gives $I = I_c \sin \phi$, meaning physically that the ground-state corresponds to when all the current flows as a supercurrent.

Before moving on to the case with anomalous phase-difference ϕ_0 , we note two things. Firstly, the anomalous phase-difference ϕ_0 is in itself a gauge-invariant quantity as it depends on gauge-invariant quantities such as magnetization vector components and spin-orbit coupling strengths. Secondly, the relation

$$V = \frac{\dot{\phi}}{2} \quad (12.244)$$

where ϕ is the gauge-invariant superconducting phase holds even in the presence of an anomalous phase-difference, because this relation is derived from local gauge-invariance inside a superconductor (see earlier sections in these lecture notes).

Now we consider the case with an anomalous phase-difference. Bobkova *et al.* showed that the resistive current through an anomalous Josephson junction where only one spin-type is considered (half-metal) with spin-orbit coupling has the form

$$I_N = \frac{\dot{\phi} - \dot{\phi}_0}{2R} \quad (12.245)$$

by deriving this result via quasiclassical theory. The extra term $\dot{\phi}_0$ thus modifies Ohm's law and can be understood as a magnetoelectric effect where magnetization dynamics induces an extra electric current. The total current through the system is now

$$I = I_c \sin(\phi - \phi_0) + I_N. \quad (12.246)$$

Recall that the power dissipated is equal to the potential energy lost as charge move across the resistor. The change in energy by electrons dQ_N in the normal current as they travel across the junction when the voltage difference is $V = \dot{\phi}/2$ is:

$$dE = V dQ_N = \dot{\phi} \frac{dQ_N}{2}. \quad (12.247)$$

Thus, the change in energy per time from the Joule heating is

$$P_{\text{Joule}} = I_N V = \frac{\dot{\phi}}{2} \frac{\dot{\phi} - \dot{\phi}_0}{2R} \quad (12.248)$$

and corresponds to the dissipated power from Joule heating. Note how it is $\dot{\phi}$, and not $\dot{\phi} - \dot{\phi}_0$, that enters the equation. However, for the rest of the derivation below, it is not important what the specific form of I_N is.

Like before, we should have in general (assuming $\partial_t F = 0$):

$$\begin{aligned} \frac{dF}{dt} &= \frac{\partial F}{\partial \mathbf{m}} \frac{\partial \mathbf{m}}{\partial t} - I_N V \\ &= + \frac{\partial F}{\partial \mathbf{m}} \frac{\partial \mathbf{m}}{\partial t} - \frac{\dot{\phi}}{2} [I - I_c \sin(\phi - \phi_0)]. \end{aligned} \quad (12.249)$$

But for $F = F(\phi, \mathbf{m})$, we also have in general

$$\frac{dF}{dt} = \frac{\partial F}{\partial \phi} \frac{\partial \phi}{\partial t} + \frac{\partial F}{\partial \mathbf{m}} \frac{\partial \mathbf{m}}{\partial t}. \quad (12.250)$$

Note that ϕ_0 in general will depend on components of $\mathbf{m}$ and should thus be differentiated if one computes $\partial_{\mathbf{m}} F$. Thus, we identify

$$\frac{\partial F}{\partial \phi} = -[I - I_c \sin(\phi - \phi_0)]/2. \quad (12.251)$$

This can now be solved for the effective energy functional for an anomalous Josephson junction:

$$F = G(\mathbf{m}) + \text{constant} - \frac{1}{2} I_c \cos(\phi - \phi_0) - I \frac{\phi}{2}. \quad (12.252)$$

Note how we have a term $I\phi$ regardless of whether an anomalous phase is present or not.

This can then be differentiated with respect to magnetization to obtain the effective field that enters the LLG equation. Note that both ϕ and ϕ_0 will in general be time-dependent. Therefore, we also need an equation which tells us what the time-dependence of ϕ is. This is obtained from Eq. (12.246) by writing it as

$$I = I_c \sin(\phi - \phi_0) + \frac{\dot{\phi} - \dot{\phi}_0}{2R}. \quad (12.253)$$

in the case of a half-metal with spin-orbit coupling. This should correspond to Eq. (11) in <https://arxiv.org/pdf/1907.08454.pdf>. The last term in the equation above is more generally written I_N .

The free energy Eq. (12.252) thus properly takes into account Joule heating and is consistent with the loss of energy via magnetization dynamics in the system. We note that the free energy properly accounts for the torque induced by the supercurrent in the system. The torque induced by the spin-polarized resistive current has to be added as a separate spin-transfer torque in the LLG equation. Bobkova *et al.* show in some papers [see <https://arxiv.org/pdf/2007.01572.pdf> and <https://arxiv.org/pdf/1804.00718.pdf>] that the supercurrent part of the torque can be computed both via the effective field method shown above or by including explicit spin-transfer torque terms in the LLG equation from the supercurrent: both methods are equivalent. The spin-transfer torque from the resistive current can be neglected in the limit of very slow magnetization dynamics, such that $\dot{\phi}$ and $\dot{\phi}_0$ become negligible, giving $I_N \simeq 0$.

12.21.3 Voltage bias/phase bias

Consider now the case where the current is not the independent variable, but rather the voltage $V \propto \dot{\phi}$. This means that the time-dependence of the phase-bias is the fixed variable, which also includes the case of a static phase-difference $V = 0$.

In such a scenario, we have $I_N = V/R$ being constant assuming that the normal-state resistance R is independent of ϕ , as is reasonable. In this case, if we were to use the same approach as in the current-biased case, we obtain

$$\frac{\partial F}{\partial \phi} \frac{\partial \phi}{\partial t} = -I_N V = -\frac{\hbar \dot{\phi} V}{2eR}. \quad (12.254)$$

Cancelling $\dot{\phi}$ on both sides of the equation, we get $\partial F/\partial \phi = -\hbar V/(2eR)$ which can be integrated with respect to ϕ with the result

$$F(\phi) = f(t) - \frac{\hbar \phi V}{2eR}. \quad (12.255)$$

So, the free energy has a dissipation term corresponding to Joule heating described by $\phi V/R \propto I_N \phi$ rather than $I\phi$ in the current biased case. For a magnetoanisotropic resistance $R = R(\mathbf{m})$, this means that the effective field $-\delta F/\delta \mathbf{m}$ will get a contribution from the second term if V is finite. If one uses phase-bias $\phi(t)$ to a Josephson junction where the bias is constant and then rapidly changes to a different constant value, then the second term only gives a contribution during the transition between the two constant values.

However, the derivation above has a weakness. It does not reduce to the correct free energy expression in the case of $V = 0$, since $f(t)$ is not the static Josephson energy then. One potential source for this discrepancy is that in the fixed voltage case, the supercurrent will oscillate due to the AC Josephson effect. This gives to radiation, which is an extra source of energy loss. Therefore, it is possible that $\frac{\partial F}{\partial \phi} \frac{\partial \phi}{\partial t}$ should not equal just the Ohmic loss, but also take into account the radiation losses somehow. This would give rise to a different expression.

Therefore, a practical solution could be to instead do what Konschelle and Buzdin do in their PRL 2008 in the case of a slowly time-dependent phase $\phi = \omega t$ with $\omega = 2eV$. One may then use the static expression for the Helmholtz free energy of the Josephson junction with $\phi = \omega t$ as an approximation. Under such circumstances, the dissipation term $-\hbar \phi V/(2eR)$ would be very small anyway since V is small for a slowly varying phase, i.e. $\dot{\phi}$ is small.

12.21.4 Dissipative current spin-torque not accounted for

In neither of the two above approaches (constant current bias or constant voltage/phase bias) is a possible spin-transfer torque provided by the dissipative part of the current taken into account. This must be added as a separate torque term in the LLG equation. Only the supercurrent-induced torque is accounted for via the effective field analysis. However, note that when the resistive current is flowing directly through a homogeneously magnetic material, it should become spin-polarized in the same direction as the magnetization, and thus not provide any torque, making it negligible. Moreover, in the case of supercurrent-induced dynamics in an AFM (even with SOC), the resistive current should not be spin-polarized and thus be negligible. One possible exception here could be a spin-orbit torque induced by the dissipative current.

12.22 Energy loss for supercurrent-induced domain wall motion and induced magnon spin current

Supercurrents may also induce domain wall motion [Phys. Rev. B 96, 121203(R) (2017)] or induce magnon spin currents [Phys. Rev. Lett. 127, 207001 (2021)]. Consider first domain wall motion. This is also a scenario with magnetization dynamics (time-dependent magnetization) which has Gilbert damping involved. Due to the energy loss via Gilbert damping, there has to be an injection of energy somewhere else in the system to maintain domain wall motion. This injection of energy is manifested through the necessity of a voltage to be applied to the Josephson junction. In other words, the domain wall motion causes the phase of the superconductor to be time-dependent, which in turn creates a voltage drop across the Josephson junction and a resistive component of the current. Only when this voltage is compensated by an external power source can the domain wall motion be sustained. So the magnetization dynamics generated in this way by the supercurrent by necessity generates an electric field and Ohmic losses, similarly to what happens with Abrikosov vortex motion under an applied current in a type II superconductor in the mixed state.

Consider now the supercurrent-induced magnon spin current. If Gilbert damping is present, the magnon spin current will eventually decay (finite propagation distance). But a difference from the domain wall motion case is that Gilbert damping is not required to have a steady-state magnon spin current. Therefore, in principle a supercurrent without any resistive component is sufficient to induce the effect. Only a detailed account of the energy balance can reveal if an applied voltage is required as well: if the kinetic energy of the supercurrent alone is sufficient to account for the energy-difference in the magnon population with zero and finite spin current, no resistive part of the current is required.

12.23 Anomalous Josephson effect: ϕ_0 -junction

12.23.1 Analogue between magnetic vector potential and SU(2) spin-orbit gauge field to understand anomalous Josephson effect

We know that presence of a magnetic vector potential $\mathbf{A}$ modifies the gauge-invariant superconducting phase difference by an additional contribution $\int \mathbf{A} \cdot d\mathbf{l}$. Interestingly, the Hamiltonian when including spin-orbit interactions in the form of a SU(2) gauge-like form looks very similar to the form of a magnetic vector potential. In the latter case, the vector potential terms look like

$$\begin{pmatrix} \mathbf{p} \cdot \underline{\mathbf{A}} & 0 \\ 0 & \mathbf{p} \cdot \underline{\mathbf{A}} \end{pmatrix}. \quad (12.256)$$

In the SOC case, one obtains instead

$$\begin{pmatrix} \mathbf{p} \cdot \underline{\mathbf{A}} & 0 \\ 0 & \mathbf{p} \cdot \underline{\mathbf{A}}^* \end{pmatrix} \quad (12.257)$$

where $\mathbf{A} = \mathbf{n} \times \boldsymbol{\sigma}$. If we for simplicity consider a situation where $\mathbf{p} \parallel \mathbf{x}$ and $\mathbf{n} \parallel \mathbf{y}$, then $\underline{\mathbf{A}} \propto \sigma_z$. The SOC effectively acts like a spin-dependent vector potential with opposite sign for the two spin species. It thus gives rise to an opposite phase-shift for spins carried by $\uparrow\uparrow$ and $\downarrow\downarrow$ Cooper pairs. If the magnitude of the currents carried by these two types of pairs is the same, there is no net anomalous

phase-difference since the currents cancel when the intrinsic phase difference $\Delta\phi = 0$. However, if we additionally have a different magnitude of these currents, a finite anomalous phase exists. The different magnitude can be accomplished via an exchange field that points in a suitable direction. In general, to have an anomalous phase the exchange field should not point in the direction of the inversion symmetry breaking. In the above example, an exchange field in the z -direction should thus work.

12.24 Andreev reflection and the proximity effect

The proximity effect is usually described as the leakage of Cooper pairs into a non-superconducting region such as a normal metal. Here, we analyze in detail what this statement really means and how superconducting correlations appear in a normal metal via the process of *Andreev reflection*.

12.24.1 Detailed microscopic description of Andreev reflection

We start then by introducing Andreev reflection. This effect is often described by considering an incoming electron from the N side of an N/S bilayer. The electron has an energy $E < \Delta$ where Δ is the bulk superconducting gap. We have set the superconducting phase to zero here since it plays no role. As there are no available quasiparticle states in the bulk of the superconductor for $E < \Delta$, one possibility is that the electron is normally reflected by a barrier potential at N/S interface. But let us assume that no such barrier exists. What happens with the electron then? It cannot be reflected and cannot be transmitted, so we seem to have reached an impasse.

The resolution is that the electron can be reflected as a hole by the superconducting order parameter. We shall see precisely how this occurs, but let us first make an argument for why only a small momentum change is permitted for the incoming electron when it is reflected by the superconducting gap. A normal reflection would require a large momentum change $k_F \rightarrow -k_F$ since the electron would change its direction completely. This can occur at a sharp interface (rapidly rising), but it is very unlikely for a slowly increasing potential. We can estimate the change in momentum δk that the superconducting gap can provide in the following way [37].

The quantity δk should be of order the force $F = dp/dt$ acting on the electron multiplied by the time dt the electron spends in the interface region. Now, the superconducting gap should rise from zero up to a significant portion of its bulk value over a distance of the coherence length ξ_S (the "healing" length of the superconducting order parameter). Therefore,

$$dt \sim \xi/v_F \quad (12.258)$$

since the electron moves with the Fermi velocity. As for the force acting on the electron, we can also express it as $F = -dV/dx$, i.e. the differential change in potential with position. Since Δ rises over a distance ξ , we then have $-dV/dx \sim \Delta/\xi$ and thus:

$$F \sim \Delta/\xi. \quad (12.259)$$

Using now that $\delta k = F \cdot dt$, we find

$$\delta k \sim \frac{\xi_S}{v_F} \frac{\Delta}{\xi_S} \sim p_F \frac{\Delta}{p_F v_F} \sim p_F \frac{\Delta}{E_F} \ll p_F \quad (12.260)$$

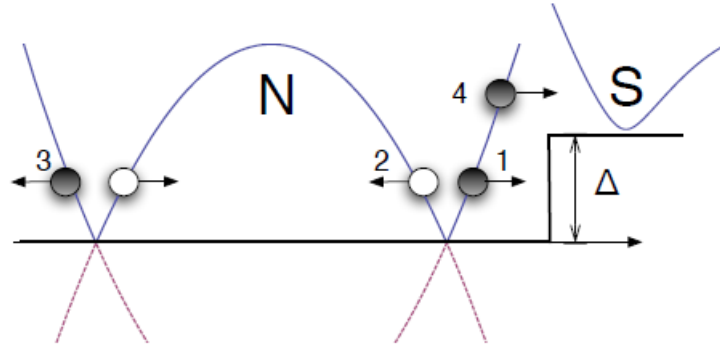


Figure 12.1: Illustration of Andreev reflection of an incoming electron toward an N/S interface. The electron and hole energy bands are drawn (blue color means excitation) with energy increasing upwards. Electrons are represented as black balls, holes as white balls and the arrows show the direction of propagation. The electron #4 can enter the superconductor as a quasiparticle since it has an energy $E > \Delta$. The electron #1 cannot, however. It can be reflected as an electron #3, but this is not possible in the absence of a barrier at the interface since we show in the main text that the superconducting gap can only provide a very small momentum change δk compared to the Fermi momentum. However, the electron #3 can also be Andreev reflected as a hole #2. In this case, the electron has paired up with another electron at energy $-E$ and entered the superconductor as a Cooper pair. Taken from Ref. [38].

since $\Delta/E_F \ll 1$ for conventional superconductors. This means that the change δk in momentum provided by reflection via the superconducting order parameter must be much smaller than the momentum k_F itself. Still, the motion of the incoming particle must after reflection be directed away from the interface.

We can satisfy both of these criteria in one way: namely, if the incoming electron with energy E and momentum $k_e \simeq k_F + 2E/v_F$ is reflected as a hole with energy E and momentum $k_h \simeq k_F - 2E/v_F$. Since the crystal momentum is opposite to the group velocity for a conduction band hole, this means that the hole is indeed physically moving away from the interface.

Andreev reflection thus provides a mechanism for converting an electron into a hole. Let us examine the transport of charge in this process. We initially have $-|e|$ moving in the right direction. The Andreev reflected hole has charge $|e|$ and is moving on the left direction. In effect, this constitutes a total current of $-2|e|$ in the right direction. This can only make sense if this charge is transmitted to the superconductor of a Cooper pair current which carries precisely a charge $-2|e|$. Let us therefore examine more carefully how this occurs. In particular, is it possible to understand why an electron with momentum $-\mathbf{k}$ tunnels in the $+\hat{x}$ -direction along with the incident electron and leaves behind a hole with momentum $+\mathbf{k}$ propagating in the $-\hat{x}$ direction?

The explanation is illustrated in Fig. 12.2. Consider an 1D geometry with an NS interface at $x = 0$. The incoming electron with energy E and momentum k feels a gradually increasing superconducting order parameter $\Delta(x)$: the gap starts at zero and gradually increases as one moves into the superconductor until it reaches the bulk value $\Delta_0 = \Delta(x \rightarrow \infty)$. But since the gap increases as the electron moves into the superconductor, the momentum of the electron has to decrease. We can see

this from the dispersion relation

$$E = \sqrt{(\epsilon_k - \mu)^2 + |\Delta(x)|^2}. \quad (12.261)$$

Since the energy E is constant and the gap increases, ϵ_k has to decrease meaning that k decreases. Keep in mind that the charge q_k of a quasiparticle in a superconductor depends on the momentum of the quasiparticle: at the Fermi momentum one has $\epsilon_k = \mu$ so that $E = \Delta(x)$ and $q_k = 0$, while for large momenta where $E \simeq \epsilon_k - \mu$ one has $q_k = -|e|$.

If the electron is now reducing its momentum, it means that it is transferring charge to the superconducting condensate as it moves into the superconductor. This happens continuously up to the point where the electron reaches a position x_0 where its energy is equal to the local gap value, i.e. $E = \Delta(x_0) < \Delta_0$ (see Fig. 12.2). At this point, the incoming electron has given up all its charge to the condensate $-|e|$. But a total charge of $-|e|$ cannot be absorbed by itself in a superconductor when $E < \Delta_0$ since there are no available quasiparticle states. Therefore, the electron (which is by now a quasiparticle inside the superconductor) has to continue reducing its momentum so that it turns into a hole-like quasiparticle with a momentum such that $\epsilon_k - \mu < 0$. The electron thus turned into an ELQ and gradually, by reducing its momentum, performed a branchcrossing and turned into a HLQ.

The HLQ now moves back toward the normal metal again and thus experiences a gradually weaker superconducting gap $\Delta(x)$. As it enters the normal metal, it is now a hole with charge $|e|$. In the process of moving back through the superconducting interface to the normal metal, it has increased its charge from 0 to $|e|$ which means that the superconducting condensate must have decreased its charge by $-|e|$. In total, a net charge of $-2|e|$ has now been absorbed by the superconductor and this happens precisely via creation of a Cooper pair. The electrons in the Cooper pair thus come from the originally incident electron with $+\mathbf{k}$ and another electron near the interface with $-\mathbf{k}$, the latter entering the superconductor due to the reflected hole tunneling into the normal metal from the superconductor.

Just like electron excitations can tunnel into a material, so can hole excitations. This is how we can make sense of an electron with momentum $-\mathbf{k}$ effectively tunneling in the $+\hat{x}$ -direction: it is because a hole with $+\mathbf{k}$ tunneled into the normal metal, which corresponds to transfer of an electron from the N part to the S part. The net result is that two electrons are transferred from the normal part to the superconductor, entering as a Cooper pair. This only becomes clear when we do as above, namely analyzing the fate of the incoming electron all the way up to being reflected by the superconducting gap through a branch-crossing.

Finally, we note that an incoming hole from the normal metal side can also be Andreev reflected: in this case, it is converted into a left-going electron. Accompanying this process, a Cooper pair is annihilated in the superconductor. In effect, we can think of Andreev reflection of a hole as a Cooper pair tunneling out of the superconductor into the normal metal: one electron fills the hole whereas the other electron in the pair enters as a left-going excitation with energy E . Also note that in equilibrium, there has to be as many electron excitations as hole excitations in the N part. Therefore, there is as many Cooper pairs transmitted into the superconductor from AR of an electron as there are Cooper pairs transmitted out of the superconductor due to AR of a hole. No net current flows, as expected in equilibrium.

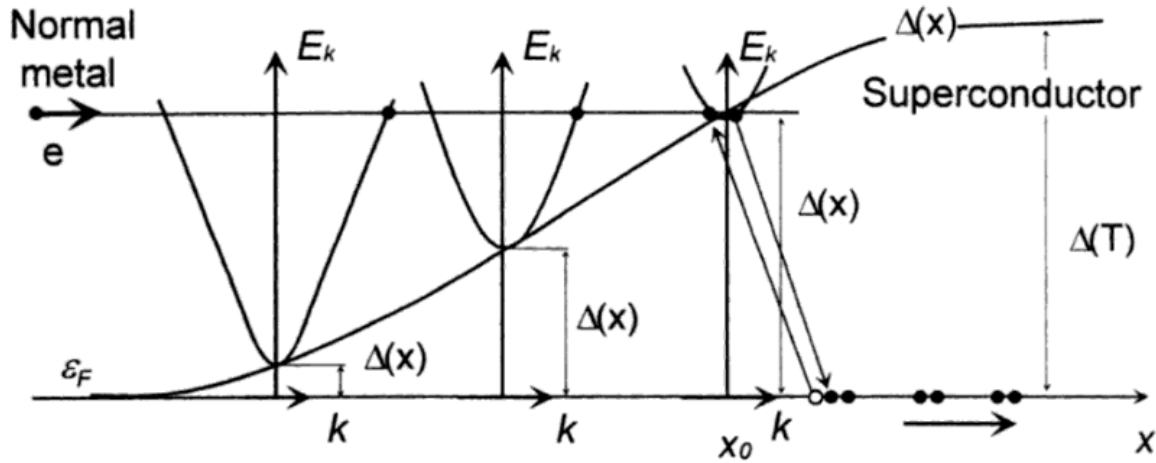


Figure 12.2: Illustration of how an incoming electron is reflected as a hole by the superconducting gap Δ after transferring its charge to the superconducting condensate. Taken from Ref. [39].

12.24.2 Microscopic understanding of the superconducting proximity effect in a normal metal

What about the relation between Andreev reflection and the proximity effect? The first thing to note is that Andreev-reflection gives to electron-hole correlations. This can be seen by noting that the phases of an incoming electron wavefunction and the Andreev-reflected hole wavefunction are distinguished only by a constant ϕ , namely the superconducting phase. More precisely, this is the case exactly at the Fermi level $E = 0$. If $E \neq 0$, the relative phases between the electron and the hole differ by $2Ex/v_F + \phi$ where the first term comes from the fact that $k_e = k_F + E/v_F$ whereas $k_h = k_F - E/v_F$. Thus, as one moves away from the interface at $x = 0$ the electron and hole gradually dephase and lose their correlation.

Let us now connect this to the usual measure of superconducting correlations, namely the anomalous Green function F . The normal and anomalous Green functions G and F and their meaning are discussed in Fig. 12.3. At first glance, it might seem like the anomalous Green function describes something different than electron-hole correlations, namely *electron pair* correlations since it has the form $F \sim \langle \Psi_\uparrow \Psi_\downarrow \rangle$. We note in passing that this expectation value measures the overlap between the state of the system and a state where two electrons have been removed from the system: it will be non-vanishing if Cooper pairs are present and if the system state consists of a superposition of different Cooper pair numbers N (i.e. the number of Cooper pairs is not sharply defined). Such a property is in accordance with the wavefunction having a sharply defined phase ϕ , since one can show that $\Delta N \Delta \phi \geq \hbar/2$ due to them being canonical variables. This is similar to the superfluid and Mott insulating phase in a Bose-Einstein condensate: in the superfluid phase, which has phase-coherence like a superconductor, the atoms are spread out over the lattice with no definite number of atoms per lattice site. In contrast, in the Mott insulating phase the atoms are localized and there is a definite number of particles per site - in turn, there is no longer any phase coherence since $\Delta \phi \rightarrow \infty$.

But how does the presence of electron-hole correlations due to Andreev reflection render F non-zero, thus inducing true superconducting correlations in the form of Cooper pairs consisting of electrons (instead of electrons and holes)? The mathematical derivation of how this occurs is shown in Ref.

[41], but the key point is that the wavefunction in the normal part of an N/S junction where Andreev reflection occurs is a two-component spinor (u, v) . In the event of an incoming hole, described by the lower part v , which is Andreev-reflected as an electron, described by the upper part u , the electron-hole correlations dictate that these two parts of the wavefunction are coherent (except for a small deviation at $E \neq 0$). But this also renders F non-zero, which can be understood physically because if the incident hole and Andreev-reflected electron are correlated, then so are also the (i) electron filling the spot of the hole and (ii) the Andreev-reflected electron - and it is these two electrons that give rise to $F \neq 0$. The phase of the electron filling the spot of the hole is determined by the phase of the hole that is annihilated and thus the two electrons are phase-coherent as well. Similarly, correlations also exist between an incoming electron that is Andreev-reflected and the electron that combines with this electron and forms a Cooper pair inside the superconductor.

Mathematically, the link between the field operators Ψ and the wavefunction scalars u and v , which are eigenfunctions of the BdG equations, is obtained by expanding the field operators in precisely these eigenfunctions. For instance, one could write [42]:

$$\Psi_{\uparrow} = \sum_n [\alpha_{n,\uparrow} u_n e^{-iE_n t/\hbar} - \alpha_{n,\downarrow}^{\dagger} v_n^* e^{iE_n t/\hbar}], \quad (12.262)$$

$$\Psi_{\downarrow}^{\dagger} = \sum_n [\alpha_{n,\uparrow} v_n e^{-iE_n t/\hbar} - \alpha_{n,\downarrow}^{\dagger} u_n^* e^{iE_n t/\hbar}], \quad (12.263)$$

where the summation over n is taken over all eigenstate energies E_n while $\alpha_{n,\sigma}$ is a fermion annihilation operator for the quasiparticle with energy E_n . By inserting these field operators Ψ_{σ} into $F \sim \langle \Psi_{\uparrow} \Psi_{\downarrow} \rangle$, it is clear that the anomalous Green function will be determined by the eigenstates u and v for the system. When we are considering an NS system, one can show that for an incoming electron ψ_e with energy E which is Andreev-reflected as a hole ψ_A we have

$$\begin{pmatrix} u \\ v \end{pmatrix} = \psi_e + r_A \psi_h \simeq \begin{pmatrix} e^{iEx/\hbar v_F} \\ e^{-i\phi - i\cos(E/\Delta) - iEx/\hbar v_F} \end{pmatrix} e^{ik_F x} \quad (12.264)$$

where r_A is the Andreev reflection coefficient and ϕ is the superconducting phase. As also discussed on page 190 in [43], the energy-resolved anomalous Green function $F(E)$ at point x will then be determined by products such as:

$$uv^* \propto e^{2iEx/\hbar v_F + i\phi}. \quad (12.265)$$

Therefore, the electron-hole coherence generated by Andreev-reflection does give rise to an anomalous Green function involving correlations between an *electron pair* inside a normal metal in contact with a superconductor. For $E = 0$, the relative phase does not change with x and coherence is maintained throughout the entire normal metal (in practice limited by inelastic scattering).

Infinite penetration for $f(E)$ but finite penetration for total order parameter

An important distinction to be made is the following. It is often stated in the literature that the electrons and holes maintain their coherence up to a finite length $L_E \sim \hbar v_F/E$, but this seems somewhat misleading. In fact, the electron-hole correlation at one particular energy E will *not* decay inside the N part of a clean S/N bilayer regardless of how long the N part is. The reason is that $F(E)$, as shown above, goes like $e^{2iEx/\hbar v_F + i\phi}$. The extra phase gained by the electrons and holes thus disappears at periodic intervals and in general $F(E)$ simply oscillates throughout the normal metal. This is valid only in the hypothetical limit of zero inelastic scattering, but it shows an important principle. Namely, that the energy-resolved correlations persist indefinitely throughout

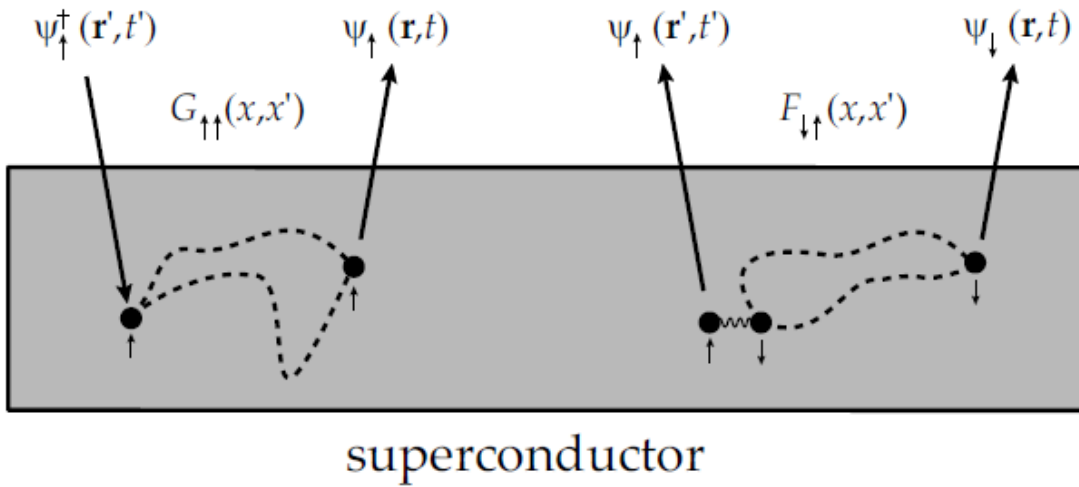


Figure 12.3: **Left:** the normal retarded Green function G represents the probability that if a spin- $\uparrow$ electron is added to the superconductor at $(\mathbf{r}', t')$, an electron with spin- $\uparrow$ will be located at $(\mathbf{r}, t)$ at a later time $t > t'$. The Green function is a statistical average over all possible paths from $\mathbf{r}'$ to $\mathbf{r}$. G thus can be thought of as describing the probability amplitude for a particle to move between two points in space and time in a coherent way (so that the initial and final states do not become orthogonal due to different phases). **Right:** the anomalous retarded Green function F is a measure of the probability that if a spin- $\uparrow$ electron of a Cooper pair is removed at $(\mathbf{r}', t')$, then the other spin- $\downarrow$ electron of the Cooper pair is found at $(\mathbf{r}, t)$. In other words, it measures the overlap between states which differ by one Cooper pair. This makes sense, because we know that the number of Cooper pairs N and the phase ϕ are canonical variables, meaning that if ϕ is sharply defined, N cannot be. Therefore, the BCS wavefunction describing the superconducting state must be a superposition of many different states with different numbers of Cooper pairs. If no Cooper pairs exist, $F = 0$. Taken from Ref. [40].

N. However, the *total superconducting order parameter* takes into account the contribution from all energies. This is seen in the BdG formalism from the summation over all eigenvalues n or in the Usadel formalism from the integration over all energies. The physical reason can be understood by considering the addition of several waves (the energy-resolved $F(E)$ functions) which become totally incoherent at large distances. At small distances, they add constructively, but at large distances the total superconducting order parameter must vanish (along with any supercurrent screening currents, for instance) despite the fact that the energy-resolved $F(E)$ survives indefinitely.

In conclusion, Andreev reflection can be compactly described as an incoming electron above the Fermi sea picking up an electron with opposite momentum below the Fermi sea and tunneling into the superconductor to form a Cooper pair. However, only when analyzing the process in detail, in particular the conversion of the electron into the hole, can we understand the apparent peculiarity that an electron with $-\mathbf{k}$ should tunnel in the $+\hat{x}$ -direction. Andreev reflection can also take place for an incident hole, in which case an electron is reflected and a Cooper pair is annihilated in the superconductor (transmitted to the normal region).

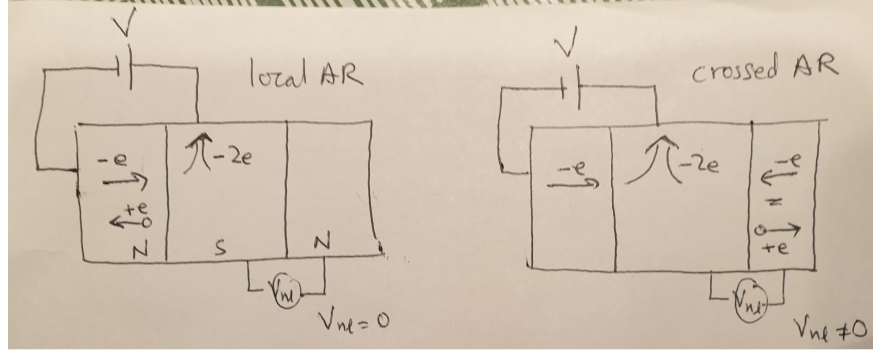


Figure 12.4: For CAR, we need an incoming current of $-e$ from the right N toward the interface in order to transmit a total supercurrent $-2e$ to the superconductor. This is equivalent to an outgoing hole of charge $+e$ in the right N.

12.24.3 Crossed Andreev reflection (CAR)

It is also possible to spatially separate the incoming electron and Andreev-reflected hole into different leads attached to the superconductor. Regardless of exactly where the leads are attached, the rule is that the incoming electron can only give rise to outgoing particles, whether it is an electron or hole that comes out on the other side. This is the only way to ensure that charge is conserved, so that $-2e$ is transferred to the superconductor in the case of a CAR-process.

For instance, if one considers a linear NSN structure, the incoming electron on the left side would be e^{ikx} whereas an Andreev-reflected hole on the left side would also be e^{ikx} . A transmitted electron on the right side would be e^{ikx} , but a crossed Andreev-reflected hole on the right side would be e^{-ikx} in order to describe a hole propagating towards right (away from the interface, so outgoing). In this way, we have a current of $-e$ incoming from both the left and right, transmitting $-2e$ to the superconductor. This is shown in the figure below.

It is instructive to consider the various sign of conductances for non-local and local transport processes in an NSN structure. Consider Fig. 12.5 where a bias voltage is applied between a left normal metal reservoirs and a superconducting reservoir, and another bias voltage between the right normal metal reservoir and a superconducting reservoir. In an open-circuit geometry to detect non-local conductance, I_2 would have to be zero which determines what V_2 is, as we shall see below. Assume now identical left and right interfaces for simplicity. The analysis below can be generalized to different interfaces straightforwardly. Now recall that positive current is defined as the direction in which positively charged particles move. Such particles move from high to low voltage V . This means electrons move from low to high voltage V . Consider now the left NS interface in the figure. If $V_S > V_1$, there should thus flow a positive current from S to N. To linear response, we can now write down the contribution to the currents I_1 and I_2 from all possible processes for subgap voltages. Then, we can only have AR, CAR, and EC contributing to transport since there are no long-lived quasiparticle states in the superconductor. Consider first AR. We get:

$$\begin{aligned} I_1 &= G_A(V_S - V_1), \\ I_2 &= G_A(V_S - V_2). \end{aligned} \quad (12.266)$$

All conductances G_i are defined to be positive. A quick consistency check of the above equation is in order: if $V_S > V_1$, electrons should be trying to move from the left N to S. This can induce AR, yielding electron transfer from N to S, corresponding to a positive current from S to N. Same

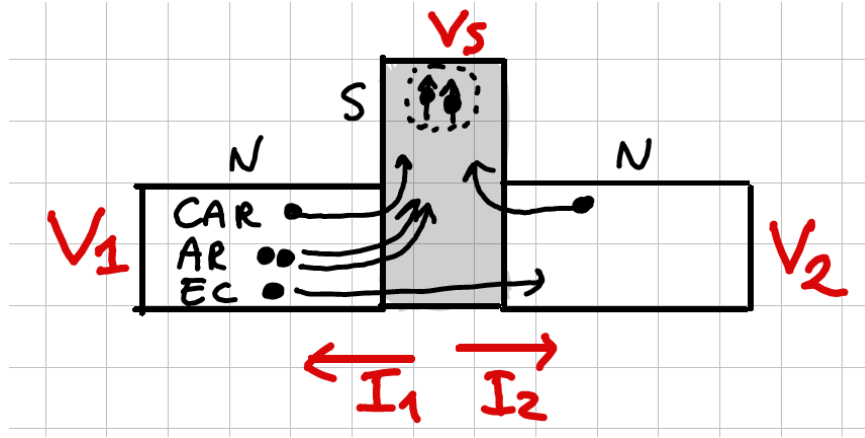


Figure 12.5: Typical experimental setup to detect non-local transport. In the CAR process, an electron is taken from each N to form a Cooper pair in S.

reasoning at the right interface.

Now consider the contribution from CAR. We get for the left interface:

$$I_1 = G_{\text{CAR}}(V_S - V_1) + G_{\text{CAR}}(V_S - V_2). \quad (12.267)$$

There are two contributions to I_1 : the first is due to an incoming electron from the left N which gives rise to a CAR-hole in the right N, and the second is due to an incoming electron from the right N toward S giving rise to a CAR-hole in the left N. The latter would induce an electron current flowing from right to left across the right interface when $V_S > V_2$, meaning a positive current flowing from left to right (corresponding to $I_2 > 0$, in agreement with the above formula). In the same way, we get

$$I_2 = G_{\text{CAR}}(V_S - V_2) + G_{\text{CAR}}(V_S - V_1) \quad (12.268)$$

We finally have the case of EC. We get

$$\begin{aligned} I_1 &= G_{\text{EC}}(V_S - V_1) - G_{\text{EC}}(V_S - V_2) = G_{\text{EC}}(V_2 - V_1), \\ I_2 &= -G_{\text{EC}}(V_S - V_1) + G_{\text{EC}}(V_S - V_2) = G_{\text{EC}}(V_1 - V_2). \end{aligned} \quad (12.269)$$

These relations can be summarized in matrix form if we keep the superconducting reservoir grounded at $V_S = 0$:

$$\begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} -G_A - G_{\text{CAR}} - G_{\text{EC}} & G_{\text{EC}} - G_{\text{CAR}} \\ G_{\text{EC}} - G_{\text{CAR}} & -G_A - G_{\text{CAR}} - G_{\text{EC}} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}. \quad (12.270)$$

This proves that CAR and EC contribute to the non-local transport (off-diagonal elements in the above matrix) with opposite sign.

12.24.4 Scaling of Andreev reflection, elastic cotunneling, and crossed Andreev reflection with tunneling amplitude

Let t be the normal-state transmission coefficient. A normal tunneling process for an electron across an interface will then have a probability (or conductance) scaling like $|t|^2$.

An Andreev-reflection process, however, will scale like $|t|^4$. This can be understood by considering the phenomenological theory for zero-energy states in superconductors published by Asano et al. PRB 2004 <https://arxiv.org/pdf/cond-mat/0307345> (although note that there is an inconsequential error there in that holes tunneling from right to left should also have t_N rather than t_N^* , which can be seen by considering the incident and scattered waves). The point is that in the Andreev-reflection process, an electron first tunnels through the interface into the superconductor, is then relected as a hole by the order parameter Δ , before finally tunneling back across the interface into the normal metal as a hole. These are two tunneling processes, so in total the probability for Andreev reflection $|r_{eh}|^2$ will scale as $|t|^4$.

Let us now consider non-local transport in an NSN junction. There are two processes: elastic cotunneling (EC) and crossed Andreev reflection (CAR). In <https://arxiv.org/pdf/cond-mat/0011339> it is derived that both of these processes scale as $|t|^4$. This can be understood as follows. For EC, it is easy to see: the electron tunnels over two interfaces, so we get $|t|^2 \times |t|^2 = |t|^4$. For CAR, the only difference from local AR is that the hole emerges into a different electrode, but it still involves transmission of an electron across an interface and transmission of a hole across an interface, so we also get $|t|^2 \times |t|^2 = |t|^4$.

12.24.5 Microscopic understanding of the superconducting proximity effect in a ferromagnet

In a ferromagnet, as in normal metals, the spatial dimensionality is not crucial in order to understand the nature of the superconducting proximity effect. For simplicity, we thus consider a 1D system extended along the x -axis. In the ferromagnet, the electron bands are not spin-degenerate, but split vertically with $2h$. This can be seen from the dispersion relations $\epsilon_\sigma(k) = k^2/2m - \mu + \sigma h$. In order for two electrons with opposite spin to form a Cooper pair at the Fermi level, the momenta of the electrons necessarily have to be different: $k_\uparrow$ and $k_\downarrow$ where $k_\sigma = \sqrt{2m(\mu + \epsilon + \sigma h)}$. This results in the singlet Cooper pairs acquiring a finite center-of-mass momentum $k_\uparrow - k_\downarrow$ and thus oscillating as a function of the center of mass coordinate X in the ferromagnet.

This can be seen formally as follows.

12.24.6 Microscopic understanding of the superconducting proximity effect in a metal with Rashba spin-orbit coupling

In the ferromagnetic case, we see that the oscillations of the pairing amplitude is a direct consequence of the broken time-reversal symmetry in the eigenvalues: $E_{\mathbf{k},\uparrow} \neq E_{-\mathbf{k},\downarrow}$. Pairing states with opposite spins must have a finite total momentum.

Consider now an 1D Rashba metal for simplicity with $\vec{g}_{\mathbf{k}} = (0, 0, -ik_x)$. This looks like a ferromagnet with a k -dependent exchange field in the z -direction. The eigenvalues now satisfy $E_{\mathbf{k},\uparrow} = E_{-\mathbf{k},\downarrow}$ and pairing can occur between particles of opposite momenta without any total center of mass momentum. Similarly to the ferromagnetic case, however, triplet pairing occurs in the SOC case because spin-degeneracy has been lifted: $E_{\mathbf{k},\uparrow} \neq E_{\mathbf{k},\downarrow}$. This can be shown by a general calculation of a 1D X/S bilayer where X has lifted spin-degeneracy so that $k_\uparrow \neq k_\downarrow$ (as in Appendix A of Reeg *et al.* PRB 2015). Physically, this can be understood as ...

In 2D, the proximity effect between S and SOC becomes qualitatively different. When the $\vec{g}_{\mathbf{k}}$ vector lies in the xy -plane, each energy band cannot be associated with a determined spin direction: the spin rotates as one moves around the Fermi surface. Therefore, interband transitions are allowed upon

Andreev reflection and the induced pairing amplitude will be a sum of non-oscillatory (intraband processes) and oscillatory (interband processes) terms.

12.24.7 Microscopic understanding of the superconducting proximity effect in an antiferromagnet

Regardless of whether one considers periodic boundary conditions or hard wall boundary conditions on a lattice, one will find that there are odd-frequency triplet correlations induced in a compensated AF/SC bilayer near the interface. These alternate in sign with each lattice site, just like the staggered magnetization in the AFM. However, to see this, one needs to plot the correlation function in real space. If one Fourier transforms along the y -direction to implement periodic boundary conditions and then plots a correlation function averaged over all lattice sites in the y -direction, $\sum i_y \langle c_{i_x i_y \uparrow}(\tau) c_{i_x i_y \downarrow}(0) \rangle + (\downarrow \rightarrow \uparrow)$, the correlation function will vanish for an equal number of lattice sites. The reason is precisely the atomic oscillations in the triplet component, which causes the average of the correlation function along y to vanish. This is the type of correlation function that was considered in Johnsen *et al.* PRB Rapid (2020), whereas the real-space one was considered in Bobkova PRB (2022). The latter one thus shows the triplet, whereas the former one does not, but both results are correct: the triplet correlation function, as it was defined in Johnsen's paper, is indeed zero since it is an average over all sites in the y -direction.

12.25 Derivation of the BTK-formula for current in an NS junction

It is instructive to consider an approach where the normal metal and superconductor are divided into two leads each: electron-like and hole-like leads. This approach is in turn based on a Landauer-like model with transport in different channels. Since we want to derive an expression for the charge current, we have the luxury of being able to evaluate it wherever we like since it has to be conserved. For reasons we will explain shortly, we choose to evaluate the charge current on the normal metal side rather than the superconductor.

We start with a brief note regarding the inclusion of group velocity in the normalization factor for the scattering wavefunctions. Consider 1D and two normal metals for simplicity. Assume the wavevectors k_L and k_R can be different on each side of the interface. The probability current is obtained from

$$j_P = \frac{\hbar}{m} \text{Im}\{\psi^* \partial_x \psi\}. \quad (12.271)$$

Now, the wavefunction on the left and right side can be written

$$\begin{aligned} \psi_L &= e^{ik_L x} + r e^{-ik_L x}, \\ \psi_R &= t e^{ik_R x}. \end{aligned} \quad (12.272)$$

for an incoming wave from the L side. This gives

$$\begin{aligned} j_L &= \frac{k_L}{m} (1 - |r|^2), \\ j_R &= \frac{k_R}{m} |t|^2. \end{aligned} \quad (12.273)$$

From probability current conservation at the interface, $j_L = j_R$ at $x = 0$, we obtain the following equation after dividing on k_L/m :

$$1 = \frac{k_R}{k_L}|t|^2 + |r|^2. \quad (12.274)$$

The transmission coefficient T is therefore $\frac{k_R}{k_L}|t|^2$ whereas the reflection coefficient R is $|r|^2$. Note that $T + R = 1$.

Instead, some authors choose to normalize the wavefunctions with a factor $1/\sqrt{k_{L,R}}$. An advantage of doing so is that it gives a unitary scattering matrix S , which is a desirable property. In this way, the particle flux carried by an incoming particle is identical regardless of whether it is incoming from the left or right region. In other words, one writes

$$\begin{aligned} \psi_L &= \frac{1}{\sqrt{k_L}}(e^{ik_L x} + r e^{-ik_L x}), \\ \psi_R &= \frac{1}{\sqrt{k_R}} t e^{ik_R x}. \end{aligned} \quad (12.275)$$

In this case, we get

$$\begin{aligned} j_L &= \frac{1}{m}(1 - |r|^2), \\ j_R &= \frac{1}{m}|t|^2, \\ 1 &= |t|^2 + |r|^2 \equiv T + R. \end{aligned} \quad (12.276)$$

Note that regardless of whether one includes the $1/\sqrt{k}$ normalization factor or not, the probability currents normalized to the incident probability current will be identical.

Now, back to the NS junction. The total current flowing in the e lead on the normal metal side is given by the totality of all processes that give rise to electron flow on the normal metal. Consider first an incoming particle toward the NS interface. This can be either from the N or S side. This particle will give rise to a charge current J in the e channel on the N side which is determined as follows. J is equal to the number of incoming particle states dN in the interval $[E, E + dE]$ times the occupation number $f(E)$ for such a state times the charge current j_Q that is *induced* in the e lead as a result of the incoming particle. The latter is computed from the wavefunction of a single such state using the quantum mechanical formula

$$j_Q = -\frac{e\hbar}{m} \text{Im}\{f^* \nabla f + g^* \nabla g\} \quad (12.277)$$

for a wavefunction in the BTK formalism of the form

$$\psi = \begin{pmatrix} f \\ g \end{pmatrix}. \quad (12.278)$$

Thus:

$$J = j_Q f(E) dN = j_Q \frac{dN}{dE} f(E) dE \quad (12.279)$$

where j_Q is the *resulting charge current in the e lead* due to the incoming particle.

Let us evaluate the total current in this way. Doing so, we will show that it reproduces the BTK formula. The advantage of using the above recipe for obtaining the charge current, rather than probability current densities as done in BTK, is that one avoids potential confusion regarding how to obtain a charge current flow from a probability current flow. The general formula for the conserved probability current j_P is:

$$j_P = \frac{\hbar}{m} \text{Im}\{f^* \nabla f - g^* \nabla g\} \quad (12.280)$$

To see why confusion may occur if one insists on writing down an expression for the charge current in terms of probability currents, consider first an electron in N. Its wavefunction is

$$\psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_F x}. \quad (12.281)$$

The probability and charge currents are:

$$j_P = \frac{\hbar}{m} k_F, \quad (12.282)$$

$$j_Q = \frac{-e\hbar}{m} k_F. \quad (12.283)$$

so that $j_Q = -ej_P$. For a electron-like quasiparticle (ELQ) in a superconductor, one might be tempted to think that the generalization of this formula can be obtained by instead multiplying the probability current with the fractional charge $q = -e(|u|^2 - |v|^2)$ carried by a quasiparticle. To check this, consider the ELQ wavefunction in S:

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix} e^{ik_F x}. \quad (12.284)$$

We considered supergap energies $E > \Delta$ for simplicity and thus approximated the wavevector as $k_F = \sqrt{2m\mu}$ rather than $\sqrt{2m(\mu + \sqrt{E^2 - \Delta^2})}$. Now, we get

$$j_P = \frac{\hbar}{m} k_F (|u|^2 - |v|^2), \quad (12.285)$$

$$j_Q = \frac{-e\hbar}{m} k_F. \quad (12.286)$$

Clearly, we don't have $j_Q = qj_P$. It might seem surprising that the charge current carried by a quasiparticle with fractional charge q and group velocity $v_F(|u|^2 - |v|^2) = v_F q$ carries *the same* current as an electron in a normal metal. This can be understood as follows. The electron part of the ELQ wavefunction carries charge $-e|u|^2$ with wavevector k_F toward the right, whereas the hole part of the ELQ wavefunction carries charge $e|v|^2$ with wavevector k_F toward the left (since momenta and phase velocity, as well as group velocity, are opposite for holes). The total current is therefore $-ek_F/m(|u|^2 + |v|^2) = -ek_F/m$.

Due to the above, it seems more appropriate to use the charge current expression directly to evaluate currents flowing in hybrid structures involving superconductors. Consider now the NS junction. Both N and S can be split up into two current-carrying channels: the e lead and h lead. There are five possible contributions to current in the e lead on the N side: an incoming e from the N side, a reflected e on the N side, an incoming h from the N side, an incoming electron-like qp from the S

side, an incoming hole-like qp from the S side. We label these contributions 1 – 5.

Before proceeding to calculate them, let us make a conceptual remark. Shouldn't we take into account the possibility of an incoming supercurrent from the S side toward the normal metal? The above procedure, considering only incoming quasiparticles, actually does so and the reason is as follows. A supercurrent incoming from the bulk of the superconductor will be gradually converted into a quasiparticle current as it approaches the interface. Precisely at the interface position, the current carried by the condensate in the superconductor must equal zero because no such current exists in the normal metal. So just like an incoming resistive current from N to S first enters S as a quasiparticle current which is gradually converted into a supercurrent, an incoming supercurrent from S to N is gradually converted into a quasiparticle current near the interface which then enters N in the form of a quasiparticle current in the e and h leads. However, note that for $E < \Delta$, there are no available quasiparticle states in the superconductor (including near the interface): their density of states is zero. Therefore, the contribution from quasiparticles coming in from the superconducting side (due to an incoming supercurrent being converted to quasiparticle current near the interface, as explained above) should be zero for $E < \Delta$. This is consistent with the treatment below where we shall see that the current contribution from a given incoming quasiparticle is proportional to its density of states.

In addition, we will see below that the formula for electric current flowing in N includes the possibility that an incoming hole from the N side is Andreev-reflected into the electron channel of the normal metal. When this happens, a Cooper pair is transmitted from the superconductor, which makes the contribution from the supercurrent in the junction accounted for via this channel as well.

Let us now compute the contributions 1-5 according to our reasoning above where we use the quantum mechanical charge current density rather than the quantum mechanical probability current density. Assume that a voltage is applied across the junction so that distribution function for electrons is $f(E - eV)$ on the N side while it is $f(E)$ on the S side. Since $dN/dE = \mathcal{N}$ where $\mathcal{N}$ is the density of states, we find:

- 1: incoming electron on N side has $j_Q = -ek_F/m$ and so contributes to the total charge current density in the e channel on the N side with $\mathcal{N}_N(-ek_F/m)f(E - eV)$.
- 2: incoming electron on N side can produce a reflected electron which has $j_Q = ek_F/m|b|^2$ and so contributes to the total charge current density in the e channel on the N side with $\mathcal{N}_N(ek_F/m)|b|^2f(E - eV)$.
- 3: incoming hole on N side produces via Andreev-reflection an electron wavefunction (with coefficient a_h) moving away from the interface on the N side, and thus an accompanying current $j_Q = ek_F/m|a_h|^2$. Thus, total contribution is $\mathcal{N}_N(ek_F/m)|a_h|^2[1 - f(-E - eV)]$ since the DOS for holes is the same as for electrons and since the occupation number for a hole with energy E is equal to the occupation of a missing electron at energy $-E$, giving the $1 - f$ factor.
- 4: incoming ELQ from S side can produce an electron wavefunction (with coefficient c') moving away from the interface on the N side. The accompanying charge current is $j_Q = ek_F/m|c'|^2$, so we get the total contribution $\mathcal{N}_S(ek_F/m)|c'|^2f(E)$.
- 5: incoming HLQ from S side can produce an electron wavefunction (with coefficient d') moving away from the interface on the N side. The accompanying charge current is $j_Q = ek_F/m|d'|^2$,

so we get the total contribution $\mathcal{N}_S(ek_F/m)|d'|^2 f(E)$.

The DOS factor can also be seen to arise from the fact that we are supposed to integrate over all possible wavevectors of incoming particles, $\int dk_{\text{inc}}$. But this can be converted into an energy integral via $\int dE \frac{dk_{\text{inc}}}{dE}$. The latter factor is proportional to the DOS in 1D. Note that this factor then becomes different depending on which incoming particle we have. For instance, in the normal metal we have

$$\frac{dk_{\text{inc}}}{dE} \propto 1/k \quad (12.287)$$

and in the superconductor we have

$$\frac{dk_{\text{inc}}}{dE} \propto N(E)/k \quad (12.288)$$

where $N(E) = E/\sqrt{E^2 - \Delta^2}$ is the ratio between the superconducting DOS and normal state DOS. The factors k in the two above expressions are different, but close to the Fermi level they are well approximated by k_F .

We thus have the total electric current j_e flowing in the e lead:

$$\begin{aligned} j_e &= \mathcal{N}_N(-ek_F/m)f(E - eV) + \mathcal{N}_N(ek_F/m)|a_h|^2[1 - f(-E - eV)] + \mathcal{N}_N(ek_F/m)|b|^2 f(E - eV) \\ &\quad + \mathcal{N}_S(ek_F/m)|c'|^2 f(E) + \mathcal{N}_S(ek_F/m)|d'|^2 f(E) \\ &= -ek_F/m \mathcal{N}_N \left(f(E - eV) - |a_h|^2[1 - f(-E - eV)] - |b|^2 f(E - eV) \right. \\ &\quad \left. - \frac{\mathcal{N}_S}{\mathcal{N}_N}|c'|^2 f(E) - \frac{\mathcal{N}_S}{\mathcal{N}_N}|d'|^2 f(E) \right). \end{aligned} \quad (12.289)$$

Note that the $\mathcal{N}_N$ factor goes like $1/k$, and so will cancel the k_F factor inside the integrand as long as we are close to the Fermi level.

We can compute the total current in the hole lead j_h similarly, providing a total current

$$j = j_e + j_h \quad (12.290)$$

on the normal metal side. A calculation shows that $j_e = j_h$, so it suffices to consider j_e (we comment on why this is so later). Note that we cannot use this method to evaluate the current on the superconducting side, because of the presence of a *supercurrent* there. In effect, if we try to compute the current on the S side as only carried by electron- and hole-like quasiparticles in the e and h leads of the superconductor, one obtains 0 for subgap energies. However, this must be wrong because a current can exist on the N side for subgap energies. We can thus only use this method of e and h leads in non-superconducting materials where there is no condensate that can carry part of the current.

Based on the above presentation, we can now understand the expression for current that BTK writes down in their original paper. There isn't much explanation accompanying that expression in the paper, but we are now in a position to understand why it looks like it does. BTK writes that the current is given by (omitting a constant prefactor):

$$j \propto \int dE [f_{\rightarrow}(E) - f_{\leftarrow}(E)] \quad (12.291)$$

where $f_{\rightarrow}(E)$ is the distribution function for right-moving electrons and $f_{\leftarrow}$ is the distribution function for left-moving electrons. BTK writes that

$$f_{\rightarrow}(E) = f(E - eV), \quad (12.292)$$

while

$$f_{\leftarrow}(E) = [1 - f(-E - eV)]A_h(E) + B(E)f(E - eV) + [C(E) + D(E)]f(E). \quad (12.293)$$

Here, BTK states that the coefficients $\{A_h, B, C, D\}$ represent the probabilities for (respectively) Andreev reflection of an incoming hole from the left side with energy E , normal reflection of an incoming electron from the left side with energy E , and transmission of an electron- and hole-like quasiparticle incoming from the right side with energy E . More precisely, $\{A_h, B, C, D\}$ are the probability density currents for the different scattering processes that can take place due to an incoming electron from the N side.

The point is that all processes included in $f_{\leftarrow}$ contribute to a left-going current in the electron channel of the normal metal whereas $f_{\rightarrow}$ contains all processes that contribute to a right-going current in the electron channel of the normal metal. Thus, BTK only considers the electron channel on the normal metal side and do not compute the corresponding current in the hole channel. However, doing so should produce exactly the same current as in the electron channel and thus merely a total factor of 2. The reason for why the hole current gives the same contribution as the electron current can be understood qualitatively by considering a bilayer where the chemical potential is raised with eV on one side. Electrons will spill over to the other side due to the raised chemical potential. But if we draw the corresponding bands for hole excitations, it is clear that holes will spill over to the side where the chemical potential is raised, i.e. in the opposite direction of electrons. Since holes carry opposite charge, the electric current is the same in both cases. We also show this with a direct calculation at the end of this section.

Let us now compare our Eq. (12.289) with (12.291) to see if they are really the same up to a constant of proportionality. The incident electron is the same as well as the normal-reflection term $|b|^2 = B$. For the quasiparticles on the superconducting side, the question is if

$$\frac{\mathcal{N}_S}{\mathcal{N}_N}|c'|^2 = C \text{ and } \frac{\mathcal{N}_S}{\mathcal{N}_N}|d'|^2 = D. \quad (12.294)$$

Recall that c', d' are the scattering coefficients for incoming quasiparticles from the S side, whereas C and D are computed for an incoming electron on the N side. To check if the above relations are valid, we perform an explicit calculation. Consider the barrierless case for simplicity. For an incoming e from the N side, we have

$$\begin{aligned} \psi_N &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ikx} + a \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ikx} + b \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx}, \\ \psi_S &= c \begin{pmatrix} u \\ v \end{pmatrix} e^{ik^+x} + d \begin{pmatrix} v \\ u \end{pmatrix} e^{-ik^-x} \end{aligned} \quad (12.295)$$

and obtain

$$\begin{aligned} a &= v/u, \quad b = 0, \quad c = 1/u, \quad d = 0, \\ C &= |c|^2(|u|^2 - |v|^2) = \frac{|u|^2 - |v|^2}{|u|^2}. \end{aligned} \quad (12.296)$$

We used that $k^\pm \simeq k$ in computing the coefficients. For an incoming ELQ from the S side, we have

$$\begin{aligned}\psi_N &= c' \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx} + d' \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx}, \\ \psi_S &= \begin{pmatrix} u \\ v \end{pmatrix} e^{-ikx} + a' \begin{pmatrix} v \\ u \end{pmatrix} e^{-ikx} + b' \begin{pmatrix} u \\ v \end{pmatrix} e^{ikx}.\end{aligned}\quad (12.297)$$

and obtain

$$\begin{aligned}a' &= -v/u, \quad b' = 0, \quad c' = \frac{u^2 - v^2}{u}, \quad d' = 0, \\ C' &= \frac{|c'|^2}{|u|^2 - |v|^2}.\end{aligned}\quad (12.298)$$

Moreover, we know that:

$$\frac{\mathcal{N}_S}{\mathcal{N}_N} = \text{Re} \left\{ \frac{E}{\sqrt{E^2 - \Delta^2}} \right\} = \begin{cases} 0 & \text{for } E < \Delta \\ \frac{1}{|u^2 - v^2|} & \text{for } E > \Delta \end{cases} \quad (12.299)$$

Therefore, we see that

$$C = \begin{cases} 0 & \text{for } E < \Delta \\ \frac{|u|^2 - |v|^2}{|u|^2} & \text{for } E > \Delta \end{cases}, \quad |c'|^2 \frac{\mathcal{N}_S}{\mathcal{N}_N} = \begin{cases} 0 & \text{for } E < \Delta \\ \frac{u^2 - v^2}{|u^2|} & \text{for } E > \Delta \end{cases} \quad (12.300)$$

Since u and v are both real for $E > \Delta$, we have shown that $C = |c'|^2 \frac{\mathcal{N}_S}{\mathcal{N}_N}$. The same proof holds for the relation between D and d' . This proves that Eq. (12.289) and (12.291) are equivalent.

Since the coefficients $\{A, B, C, D\}$, where now A (in contrast to A_h) corresponds to Andreev-reflection of an incident electron to a hole, are the probability current densities normalized on the incident probability current density of the incoming electron, one can show that $A + B + C + D = 1$. Using this conservation of probability, we can rewrite j to

$$\begin{aligned}j &\propto \int dE \left(f(E - eV) - f(E + eV)A_h(E) - B(E)f(E - eV) - [1 - A(E) - B(E)]f(E) \right) \\ &= \int dE \left(f(E - eV)[1 + A_h(-E) - B(E)] - f(E)[1 + A(-E) - B(E)] \right) \\ &= \int dE \left(f(E - eV)[1 + A_h(-E) - B(E)] - f(E)[1 + A(-E) - B(E)] \right).\end{aligned}\quad (12.301)$$

Here, we used that $1 - f(-x) = f(x)$ for the Fermi-Dirac distribution function. Note how we have $A_h = |a_h|^2$ for the incoming hole from the N side, whereas we have $A = |a|^2$ for the incoming electron on the N side. BTK then states that one may use $A(-E) = A(E)$ which leads to the final form of the BTK equation. This is somewhat confusing since inspection of the general formula for $A(E)$ in the BTK paper table does not have this property.

To clarify this point, we first note a fundamental symmetry of the BdG equations. Namely, if (u, v) is an eigenstate for positive energy E , then $(-v^*, u^*)$ is an eigenstate for the negative energy $-E$. However, note that the values for v^* and u^* that enter the above expression should be the ones obtained for $E > 0$. Therefore, if we use the analytical expression $u, v = \sqrt{\frac{1}{2}(1 \pm \xi/E)}$, we should therefore write the negative energy solution as $(-u^*, v^*)$ to get the correct result since for negative

energies u has the value v has for positive energies.

The complex conjugation is necessary even for a real gap since u, v are complex for subgap energies $|E| < \Delta$. Therefore, we can obtain the Andreev-reflection probability current density for an incoming electron with $E < 0$ simply by replacing $u \rightarrow -u^*$ and $v \rightarrow v^*$. Since we found $a = v/u$ for $E > 0$, we get $a = -v^*/u^*$ for $E < 0$. Therefore, $|a|^2$ is invariant under $E \rightarrow -E$. This proves that $A(E) = A(-E)$ when using the appropriate expression for A for negative energies (in contrast to BTK). The same argument holds for $A_h = |a_h|^2$. What remains to be proven is that $A_h(E) = A(E)$. This is done with an explicit calculation when considering an incoming hole with positive energy, including also the effect of a barrier Z :

$$\begin{aligned}\psi_N &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ikx} + a_h \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx} + b_h \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx}, \\ \psi_S &= c_h \begin{pmatrix} u \\ v \end{pmatrix} e^{ik^+x} + d_h \begin{pmatrix} v \\ u \end{pmatrix} e^{-ik^-x}\end{aligned}\quad (12.302)$$

Determining the coefficients using Maple (not shown here), one verifies that $A_h(E) = A(E)$. In this way, due to the relations $A_h(E) = A(E)$ and $A(E) = A(-E)$, one may write the integrand of BTK as $1 + A(E) - B(E)$ where A and B are the coefficients evaluated only for an incoming electron, and we end up with:

$$j = \int dE [1 + A(E) - B(E)] [f(E - eV) - f(E)]. \quad (12.303)$$

Finally, we note that $j_h = j_e$ can be seen to hold by starting with the equation for the total electric current flowing in the hole channel:

$$j_h = - \int dE [f(E + eV) - Af(E - eV) - B_h(E + eV) - (1 - A_h - B_h)f(E)] \quad (12.304)$$

where B_h is the probability coefficient for an incoming hole to be reflected normally, and using that $B_h(E) = B_h(-E)$ as well as the above symmetries for A and A_h .

12.25.1 Relation between probability coefficients due to unitarity of scattering matrix

Consider an NS junction. We are used to the following equation describing conservation of probability:

$$1 = R(e_N \rightarrow e_N) + R(e_N \rightarrow h_N) + T(e_N \rightarrow e_S) + T(e_N \rightarrow h_S) \quad (12.305)$$

meaning that an incoming electron from the N side must be either reflected to an electron in N (e_N), Andreev-reflected to a hole in N (h_N), or transmitted as electron or hole in S (e_S and h_S). This makes sense intuitively: an incoming electron must be scattered somewhere.

The question is now if/why the following equation is also true:

$$1 = R(e_N \rightarrow e_N) + R(h_N \rightarrow e_N) + T(e_S \rightarrow e_N) + T(h_S \rightarrow e_N) \quad (12.306)$$

This corresponds to the equation below eq 19 in <https://journals.aps.org/prb/pdf/10.1103/PhysRevB.67.094515>. This expresses that the sum of all scattering probabilities that lead to an electron flowing on the N side are equal to unity. It is perhaps less obvious intuitively why this must be the case.

I suspected during our meeting that this equation holds because of the unitarity of the scattering matrix S which connects incoming and outgoing waves. As far as I can see, this is indeed the case. To see this, consider eq. 1.58 here: <http://assets.press.princeton.edu/chapters/s8695.pdf> (r, t) are the reflection and transmission coefficients for incoming waves from one side of the interface (for instance N), whereas (r', t') are the same coefficients for incoming waves from the other side of the interface (for instance S). The crucial point is now that in order to conserve probability current (section 1.2.1), the S-matrix must be unitary: $S^\dagger = S^{-1}$. Now, due to this property alone, it is derived in the above document (see equations 1.24-1.31) that

$$|S_{12}| = |S_{21}||S_{11}| = |S_{22}| \quad (12.307)$$

If we now translate this to a N/S bilayer, it follows that for instance:

$$R(e_N \rightarrow h_N) = R(h_N \rightarrow e_N) \quad (12.308)$$

It expresses that the probability for scattering from one channel to another is the same as for the opposite process. In more complicated systems, where e.g. time-reversal symmetry is broken, there can be other processes which have the same probability. But the point is that due to the unitarity of S , it is possible to equate certain probabilities [such as $R(e_N \rightarrow h_N)$] to other probabilities [such as $R(h_N \rightarrow e_N)$].

Once we have such relations, the equation below eq 19 which we did not understand now makes sense:

we simply take the equation we are used to, $1 = R(e_N \rightarrow e_N) + R(e_N \rightarrow h_N) + T(e_N \rightarrow e_S) + T(e_N \rightarrow h_S)$, and use that $R(e_N \rightarrow h_N) = R(h_N \rightarrow e_N)$ and similarly for the T -coefficients. Then, the equation we wanted to understand follows immediately.

To do: write down scattering matrix for NS bilayer, and show explicitly that e.g. $T(e_N \rightarrow h_S) = T(h_S \rightarrow e_N)$.

12.25.2 Current carried by continuum and Bagwell formula

The current carried by the continuum in Josephson junctions ($E > \Delta$) can be computed using the Bagwell formula from BdG, see eq. 2.90 in https://mycourses.aalto.fi/pluginfile.php/1414652/mod_resource/content/13/theory_sc.pdf and eq. 10 in <https://journals.aps.org/prb/pdf/10.1103/PhysRevB.49.6841>. These are formally derived using BdG theory. Note that the same charge e is used for both the u and v terms and regardless of what the injected quasiparticle is. Moreover, a special mention regarding how to choose $f(E)$ is required. First, note that the same $f(E)$ term should be used for both the u and v -terms. Secondly, note that the distribution function that should be used corresponds to the incident quasiparticle, since this is the excitation $\gamma^\dagger \gamma$ that we are considering. Therefore, for an injected electron from a normal metal with bias voltage eV , we have $f(E) = n(E - eV)$ where n is FD. But for an injected hole from a normal metal, we have $f(E) = n(E + eV) = 1 - n(-E - eV)$. As mentioned above, the charge is still the same. By using this procedure, one derives exactly the same electron and hole currents as when one uses the procedure described in the subsection above. Note how we get $1 - f(E + eV)$ in front of the v terms for injected holes, but the 1's cancel in the end as one obtains the prefactor $A - 1 + B + D + C = 0$ in front of the ones when taking into account both injected electrons and holes. To be concrete,

using the Bagwell formula for an NS junction we get

$$\begin{aligned}
j &= f(E - eV)(1 - B_{e \rightarrow e}) + [1 - f(E - eV)]A_{e \rightarrow h} \\
&\quad f(E + eV)(-A_{h \rightarrow e} + [1 - f(E + eV)](-1 + B_{h \rightarrow h})) \\
&\quad f(E)(-T_{e \rightarrow e}) + [1 - f(E)]T_{e \rightarrow h} \\
&\quad f(E)(-T_{h \rightarrow e} + [1 - f(E)]T_{h \rightarrow h}).
\end{aligned} \tag{12.309}$$

The first line is for injected electrons from N, second line for injected holes from N, third line injected ELQ from S, fourth line injected HLQ from S. Looking now at the current flowing in the e channel, it reads

$$\begin{aligned}
j_e &= f(E - eV)(1 - B_{e \rightarrow e}) - f(E + eV)A_{h \rightarrow e} - (T_{e \rightarrow e} + T_{h \rightarrow e})f(E) \\
&= f(E - eV)(1 - B_{e \rightarrow e}) - f(E + eV)A_{h \rightarrow e} - (1 - B_{e \rightarrow e} - A_{h \rightarrow e})f(E).
\end{aligned} \tag{12.310}$$

This is exactly the expression for electron lead current in the above subsection when taking into account that $A_{h \rightarrow e} = A_{e \rightarrow h}$. In the h channel, it reads

$$\begin{aligned}
j_h &= -f(E - eV)A_{e \rightarrow h} + f(E + eV) - f(E + eV)B_{h \rightarrow h} \\
&\quad - (T_{e \rightarrow h} + T_{h \rightarrow h})f(E) + (A_{e \rightarrow h} + B_{h \rightarrow h} + T_{e \rightarrow h} + T_{h \rightarrow h} - 1) \\
&= f(E + eV) - f(E - eV)A_{e \rightarrow h} - f(E + eV)B_{h \rightarrow h} - [1 - A_{e \rightarrow h} - B_{h \rightarrow h}]f(E).
\end{aligned} \tag{12.311}$$

Again, this is exactly the expression for the hole current above.

We underline that the usage of this formula in Paolas PRB from 2022 appears to be incorrect in several respects: using q_l inside the summation for different injections and using $1 - f_{-\varepsilon}$ for the v -terms.

12.25.3 The importance of the DOS factor

To illustrate the importance of the DOS factor in the expression for the current and conductance, including where it comes from and what its expression is, consider an N/F junction. Set $Z = 0$ for simplicity. Boundary conditions are then continuity of ψ and ψ' . Let the magnetization in F point in the z -direction. Consider 1D for simplicity.

Let r_σ^N be reflection coefficients in the wavefunctions in the normal metal for spin σ . Similarly for r_σ^F in the F. Also, let $t_\sigma^{N,F}$ be transmission coefficients in the wavefunction on the N and F side.

Considering incoming particles from the N side, I get

$$\begin{aligned}
r_\sigma^N &= (k - k_\sigma)/(k + k_\sigma), \\
t_\sigma^F &= 2k/(k + k_\sigma)
\end{aligned} \tag{12.312}$$

where k and k_σ are the wavevectors on the N and F side for spin σ .

Consider incoming particles from the F side, I get

$$\begin{aligned}
r_\sigma^F &= (k_\sigma - k)(k_\sigma + k), \\
t_\sigma^N &= 2k_\sigma/(k + k_\sigma)
\end{aligned} \tag{12.313}$$

Now let us construct the total current on the N side. Consider the current flowing in the up channel. The current j_Q is essentially determined by the wavevector of each contribution. Thus, I get

$$I_{\uparrow} = -e \int dk_{\text{inc}} [f(E - eV)k - f(E - eV)k|r_{\uparrow}^N|^2 - f(E)k|t_{\uparrow}^N|^2] \quad (12.314)$$

when assuming a voltage difference eV is applied between N and F. The spin down current $I_{\downarrow}$ is constructed in the same way. Note that when a voltage difference is applied, strictly speaking the wavevector in the region should also be modified according to $E \rightarrow E - eV$.

Here, k_{inc} is the incoming wavevector and we want to integrate over all possible contributions. Now, k_{inc} is different depending on whether the particle is incoming from N or F side. But we can switch from integration over k_{inc} to integration over energy by using

$$\int dk_{\text{inc}} = \int dE (dk_{\text{inc}}/dE) \quad (12.315)$$

This is how we get the density of states factor into the expression, since in 1D the DOS is simply (proportional to) dk_{inc}/dE . Using energy dispersion in N and F, respectively, we find DOS factor

$$\begin{aligned} D_{N,\sigma} &= 1/k \equiv D_N, \\ D_{F,\sigma} &= 1/k_{\sigma} \end{aligned} \quad (12.316)$$

A common factor $\propto m$ was omitted for brevity. Thus, we find the total current

$$I = I_{\uparrow} + I_{\downarrow} = -e \int dE k \left([2 - |r_{\uparrow}^N|^2 - |r_{\downarrow}^N|^2] D_N f(E - eV) - [D_{F,\uparrow} |t_{\uparrow}^N|^2 + D_{F,\downarrow} |t_{\downarrow}^N|^2] f(E) \right) \quad (12.317)$$

Looking at the expressions for the scattering coefficients r, t that I wrote above, we see why the DOS factors are crucial. Namely, we have

$$D_N (1 - |r_{\sigma}^N|^2) = D_{F,\sigma} |t_{\sigma}^N|^2 \quad (12.318)$$

This is what allows us to write the final current in the form

$$I = \int dE i(E) [f(E - eV) - f(E)] \quad (12.319)$$

where $i(E)$ is an integrand depending on the scattering coefficients. It is clear that $I = 0$ for $eV = 0$.

Let us now look at the 2D case for N/F. One has to consider carefully the expression for DOS that is used. Namely, to begin with we should integrate over all possible incoming states for both k_x and k_y :

$$\int dk_{x,\text{inc}} dk_{y,\text{inc}} \quad (12.320)$$

We start by converting the $\int dk_{x,\text{inc}}$ integral to an integral over E . This assumes a fixed k_y -value. Then, we have

$$\int dk_{x,\text{inc}} = \int dE (dk_{x,\text{inc}}/dE) \quad (12.321)$$

Define the factor $N(E, \theta) = dk_{x,\text{inc}}/dE$. This is different from the 2D expression for density of states, even if we're considering a 2D junction.

For inc particles from N side, we now get

$$dk_{x,\text{inc}}/dE = 1/k_x^N \quad (12.322)$$

where k_x^N is the k_x on the N side, whereas for inc particles from the F side we get

$$dk_{x,\text{inc}}/dE = 1/k_{x,\sigma}^F \quad (12.323)$$

where $k_{x,\sigma}^F$ is the x -component of wavevector on the F side for incoming spin σ .

So the DOS factor which should be used for a 2D N/F bilayer is, for instance, for an incoming spin- $\uparrow$ particle from the F side with dispersion $E = k^2/2m - \mu - h$ given by:

$$N(E, \theta) = \frac{dk_{x,\text{inc}}}{dE} = \frac{m}{k_x}. \quad (12.324)$$

In an AM, one would get for an incoming $e, \uparrow$ in the $k_x^2 - k_y^2$ case that

$$N(E, \theta) = \frac{1}{k_x/m + \alpha k_x}. \quad (12.325)$$

The k_y integration now remains. Importantly, our 1D analysis of the N/F junction can be done for any finite k_y value. A 2D junction can be viewed as N 1D junctions, each characterized by a mode index k_y . Therefore, the current should vanish for $eV = 0$ also in 2D, as can be seen analytically from this argument.

We convert the k_y integral to angular integration via

$$\int dk_{y,\text{inc}} = \int d\theta (dk_{y,\text{inc}}/d\theta) \quad (12.326)$$

But here one has to be careful. Namely, k_y is a conserved quantity when we have translational invariance along the y -direction. Therefore, the allowed k_y -values are the same for each particle, whether they are incoming on the left or right side.

To illustrate this, consider a 2D N/F junction without barrier and let us write down the complete expression for the charge current. An incoming wave from N is written $\psi = e^{ik_x^N x}$ whereas an incoming wave from F is written $\psi = e^{-ik_x^F \sigma x}$ for spin σ .

We want to sum over all possible incoming modes: $\int dk_y \int dk_x$ where k_y and k_x denote the wavevectors for each incoming mode. In effect, they are different for different incoming modes. Translational invariance (conservation of k_y) must be taken into account by integrating over exactly the same k_y values for all incoming modes. This is in contrast not a requirement for the integration over k_x since it is not conserved.

To be clear about the k_y integration, consider an inc particle from N with $k_y = k_N \cos \theta$ and $k_N = \sqrt{\mu + E}$. We have

$$\int dk_y = \int \frac{dk_y}{d\theta} d\theta. \quad (12.327)$$

The integration over θ goes from $-\pi/2$ to $\pi/2$ here and below unless otherwise indicated. Using these limits requires using the correct expression for the quantum mechanical charge current density so that only real wavevectors contribute.

Consider instead an inc particle from F with $k_y = k_{\uparrow} \cos \theta_{\uparrow}$ and $k_{\uparrow} = \sqrt{\mu + E - J}$. We have

$$\int dk_y = \int \frac{dk_y}{d\theta_{\uparrow}} d\theta_{\uparrow}. \quad (12.328)$$

Here comes the crucial point: the actual numerical evaluation of the integral over $\theta_{\uparrow}$. Namely, since we have

$$k_N \sin \theta = k_{\uparrow} \sin \theta_{\uparrow} = k_{\downarrow} \sin \theta_{\downarrow} \quad (12.329)$$

there exist a relation between $d\theta$ and $d\theta_{\uparrow}$. In the numerical code, one can therefore *not* use the same 'steptheta' variable for all types of incoming particles. If we use a particular value for 'steptheta' for incoming particles from N (for instance 0.01), we must use a different one for incoming particles from F according to

$$d\theta_{\uparrow} = \frac{k_N \cos \theta}{k_F \cos \theta_{\uparrow}} d\theta \quad (12.330)$$

So when we do the integration over k_y for incoming particles from F, we have to use a 'steptheta' value equal to $0.01 \times \frac{k_N \cos \theta}{k_F \cos \theta_{\uparrow}}$. Note how the modifying prefactor varies depending on the value of $\theta_{\uparrow}$ and θ .

Thus, in the actual numerical evaluation of the integral $\int d\theta_{\uparrow} \frac{dk_y}{d\theta_{\uparrow}}$, we can integrate from $-\pi/2$ to $\pi/2$, but we have to use a value for $d\theta_{\uparrow}$ given by the above expression. Then, the current should vanish at zero voltage or spin pumping frequency.

The total charge current at zero voltage in a 2D N/F case, evaluated on the N side, should then be:

$$\begin{aligned} I_Q \propto & \overbrace{\int_{-\mu}^{\infty} dE \int d\theta \frac{dk_y}{d\theta} \frac{1}{k_x^N} (k_x^N)}^{\text{inc spin-}\uparrow \text{ from N}} + \overbrace{\int_{-\mu}^{\infty} dE \int d\theta \frac{dk_y}{d\theta} \frac{1}{k_x^N} (k_x^N)}^{\text{inc spin-}\downarrow \text{ from N}} \\ & + \overbrace{\int_{-\mu}^{\infty} dE \int d\theta \frac{dk_y}{d\theta} \frac{1}{k_x^N} (-k_x^N |r_{\uparrow}|^2)}^{\text{reflected spin-}\uparrow \text{ in N}} + \overbrace{\int_{-\mu}^{\infty} dE \int d\theta \frac{dk_y}{d\theta} \frac{1}{k_x^N} (-k_x^N |r_{\downarrow}|^2)}^{\text{reflected spin-}\downarrow \text{ in N}} \\ & + \overbrace{\int_{-\mu+J}^{\infty} dE \int d\theta_{\uparrow} \frac{dk_y}{d\theta_{\uparrow}} \frac{1}{k_x^{F\uparrow}} (-k_x^N |t_{\uparrow}|^2)}^{\text{transmitted spin-}\uparrow \text{ into N from F}} + \overbrace{\int_{-\mu-J}^{\infty} dE \int d\theta_{\downarrow} \frac{dk_y}{d\theta_{\downarrow}} \frac{1}{k_x^{F\downarrow}} (-k_x^N |t_{\downarrow}|^2)}^{\text{transmitted spin-}\downarrow \text{ into N from F}}, \end{aligned} \quad (12.331)$$

but where attention has to be paid to the numerical evaluation of the $\int d\theta_{\sigma}$ vs. $\int d\theta$ integrals.

In this way, we will have exactly the same prefactor coming from the transverse modes in front of every incoming contribution when we integrate over $d\theta_{\uparrow}$ and since the prefactor is the same for every incoming particle, the current will still be zero for each value of k_y when there is no applied voltage.

Easier to integrate over $\int dk_y$

With all this said, it turns out to be easier and more general to actually just integrate directly over k_y . The max and min values for a given E are then dictated by the Fermi surface, *e.g.* for a spin- $\uparrow$ in F the integration over k_y should be from $-\sqrt{\mu + E - J}$ to $+\sqrt{\mu + E - J}$. Note that the same dk_y -step should be used in the numerics for all incoming particles if one approximates the integral as a sum, as discussed above. If the wavefunctions have superconducting gaps which are anisotropic, such as p -wave or d -wave, the angle which should be inserted into the gap is computed simply from $\tan \theta = k_y/k_x$. Moreover, integrating directly over $\int dk_y$ instead of going via angles makes it easier to deal with non-spherical Fermi surfaces such as in the altermagnetic case in this way. Otherwise, one would have to solve a highly non-linear equation $k_{\uparrow}(\theta_{\uparrow}) \sin \theta_{\uparrow} = k_{\downarrow}(\theta_{\downarrow}) \sin \theta_{\downarrow}$ to relate the angles θ_{σ} .

Note that the integration limits for k_y for different incoming particles do not have to be the same: only the step dk_y must be the same so that the actual k_y values that overlap between the incoming particles are identical. If one Fermi surface is larger than another, so that particles incoming from the largest Fermi surface can take on a larger range of k_y values than the ones incoming from the smaller Fermi surface, that is fine since such particles will be fully reflected in any case and not contribute to current or conductance.

Let us consider in more detail what happens when we have an incoming wave from the right side, *i.e.* which is written e^{-ikx} . In order to keep the integration range for the energy E the same for all incoming particles, an extra minus sign then appears in the factor dk/dE .

To see this, consider first an incoming wave from N side in an N/F junction. We write this as $e^{ik_x x}$. We have $k_x = \sqrt{\mu + E}$. Then:

$$\begin{aligned}
 \int dk_{\text{inc}} &= \int_0^{\infty} dk_x \\
 &= \int_{-\mu}^{\infty} dE \frac{dk_x}{dE} \\
 &= \int_{-\mu}^{\infty} dE \frac{1}{k_x}.
 \end{aligned} \tag{12.332}$$

Note that if we wanted, we *could* instead write the incoming wave from the N side as e^{-iKx} so that

$k_x = -K$. We have $K = -\sqrt{\mu + E}$. Then:

$$\begin{aligned}
 \int dk_{\text{inc}} &= \int_0^\infty dk_x \\
 &= -\int_0^\infty (-dk_x) \\
 &= -\int_0^{-\infty} dK \\
 &= \int_{-\infty}^0 dK \\
 &= \int_{-\infty}^{-\mu} dE \frac{dK}{dE} \\
 &= \int_{-\mu}^\infty dE \frac{-dK}{dE} \\
 &= \int_{-\mu}^\infty dE \frac{-1}{K}.
 \end{aligned} \tag{12.333}$$

Now, to obtain this result directly by integrating over K instead of going via k_x , the rationale is as follows. With a plane-wave e^{-iKx} on the right side of the interface, we want to perform a summation over all modes $K < 0$ in order to describe propagation toward the interface. A summation $\sum_{K<0}$ is converted to an integral via

$$\int_{-\infty}^0 dK \tag{12.334}$$

which is identical to the above result. The above shows that has to pay attention to the limits of the integral when performing the variable change from wavevector to energy, but there is no need to enforce an absolute value on the DOS factor (the derivative of momentum with respect to energy) by hand to keep this quantity positive: the correct sign is taken care of automatically by paying attention to the integration limits.

Consider now a slightly more complicated case where the energy dispersion is not simply quadratic in k . We consider an incoming spin-up particle from a $k_x k_y$ oriented altermagnet in a N/AM junction. We may then write:

$$\psi = e^{ik_{e,\uparrow,-}x} \tag{12.335}$$

where

$$k_{e,\uparrow,-} = -\sqrt{2m(\mu + E) - k_y^2 + \alpha^2 m^2 k_y^2} - \alpha m k_y \tag{12.336}$$

. Define for brevity $R \equiv \sqrt{\dots}$. Now, we want to perform a summation over all possible incoming modes toward the interface. This amounts to a summation over all possible negative group velocities. The group velocity is determined by $v_g = \partial E / \partial k_x$ where $E = (k_x^2 + k_y^2)/2m - \mu + \alpha k_x k_y$, giving $v_g = k_x/m + \alpha k_y$. This shows that $v_g = -R$ for the above wavevector. Therefore, we must perform a summation over all positive R :

$$\sum_{R>0} \rightarrow \int_0^\infty dR = \int_{-E_c(\theta)}^\infty dE \frac{dR}{dE} \Big|_{k_x=k_{e,\uparrow,-}} \tag{12.337}$$

where $-E_c(\theta)$ is the energy which makes $R = 0$.

The final step is just to compute dR/dE . From the expression for E , we obtain:

$$\left. \frac{dR}{dE} \right|_{k_x=k_{e,\uparrow,-}} = R/m. \quad (12.338)$$

Therefore, the integral is simply

$$\int dE \frac{m}{R}. \quad (12.339)$$

One obtains exactly the same result for an incoming spin-down particle from the AM side. However, note that we would obtain precisely the same result also by just doing:

$$\int dk_x = \int dE \left. \frac{dk_x}{dE} \right|_{k_x=\text{value corresponding to positive group velocity}} \quad (12.340)$$

so there is no need to go via the R -route unless one wants.

In 2D, the angular weight of the various incoming particles is $\cos \theta$ -like. This can be seen especially easily in a 2D N/N junction where we may write

$$I \propto \sum_{n,k_x,k_y} i_{k_x,k_y}^n f^n(k_x, k_y). \quad (12.341)$$

Here, i^n is the current carried by mode n which has momenta k_x, k_y and f^n is the distribution function for that mode. Applying a voltage on the left side, so that $f^L(k_x, k_y) = f[E(k_x, k_y) - eV]$. Converting to integrals, we obtain

$$\begin{aligned} I &\propto \int dk_x dk_y k_x (1 - |r|^2) [f(E - eV) - f(E)] \\ &= \int dE \frac{dk_x}{dE} d\theta \frac{dk_y}{d\theta} k_x (1 - |r|^2) [f(E - eV) - f(E)] \\ &= \int dE \frac{m}{k_x} d\theta k_x k_x (1 - |r|^2) [f(E - eV) - f(E)] \\ &= \int dE d\theta m k_F \cos \theta (1 - |r(E, \theta)|^2) [f(E - eV) - f(E)]. \end{aligned} \quad (12.342)$$

Note that in Chi and Linder, PRB 2023 where spin-pumping with a d -wave superconductor is considered, there is an additional $\cos \theta$ factor inside the expression for the spin current which strictly speaking should not be there. The reason is that $dk_y = d\theta (dk_y/d\theta) \simeq d\theta k_x$ and k_x will cancel the $1/k_x$ factor appearing in the DOS expressions. However, the extra $\cos \theta$ factor should have very little impact since it simply means that the normally incident particles (which are the most important in any case) are weighted a little extra.

Finally, we comment on how incident holes can be handled. In the BTK approach, one integrates over the same energy range E for both electrons and holes, but this is only valid when one also takes into account a background contribution to the charge-current which exists due to the fact that we have expanded our Hamiltonian to electron-hole basis: there is a background of filled electron

states (see Sun and Linder, PRB 2023).

To show that the background contribution is needed to get the correct total current when one expands to particle-hole space, consider an N/N junction and an incident current from the left N. The electron contribution is (with $E = k_x^2/2m - \mu$)

$$I_e = \int_{-\mu}^{\infty} dE \frac{dk_x}{dE} \big|_{k_x=k_e} k_e (1 - |r|^2) f(E - eV). \quad (12.343)$$

The point is now that the hole contribution + the background contribution are equal to the electron contribution. To see this, first consider the background contribution corresponding to a completely filled electron sea at all energies:

$$I_{bg} = \int_{-\mu}^{\infty} dE \frac{1}{k_e} k_e (1 - |r|^2). \quad (12.344)$$

The hole contribution, on the other hand, is:

$$\begin{aligned} I_h &= \int_0^{-\infty} dk_x f_{k_x}^h (1 - |r_h|^2) \\ &= \int_{\mu}^{-\infty} dE \frac{dk_x}{dE} \big|_{k_x=-k_h} (-k_h) (1 - |r_h|^2) f(E + eV) \\ &= - \int_{-\infty}^{\mu} dE \left(-\frac{1}{k_h}\right) (-k_h) (1 - |r_h|^2) f(E + eV) \\ &= - \int_{\infty}^{-\mu} (-dx) (1 - |r_e|^2) f(-E + eV) \\ &= - \int_{-\mu}^{\infty} dE (1 - |r_e|^2) [1 - f(E - eV)] = -I_{bg} + I_e. \end{aligned} \quad (12.345)$$

However, if one is only interested in computing the conductance (the derivative of current with respect to voltage), one can observe the following with regard to the integration limits. Consider the contribution to the current from an incident hole on the right side of the interface. This hole has $\psi = e^{ikx}$ and $E = \mu - k^2$ so that $v_g = -k$. Thus, $k > 0$ and we want to integrate over all possible incoming modes $k > 0$. This gives

$$\begin{aligned} \sum_{k>0} &\rightarrow \int_0^{\infty} dk = \int_{\mu}^{-\infty} dE \frac{dk}{dE} \\ &= \int_{\mu}^{-\infty} dE \frac{-1}{k} = \int_{-\infty}^{\mu} dE \frac{1}{k}. \end{aligned} \quad (12.346)$$

The associated distribution function inside the integrand is $f(E + eV)$ if a voltage is applied, giving a Dirac-delta function contribution inside the integration range (at $E = -eV$). Thus, it doesn't matter that the integration range for the electron and hole currents are different as one computes the conductance, because the range easily includes any voltage $\ll \mu$. The background contribution to the conductance is zero since it has no distribution function.

12.25.4 Modified boundary conditions in the presence of SOC

Consider a 1D system with $H = E = k^2/2m - \mu + \alpha k$. If we have a hybrid system SOC/N, the H should be symmetrized to $H = E = k^2/2m - \mu + \frac{\alpha}{2}\{k, \theta(-x)\}$. One can now derive a continuity

equation for the probability density $P = |\psi|^2$ by using the time-dependent SE. One obtains an equation $\partial_t P + \partial_x j_P = 0$ where

$$j_P = \frac{\hbar}{2m} \text{Re}(\psi^\dagger \partial_x \psi) - \theta(x) \alpha |\psi|^2. \quad (12.347)$$

So probability current is still conserved, as it should, and we can apply continuity of the probability current across the interface as a way to extract reflection and transmission probabilities (by dividing on the incoming wave). A general boundary condition is nevertheless obtained in the standard way of integrating the BdG equations over a small interval $-\epsilon$ to ϵ across the interface. Note that the boundary conditions and probability current will be further modified whenever there is a component of momentum perpendicular to the interface in the Hamiltonian, such as for altermagnets, depending on whether we have $k_x^2 - k_y^2$ or $k_x k_y$ lobes relative the interface.

12.25.5 Decaying quasiparticles and Fermi-vector mismatch

Consider an N/S junction with the standard ELQ and HLO on the S side:

$$\psi = c \begin{pmatrix} u \\ v \end{pmatrix} e^{iq_e x} + d \begin{pmatrix} v \\ u \end{pmatrix} e^{-iq_h x} \quad (12.348)$$

where

$$q_e = \sqrt{2m(\mu + \sqrt{E^2 - \Delta^2}) - k_y^2}, \quad q_h = \sqrt{2m(\mu - \sqrt{E^2 - \Delta^2}) - k_y^2}. \quad (12.349)$$

For unconventional superconductors, u and v can also depend on angle θ as well as have phase factors. There are two key points to consider with regard to the choice of wavevectors and angle here.

Consider first $E < \Delta$. In this case, $q_{e,h}$ will be complex, thus containing a decaying part. The propagation direction and decay as one moves into the bulk of the superconductor are still correct, regardless of how large k_y is. So the values of $q_{e,h}$ can be used as they stand. However, if k_y is so large that there exists no point on the normal-state Fermi surface of the superconductor with this k_y value, one should use $\theta = \pi/2$ in u, v and $\Delta(\theta)$ since the small $\sqrt{E^2 - \Delta^2}$ term can be neglected in the wavevector, making it purely imaginary when k_y is large enough so that $q_{e,x} = 0$.

Consider next $E > \Delta$. In this case, $q_{e,h}$ is purely real or purely imaginary, depending on the size of k_y . If k_y is small enough to make the wavevector real, the expressions for $q_{e,h}$ can be used as they stand. However, care must now be taken if k_y is large enough that $q_{e,h}$ becomes purely imaginary. To ensure decay of the quasiparticle into the superconductor, we now have to use

$$q_h = -\sqrt{2m(\mu - \sqrt{E^2 - \Delta^2}) - k_y^2}. \quad (12.350)$$

This is because of the extra minus sign the exponent of the HLQ in the wavefunction. Note that we are mathematically allowed to change the sign of q_h , since the general solution of q_h is $\pm\sqrt{\dots}$. Interestingly, the expression for charge conductance and probability appears to give identical results to the procedure above if one for supergap energies instead simply set $q_e = q_h = 0$. There appears to be some cancellation of the superconducting wavevectors for supergap energies which makes both approaches the same.

12.26 Odd-frequency superconductivity

Intro ...

Let us comment on how odd-frequency superconductivity is treated using the anomalous Green functions in quasiclassical theory. The Pauli principle in a diffusive system (*s*-wave) states that

$$f_{\alpha\beta}^M(i\omega_n) = -f_{\beta\alpha}^M(-i\omega_n). \quad (12.351)$$

Here, f^M is the Matsubara Green function, ω_n is the Matsubara frequency, and $\{\alpha, \beta\}$ are the spin indices. One can prove directly from this relation that in terms of real-energy Green functions, the Pauli principle reads

$$f_{\alpha\beta}^R(E) = -f_{\beta\alpha}^A(-E). \quad (12.352)$$

Here, $f^{R,A}$ are the retarded and advanced Green functions. They are obtained from the Matsubara in the usual manner

$$\lim_{i\omega_n \rightarrow E \pm i0^+} f^M(i\omega_n) = f^{R,A}(E). \quad (12.353)$$

Alternatively, Eq. (12.352) can be proven directly by Fourier-transformation of the basic definition of the retarded and advanced Green functions. Eq. (12.352) is also consistent with PRL 2007 by Tanaka and Golubov. Now, how do we know if an anomalous Green function describes even or odd-frequency pairing? In the Matsubara language, it is easy: f^M is antisymmetric in ω_n if it is an odd-frequency correlation, $f_{\alpha\beta}^M(i\omega_n) = -f_{\alpha\beta}^M(-i\omega_n)$. Performing the operation $i\omega_n \rightarrow E + i0^+$ on this equation, we find that

$$f_{\alpha\beta}^R(E) = -f_{\alpha\beta}^A(-E) \text{ for odd-frequency pairing.} \quad (12.354)$$

Similarly, one finds that

$$f_{\alpha\beta}^R(E) = f_{\alpha\beta}^A(-E) \text{ for even-frequency pairing.} \quad (12.355)$$

Again, this is consistent with the equations in Tanaka and Golubov PRL 2007.

We can check that the BCS superconductor anomalous Green function satisfies the even-frequency condition. It is given by (see *e.g.* JP Morten thesis):

$$\begin{aligned} f_{\uparrow\downarrow}^R(E) &= \frac{\Delta \text{sign}(E)}{\sqrt{E^2 - |\Delta|^2}} \Theta(E^2 - |\Delta|^2) - \frac{i\Delta}{\sqrt{|\Delta|^2 - E^2}} \Theta(|\Delta|^2 - E^2), \\ f_{\uparrow\downarrow}^A(E) &= -\frac{\Delta \text{sign}(E)}{\sqrt{E^2 - |\Delta|^2}} \Theta(E^2 - |\Delta|^2) - \frac{i\Delta}{\sqrt{|\Delta|^2 - E^2}} \Theta(|\Delta|^2 - E^2). \end{aligned} \quad (12.356)$$

It is seen that Eq. (12.355) is satisfied. This also suggests how we may in the simplest way possible describe an odd-frequency bulk superconductor quasiclassically: simply by letting $\Delta \rightarrow \Delta(E)$ where $\Delta(E) = -\Delta(-E)$ must be an odd function in E . In that case, we obtain:

$$\begin{aligned} f_{\uparrow\downarrow}^R(E) &= \frac{\Delta(E) \text{sign}(E)}{\sqrt{E^2 - |\Delta(E)|^2}} \Theta(E^2 - |\Delta(E)|^2) - \frac{i\Delta(E)}{\sqrt{|\Delta(E)|^2 - E^2}} \Theta(|\Delta(E)|^2 - E^2), \\ f_{\uparrow\downarrow}^A(E) &= -\frac{\Delta(E) \text{sign}(E)}{\sqrt{E^2 - |\Delta(E)|^2}} \Theta(E^2 - |\Delta(E)|^2) - \frac{i\Delta(E)}{\sqrt{|\Delta(E)|^2 - E^2}} \Theta(|\Delta(E)|^2 - E^2). \end{aligned} \quad (12.357)$$

In this case, we see that Eq. (12.354) is satisfied.

It is also possible to discuss symmetry relations that the retarded Green function alone has to satisfy (see PRB 2023, Giil and Linder). These are established by looking at the energy symmetry of the retarded BCS singlet correlator (drop the superscript R for brevity): $f_s(E, \phi) = -f_s(E, -\phi)$. Here, ϕ is the superconducting phase of the order parameter. The corresponding symmetry for the triplet $\mathbf{d}$ -vector is $\mathbf{d}(E, \phi) = \tilde{\mathbf{d}}(E, -\phi)$. Note that this means that the individual triplet components $f_{\alpha\beta}$ do not have any definite energy symmetry, at least when using the KL boundary conditions. For instance for an S/F junction, we will have $f_{\sigma\sigma} = \tilde{f}_{\sigma\sigma}$ if the magnetization points in the x -direction, but instead $f_{\sigma\sigma} = -\tilde{f}_{\sigma\sigma}$ if it points in the y -direction.

However, even the above $\mathbf{d}$ -vector symmetry appears to break down if one uses fully polarized boundary conditions. For instance, consider an S/F/fully polarized interface along z /N structure. The magnetization in F points in the x -direction. Thus, both $f_{\uparrow}$ and $f_{\downarrow}$ are induced in F. Only the $f_{\uparrow}$ are induced in N due to the fully polarized interface. Therefore, it is impossible to satisfy both $d_x = \tilde{d}_x$ and $d_y = \tilde{d}_y$ simultaneously. A possible reason for this is that $f_s = 0$ in the N metal. Therefore, there is no guiding relation of the type $f_s = -\tilde{f}_s$ which imposes a restriction on the corresponding symmetry of the components of the $\tilde{\mathbf{d}}$ -vector, as seen *e.g.* from the linearized Usadel equation.

12.27 Paramagnetic Meissner effect

One of the most fascinating and well-known consequences of superconductivity is the ability of a superconductor to repel magnetic flux, which results in magnetic levitation. This occurs due to the Meissner effect that was first reported by Meissner and Ochsenfeld in 1933. This discovery was critical in formulating the fundamental theory of superconductivity, which led to Bardeen, Cooper, and Schrieffer receiving the 1973 Physics Nobel Prize.

In the 1990s a series of experimental papers (e.g. [5]) claimed an unconventional Meissner effect in which certain superconducting materials appeared to attract rather than repel magnetic flux — the paramagnetic Meissner effect. This work generated enormous excitement from the scientific community as a paramagnetic response of a superconductor implied a compatibility between magnetic and superconducting quantum states. However, it was later shown [6] that this effect was not an intrinsic property of superconductivity but a consequence of surface defects that allow additional flux to penetrate the surface of a superconducting material.

Recently, an intrinsic paramagnetic Meissner effect was predicted in exotic (s-wave, odd frequency) superconductors in which time reversal symmetry is broken. Although odd frequency superconductivity has not been observed in bulk materials, it can appear at superconductor / magnet interfaces, but so far the paramagnetic Meissner effect has not yet been observed to the best of our knowledge. This is most likely since detecting this effect requires a sensitivity to magnetic flux that cannot be resolved by standard magnetometry techniques. Di Bernardo *et al.* have used low energy muons at the Paul Scherrer Institut in Switzerland to probe the Meissner effect in a thin film of Au proximity coupled to an antiferromagnetic / superconductor structure and have directly observed the paramagnetic Meissner effect [7]. This would be the first evidence for an intrinsic paramagnetic Meissner effect. The results will necessarily excite the development of new first principle calculations in order to understand the science in more detail. The idea that a superconductor can attract rather than

expel magnetic flux is in stark contrast with well-known effects like magnetic levitation that are usually tantalising for readers with a broad range of scientific backgrounds.

In a bulk superconductor, a paramagnetic Meissner effect leads to a thermodynamically unstable state with no lower bound on the free energy. This can be seen from the Landau expansion of the (Gibbs) free energy in the complex order parameter:

$$F = \int \left[\alpha(T)|\psi|^2 + \frac{1}{2}\beta(T)|\psi|^4 + \gamma(T)|(\nabla + 2ie/\hbar c)\psi|^2 + B^2/8\pi \right] d^3x. \quad (12.358)$$

This free energy must be minimized with respect to variations of ψ and $\mathbf{A}$. Minimization with respect to $\mathbf{A}$, $\delta F/\delta \mathbf{A} = 0$, gives

$$\nabla \times \mathbf{B} = (4\pi/c)\mathbf{j} \quad (12.359)$$

where the supercurrent is

$$\mathbf{j} = -(4e\gamma/\hbar)|\psi|^2(\nabla\phi + 2e\mathbf{A}/\hbar c). \quad (12.360)$$

For $\gamma > 0$, we have a diamagnetic Meissner effect and the London penetration depth is

$$\lambda^{-2} = 32\pi(e^2/\hbar^2 c^2)\gamma|\psi|^2. \quad (12.361)$$

The superfluid density is then $n_s \propto \gamma|\psi|^2$. The above equations demonstrate why a paramagnetic Meissner effect becomes thermodynamically unstable. To reverse the supercurrent response due to $\mathbf{A}$, we must set $\gamma < 0$. We note that this makes the superfluid density negative. The problem is now that the free energy term $\propto \gamma$ can be made increasingly negative by making $\nabla\psi$ larger and larger in magnitude. There is no lower bound as ψ becomes ever more inhomogeneous, which is unphysical.

However, in hybrid structures where a conventional superconductor provides a diamagnetic Meissner effect, the proximity-induced correlations may still yield a paramagnetic response in a neighboring material.

12.28 Bound-states in superconductors: impurities and vortices

The bound-states forming in superconductors with vortices or with surface impurities give rise to a DOS that breaks particle-hole symmetry, either in the form of just one resonant state at positive or negative energy inside the gap or in the form of two states at opposite energies but with unequal height.

The physical reason for the breaking of p-h symmetry in the impurity case is the impurity potential itself, which enters in the usual $Uc^\dagger c$ way and thus affects electrons and holes differently. Without impurity potential and chemical potential $\mu = 0$, we have particle-hole symmetry in a tight-binding model in the sense that the kinetic term is invariant under the transformation $d_{i\sigma}^\dagger = (-1)^i c_{i\sigma}$. However, both a finite U and μ induce a particle-hole asymmetry.

In the vortex case, the physical reason can be understood intuitively based on how states are pushed out of the superconducting gap. First, note that the discreteness of the level separation of quasiparticle states in a vortex core can only be observed when temperature T is so low that thermal smearing is smaller than the level spacing. The level spacing of vortex core states is typically of order Δ_0^2/E_F where Δ_0 is the bulk superconducting gap. This is (up to a constant prefactor of order

unity) equal to $\Delta_0/k_F\xi$. Therefore, the discreteness is observed in a regime where $T < \Delta_0/k_F\xi$, or roughly

$$\frac{T}{T_c} \leq \frac{1}{k_F\xi}. \quad (12.362)$$

The smaller $k_F\xi$ is, the easier this condition is to meet. This means that we need materials with a small ratio of Δ_0/E_F , like the high- T_c cuprates. This can now finally be linked to an intuitive understanding of the particle-hole asymmetry of the DOS in the vortex core.

As an approximation, imagine the gap as a forbidden region around a circular Fermi surface in $\mathbf{k}$ -space in some region of space inside the vortex. The gap Δ_{local} here is smaller than the bulk gap, but there is still a gap in the spectrum (except for the very center of the vortex). All states that normally would have occupied this region are pushed out and end up at energies right above or below the gap. Note that this will still be subgap states in the sense that their energies are smaller than the bulk gap Δ_0 . Now, if Δ_{local} is much smaller than E_F , the surfaces $E_F + \Delta_{\text{local}}$ and $E_F - \Delta_{\text{local}}$ are approximately equal and the density of states above and below the gap is similar. If $E_F \sim \Delta_{\text{local}}$ this is no longer true, and the states which are being pushed into the Fermi surface will be packed together more closely than those pushed away from it. The same reasoning may actually be applied also to the bulk of the superconductor, meaning that the DOS will not be symmetric relative each side of the coherence peaks in the bulk superconducting DOS.

12.29 Thermoelectric effects

12.29.1 General considerations

A key concept when treating thermoelectric effects, such as an electric current or voltage induced by a temperature gradient (Seebeck effect), is *particle-hole asymmetry*. Consider a bilayer of two semiconductors that have perfectly symmetric valence and conduction bands, as shown in Fig. 12.6(a). Let the cold material be at $T = 0$ for simplicity, whereas the hot material has some thermally excited electrons in the conduction band due to $T + \Delta T \neq 0$. A temperature difference ΔT thus exists across the junction. The thermally excited electrons in the hot material can tunnel into the empty conduction band of the cold material. However, simultaneously there are available electron states in the valence band of the hot material which can be filled by electrons in the full valence band of the cold material. Due to charge conservation, there must be equally many empty electron states in the hot material valence band as there are excited electron states in the hot material conduction band. Therefore, the net flow of electrons across the junction is zero and there is no charge current. One can also think about this in the *excitation picture* where the missing electrons in the valence band of the hot material are represented as positive energy hole excitations [Fig. 12.6(b)]. The electron and hole current across the junction is equally large and there is no net charge flow.

However, as soon as we introduce a particle-hole asymmetry on at least one of the two sides (the hot or the cold one), a thermoelectric effect comes into play [Fig. 12.6(c)]. Above, we have doped the cold material side in a manner which has made the conduction band effective mass larger and the valence band mass smaller. Moreover, doping changes the position of the bands relative to the Fermi level. For instance, n -doping will bring the conduction band closer to the Fermi level (as indicated in the figure). It is a common scenario that the effective electron and hole masses are different (corresponding to the curvature of the bands). Since the density of states associated with the edges of the conduction and valence bands are now different, there is an imbalance between how

many electron and hole excitations that cross the junction. As a result, the temperature difference has induced a flow of electric current.

Surprisingly, superconductors can actually be used to yield very large spin-dependent thermoelectric effects. Before showing how this takes place, let us establish some additional fundamental principles regarding heat transport in hybrid structures.

First, recall that applying a voltage to one side in a hybrid structure shifts the entire energy band along with the Fermi level as shown in the below figure. Thus, it is different from changing *only* the effective Fermi level as done via electric gating in 2DEGs where the energy band bends while the Fermi level remains the same. We previously derived the tunneling current between two metals separated by a barrier. It might be tempting to generalize this expression by simply adding an energy term E under the integral, computing effectively the energy current, and say that this is the amount of heat transferred. However, this is incorrect. As we will explain below, the correct expression for the heat current must measure energy relative the Fermi level:

$$\mathbf{j}_Q = \mathbf{j}_E - \mu \mathbf{j} \quad (12.363)$$

where $\mathbf{j}_Q$ is the heat current, $\mathbf{j}_E$ is the energy current, and $\mathbf{j}$ is the particle current (so that the charge current is $\mathbf{j}_{\text{charge}} = -|e|\mathbf{j}$). The key to realizing why energy current is not the same as heat current can be understood by realizing that the temperature in a system can be changed in two ways: removing/adding hot electrons or removing/adding cold electrons. This is illustrated in the figure.

Heating: increasing the temperature of the system means that the distribution function becomes less step-like. This can be achieved by either adding a hot electron with energy $E > \mu$ or removing a cold electron with energy $E < \mu$.

Cooling: lowering the temperature of the system means that the distribution function becomes more step-like. This can be achieved by either adding a cold electron with energy $E < \mu$ or removing a hot electron with energy $E > \mu$.

It is clear that the heating effect of electrons that are moving across the junction is determined by their energy relative the local chemical potential, which is ultimately the reason for why we

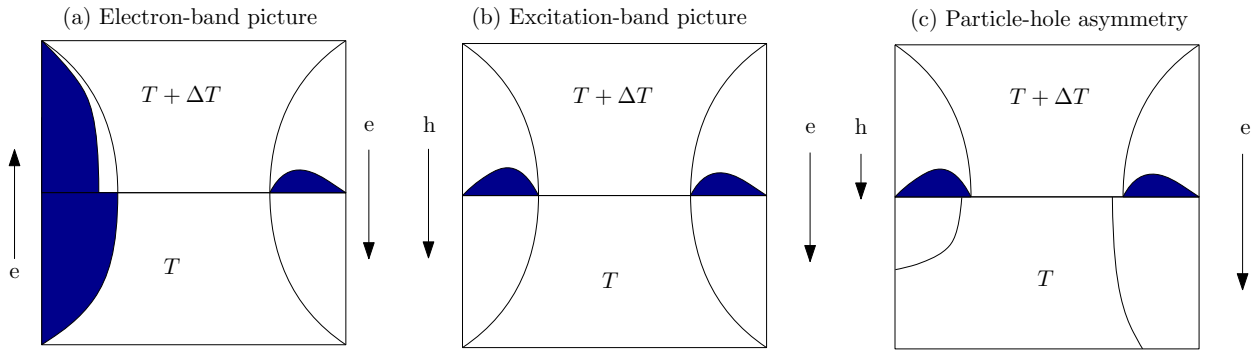


Figure 12.6: A temperature gradient exists from a hot to a cold material, the latter at $T = 0$. If one has particle-hole symmetry, there is no net charge flow across the junction since the electron and hole flow is equally large.

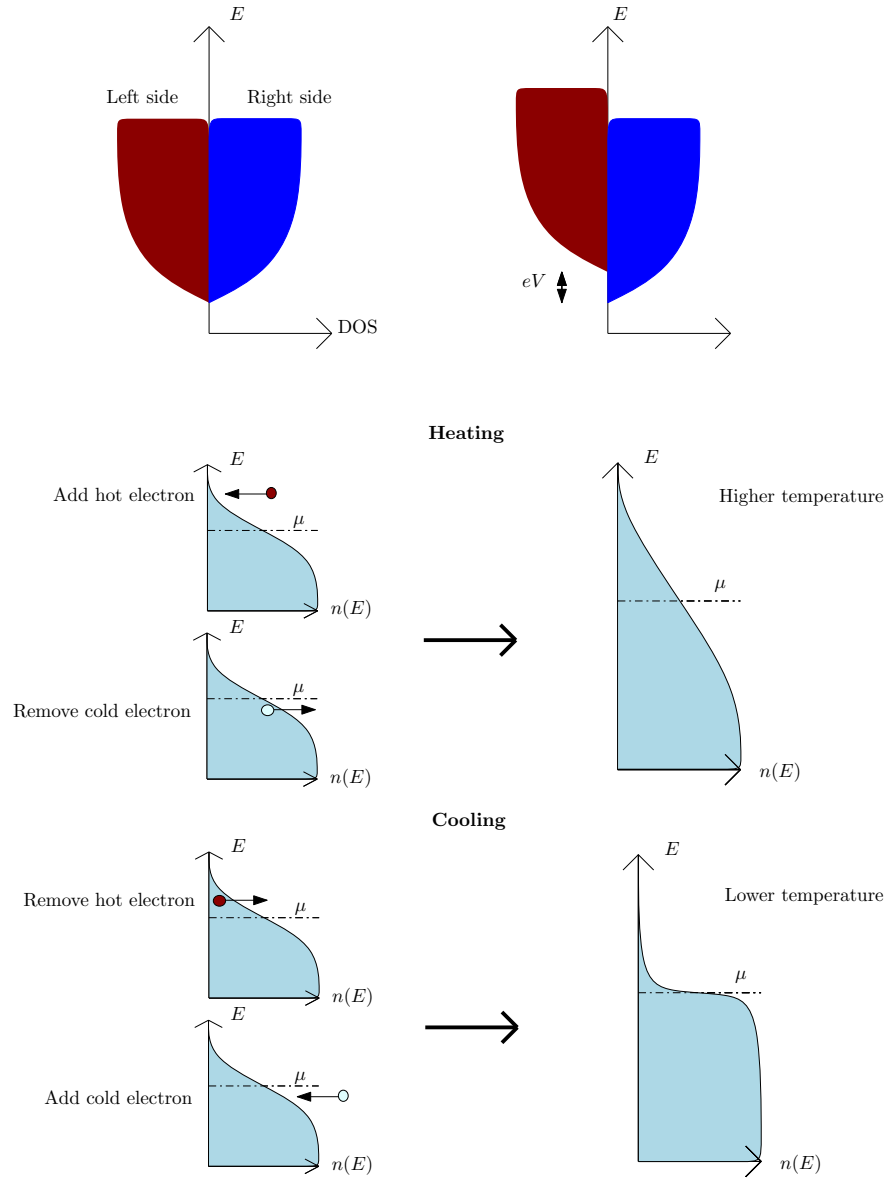


Figure 12.7: Top row: demonstrating the effect of applying a bias voltage, which raises the entire energy band on one side. Middle row: two ways to achieve heating. Bottom row: two ways to achieve cooling.

subtract $\mu \mathbf{j}$ to find the heat current. In terms of our previous treatment of tunneling currents, the correct expression for the heat current flowing out of the left lead (which is biased at $+eV$) reads:

$$\dot{Q}_L \propto \int_{-\infty}^{\infty} (E - eV) N_L(E - eV) N_R(E) [f(E - eV) - f(E)] dE, \quad (12.364)$$

where the energy is measured relative the chemical potential in the right lead. One could also write this as:

$$\dot{Q}_L \propto \int_{-\infty}^{\infty} (E' - \mu_L) N_L(E' - \mu_L) N_R(E' - \mu_R) [f(E' - \mu_L) - f(E' - \mu_R)] dE', \quad (12.365)$$

by using that $eV = \mu_L - \mu_R$ and introducing the variable $E' = E + \mu_R$, i.e. the energy measured relative zero. This is the heat current coming from the left side, as is clear from the subtraction of μ_L . It is *not* equal to the total heat current in the system, i.e. the rate of heat deposited on the L and R side, which always has to equal the dissipation $P = IV$ coming from Joule heating. This can be seen by considering the heat current flowing into the right lead, which is

$$\dot{Q}_R \propto \int_{-\infty}^{\infty} (E' - \mu_R) N_L(E' - \mu_L) N_R(E' - \mu_R) [f(E' - \mu_L) - f(E' - \mu_R)] dE'. \quad (12.366)$$

The rate of heat deposited in the L part is $-\dot{Q}_L$ and the rate of heat deposited in the R part is $\dot{Q}_R$. We see that $-\dot{Q}_L + \dot{Q}_R$ cancels the contribution from E' inside the integrand and gives precisely $(\mu_L - \mu_R) = eV$ times the particle current. In effect, the total rate of heat change into each of the reservoirs (heat current going into left reservoir pluss heat current going into right reservoir) equals the Joule dissipation. For high voltages eV , the heat dissipation should distribute evenly between the two leads so that $\dot{Q}_L < 0$ (gains heat from Joule dissipation) and $\dot{Q}_R > 0$ (gains heat from Joule dissipation).

In the presence of Andreev reflection, an important observation must be made. Transferring a Cooper pair to a superconductor does not add any heat to the superconductor since the average electron energy of the two added electrons is at the Fermi level. However, it does increase the Joule heating in the normal metal since the current is increasing there (recall that the conductance doubles compared to the normal-state for perfect Andreev reflection). We are removing cold electrons from the normal metal via Andreev reflection, and thus it is heating. If the left reservoir is the normal metal and the right one is a superconductor, then we must take into account the additional Joule heating from the Andreev current I_A by writing:

$$\dot{Q}_L \rightarrow \dot{Q}_L - I_A V. \quad (12.367)$$

We emphasize that electrons, like any other particle, will always move from higher potential energy U to lower potential energy. Since the electron charge is negative, it means that electrons move from lower electric potential V to higher electric potential. When we write $\mu_L - \mu_R = eV$, it means that the electron have highest potential energy on the left side and the current thus goes from left to right.

12.29.2 Thermoelectric effects in S/F structures

Let us consider some aspects of spin-dependent thermoelectric effects in S/F structures. The key to achieving this is to create a large spin-dependent particle-hole asymmetry, even if the total (summed over both spins) particle-hole asymmetry is zero (which is always the case quasiclassically). For concreteness, say we have a ferromagnet on the left side and superconductor on the right side. The electric current I_σ and heat current $\dot{Q}_\sigma$ carried by spin- σ electrons from the ferromagnet are then given by:

$$\begin{aligned} I_\sigma &= \frac{G_\sigma}{e} \int dE N_\sigma(E) [f_F(E - \mu_F) - f_S(E)], \\ \dot{Q}_\sigma &= \frac{G_\sigma}{e^2} \int dE (E - \mu_F) N_\sigma(E) [f_F(E - \mu_F) - f_S(E)]. \end{aligned} \quad (12.368)$$

Here, we have set the DOS in the ferromagnet to be constant for each spin band and absorbed into the spin-dependent conductivity coefficients G_σ . The energy E is measured relative the Fermi level

in the superconductor while $N_\sigma(E)$ is the DOS for spin- σ in the superconductor. However, should we wish to address a situation where we allow the DOS in the non-superconducting part to depend on energy as well, we would have written:

$$\begin{aligned} I_\sigma &= \frac{G_0}{e} \int dE N_{N,\sigma}(E - \mu_N) N_{S,\sigma}(E) [f_N(E - \mu_N) - f_S(E)], \\ \dot{Q}_\sigma &= \frac{G_0}{e^2} \int dE (E - \mu_N) N_{N,\sigma}(E - \mu_N) N_{S,\sigma}(E) [f_N(E - \mu_N) - f_S(E)]. \end{aligned} \quad (12.369)$$

Let us for now continue with Eq. (12.368) and set $\mu_F = -eV$. This means that current will flow from the superconductor to the ferromagnet.

We introduce various useful quantities such as the polarization, spin-polarized currents, and total conductance as follows:

$$\begin{aligned} P &= \frac{G_\uparrow - G_\downarrow}{G_\uparrow + G_\downarrow}, \quad I = I_\uparrow + I_\downarrow, \quad I_S = I_\uparrow - I_\downarrow, \quad G_T = G_\uparrow + G_\downarrow, \\ \dot{Q} &= \dot{Q}_\uparrow + \dot{Q}_\downarrow, \quad \dot{Q}_S = \dot{Q}_\uparrow - \dot{Q}_\downarrow, \\ N_0 &= \frac{N_\uparrow + N_\downarrow}{2}, \quad N_z = N_\uparrow - N_\downarrow. \end{aligned} \quad (12.370)$$

Note that the heat current $\dot{Q}$ defined in this way is the heat current going out of the ferromagnet (it can still be negative, meaning that heat is absorbed by F) and is thus not in general equal to the total Joule power dissipated.

12.29.3 Onsager matrix symmetries

The relation between applied voltages or temperature gradients and currents of charge or heat can be conveniently expressed through Onsager reciprocal relations in the linear response regime. Formally, one may define a response matrix with elements L_{ij} which describe how a thermodynamic force F_j associated with a variable q_j produces a response in a different variable q_i . Conversely, a thermodynamic force F_i producing a change in the quantity q_j is the reciprocal process. In our case, the forces F may be the applied voltage V or the temperature difference ΔT while the variable q denotes for instance the charge or heat current. The linear response coefficients of reciprocal phenomena are related through the so called Onsager symmetries:

$$L_{ij} = (\mathbf{M}, \mathbf{H}) = \sigma_i \sigma_j L_{ji}(-\mathbf{M}, -\mathbf{H}) \quad (12.371)$$

where $\sigma_i = +1$ if the quantity q_i is even under time reversal and $\sigma_i = -1$ if the quantity q_i is odd under time-reversal. Above, $\mathbf{M}$ and $\mathbf{H}$ is the intrinsic magnetization and externally applied field.

It is thus noteworthy that the matrix defined in [14] satisfies the proper Onsager symmetries whereas the statement concerning the matrix involving the spin current in [13] is incorrect.

12.30 Boundary conditions for superconducting order parameter at edges

Consider first the non-superconducting case. For the particle-in-a-box problem, it is customary to set $\psi = 0$ at the hard wall since $V \rightarrow \infty$ there, meaning that ψ must vanish beyond the hard wall.

Continuity of the wavefunction then requires that $\psi = 0$ right at the wall. If we instead of a hard wall had an infinitely high δ -function potential, and then a normal metal on the other side of the barrier, it is interesting to note that we do not need $\psi = 0$ at the barrier as the wavefunction in principle can exist on the other side of the barrier. Having said that, the reflection coefficient becomes unity in magnitude for an infinite δ -function barrier, but this means that $\partial_x \psi = 0$ rather than $\psi = 0$: the probability current at the barrier is zero. A fully reflective barrier with non-vacuum on the other side is thus described by the boundary condition $\partial_x \psi = 0$ whereas the onset of vacuum is described by $\psi = 0$. This is true even if a vacuum edge can be thought of as a fully reflective barrier, the difference being that a wavefunction can in principle exist on the other side of the barrier if the system *e.g.* is prepared in that way (the barrier is suddenly turned on).

This difference is conceptually important when it comes to doing *e.g.* STM measurements. If $\psi = 0$, there shouldn't be any states to tunnel into from the STM tip at all. Instead, the STM-scenario is better thought of as a barrier (the vacuum between the STM tip and the material) separating two conducting materials. Thus, we should not set $\psi = 0$ at the vacuum edge when the vacuum does not extend infinitely far away from the edge.

Consider now the superconducting case. We have to distinguish between the wavefunction ψ entering the BdG-equations, which describes quasiparticles, and the superconducting order parameter Ψ , which describes the macroscopic condensate of Cooper pairs and enters the GL-equations. A commonly used boundary condition for Ψ at vacuum edges is that $\partial_x \Psi = 0$, which means that no supercurrent can flow into vacuum, as is reasonable. However, Ψ can still be finite at the edge, meaning that the superconducting gap is not suppressed by scattering of a reflective barrier. This is in agreement with the general notion that *s*-wave Cooper pairs are immune to elastic scattering.

However, an apparent paradox arises if we look at the BdG equations for ψ . If there is a true vacuum edge (vacuum extending far away from the edge), then clearly $\psi = 0$ at the edge according to our above reasoning. But the gap Δ is determined selfconsistently from the u and v coherence factors that make up the wavefunction $\psi = (u, v)$. Thus, if $u = v = 0$ at the edge, then $\Delta = 0$ as well. So at a true vacuum edge, it does seem reasonable that the order parameter itself should go to zero. Quasiclassically, we cannot capture this phenomenon because $\hat{g}^2 = \hat{1}$ and we cannot set $\hat{g} = 0$. This means that the wavefunction should go to zero over an atomic distance near the edge, which cannot be captured quasiclassically. Instead, the best we can do there is to set $\partial_x \hat{g} = 0$ so that no current flows out of the interface (a fully reflective interface). In this case, there is indeed no suppression of the SC order parameter since Cooper pair scattering causes no suppression of the isotropic Δ .

12.31 Further aspects of non-equilibrium superconductivity

12.31.1 Electron-phonon interaction

The physical origin of the electron-phonon interaction is the coupling between electrons and ions via the Coulomb interaction. Since phonons represent excitations that disturb the ion lattice, this displacement of ions will couple to the electrons since it modifies the Coulomb interaction.

12.31.2 Charge imbalance

Following [23] and [24], we start by considering the total electric charge Q_{tot} of a superconductor. From BCS theory, one derives that ($e > 0$)

$$Q_{\text{tot}} = (-e) \sum_{k\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle = -\frac{2e}{\Omega} \sum_k [u_k^2 f_k + v_k^2 (1 - f_k)]. \quad (12.372)$$

Here, Ω is the volume of the superconductor, u_k and v_k are the regular coherence factors, and f_k is the distribution function for state k . In thermal equilibrium, f_k is the Fermi-Dirac distribution function. The sum over k runs over states above and below k_F . We have omitted a prefactor $-|e|$ for the charge of the original fermions $\{c_{k\sigma}\}$.

We will rewrite the above expression below to a form which shows explicitly the contribution to Q_{tot} from the Cooper pairs and from the quasiparticles. We note that

$$u_k(v_k) = \sqrt{\frac{1}{2}(1 \pm \xi_k/E_k)} \quad (12.373)$$

where

$$\xi_k = k^2/2m - \mu_S, \quad E_k = \sqrt{\xi_k^2 + |\Delta|^2}. \quad (12.374)$$

Above, ξ_k is the kinetic energy of an electron in the state k relative the chemical potential μ_S . It is *convenient* to think of μ_S as the chemical potential associated with the Cooper pair condensate. This might not be entirely intuitive as it appears in the single-particle energy. However, we will show that it is useful to work with two electrochemical potentials in the superconducting state: the Cooper pair chemical potential μ_S and the quasiparticle excitation chemical potential μ_{qp} . In thermal equilibrium, they are equal. Below, we explain why μ_S can be interpreted as the Cooper pair chemical potential. We underline that μ_S should not be thought of as a chemical potential for "bosonic" Cooper pairs: we will in fact define μ_S in the usual fermionic way below.

From BCS theory, we know that u_k^2 is the probability that a state k is not occupied by a Cooper pair whereas v_k^2 is the probability that the state k is occupied by a Cooper pair. The chemical potential of the pairs μ_S is the "mean band energy" of the condensate: the energy which gives a pair state with occupation probability 0.5 (similarly to how chemical potential is defined for single particles). This occurs when $v_k^2 = 0.5$, which is the case when $\xi_k = 0$, so it is clear that μ_S must be the chemical potential that enters ξ_k . In equilibrium $\mu_S = \mu$ where μ is the normal-state chemical potential.

The expression for the total charge Eq. (12.372) can then be understood physically. The total expression inside the square bracket is the probability that a state k is occupied, either by an electron in a pair state or a quasiparticle. The first term inside the square bracket is the probability that a pair-state $(k, -k)$ is empty, u_k^2 , times the probability that a quasiparticle state is occupied, f_k . The second term is the probability that a pair-state $(k, -k)$ is occupied, v_k^2 , times the probability that a quasiparticle state k is empty, $1 - f_k$.

We can rewrite Q_{tot} in a way which makes it clear why it is correct:

$$Q_{\text{tot}} = Q_S + Q_N = -\frac{2e}{\Omega} \sum_k v_k^2 + \frac{2}{\Omega} \sum_k q_k f_k, \quad (12.375)$$

where $q_k = -e(u_k^2 - v_k^2)$ is the fractional quasiparticle charge while $f_k = f(E_k)$ is the Fermi-Dirac distribution function. The first term Q_S is then clearly the Cooper pair charge while the second term Q_N is the quasiparticle charge. The quasiparticle contribution Q_N to the charge is called the *charge imbalance* of the system. In thermal equilibrium, $Q_N = 0$ even at finite temperatures. This can be seen by noting that $q_k = u_k^2 - v_k^2 = \xi_k/E_k$ is antisymmetric for k -values above and below the Fermi level, whereas $f_k = f(E_k) = f(\sqrt{\xi_k^2 + |\Delta|^2})$ is clearly symmetric for such k -values. The overall summation thus always vanishes (disregarding here particle-hole asymmetry above and below the Fermi level).

However, note that $Q_N = 0$ does *not mean* that there are no quasiparticles in the system. Instead, charge imbalance $Q_N \neq 0$ comes about when there is an *imbalance between the k^+ and k^- branches* of quasiparticles, using the BTK notation where $k^\pm = \sqrt{2m(\mu_S \pm \sqrt{E^2 - \Delta^2})}$. We see that $k^- < k_F$ and $k^+ > k_F$ where $k_F = \sqrt{2m\mu_S}$. Also note that in much literature, one uses the notation Q^* instead of Q_N . Now, in non-equilibrium, Q_N need not be zero since f_k is no longer the Fermi-Dirac distribution function. In fact, it turns out that Q_N induces a change in the Cooper pair chemical potential μ_S in order to maintain charge neutrality, as we shall discuss below.

Note that at $T = 0$, $f_k = 0$ for any k due to the properties of f_k , so that the total charge in the superconductor is $-\frac{2e}{\Omega} \sum_k v_k^2$ at $T = 0$. Due to conservation of charge, it should be equal to this value for any temperature.

The conservation of total charge holds also out of equilibrium. Imagine for instance that we inject charge into a region of the superconductor. This means that we excite quasiparticles in the $k > k_F$ branch of the dispersion relation. To maintain charge neutrality, we have to remove Cooper pairs with equivalent charge from the system. Therefore, the chemical potential μ_S changes to from μ to $\mu + \delta\mu_S$ where $\delta\mu_S < 0$, and is thus reduced from its equilibrium value, since the chemical potential μ_{qp} for quasiparticles is increasing with the addition of excitation. As seen in the left panel of Fig. 12.8 below, this reduces the probability to find a Cooper pair at a given momentum k . At the same time, the excitation spectrum for quasiparticle shifts since its minimum still occurs at the chemical potential of the Cooper pairs, in effect at $\mu_S = \mu + \delta\mu_S$. Thus, adding a single electron-like excitation ($k > k_F$) shifts the dispersion curve E vs. k toward smaller k (left), since the minimum of E should now occur at $k^2/2m = \mu_S = \mu + \delta\mu_S$. This has two effects. The first effect is that it causes some quasiparticles to change branch: as one moves the dispersion curve, particles at a given k that were previously in the hole branch $k^- < k_F$ now become part of the electron branch. Secondly, it causes a small increase of the effective charge of all electron-like quasiparticles and a small decrease in charge of all hole-like quasiparticles. In order to introduce a chemical potential for the quasiparticles in the presence of charge imbalance, we assume that the quasiparticles are in equilibrium with *themselves* even if they are not in equilibrium with the condensate. We illustrate these effects in Fig. 12.8 (taken from K. Gray, *Nonequilibrium superconductivity* in the J. Clarke chapter).

Charge neutrality then dictates that $Q_S + Q_N$ in the above out of equilibrium situation must equal the equilibrium value $\frac{2e}{\Omega} \sum_k v_k^2$. We may thus write:

$$Q_N|_{\delta\mu_S \neq 0} + Q_S|_{\delta\mu_S \neq 0} = -\frac{2e}{\Omega} \sum_k v_k^2, \quad (12.376)$$

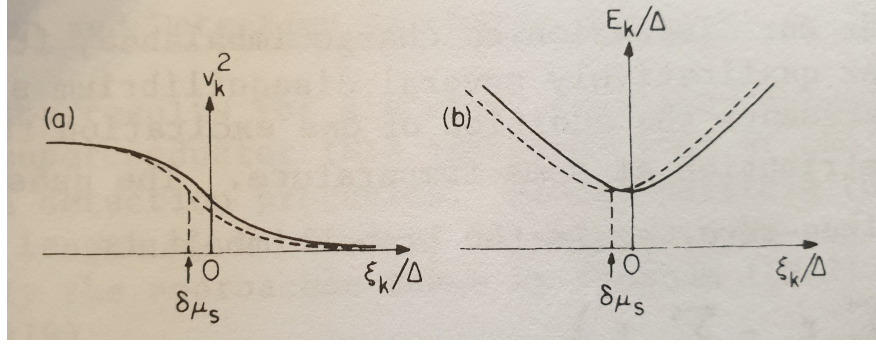


Figure 12.8: (a) The effect on the condensate density and (b) the quasiparticle excitation spectrum when ELQ are added to the superconductor. The solid and dashed lines represent equilibrium and non-equilibrium, respectively. Remember that in equilibrium, we have $\mu_S = \mu$, whereas out of equilibrium $\mu_S = \mu + \delta\mu_S$. In the figure, $\xi_k = k^2/2m - \mu$. Note that the quasiparticle charge is now determined by $q_k = -e[k^2/2m - (\mu - \delta\mu_S)]/E_k(\mu_S) = -e(\xi_k - \delta\mu_S)/E_k(\mu_S)$.

which gives the total quasiparticle charge out of equilibrium:

$$Q_N|_{\delta\mu_S \neq 0} = -\frac{2e}{\Omega} \sum_k (v_k^2|_{\delta\mu_S=0} - v_k^2|_{\delta\mu_S \neq 0}). \quad (12.377)$$

From now on, we simply write Q_N for the charge imbalance and drop the subscript.

We can convert the summation over k to an integral over the kinetic energy $\epsilon = k^2/2m$ via

$$\frac{1}{\Omega} \sum_k \rightarrow \int d\epsilon N(\epsilon) \quad (12.378)$$

where $N(\epsilon)$ is the single-spin normal-state density of states. Assuming that $\delta\mu_S$ is small compared to μ , we then get:

$$\begin{aligned} Q_N &= -2e \int_0^\infty d\epsilon N(\epsilon) (v_k^2|_{\delta\mu_S=0} - v_k^2|_{\delta\mu_S \neq 0}) \\ &= 2e \int_{-\mu_S}^\infty d\xi_k N(\xi_k) \frac{\partial(v_k^2)}{\partial(\delta\mu_S)} \delta\mu_S \end{aligned} \quad (12.379)$$

after a change of integration variable from ϵ to ξ_k . In v_k , it is only

$$\xi_k = \epsilon - \mu_S = \epsilon - \mu - \delta\mu_S \quad (12.380)$$

that depends on $\delta\mu_S$, and we may therefore write

$$\begin{aligned} \frac{\partial(v_k^2)}{\partial(\delta\mu_S)} &= \frac{\partial(v_k^2)}{\partial\xi_k} \frac{\partial\xi_k}{\partial(\delta\mu_S)} \\ &= \frac{\partial(v_k^2)}{\partial\xi_k} \times (-1). \end{aligned} \quad (12.381)$$

The integral for Q_N then takes the form:

$$Q_N = -2e\delta\mu_S \int_{-\mu_S}^\infty N(\xi_k) \frac{\partial(v_k^2)}{\partial\xi_k} d\xi_k. \quad (12.382)$$

The quantity $\frac{\partial(v_k^2)}{\partial\xi_k}$ is largest near $\xi_k = 0$, so we perform an approximation where we pull the density of states factor outside of the integral and replace it with its value N_0 at the Fermi level $\xi_k = 0$ since the DOS varies slowly. We then obtain

$$\begin{aligned} Q_N &= -2e\delta\mu_S N_0 [v_k^2]_{\xi_k=-\mu_S}^{\xi_k \rightarrow \infty} \\ &= 2e\delta\mu_S N_0 \end{aligned} \quad (12.383)$$

where we used that $v_k^2 = \frac{1}{2}(1 - \xi_k/\sqrt{\xi_k^2 + |\Delta|^2})$ and $v_k^2(\xi_k \rightarrow \infty) = 0$ and $v_k^2(\xi_k = -\mu_S) \simeq 1$ since $\mu \gg |\Delta|$. Thus, for an excess of electron-like excitations, we have $Q_N < 0$ and $\mu_S < \mu$ is reduced compared to its normal-state value (opposite for excess of holes). One can show (see textbook by Tidecks) that for $T \simeq T_c$, we have $\mu_q \simeq \mu$, so that in that case one may write $Q_N \propto \mu_q - \mu_S$: the charge imbalance is then a direct measure of the difference between the chemical potentials of the quasiparticles and the Cooper pairs. For $T \simeq T_c$, we can even write $Q_N \propto \mu_{ec,q} - \mu_{ec,S}$ where μ_{ec} is the electrochemical potential (taking into account the electrostatic potential $-q\phi$) which we will discuss later, since the ϕ just cancels out. However, we will show that Q_N is also proportional to ϕ later on, so that $\delta\mu_S \propto \phi$.

Therefore, the equation we started with:

$$Q_{\text{tot}} = -\frac{2e}{\Omega} \sum_k v_k^2 + \frac{2}{\Omega} \sum_k q_k f_k, \quad (12.384)$$

is a self-consistency equation for $\delta\mu_S$. For any non-equilibrium quasiparticle distribution f_k , the constancy of Q_{tot} determines the change $\delta\mu_S$ in the pair chemical potential that enters q_k and v_k in the above equation. This is similar to the BCS gap equation, where for any given f_k the self-consistency equation determines Δ .

Steady state

In a steady state situation where a constant current goes into the superconductor, a charge imbalance is continuously injected at a rate $\dot{Q}_N^{\text{in}}$. This excess charge, described by a non-equilibrium distribution function f_k , relaxes to a Fermi-Dirac distribution at a rate denoted τ_Q^{-1} . This produces a steady state charge imbalance Q_N . We have

$$\tau_Q^{-1} = \frac{\dot{Q}_N^{\text{in}}}{Q_N}. \quad (12.385)$$

This equation can be understood as follows. To have a steady state (constant in time) charge imbalance Q_N , the relaxation rate has to equal the rate of injection. The decay of charge imbalance to relaxation processes that occur with a rate τ_Q^{-1} can be described in the standard way

$$\left. \partial Q_N / \partial t \right|_{\text{relax}} = -\tau_Q Q_N. \quad (12.386)$$

Solving this differential equation would give an exponentially decaying $Q_N(t) = Q_N(t=0)e^{-t/\tau_Q}$. But in steady state, we have $\partial Q_N / \partial t = 0$. This is because the decay is balanced by the injection rate $\dot{Q}_N^{\text{in}}$:

$$\partial Q_N / \partial t = 0 = -\tau_Q Q_N + \dot{Q}_N^{\text{in}}. \quad (12.387)$$

This immediately gives Eq. (12.385).

Presently, we have simply introduced τ_Q^{-1} as a phenomenological quantity, but it can be measured experimentally and we shall discuss the physical processes that are responsible for the relaxation of the charge imbalance later.

We also note that one can define a branch imbalance B which gives information about the quasiparticle *population* of the e- and h-like branches of the spectrum, irrespective of the quasiparticle charge of this population:

$$B = \frac{2}{\Omega} \left(\sum_{k > k_F} f_k - \sum_{k < k_F} f_k \right). \quad (12.388)$$

What about the quasiparticle chemical potential μ_{qp} ?

Where does the quasiparticle chemical potential μ_{qp} enter? It enters in the distribution function f_k : specifically, the occupation probability of a quasiparticle in the presence of charge imbalance can be described by a Fermi function $f(E_k)$ in which μ_S in the quasiparticle energy E_k has been replaced by μ_{qp} :

$$E_k = \sqrt{[k^2/2m - \mu_{qp}]^2 + |\Delta|^2}. \quad (12.389)$$

However, note that the potential μ_{qp} does *not* enter the expression for the effective quasiparticle charge q_k , and thus u_k and v_k , since these have to be computed with the actual local value of the pair chemical potential μ_S .

We underline that in order to be able to introduce a chemical potential for the quasiparticles at all in the presence of a charge imbalance, one has to assume that the quasiparticles are in equilibrium with themselves although they are not in equilibrium with the condensate (in the sense that the occupation probability of a quasiparticle state is not given by a Fermi function $f(E_k)$ using the local value of μ_S).

We can derive an explicit expression for μ_{qp} . Let $\delta f = f_k - f_k^{\text{eq}}$, where f_k^{eq} is the equilibrium Fermi-Dirac distribution function and $f_k^{\text{non-eq}}$ is a general, non-equilibrium distribution. Out of equilibrium, we may then write the charge imbalance $Q_N = \frac{2}{\Omega} \sum_k q_k f_k$ as

$$Q_N = \frac{2}{\Omega} \sum_k q_k \delta f_k \quad (12.390)$$

since the equilibrium term gives no contribution to the charge imbalance. Now, let $\delta\mu_{qp} = \mu_{qp} - \mu_S$ be the deviation in quasiparticle chemical potential from the condensate chemical potential out of equilibrium. Since the quasiparticle chemical potential enters f_k as

$$f_k = f(\sqrt{[k^2/2m - \mu_{qp}]^2 + |\Delta|^2}), \quad (12.391)$$

we can write to first order in $\delta\mu_{qp}$:

$$\delta f_k = \frac{\partial f_k}{\partial E_k} \frac{\partial E_k}{\partial \mu_S} \delta\mu_{qp}. \quad (12.392)$$

We have

$$\frac{\partial E_k}{\partial \mu_S} = q_k/e \quad (12.393)$$

where q_k is the fractional charge of quasiparticles. Plugging all of this back into Eq. (12.390) gives

$$\delta\mu_{\text{qp}} = \frac{Q_N}{2/\Omega e} \frac{1}{\sum_k q_k^2 \partial f_k / \partial E_k}. \quad (12.394)$$

In equilibrium where $Q_N = 0$, we see that $\delta\mu_{\text{qp}} = 0$ so that $\mu_{\text{qp}} = \mu_S = \mu$.

From the above definition of the quasiparticle chemical potential, it is clear that $\mu_{\text{qp}} = \mu_S$ in equilibrium. In the presence of a charge imbalance, the pair chemical potential is reduced while the quasiparticle chemical potential increases, or vice versa (depending on whether $Q_N < 0$ or $Q_N > 0$). μ_S is used to compute effective quasiparticle charges and the coherence factors u_k and v_k , whereas μ_{qp} is used in the quasiparticle energy entering the distribution function.

In recent years, experimental papers on charge and spin imbalance in superconductors have used a modelling where they seem to simply shift E itself by a chemical potential $\delta\mu$ in the Fermi-Dirac distribution function, i.e. $f(E_k \pm \delta\mu)$. One way to justify this is to assume that the deviation of μ_{qp} from its equilibrium value μ , $\delta\mu = \mu_{\text{qp}} - \mu$, is small and then Taylor-expand E_k so that one obtains $f[E_k(\delta\mu = 0) + \delta\mu]$.

Thus, *charge relaxation* in a superconductor refers to the fact that when you inject a non-polarized current from a normal metal into a superconductor, you generate a charge accumulation of quasiparticles at the interfaces which decays as the particles recombine into Cooper pairs in the bulk of the superconductor.

12.31.3 Converting quasiparticle current driven by charge imbalance into supercurrent flowing in the bulk

We now wish to understand in more detail how the charge imbalance that occurs on the S side gives rise to a quasiparticle current which decays over a length scale λ_Q and instead converts into supercurrent. In this way, we explain the physics behind how supergap quasiparticles $E > \Delta$ are converted into supercurrent even without Andreev reflection.

In other words, the proximity effect in a normal metal always requires Andreev reflection, but the conversion from normal current to supercurrent does *not* require Andreev reflection: it can also occur via a decaying charge imbalance. This is what we will show.

The starting point is to force $\mathbf{F}$ exerted on superconducting electrons, which are part of the Cooper pairs:

$$\begin{aligned} \mathbf{F} &= \frac{d}{dt}(m\mathbf{v}_S) = q\mathbf{E} - \nabla\mu_S \\ &= e\nabla\phi + e\frac{d\mathbf{A}}{dt} - \nabla\mu_S. \end{aligned} \quad (12.395)$$

Here, we have expressed the gauge-invariant electric field in terms of its potentials and also, importantly, added a possible gradient in the chemical potential μ_S for superconducting electrons. A

gradient in this potential results in a force on the electrons. This is understood by noting that the appropriate potential energy to use in a problem where there is a concentration gradient of electrons and an electrostatic field present is the *electrochemical potential*

$$\mu_{ec} = q\phi + \mu \quad (12.396)$$

The force is generally minus the gradient of the potential energy, which gives Eq. (12.395) (when one also includes the $\mathbf{A}$ -part to ensure gauge invariance). The component $-\nabla\mu_S$ thus corresponds to a driving force for diffusion pointing from high concentration to low concentration. Note that our derivation of $Q_N \propto \delta\mu_S$ is still correct, where μ_S and $\delta\mu_S$ is the chemical (not electrochemical) potential in the superconductor since these were defined using the excitation energies and not Fermi-Dirac distribution functions.

This above expression for the force allows us to consider a non-equilibrium situation where $\nabla\mu_S \neq 0$. Under stationary, but non-equilibrium, conditions, we must have $\frac{d}{dt}(m\mathbf{v}_S) = 0$. The superconducting electrons, which make up the Cooper pairs, should not accelerate under stationary conditions. Importantly, this does not oppose the existence of an electric field. The reason is that the gradient in μ_S can cancel $\mathbf{E}$. In fact, we get

$$\mathbf{E} = -\nabla\phi - \frac{d\mathbf{A}}{dt} = -\nabla\mu_S/e. \quad (12.397)$$

In other words, the charge imbalance first causes a gradient in μ_S due to charge neutrality. Under stationary conditions, this means that an electric field exists in the non-equilibrium region with charge imbalance. Now, we derived earlier that $Q_N = 2eN_0\delta\mu_S = 2eN(0)(\mu_S - \mu)$. Therefore, $\nabla\mu_S = \nabla Q_N/2eN_0$, and we have obtained

$$\mathbf{E} = -\frac{1}{2e^2N_0}\nabla Q_N. \quad (12.398)$$

A gradient in the charge imbalance Q_N thus brings about an electric field. But does this field does not cause the Cooper pairs to accelerate, due to the compensating gradient $\nabla\mu_S$. So, setting $\mathbf{A} = 0$, the potential ϕ is determined by the deviation of the pair chemical potential $\delta\mu_S$ from its equilibrium value:

$$\phi = -\delta\mu_S/e \propto Q_N, \quad (12.399)$$

and also gives the electric field via $\mathbf{E} = -\nabla\phi$.

We note in passing that the comment about charge neutrality in RMP 2017 by Bergeret *et al.* can be understood in this light. Their ρ is the non-equilibrium charge in the system. They say that when charge neutrality is maintained, the charge imbalance [μ in their notation and it is the difference between electron and hole excitations in the system, just like for us] is always accompanied by a finite electrostatic potential ϕ . Therefore, a gradient in charge imbalance gives rise to a gradient in ϕ and thus static electric fields, just as in our case. Moreover, when Bergeret *et al.* refer to the condensate potential μ_S and set this to zero, this should be understood as setting our μ_{ec} to zero since under stationary conditions there is no acceleration of Cooper pairs ($\nabla\mu_{ec} = 0$).

So how do we now actually see the conversion from normal quasiparticle current to supercurrent? The first step is to note that since the total current has to be conserved, we have that $\nabla \cdot \mathbf{J} = 0$

where $\mathbf{J} = \mathbf{J}_N + \mathbf{J}_S$. We can get an expression for $\nabla \cdot \mathbf{J}_N$ from the continuity equation for the charge imbalance Q_N :

$$\partial Q_N / \partial t + \nabla \cdot \mathbf{J}_N = \mathcal{S}_Q \quad (12.400)$$

Here, $\mathcal{S}_Q = \partial Q_N / \partial t|_{\text{relax}}$ is a source term which accounts for relaxation processes. We know that Q_N relaxes, via different relaxation mechanisms which will be treated in detail later, according to

$$\mathcal{S}_Q = -Q_N / \tau_Q. \quad (12.401)$$

Therefore, we get at steady state ($\partial Q_N / \partial t = 0$):

$$\nabla \cdot \mathbf{J}_N = -Q_N / \tau_Q. \quad (12.402)$$

Close to T_c , where there are mostly normal electrons in the superconductor, we should expect Ohm's law to be approximately valid for the normal current, $\mathbf{J} = \sigma \mathbf{E}$. In general, since there is a gradient in the quasiparticle chemical potential as well, this should also give a diffusion contribution to the normal current $\mathbf{J}$. However, we disregard it here since we are close to T_c where Ohm's law should be close to valid for the normal current. Inserting this into the above equation gives

$$-\frac{\sigma}{2e^2 N_0} \nabla \cdot \nabla Q_N = -Q_N / \tau_Q \quad (12.403)$$

which can be rearranged into

$$\nabla^2 Q_N - Q_N / \lambda_Q^2 = 0 \quad (12.404)$$

where we defined the *charge relaxation length* λ_Q according to:

$$\frac{1}{\lambda_Q^2} \equiv \frac{2e^2 N_0}{\sigma \tau_Q}. \quad (12.405)$$

The differential equation for Q_N can be solved straightforwardly. Consider 1D for simplicity where we get:

$$Q_N = Q_0 e^{-x/\lambda_Q} \quad (12.406)$$

with Q_0 determined by boundary conditions at the interface.

We can now also show how the normal current decays on the length scale λ_Q . Going back to Eq. (12.402) and considering 1D, we get the equation

$$\partial_x J_N = -\frac{Q_0}{\tau_Q} e^{-x/\lambda_Q} \quad (12.407)$$

which gives the solution for the current:

$$J_N(x) = \frac{\lambda_Q}{\tau_Q} Q_0 e^{-x/\lambda_Q} + \text{constant}. \quad (12.408)$$

The constant is zero based on the boundary condition that $J_N \rightarrow 0$ deep inside the superconductor since the charge imbalance vanishes there.

We can now also determine the spatial behavior of the supercurrent, based on the conservation of the total charge current $J = J_N + J_S$, which is $\partial_x J = 0$. Therefore, $\partial_x J_N = -\partial_x J_S$ and we get:

$$J_S(x) = -\frac{\lambda_Q}{\tau_Q} Q_0 e^{-x/\lambda_Q} + \text{constant}. \quad (12.409)$$

Here, the constant term is not zero. Right at the interface, there should be no supercurrent since the charge imbalance has not had time to relax yet, so $J_S(0) = 0$. This determines the constant and we get

$$J_S(x) = \frac{\lambda_Q Q_0}{\tau_Q} (1 - e^{-x/\lambda_Q}). \quad (12.410)$$

which increases until it reaches a constant value in the bulk.

We finally comment on the relation to a gradient in the superconducting order parameter, which should be present in the bulk due to the supercurrent. First, we show that it is possible to get a gradient in the superconducting phase even if $\delta\mu_S \rightarrow 0$ in the bulk, so that $\mu_S \rightarrow \mu$. We start by recalling that the London equations are normally written

$$\begin{aligned} \nabla \times (\lambda \mathbf{J}_S) &= -\mathbf{B}, \\ \frac{d}{dt} (\lambda \mathbf{J}_S) &= \mathbf{E} = -\dot{\mathbf{A}} - \nabla\phi, \end{aligned} \quad (12.411)$$

where λ is the penetration depth (the London parameter) which is inversely proportional to the superfluid density n_S , while $\mathbf{J}_S$ is the supercurrent. The equations are independent and each connected with an important superconducting property. The first one predicts the Meissner effect, whereas the second one shows that for a constant supercurrent, the electric field is zero. These are the two main properties of a superconductor.

The question is now if London's equations should be modified in the presence of a charge imbalance. In normal metals, we know that the driving force for electrons is not just an electric field, but more generally the gradient of an electrochemical potential μ_{ec} . We have

$$\mu_{ec} = q\phi + \mu \quad (12.412)$$

so that

$$\nabla\mu_{ec} = -q\mathbf{E} + \nabla\mu, \quad (12.413)$$

meaning that a gradient $\nabla\mu$ in the chemical potential for the fermions can also drive a current. From our above analysis, it thus seems reasonable that we should modify the second of London's equations to incorporate the possible presence of a gradient in the pair chemical potential $\nabla\mu_S$ which should act similarly to the electric field. In effect, we perform $q\mathbf{E} \rightarrow q\mathbf{E} - \nabla\mu$ in order to get:

$$\frac{d}{dt} (\lambda \mathbf{J}_S) = -\dot{\mathbf{A}} - \frac{1}{q} \nabla\mu_{ec} \quad (12.414)$$

as the generalized second London equation where now μ_{ec} is the appropriate electrochemical potential for the Cooper pairs. By now taking the first London equation and combining it with the GL

equation for the supercurrent $\mathbf{J}_S$, we obtain the following two equations:

$$\begin{aligned}\frac{d}{dt}(\lambda \mathbf{J}_S) &= -\dot{\mathbf{A}} - \frac{1}{q} \nabla \mu_{ec}, \\ \frac{d}{dt}(\lambda \mathbf{J}_S) &= -\dot{\mathbf{A}} + \frac{\hbar}{2q} \nabla \dot{\theta}.\end{aligned}\tag{12.415}$$

Clearly, it follows that the Josephson relation for the phase θ of the OP $\Delta = |\Delta|e^{i\theta}$ at a given point in space and time is then:

$$\frac{d\theta}{dt} = -2(\mu_S + q\phi) + \text{constant}\tag{12.416}$$

Under stationary conditions, $\dot{\theta} = 0$ and thus the right-hand side should vanish. Assuming that charge imbalance is the only source of an electrostatic potential, we can set $\phi = 0$ in the bulk of the superconductor. This means that the constant is equal to 2μ since $\mu_S = \mu$ in the bulk of the superconductor. Therefore, we have in general:

$$\dot{\theta} = -2(\delta\mu_S + q\phi)\tag{12.417}$$

The point is now that this equation does not preclude that $\theta = \theta(\mathbf{r})$. Even if $\dot{\theta} = 0$, the phase θ can still have a gradient in space, which corresponds to a supercurrent. So long as μ_{ec} is constant and equal to μ , so that $\mu_S + q\phi = \mu$, we have $\dot{\theta} = 0$. This scenario still covers charge imbalance and conversion from resistive to supercurrent, since μ_S can still have a spatial gradient which is cancelled by the gradient in the electrostatic potential ϕ under stationary conditions. In other words, we can have μ_{ec} constant throughout a non-equilibrium, stationary superconductor.

A microscopic derivation of Eq. (12.416) beyond a modification of the (phenomenological) London equations is discussed in detail in <https://royalsocietypublishing.org/doi/pdf/10.1098/rspa.1975.0133>.

What about literature saying that μ_{ec} relaxes over ξ_S ?

In previous literature, one finds that the statement (such as in <https://iopscience.iop.org/article/10.1088/1367-2630/9/5/116/pdf>) that the Cooper pair electrochemical potential recovers its bulk value over a distance ξ_S . This is much shorter than λ_Q and in practice one can take μ_{ec} for the Cooper pairs as constant throughout the superconductor, as long as one is not close to T_c . The reason for this statement is probably the variation of the superconducting gap near the interface which recovers over a distance ξ_S , which we have not taken into account (i.e. the spatial variation of $|\Delta|$) in our treatment above. However, note that even if μ_{ec} relaxes much quicker than μ_{qp} , this does not contradict current conservation: the supercurrent is driven by a phase gradient, not a gradient in μ_{ec} , so that a supercurrent can flow even if μ_{ec} is constant. On the other hand, a quasiparticle current can only flow when there exists a gradient in μ_{qp} , and as a result there exists an associated electric field and voltage drop.

What is the value of the charge relaxation length λ_Q ?

The length-scale for conversion from resistive current to supercurrent in a superconductor was denoted λ_Q above: the charge relaxation length. How long this length is depends on the properties of the superconductor.

Saja and Lofwander in PRB 2021 showed precisely this by solving the Eilenberger equation self-consistently in a superconductor. In their fig. 10, they consider a clean superconductor with mean

free path $l_{\text{mfp}}/\xi_0 = 10$ where ξ_0 is the BCS coherence length. Their fig. 10b shows the spatial dependence of the quasiparticle and supercurrent inside S, and it is clear that the conversion takes place over a distance exceeding $10\xi_0$, in effect far exceeding the superconducting coherence length. In fig. 13, they consider a superconductor much closer to the diffusive limit. Here, $l_{\text{mfp}} = \xi_0$ is used. They also have two normal regions for $z/\xi_0 \in [0, 5], [55, 60]$, which is why the quasiparticle current is constant there. But consider now what happens at the interface $z/\xi_0 = 5$. The conversion between currents occurs over just a couple of coherence lengths. The same happens in fig. 4. We are not quite in the diffusive limit $l_{\text{mfp}} \ll \xi_0$, but the trend is clear: the charge relaxation length becomes much closer to the coherence length the more dirty the superconductor is. Recall that the diffusive limit coherence length is $\xi = \sqrt{l_{\text{mfp}}\xi_0}$, so that $\xi = \xi_0$ for $l_{\text{mfp}} = \xi_0$.

12.31.4 Measuring the difference between pair and quasiparticle electrochemical potential

First, recall that the pair electrochemical potential and quasiparticle electrochemical potential were defined as

$$\begin{aligned}\mu_{\text{ec},S} &= \mu_S + q\phi, \\ \mu_{\text{ec},qp} &= \mu_{qp} + q\phi.\end{aligned}\tag{12.418}$$

Here, ϕ is the electrostatic potential, $q = -e$ is the charge, μ_S and μ_{qp} are the chemical potentials for Cooper pairs and quasiparticles. The potential $\mu_{\text{ec},S}$ can be understood as expressing that pairs added to the condensate enter at an energy $2\mu_{\text{ec},S}$.

A question is now: how do we measure experimentally the difference between $\mu_{\text{ec},S}$ and $\mu_{\text{ec},qp}$? The difference can be measured using a normal metal probe. Placing this in contact with the superconductor at a point where charge imbalance exists, the electrons in the normal probe will be in equilibrium with the normal fluid (quasiparticles) in the superconductor. Therefore, a voltage difference will exist between the probe and the far end of the superconductor where the charge imbalance has relaxed and $\mu_{\text{ec},qp} = \mu_{\text{ec},S}$. In this way, the voltage is equal to precisely $\mu_{\text{ec},qp}(x) - \mu_{\text{ec},S}$ at a given point x away from the point where current is injected into the superconductor.

12.31.5 Relaxation mechanisms for charge imbalance

We have seen above that if one assumes that relaxation mechanisms exist for the charge imbalance, it will cause Q_N to decay as one moves into the supercurrent. This also means that the resistive quasiparticle current will decay as one moves into the superconductor. Current conservation tells us that a supercurrent has to take over for the quasiparticle current and the physical mechanism behind this is that the charge imbalance is actually converted to charge in the condensate by relaxation mechanisms we will discuss here.

Relaxation of charge imbalance in the presence of supercurrent flow

The supercurrent flow mechanism goes as follows: when a supercurrent flows, left- and right-moving quasiparticles will have different energies due to the Doppler shift. This means that elastic scattering, conserving energy, can scatter an ELQ at a given momentum to a HLQ at a different momentum since the energies are equal despite the gap being isotropic. In this way, a charge imbalance can even out and relax.

12.32 Calculating non-equilibrium spin and charge accumulation in the superconducting state

When computing the spin and charge accumulation via quasiclassical theory, it is common in the literature to subtract the equilibrium contribution in order to obtain the true non-equilibrium accumulation. However, it turns out that this may have been done in an erroneous manner in the literature so far. The reason is the following. The equilibrium part of the spin "accumulation", more accurately described as the proximity-induced magnetization in equilibrium, will depend on the superconducting order parameter. If one turns on a voltage or temperature-gradient, the order parameter will change if it is solved selfconsistently. Therefore, the equilibrium contribution (stemming from $\hat{g}^R$ and $\hat{g}^A$ alone and not the distribution functions) will also change and *in general not cancel the equilibrium contribution when there is no voltage or temperature-gradient applied*.

12.33 The advantage of superconductors in electronics

A commonly used selling point for superconductors in electronic circuits is that they are dissipationless. One thus reads about things like lossless electronics or diode effects et.c. However, closer examination shows that this is misleading. Consider a resistive circuit with a load R and a voltage source. If we either replace R with a superconductor or add a superconductor to the circuit, there still has to be energy loss due to the electrons moving from one side of the battery to the other. The superconductor just changes where that dissipation of energy takes place. In the case of a Josephson junction, for instance, the external load R takes care of the power dissipation so that a pure current bias is applied to the Josephson junction. There is no dissipation in the Josephson junction itself, but the power is still dissipated elsewhere! In other words, adding the superconductor just controls where in the junction the power dissipation (heating) takes place.

This can of course be a useful thing. Say we want to build a quantum computer with superconducting elements. We still have to supply power, but all the heating can take place outside of the circuit component (inside the computer) itself in principle.

Moreover, superconductors have the advantage that you can trap currents running in closed loop forever. This is used in MR-technology in hospitals, where superconductors are used to generate large magnetic fields due to large currents flowing in them. Then one could ask: ok, but you still have to generate the current by a voltage source, so haven't you just moved the dissipation elsewhere in the system (and not eliminated the dissipation)? That is true, but currents can be trapped in superconductors by using a well-defined protocol, and once you've done that there is no need for an external power source anymore. The superconducting current in the loop keeps running and sustains a magnetic field.

Finally, superconductors of course are useful even disregarding any aspect of dissipation because they offer entirely new functionality like extreme magnetic field sensitivity in SQUIDs via phase coherence and via superconducting qubits.

Chapter 13

Materials

Normal metals:

- Cu
- Au
- Ag

Heavy normal metals (boosting Rashba for thin-films):

- Pt
- W
- Ta

Insulators:

- MgO
- Al₂O₃
- Glass

Mott insulators:

- NiO
-

Ferromagnetic metals:

- Co
- Fe
- Ni

Ferromagnetic insulators:

- YIG
- EuO

- GdN

Antiferromagnetic metals:

- Cr
- FeMn
- IrMn
- Mn₃Sn

Antiferromagnetic insulators:

- NiO
- Cr₂O₃

Conventional superconductors:

- Nb
- Al

p-wave superconductors:

- Sr₂RuO₄

d-wave superconductors:

- YBCO
- ...

Iron-based superconductors:

- ...

Chapter 14

Superfluidity

Rotating the Container Suppose we pour some liquid helium into a cylindrical container. And the temperature is above the lambda point so right now it's just a normal fluid (not yet cold enough to be a superfluid). Next, we start rotating the container, and the liquid helium starts to rotate with it. We continue rotating the container at the same speed and soon the liquid comes into equilibrium with it.

Now we cool the liquid down below 2.17K. Soon as we hit 2.17K, part of the liquid begins exhibiting superfluid behavior, while part of it continues acting like a normal fluid. The colder we make it, the greater the proportion of superfluid. So let's take the temperature down to near absolute zero so that pretty much all of it is superfluid.

Once we've reached our desired temperature, we stop the container. What happens? If it were a normal fluid, then once the container stopped rotating, the liquid would also soon come to rest due to viscosity. But the superfluid? It will continue circling around a long, long time.

Quantized Angular Momentum Now suppose we perform the experiment again. We do everything exactly the same as we did it last time with only one difference: we rotate the container more slowly. This time when we cool the liquid down, the liquid will stop swirling. It will stop swirling regardless of whether we stop the container or whether we let the container continue rotating. This is in stark contrast to a normal fluid which is pulled along by the container and is forced to rotate along with it. But the superfluid doesn't necessarily rotate along with its container; instead its angular momentum is quantized. A superfluid system will enter into the state whose quantized angular velocity is closest to the angular velocity with which we were rotating our container. And if we don't rotate fast enough to put it into the first excited state, the liquid will just sit there even though the container is spinning around.

Vortices Each vortex can be thought of as a quantum of angular momentum and contains, at its center, a phase singularity around which the phase changes by a multiple of 2π . This 2π winding of the phase occurs for the same reason that deBroglie matter waves explain the quantization of angular momentum. The idea is simply that the matter wave is single valued, so that if you pick any point in space and label the phase at that point 0, then if you go around in a circle so that you come back to where you started then the phase must have changed by a multiple of 2π or not at all.

And the center of the vortex is a phase singularity. This means that the matter waves must vanish at the center. Although the normal uncondensed component of the system is free to inhabit the core. But there is no superfluid at the core of a vortex. Instead, superfluid flows with quantized circulation around each core.

14.0.1 Fountain effect

If a superfluid is placed in an open container, it will creep out and overcome gravity. This is due to attractive VdW forces between the atoms in the superfluid and the container wall, which causes the superfluid to rise at the edge. This happens also for a normal fluid where the VdW forces can overcome gravity to drag the fluid up the walls and form a thin coating (example: wine glass). However, due to the finite viscosity of a normal fluid, the fluid cannot spontaneously creep up the walls and out of the container once the coating is formed, because it would require energy for the fluid to move. In contrast, there is no energy dissipation when a superfluid moves. Therefore, as the coating is formed the VdW forces can continue to drag the superfluid up along the wall and out of the container, causing the container to eventually be emptied of the superfluid. This does not happen for a normal fluid.

Chapter 15

Insulators

An insulating material conducts electric currents poorly. But insulators can have different physical origins. We may distinguish between

- Band insulators
- Mott insulators
- Anderson insulators

In each case, the insulating properties arise due to different effects. We proceed to discuss this in more detail.

15.1 Band insulator

15.2 Mott insulator

15.3 Anderson insulator

In the thermodynamic limit (infinite system), adding an infinitesimal amount of impurities to a 1D or 2D system makes them insulating. In 3D, one requires a critical value of the disorder strength in order to trigger a metal-insulator transition. In finite systems, a critical value of disorder is also required in 2D, as seen *e.g.* for a two-dimensional square lattice treated with $U = 0$ Hubbard model when adding random impurities.

Chapter 16

Magnetism

We will here give an introduction to fundamental aspects of magnetism, focusing to begin with on its physical origin and the distinction between a quantum mechanical vs. classical treatment. After a discussion of the Heisenberg model, we will then study the Landau-Lifshitz-Gilbert equation [?] and magnetization dynamics with a special eye toward possible applications such as magnetization switching and domain wall motion. Much of the material found here has been adapted from Ref. [1].

16.1 Physical origin

The phenomenon of ferromagnetism, materials which display a spontaneous magnetization even in the absence of external fields, was reported as early as 400 B.C. in China where one observed the attraction between magnetic materials. Historically, Oersted found in 1819 that current-carrying wires could deflect magnetic materials in the same way as another magnet, which suggested that there was a relation between magnetization and permanent currents of electrons. The quantitative relation between current and magnetic induction was determined by Biot, Savart, and Ampere, whereas it fell to Maxwell to complete the classical theory of electromagnetism.

16.1.1 Classical vs. Quantum

As we are faced with the phenomenon of ferromagnetism, an important question is: do we need quantum mechanics to understand it or will classical mechanics, i.e. Maxwells equations, suffice? To investigate this, consider N classical electrons with positions $\mathbf{r}_i$ and momenta $\mathbf{p}_i$. The partition function from statistical physics for such a system reads:

$$Z \propto \int \prod_i d\mathbf{r}_i d\mathbf{p}_i e^{-\beta H(\mathbf{r}_1, \dots; \mathbf{p}_1, \dots)}, \quad (16.1)$$

where H is the classical Hamilton function

$$H = \frac{1}{2m} \sum_i (\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i))^2 + U(\mathbf{r}_1, \dots). \quad (16.2)$$

The origin of the vector potential $\mathbf{A}$ need not be specified: it can be both due to currents and external fields. Let us now substitute $\mathbf{p}_i \rightarrow \tilde{\mathbf{p}}_i = \mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i)$ in the above expression for Z :

$$Z \propto \int \prod_i d\mathbf{r}_i d\mathbf{p}_i e^{-\beta \sum_j (\tilde{\mathbf{p}}_j^2 / 2m + U)} \quad (16.3)$$

The vector potential has been eliminated from the partition function. Since the free energy is $F = -(1/\beta) \ln Z$, we find the magnetization

$$\mathbf{M} = -\frac{\partial F}{\partial \mathbf{B}} = 0. \quad (16.4)$$

This shows that we cannot obtain an equilibrium spontaneous magnetization in a classical theory where the magnetic field arises from currents in the material. The resolution to this problem lies in the property of electrons called *spin* which is an intrinsic magnetic moment carried by them. One usually states that spin is a quantum mechanical property, although there is some controversy about this for integer spins. As will become clear below, however, the fact that spin can only take certain quantized values is definitely a quantum mechanical property and at least the existence of half-integer spins can be stated to be a purely quantum mechanical phenomenon. To see this, consider the fact that the magnetic dipole moment of a current loop comprised of a circulating electron is given by:

$$\mathbf{m}_l = -\mu_B \mathbf{l} / \hbar, \quad (16.5)$$

where the subscript 'l' indicates that the magnetic moment is due to the angular momentum of a charged particle. Now, if we try to think of the spin in some classical way, we can imagine it being due to the magnetic moment of a spinning charged sphere. The resulting magnetic moment can be calculated if we assume an identical mass and charge distribution of the sphere, in which case one would get:

$$\mathbf{m}_s = -\mu_B \mathbf{s} / \hbar, \quad (16.6)$$

with $\mathbf{s}$ being its angular momentum. However, the experimental reality is that the intrinsic magnetic moment of the electron is:

$$\mathbf{m}_s = -g\mu_B \mathbf{s} / \hbar \quad (16.7)$$

with g being very close to 2 in magnitude, so twice the expected moment of a spinning sphere. Classical physics cannot offer any explanation for the factor of 2. Quantum theory in the form of the Dirac equation, however, does provide $g = 2$ since the spin naturally emerges there. One may then read off the size of the electron magnetic moment from the form of the Zeeman-coupling in *e.g.* in the Pauli limit.

16.1.2 The necessity of electric charge

Magnetism, classically speaking, can be understood as a property of moving electric charge. This is the only way to generate magnetic field classically. Therefore, magnetism is an aspect of electric charge (in motion) just as electricity is a different aspect (which is present also when the charge is at rest).

But quantum mechanically, a charged particle with spin also has an intrinsic magnetic moment which creates a magnetic field. This occurs even for particles at rest. So generally speaking, one cannot state that magnetism is a property that only arises for moving, charged particles. However, one can still state that magnetism is a property that is only associated with particles that have electric charge.

16.1.3 RKKY interaction, superexchange, and dipole-dipole interaction

RKKY interaction

RKKY stands for Ruderman - Kittel - Kasuya - Yosida and refers to a coupling mechanism of nuclear magnetic moments or localized inner d - or f -shell electron spins in a metal by means of an interaction through the conduction electrons. The theory uses second-order perturbation theory to describe an indirect exchange coupling whereby the nuclear spin of one atom interacts with a conduction electron through the hyperfine interaction, and this conduction electron then interacts with another nuclear spin, thus creating a correlation energy between the two nuclear spins. Alternatively, instead of nuclear spins coupling to conduction spins through the hyperfine interaction, another scenario is for inner electron spins to couple to conduction spins through the exchange interaction. The theory is based on Bloch wavefunctions which is applicable to crystalline systems.

Tadao Kasuya from Nagoya University later proposed that a similar indirect exchange coupling could be applied to localized inner d -electron spins interacting through conduction electrons. This theory was expanded more completely by Kei Yosida of the University of California, Berkeley.

Perhaps the most significant application of the RKKY theory has been to the theory of giant magnetoresistance (GMR). GMR was discovered when the coupling between thin layers of magnetic materials separated by a non-magnetic spacer material was found to oscillate between ferromagnetic and antiferromagnetic as a function of the distance between the layers. This ferromagnetic/antiferromagnetic oscillation is one prediction of the RKKY theory.

The physics of the oscillations can be understood from the same physics that gives rise to Friedel oscillations of the electron density near an impurity. It is essentially an interference phenomena between electron wavefunctions that have different wavevectors. At some distances from the impurity, the density corresponding to these wavefunctions interferes constructively, at other it interferes destructively. This gives rise to an oscillating electron density as one moves away from the impurity. Generalizing this to include the spin-degree of freedom, two magnetic impurities will also induce oscillations in the charge and spin densities near them. The impurities interact with the local itinerant electron spin density according to $\mathbf{S}_{\text{imp}} \cdot \mathbf{s}_{\text{itinerant}}$, and the interaction energy between them will depend on how $\mathbf{s}_{\text{itinerant}}$ is affected by both impurities. Moving one impurity away from the other will change its contribution to $\mathbf{s}_{\text{itinerant}}$ in an oscillatory manner, and thus the net interaction energy between the impurity spins $\mathbf{S}_{\text{imp}}$ will oscillate.

Let us give a simplified mathematical model to describe the essence of the physics. Consider first the Friedel oscillations of the electron (charge) density induced by a hard wall. Consider an incoming electron with energy E and momentum $k = \sqrt{2mE}$ which scatters on the hard wall at $x = 0$:

$$\psi = e^{ikx} + re^{-ikx}. \quad (16.8)$$

The reflection probability $R = |r|^2$ is unity and r is in general complex since the energy is smaller than the potential barrier. The density of the electron wavefunction is

$$\rho = |\psi|^2 = 1 + |r|^2 + 2\text{Re}\{re^{-2ikx}\}. \quad (16.9)$$

The reflection coefficient is generally:

$$r = \frac{k - q}{k + q}, \quad (16.10)$$

where $q = \sqrt{2m(E - V)}$. For $V \gg E$, as appropriate for a hard wall, the reflection coefficient is $r \simeq -1$. Therefore, we get

$$\rho = 2 + 2 \cos(2kx). \quad (16.11)$$

To find the total electron density at a point x , we have to take into account the contribution from all possible wavevectors. At zero temperature, all wavevectors from 0 to k_F will contribute:

$$\rho_{\text{tot}}(x) = \int_0^{k_F} dk \rho(x) = 2k_F + \frac{\sin(2k_F x)}{x}. \quad (16.12)$$

It is clear that an oscillating component appears which decays away from the interface. The physics behind this is that different wavelength electrons will be in phase close to the interface, but eventually start to interfere destructively since they oscillate over different length scales.

Let us now apply the same reasoning to understand RKKY oscillations in the interaction between two spin impurities. Consider first one of the two spin impurities. We may again consider incoming electrons, but now we have to distinguish between spin-up and spin-down since the reflection coefficient will be different due to the spin-dependent interaction between the electrons and the impurity:

$$\begin{aligned} \psi_{\uparrow} &= e^{ikx} + r_{\uparrow} e^{-ikx}, \\ \psi_{\downarrow} &= e^{ikx} + r_{\downarrow} e^{-ikx}. \end{aligned} \quad (16.13)$$

We consider the impurity spin to be a weak potential which does cause some reflection, but not nearly as drastic as a hard wall. Therefore, the scattering coefficients are assumed small: $|r_{\sigma}| \ll 1$. This can be seen to be the case for electron energies which are much larger than the impurity potential V from the analytical expression for r . We also note that r_{σ} is real and positive in this case.

Now, we may construct the contribution to the electron spin magnetization for a given k from the above wavefunctions according to

$$\mathbf{M} = \psi^{\dagger} \boldsymbol{\sigma} \psi, \text{ where } \psi = \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix}. \quad (16.14)$$

From this, and computing the contribution to M_z from incoming spin up and spin down contributions separately, one obtains:

$$M_z = 2(r_{\uparrow} - r_{\downarrow}) \cos(2kx) \quad (16.15)$$

upon neglecting terms $\mathcal{O}(r_{\sigma}^2)$ due to their smallness. The total spin density is obtained by integrating over all momenta and gives

$$M_{z,\text{tot}} = \int_0^{k_F} dk M_z = \frac{(r_{\uparrow} - r_{\downarrow}) \sin(2k_F x)}{x}. \quad (16.16)$$

This shows that the induced magnetization due to the electron interaction with the spin impurity oscillates as one moves away from the impurity spin. At some distances x , the magnetization is positive. If a second impurity spin is located at such distances, it will be energetically preferable for this impurity spin to point along the positive spin direction. If it is instead located at a distance where the magnetization is negative, it will prefer to point in the opposite direction.

We should also check that this is consistent by starting with the scattering off the other impurity. If we find above that the magnetization is positive, so that the other spin prefers to point in the same direction as the original impurity spin, the whole argument can be reversed by letting $k \rightarrow -k$ in the wavefunctions. This has no effect on the final result. If the magnetization instead is negative, $-|M|$, at the position of the other spin, it will point anti-parallel to the original impurity spin. Then, in addition to $k \rightarrow -k$ we have to let $r_{\uparrow} \leftrightarrow r_{\downarrow}$ for scattering of the present impurity spin since it is pointing in the opposite direction as the original spin. This causes the magnetization to be $+|M|$ at the original spin, consistent with it pointing oppositely to the other spin.

Above, we assumed implicitly that the incoming electron had a spin collinear with the impurity, since otherwise there would have been a probability for spin-flip reflection. However, there is no loss of generality in assuming since all spin quantization axes are equivalent in a normal metal.

The above treatment can in principle be generalized to a normal metal including Rashba spin-orbit interactions. In this case, the eigenstates are the helicity eigenspinors ψ_{λ} , $\lambda = \pm$ rather than $\psi_{\uparrow} = (1, 0)$ and $\psi_{\downarrow} = (0, 1)$. We can consider incident helicity eigenstates toward a spin impurity, in which case reflection both as the same helicity and opposite helicity can generally take place, depending on the orientation of the spin impurity. This depends on the precise form of the spin-orbit coupling. For instance, we can take $H_{\text{SOC}} = \alpha k_x \sigma_z$, in which case the z -component of the spin is still a good quantum number, or we can take $\alpha k_x \sigma_x$, in which case it is not. Computing the induced itinerant electron spin magnetization from reflection at the spin impurities, considering both incoming $+$ and $-$ helicity particles separately, one would find a precessing spin moving from one impurity to the other in general. Imamura *et al.* show that when transforming one of the impurity spins to rotate with a precession angle $k_{\text{SO}}R$, where k_{SO} is related to the spin-orbit strength and R is the separation distance, the final coupling ends up being $\mathbf{S}_1 \cdot \mathbf{S}_2^{\text{transformed}}$. In the original frame, this gives rise to a DMI-interaction.

One could then ask: should we also expect a DMI-term in the spin-spin interaction if one considers impurity spins in a ferromagnet, since spins that are not aligned with the magnetization can precess as well? The answer is no, as explained in Fig. ???. If one replaces the ferromagnet with a Rashba spin-orbit coupled material instead, however, the effective magnetic field depends on momentum: $\mathbf{M}(\mathbf{k}) = -\mathbf{M}(-\mathbf{k})$. Therefore, the precession in the lower row is opposite to the upper row since the electron moves in the opposite direction. Therefore, a canted spin configuration is permitted.

Comparison with dipole-dipole strength

The RKKY interaction strength, for spins separated a few lattice sites, ranges from less than a meV to tens of meV, depending on which material and doping range one considers. Metals typically lie in the upper range, whereas insulators give a very low RKKY strength, and superconductors lie in between (meV or a bit less).

Let us compare this with the potential energy from a magnetic dipole-dipole interaction which at finite distance between the dipoles has the form

$$E = -\frac{\mu_0}{4\pi r^3} [3(\mathbf{m}_1 \cdot \hat{\mathbf{r}})(\mathbf{m}_2 \cdot \hat{\mathbf{r}}) - \mathbf{m}_1 \cdot \mathbf{m}_2], \quad (16.17)$$

where $\hat{\mathbf{r}}$ is the unit vector parallel to the line joining the centers of the dipoles $\mathbf{m}_1$ and $\mathbf{m}_2$. If we

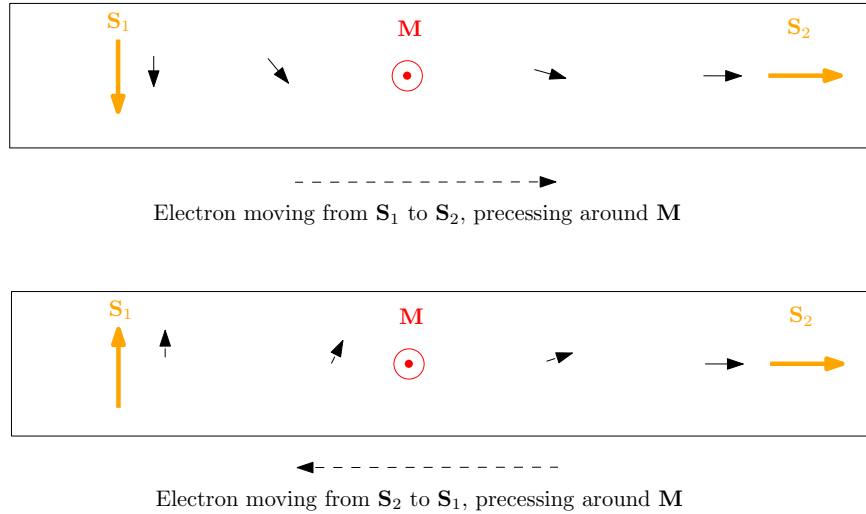


Figure 16.1: *Top row:* an electron interacting with $\mathbf{S}_1$ prefers to be aligned with it due to the exchange coupling. As it moves toward $\mathbf{S}_2$, it precesses due to the presence of $\mathbf{M}$. When it reaches $\mathbf{S}_2$, a parallel coupling between them will be favored. *Lower row:* However, for the impurity spin configuration in the top row to be the ground state, the reverse argument has to work: a spin starting from $\mathbf{S}_2$ has to end up being parallel to $\mathbf{S}_1$ after moving to it and precessing. The precession occurs in the same direction as before (this can be seen by physically rotating the system 180 degrees), but the electron starting at $\mathbf{S}_2$ then ends up being antiparallel to the $\mathbf{S}_1$ direction from the top row. Therefore, the precession prevents any non-collinear alignment of the impurity spins from being the ground state. Mathematically, this also follows from the effective RKKY interaction obtained in a ferromagnet: $F = E_I S_{1z} S_{2z} + E_H (S_{1x} S_{2x} + S_{1y} S_{2y})$. Depending on which term is largest, E_I or E_H , the spins will prefer to be aligned with the z -axis or lie in the xy -plane.

take the magnitude of the dipoles to be 10 Bohr magneton (10 electron spins), then for a separation distance of 1 nm with antiparallel dipoles (maximizing E), we find $E \simeq 0.02$ meV. Hence, it is reasonable to neglect this compared to the RKKY strength.

Superexchange

Superexchange is the strong and usually antiferromagnetic coupling between two next-to-nearest neighbour cations through a non-magnetic anion. An example of this is Mn-O-Mn where the spins couple as $\downarrow - \uparrow, \downarrow - \uparrow$ so that there in effect is an AFM coupling between the spins on the magnetic Mn ions.

Dipole-dipole interaction

A magnetic dipole can be viewed as the limit of a current loop where the radius shrinks to zero while the current increases so that the magnetic moment remains constant. Because of this analogy, one can derive that the vector potential at position $\mathbf{r}$ produced by a magnetic moment $\mathbf{m}$ is (outside the source region, i.e. away from the infinitesimal current loop)

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \frac{\mathbf{m} \times \mathbf{r}}{r^3} \quad (16.18)$$

The belonging magnetic field is

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A} = \frac{\mu_0}{4\pi} \left(\frac{3\mathbf{r}(\mathbf{m} \cdot \mathbf{r})}{r^5} - \frac{\mathbf{m}}{r^3} \right) \quad (16.19)$$

Now, the force exerted by a dipole moment $\mathbf{m}_1$ on another $\mathbf{m}_2$ when the two dipoles are separated in space by the vector $\mathbf{r}$ is

$$\mathbf{F} = \nabla(\mathbf{m}_2 \cdot \mathbf{B}_1), \quad (16.20)$$

where $\mathbf{B}_1$ is the field coming from dipole 1, and so the potential energy of the interaction between them is obtained from $\mathbf{F} = -\nabla U$:

$$U = -\mathbf{m}_2 \cdot \mathbf{B}_1 \quad (16.21)$$

and gives

$$U = -\frac{\mu_0}{4\pi r^3} [3(\mathbf{m}_1 \cdot \hat{\mathbf{r}})(\mathbf{m}_2 \cdot \hat{\mathbf{r}}) - \mathbf{m}_1 \cdot \mathbf{m}_2]. \quad (16.22)$$

This is the dipole-dipole interaction between two magnetic dipoles, such as spins. In an actual magnetic material, one has a whole distribution of spins and thus it becomes natural to let the dipole moments be dipole moment densities (i.e. magnetization) and then integrate the potential energy over the entire sample to find the total dipole-dipole free energy.

16.1.4 Dipole-dipole vs. exchange interaction as origin of magnetism

Since the magnitude of the dipole-dipole interactions apparently don't quite cut it in order to explain magnetic order at high temperatures, we need to look elsewhere to find a stronger interaction between electrons that could account for the observations. It was Heisenberg who in 1928 realized that the Coulomb repulsion between electrons can explain magnetic order at high temperatures. This might seem strange at first since this interaction is spin-independent. The point is that when combined with the intrinsic spin selectivity of quantum mechanics coming from the Pauli principle, stating that two electrons with parallel spins cannot be at the same place at the same time, a spin-dependent strong interaction is produced. Let us examine how this occurs (we have already seen an example of this in our treatment of the exchange integral in the chapter on symmetries in this book).

According to the general result in Chapter ?? for how second quantization of a two-particle operator term in the Hamiltonian should be constructed, the operators must be normal-ordered in the second quantized version of the Hamiltonian:

$$H_C = \frac{1}{2} \frac{e^2}{4\pi\epsilon_0} \int d^3r_1 d^3r_2 \sum_{\sigma\sigma'} \frac{\psi_{\sigma}^{\dagger}(\mathbf{r}_1) \psi_{\sigma'}^{\dagger}(\mathbf{r}_2) \psi_{\sigma'}(\mathbf{r}_2) \psi_{\sigma}(\mathbf{r}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (16.23)$$

If we do not normal-order the operators, a divergent term appears for $\mathbf{r}_1 = \mathbf{r}_2$ when the fermions have equal spin which is unphysical, because the Pauli principle forbids such a scenario to occur. The field operators satisfy the usual fermionic anticommutation relations such as $\{\psi_{\sigma_1}(\mathbf{r}_1), \psi_{\sigma_2}^{\dagger}(\mathbf{r}_2)\} = \delta_{\sigma_1, \sigma_2} \delta(\mathbf{r}_1 - \mathbf{r}_2)$.

The field operators ψ can be expanded into any orthonormal set of single-electron wave functions. Considering a crystal of ions as our model for a solid-state system, it is reasonable to use a set of orbital wavefunctions $\phi_{\mathbf{R}}(\mathbf{r})$ which are localized around ionic positions $\mathbf{R}$ (Wannier functions):

$$\psi_{\sigma}(\mathbf{r}) = \sum_{\mathbf{R}} \phi_{\mathbf{R}}(\mathbf{r}) c_{\mathbf{R}\sigma}, \quad (16.24)$$

where $c_{\mathbf{R}\sigma}$ are fermion annihilation operators, satisfying the same anticommutation rules as $\psi_\sigma(\mathbf{r})$. Inserting this into H_C , we obtain:

$$H_C = \frac{1}{2} \sum_{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3, \mathbf{R}_4} \langle \mathbf{R}_1, \mathbf{R}_2 | \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} | \mathbf{R}_3, \mathbf{R}_4 \rangle \times \sum_{\sigma_1 \sigma_2} c_{\mathbf{R}_1 \sigma_1}^\dagger c_{\mathbf{R}_2 \sigma_2}^\dagger c_{\mathbf{R}_3, \sigma_2} c_{\mathbf{R}_4, \sigma_1} \quad (16.25)$$

by using the orthonormality of the spinors and we have defined the quantity:

$$\langle \mathbf{R}_1, \mathbf{R}_2 | \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} | \mathbf{R}_3, \mathbf{R}_4 \rangle \equiv \int d^3 r_1 d^3 r_2 \phi_{\mathbf{R}_1}^*(\mathbf{r}_1) \phi_{\mathbf{R}_2}^*(\mathbf{r}_2) \frac{e^2}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|} \phi_{\mathbf{R}_3}(\mathbf{r}_2) \phi_{\mathbf{R}_4}(\mathbf{r}_1). \quad (16.26)$$

To make the sum over ionic position more manageable, we consider the contribution $\mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R}_3 = \mathbf{R}_4$ first, i.e. the on-site contribution of the Coulomb interaction. We then get:

$$H_{C, \text{on-site}} = \frac{1}{2} \sum_{\mathbf{R}} \sum_{\sigma_1, \sigma_2} K c_{\mathbf{R}, \sigma_1}^\dagger c_{\mathbf{R}, \sigma_2}^\dagger c_{\mathbf{R}, \sigma_2} c_{\mathbf{R}, \sigma_1}, \quad (16.27)$$

with

$$K = \int d^3 r_1 d^3 r_2 |\phi(\mathbf{r}_1)|^2 \frac{e^2}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|} |\phi(\mathbf{r}_2)|^2. \quad (16.28)$$

Using that $c_{\mathbf{R}, \sigma} c_{\mathbf{R}, \sigma} = 0$ and rearranging the operators in $H_{C, \text{on-site}}$, we obtain:

$$H_{C, \text{on-site}} = \frac{1}{2} \sum_{\mathbf{R}} K n_{\mathbf{R}} n_{\mathbf{R}}, \quad (16.29)$$

with the number operator $n_{\mathbf{R}} = \sum_{\sigma} c_{\mathbf{R}, \sigma}^\dagger c_{\mathbf{R}, \sigma}$. This is the density-density interaction of the Coulomb repulsion (the so-called Hubbard U -term).

To see how spin-dependent interactions come into play in our model, we now consider the contribution to H_C from different ionic sites $\mathbf{R}_i$. As a first-order approximation, we can assume that orbitals $\phi_{\mathbf{R}}(\mathbf{r})$ at different sites $\mathbf{R}$ have negligible overlap. In this case, we only have a contribution to the integral when $\mathbf{R}_1 = \mathbf{R}_4$ and $\mathbf{R}_2 = \mathbf{R}_3$ or if $\mathbf{R}_1 = \mathbf{R}_3$ and $\mathbf{R}_2 = \mathbf{R}_4$. Inserting this into the Hamiltonian, and using that

$$\sum_{\sigma_1, \sigma_2} c_{\mathbf{R}, \sigma_1}^\dagger c_{\mathbf{R}, \sigma_2}^\dagger c_{\mathbf{R}, \sigma_2} c_{\mathbf{R}, \sigma_1} = \frac{1}{2} n_{\mathbf{R}} n_{\mathbf{R}} + 2 \mathbf{s}_{\mathbf{R}} \cdot \mathbf{s}_{\mathbf{R}} \quad (16.30)$$

where $\mathbf{s}_{\mathbf{R}}^\alpha = \sum_{\sigma \sigma'} c_{\mathbf{R}, \sigma}^\dagger (\sigma_{\sigma \sigma'}^\alpha) c_{\mathbf{R}, \sigma'}$, we get:

$$H_{C, \text{exchange}} = \frac{1}{2} \sum_{\mathbf{R}_1, \mathbf{R}_2} \left[(K_{12} - \frac{1}{2} J_{12}) n_1 n_2 - 2 J_{12} \mathbf{s}_1 \cdot \mathbf{s}_2 \right] \quad (16.31)$$

upon defining

$$\begin{aligned} K_{12} &\equiv K_{\mathbf{R}_1, \mathbf{R}_2} = \int d^3 r_1 d^3 r_2 |\phi_{\mathbf{R}_1}(\mathbf{r}_1)|^2 \frac{e^2}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|} |\phi_{\mathbf{R}_2}(\mathbf{r}_2)|^2, \\ J_{12} &\equiv J_{\mathbf{R}_1, \mathbf{R}_2} = \int d^3 r_1 d^3 r_2 \phi_{\mathbf{R}_1}^*(\mathbf{r}_1) \phi_{\mathbf{R}_2}^*(\mathbf{r}_2) \frac{e^2}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|} \phi_{\mathbf{R}_1}(\mathbf{r}_2) \phi_{\mathbf{R}_2}(\mathbf{r}_1). \end{aligned} \quad (16.32)$$

We see that a spin-dependent interaction has arisen and in fact one may show that $J_{12} \geq 0$. This means that the Coulomb repulsion between electrons in orthogonal orbitals always leads to a ferromagnetic exchange interaction. Physically, one may think of this as follows: by making their spins parallel, the electrons cannot occupy the same position in space and thus avoid strong Coulomb repulsion. This makes their energy lower compared to if their spins were antiparallel. To see that $J_{12} \geq 0$, we use that

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \int d^3k (2\pi)^3 e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)} \frac{4\pi}{k^2} \quad (16.33)$$

we get

$$J_{12} = \int d^3k (2\pi)^3 \frac{e^2}{\epsilon_0 k^2} |I(\mathbf{k})|^2 \geq 0 \quad (16.34)$$

having defined $I(\mathbf{k}) = \int d^3r_1 \phi_{\mathbf{R}_1}^*(\mathbf{r}_1) \phi_{\mathbf{R}_2}(\mathbf{r}_1) e^{i\mathbf{k} \cdot \mathbf{r}_1}$.

Had we allowed for the possibility of multiple orbitals m per ionic site, i.e.

$$\psi_\sigma(\mathbf{r}) = \sum_{\mathbf{R}, m} \phi_{\mathbf{R}, m}(\mathbf{r}) c_{\mathbf{R}, m, \sigma}, \quad (16.35)$$

we would also have obtained an exchange integral involving wavefunctions at different orbitals even when just considering one particular ionic site $\mathbf{R}_i = \mathbf{R}$. The conclusion, similarly to before, is that electrons with parallel spins cannot occupy the same orbital and therefore avoid the strong intra-orbital Coulomb repulsion.

16.2 Can magnetic fields perform work?

According to the expression of the Lorentz-force

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (16.36)$$

the force on a charged particle moving in a magnetic field acts perpendicularly to the velocity of the particle, and thus no work can be performed by $\mathbf{B}$ since $W = \int \mathbf{F} \cdot d\mathbf{l}$. However, consider the following scenario where the magnetic field appears to do work. An electron spin sitting in a static but inhomogeneous magnetic field $\mathbf{B} = \mathbf{B}(\mathbf{r})$ will experience a potential energy $U = -\boldsymbol{\mu} \cdot \mathbf{B}$ and thus a potential gradient $\nabla U = -\boldsymbol{\mu} \cdot \nabla \mathbf{B}$. Therefore, the electron will start to move and thus gain a kinetic energy. Where did this energy come from if a magnetic field cannot perform work? The explanation is not obvious, but it turns out that the kinetic energy is taken from the *internal energy* of the electron because the rest mass changes as it moves through the field (see equation B6 here: <https://arxiv.org/pdf/0905.2391.pdf>).

The question regarding whether or not magnetic fields can perform work is also possible to raise in the context of diamagnetism and Meissner screening currents in a superconductor. We already know that diamagnetism, or any form for spontaneous magnetic order, cannot be explained classically according to the Bohr–Sommerfeld–Leeuwen theorem. Instead a quantum mechanical description is required. In the case of diamagnetism, the commonly accepted model is Landau's model of diamagnetism where the organization of electrons into Landau levels under the application of a magnetic field provides an induced magnetization which opposes the magnetic field. But is it the magnetic

field that ultimately performs work on the electrons via the Lorentz-force to generate the opposing magnetization? Quantum mechanically, the concept of "work performed" cannot be used in the same way as classical physics. In classical physics, one says that the work $W_{AB} = \int_A^B \mathbf{F} \cdot d\mathbf{r}$ performed by a force $\mathbf{F}$ between points A and B. But quantum mechanically, particles do not move along deterministic trajectories and so we cannot define a precise integral in the same way as we do classically.

Put differently, since electrons do not move classically in well-defined trajectories around atoms, we cannot compute work done on electrons by forces in the same way as we do classically. Electrons have expectation values for their distance from the atomic core and can have different quantum numbers for *e.g.* angular momentum which affects their probability distribution. Therefore, we should not expect that it is possible to use classical arguments to explain the behavior of electrons on an atomic scale, which is consistent with the fact that neither diamagnetism or superconducting screening currents can be explained classically.

On the other hand, *energy conservation* still applies quantum mechanically. Therefore, we can definitely ask: where does the kinetic energy of a supercurrent come from? Is it provided by the external magnetic field? The answer is that it comes from the magnetic energy density which is reduced near the superconducting surface because of the screening currents. In this way, energy is kept constant: the magnetic field is reduced (lowering the energy density) and the superconducting electrons gain kinetic energy. This argument is consistent with the fact that the critical field of a superconductor is determined as the field $B = B_c$ which causes the magnetic energy density $\frac{1}{2\mu_0} B^2$ to equal the superconducting condensation energy $\propto \Delta_0^2$. When this happens, the kinetic energy of the supercurrent (which comes precisely from the magnetic energy density) is larger than the energy gain that comes from the condensation energy.

16.2.1 Landau's model for diamagnetism

In short, the argument goes like this. One includes the external field via $\mathbf{A}$ in the Hamiltonian for free electrons via minimal coupling as usual. From this, one derives Landau energy eigenvalues and can consequently compute the free energy of the system which now will depend on $\mathbf{B}$ through the vector potential. Since the magnetization is the canonical variable to the magnetic field, we have $\mathbf{M} \propto \partial F / \partial \mathbf{B}$ and one finds $\mathbf{M} \neq 0$ with a direction that is opposite to $\mathbf{B}$. Additionally, we know that a thermodynamical current can be defined quantum mechanically as $\mathbf{j} \propto \partial F / \partial \mathbf{A}$ which produces precisely the diamagnetic screening current provided by the Landau levels.

Diamagnetism: always. Paramagnetism: Sometimes

It should be noted that diamagnetism is *always* present because such a response does not require any finite magnetic moment to exist: even if the electron spins and orbital motion cancel each other out completely, a diamagnetic effect occurs. In contrast, a paramagnetic effect can only take place if a net magnetic moment of the atom exists, causing this magnetic moment to align with the external field. If both paramagnetism and diamagnetism is present, paramagnetism tends to dominate.

16.2.2 Classical "motivation" for diamagnetism (albeit not strictly correct)

We have just argued that classical physics cannot explain diamagnetism. To quote Feynman:

'It is, however, possible to make some phoney classical arguments and to get some idea of what is

going on. We might put it this way. You can make some classical arguments and get guesses as to the behavior of the material, but these arguments are not "legal" in any sense because it is absolutely essential that quantum mechanics be involved in every one of these magnetic phenomena. On the other hand, there are situations, such as in a plasma or a region of space with many free electrons, where the electrons do obey the laws of classical mechanics. And in those circumstances, some of the theorems from classical magnetism are worthwhile. Also, the classical arguments are of some value for historical reasons. The first few times that people were able to guess at the meaning and behavior of magnetic materials, they used classical arguments. Finally, as we have already illustrated, classical mechanics can give us some useful guesses as to what might happen - even though the really honest way to study this subject would be to learn quantum mechanics first and then to understand the magnetism in terms of quantum mechanics. On the other hand, we don't want to wait until we learn quantum mechanics inside out to understand a simple thing like diamagnetism. We will have to lean on the classical mechanics as kind of half showing what happens, realizing, however, that the arguments are really not correct.'

We here provide a qualitative sketch which motivates diamagnetism, although the microscopic mechanism is not strictly correct.

Classically, one can easily show that a charged particle moving in a circular orbit (*e.g.* around an atomic core), its magnetic moment $\boldsymbol{\mu}$ and angular momentum $\mathbf{J}$ are proportional. One finds

$$\boldsymbol{\mu} = \frac{q}{2m} \mathbf{J} \quad (16.37)$$

where q is the charge of the particle and m is its mass. Now, imagine that we turn on a magnetic field

16.3 Magnetomechanical effects

Two particular effects illustrate the coupling between mechanical degrees of freedom and the magnetic moment of charged particles: the Einstein-Haas effect and the Barnett effect.

16.3.1 Einstein-de Haas effect

This effect was in fact predicted by Richardson in 1908, but is nevertheless attributed to Einstein and de Haas who published experimental evidence of it. It states that a change in the magnetic moment of a free body causes the body to rotate.

This phenomenon can be understood as a consequence of conservation of angular momentum. Consider a material with a macroscopic amount of magnetic moments $\boldsymbol{\mu}_i$. These can be either of spin or orbital origin. These moments then give rise to a total magnetization $\mathbf{M} = \sum_i \boldsymbol{\mu}_i / V$ where V is the volume of the body. Consider now a magnetic field $\mathbf{B}$ applied along the z -axis. All the moments are not necessarily aligned along z , for instance in a paramagnetic phase. However, there can exist no torque $\boldsymbol{\tau}$ along the z -axis as is clear from

$$d\mathbf{L}/dt = \boldsymbol{\mu} \times \mathbf{B} \quad (16.38)$$

since $\mathbf{B}$ points along the z -axis. This means that

$$dL_z/dt = 0. \quad (16.39)$$

As magnetic moments become aligned with the z -axis due to the torque exerted by $\mathbf{B}$ (initially precessing, but due to damping eventually aligning with $\mathbf{B}$), the magnetization along the z -axis increases by $\Delta\mathbf{M}$. Therefore, a compensating reduction of L_z has to take place in order to satisfy $dL_z/dt = 0$. This occurs by the body starting to rotate in a direction which cancels out the increase in angular momentum caused by $\Delta\mathbf{M}$. In effect, an increase in magnetization has caused the body to start rotating.

An interesting application of this result is that it allows for an identification of how much of a body's magnetization stems from the electron spin and how much that stems from the electron orbital motion. In elemental ferromagnets like Fe, the spin contribution completely dominates.

16.3.2 Barnett effect

This is the opposite effect of the Einstein-de Haas effect, namely that a rotating body becomes spontaneously magnetized. The effect can be explained as follows.

16.3.3 Magnetic torque: precession or alignment with external field?

It is well-known that an electron spin (magnetic moment) in an external field will precess around $\mathbf{B}$, as seen from

$$\frac{d\mathbf{L}}{dt} = \gamma \mathbf{L} \times \mathbf{B}. \quad (16.40)$$

Only in the presence of dissipation, such as Gilbert damping if the electron was part of a lattice, will the spin eventually align with $\mathbf{B}$. But a bar magnet does not precess in the Earth's magnetic field, it simply aligns with the external field. Why? Shouldn't the same equation be valid for each of the electron spins constituting the magnetization of the bar magnet?

The resolution lies precisely in the damping that is present in the bar magnet. If one places a bar magnet in an external field, the electron spins will initially precess, precisely as described by the equation above. Due to spin-lattice coupling, this precession dies out and the spins eventually align with the magnetic field. However, conservation of the angular momentum component parallel with $\mathbf{B}$ dictates that the change in this component of the spin-magnetization must be compensated by something else: namely, the mechanical rotation of the bar magnet itself. The details of this process is not necessarily easy to describe, since one has to consider effects like the demagnetization field of when the bar magnet tries to become polarized along a different direction than its direction of spatial extension. In other words, the frictional torque transfers angular momentum from the magnetization to the body of the bar magnet itself and then ultimately to the surroundings (whatever the bar magnet is attached to and surrounding air). The final result where the system stops changing is when the bar magnet has aligned its magnetization with $\mathbf{B}$.

16.4 Ferromagnetic resonance

16.4.1 Classical vs. quantum origin of FMR

Before discussing ferromagnetic resonance, which is a useful tool to characterize the magnetization, magnetization dynamics, and spin waves in ferromagnets, it is useful to compare the classical and quantum pictures of spin precession.

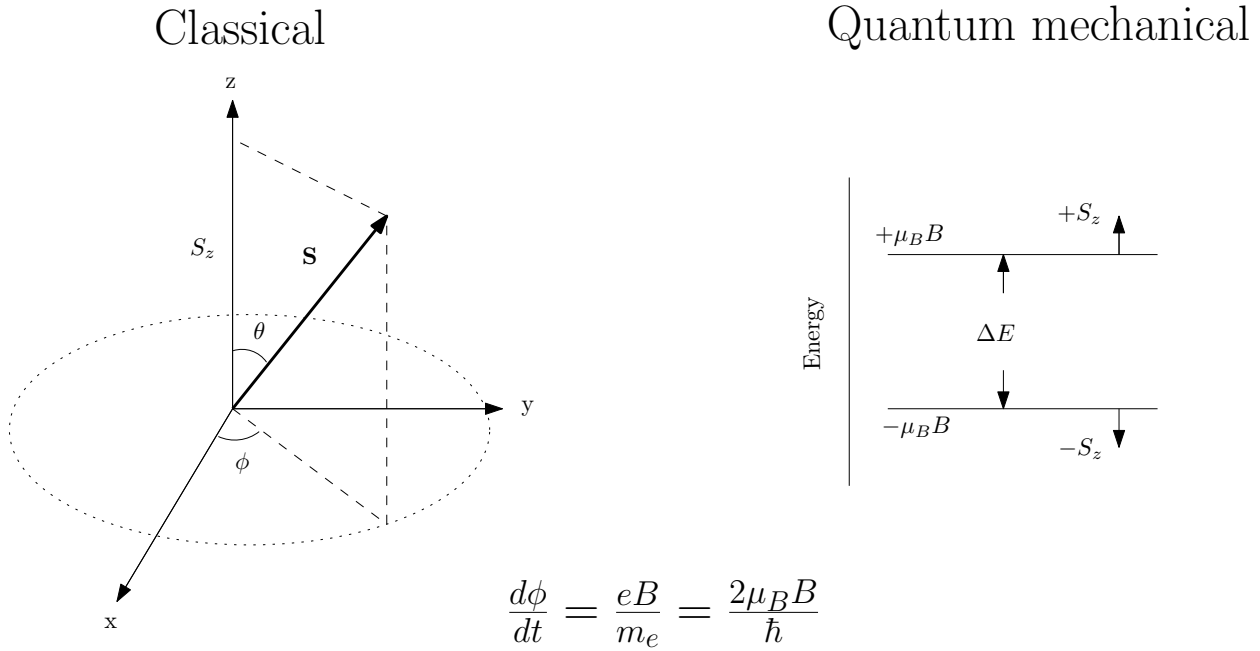


Figure 16.2: In the figure, the classical picture of precession is shown on the left and the quantum mechanical is shown on the right. One has to be careful with the signs of the magnetic moments and spins since these are proportional via the electric charge, which can be negative. In the picture above, we have assumed that $\downarrow$ is the majority spin. Consider for simplicity a positive charge so that the magnetic moment is proportional to the spin. At FMR, optical transitions occur via majority spins being excited up to minority spin levels. This means that the magnetization turns away from the magnetic field, since the minority spin component of the state increases.

The motion of an electron spin $\mathbf{s}$ in an external magnetic field $\mathbf{B}$ directed along the z -axis of the coordinate system is shown in Fig- 16.2. In the classical picture a spin that is not aligned with the field will precess about it with the Larmor frequency $\omega_L = d\phi/dt = eB/m_e$. This frequency is independent on θ . The precession direction is given by the torque $\boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B}$.

In the quantum mechanical picture, the spin-state which is misaligned to the z -direction consists of a superposition of $+s_z$ and $-s_z$ states. In effect, the system has a finite probability of being in both the spin-up state $+s_z$ and the spin-down state $-s_z$. The spin precession $d\phi/dt$ about B corresponds to the up and down spin states acquiring *time-dependent phases*, $e^{\pm i\gamma B t/2}$, in the presence of the external field. This can be seen by acting with the time-evolution operator $e^{-iHt/\hbar}$ on the state of the system, where $H = -\gamma B S_z$.

A key observation, which we will make use of later to explain why FMR occurs, is that the precession frequency is equal to the field-induced splitting caused by the magnetic field. Namely, the energy level which is degenerate without magnetic field is split into two levels a distance $2\mu_B B$ apart due to the Zeeman effect. Thus, the corresponding frequency is $\omega = d\phi/dt = 2\mu_B B/\hbar = eB/m_e$ by using the definition of the Bohr magneton. Note that in a ferromagnet, the bands (and energy levels) are already spin-split, but the magnetic field imposes an extra Zeeman-splitting.

Changes in the angle θ correspond to a change in the relative *probabilities* of the up and down states.

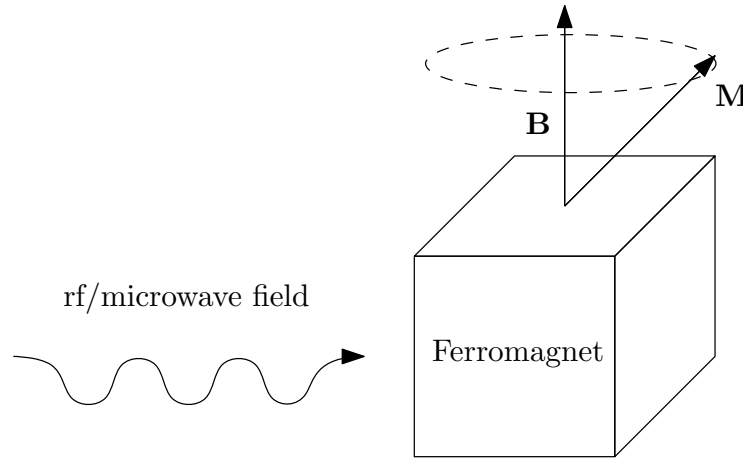


Figure 16.3: Basic idea behind FMR experiment.

Therefore, if any angular rotation $d\theta/dt$ is present, it is determined by the spin-flip frequency between the two states. Such a rotation of θ into the field direction corresponds to dissipative processes which ensure that the magnetization ultimately ($t \rightarrow \infty$) will align with B . These processes are described by the Gilbert damping term α in the LLG equation.

16.4.2 Physical picture

Let us now discuss the physics of ferromagnetic resonance. It was discovered experimentally in 1911 and explained theoretically a decade later as resulting from optical transitions due to the Zeeman splitting in a ferromagnet. Ferromagnetic resonance arises from the precessional motion of a magnetization $\mathbf{M}$ in an external magnetic field $\mathbf{B}$, as the field exerts a torque on the magnetization. The precession frequency depends on $|\mathbf{B}|$ and $|\mathbf{M}|$. The precession frequency of a ferromagnet is usually much lower in value than the precession frequency of a single free electron (EPR).

The essential setup for an FMR experiment is that a magnetic material is placed in a microwave resonant cavity (schematically shown in Fig. 16.3). The resonant cavity hosts a microwave field, in effect an ac electromagnetic field, at a fixed frequency. A detector at the end of the cavity detects the intensity of the microwaves. When the magnetic material is placed inside the cavity and $\mathbf{B}$ is swept in strength, so that the precession frequency changes, the resonant absorption intensity of the microwaves will change. Specifically, when the magnetization precession frequency and the cavity microwave frequency are the same, the absorption of microwaves by the ferromagnet increases sharply. This is experimentally observed as a decrease in the intensity at the detector. The absorption of microwave energy causes local heating in the ferromagnet. If the magnet has a local magnetic order parameter varying on the nanometer scale, FMR can be used for spatially dependent spectroscopy investigations.

The reason for why the absorption of microwaves by the ferromagnet increases strongly at the resonance frequency is that the photon energies $\hbar\omega$ of the microwave field match the difference between the Zeeman-split (caused by $\mathbf{B}$) energy levels of the electrons in the ferromagnet. This can be seen in Fig. 16.2: the precession frequency of the magnetization is determined by the splitting of the levels and when this splitting equals the photon energies, transition occurs and the absorption

increases strongly. This enables electrons to make energy transitions in the magnetic material, and thus photons are absorbed in the process.

It should be emphasized here that in a ferromagnetic material, the situation is more complex than the effective free-electron spin described above. For one thing, there already exists a magnetization and spin-splitting field. Thus, additional resonant transitions can show up in FMR power absorption spectra and thus such spectra must be carefully analyzed in order to know which information one is extracting. The resonance frequency value will in general depend on the anisotropy and demagnetization field of the ferromagnet as well. Without the ac microwave field, the magnetization dynamics in the ferromagnet will die out due to damping effects. When the ac field has a frequency which matches the natural precession frequency of the ferromagnet, the precession is maintained by force since energy is supplied by the microwaves.

Damping should also be taken into account in a realistic description. When the ac field frequency matches the FMR frequency, optical transitions occur as described above, causing the probability weights of the spin-up and spin-down states to change. This in turn, induces an increase in the tilt angle θ of the magnetization relative the external field. Nevertheless, this will be countered by damping in the material. In practice, the magnetization precession will occur steadily at a tilt angle θ at which the energy supplied by the microwaves equal the energy dissipation caused by damping. The magnetization tilt angle will also increase with increasing ac field magnitude, but so will the damping since it is proportional to the tilting angle, and a balance between the two ensues.

16.4.3 FMR in Landau-Lifshitz-Gilbert formalism

In practice, the FMR frequency can also be found in the LLG-formalism, even if the microscopic mechanism of optical transition is not accounted for there. The reason is that the FMR frequency is simply the natural frequency, or eigenfrequency, of the ferromagnet in an external field. This can readily be modelled in the LLG-formalism and the calculation goes as follows.

The LLG equation in the presence of a static field H_z takes the form

$$\frac{d\mathbf{M}}{dt} = -\gamma \mathbf{M} \times \mathbf{H}_{\text{eff}}. \quad (16.41)$$

Here, the effective field components are

$$H_{\text{eff},x} = 0, \quad H_{\text{eff},y} = 0, \quad H_{\text{eff},z} = H_z. \quad (16.42)$$

We have neglected here the influence of demagnetization (stray field). For a small precession around the z -axis, we make the ansatz that $M_{x,y}(t) = M_{x,y} e^{i\omega t}$ and identify the following equations from the LLG equation:

$$\frac{dM_x}{dt} = -\gamma H_z M_y, \quad \frac{dM_y}{dt} = -\gamma H_x M_z + \gamma M_x H_z, \quad \frac{dM_z}{dt} = 0. \quad (16.43)$$

To lowest order, we thus have $M_z \simeq M_0$ where M_0 is the saturation magnetization. Inserting our ansatz for $M_{x,y}$, we obtain the system of algebraic linear equations:

$$i\omega M_x = -\gamma(H_0 + M_0)M_y, \quad i\omega M_y = -\gamma H_0 M_x. \quad (16.44)$$

In order to find the eigenfrequency of the magnetization precession, then a nontrivial solution will exist only when the determinant of the system is equal to zero. This condition gives us:

$$\omega_0^2 = \gamma^2 H_0 (H_0 + M_0). \quad (16.45)$$

16.5 Curie and Curie-Weiss law

In textbooks on magnetism, one will read about Curie's law which is a phenomenological statement (motivated by its good match with experiments for several materials) that the magnetization $\mathbf{M}$ in a paramagnetic material is proportional to the externally applied field $\mathbf{H}$ according to

$$M = \frac{C}{T}H \quad (16.46)$$

where T is temperature and C is a material-dependent constant known as the Curie constant. Since the susceptibility of a material is generally defined as

$$\chi = \frac{M}{H} \quad (16.47)$$

we have that $\chi = C/T$. This law is modified for the paramagnetic phase of a *ferromagnetic* material, that is above the Curie temperature T_c . In this case it is known as the Curie-Weiss law and reads:

$$\chi = \frac{C}{T - T_c}. \quad (16.48)$$

According to this equation, the susceptibility should have a singularity at $T = T_c$. This is similar to the divergence of the superconducting coherence length ξ at the critical superconducting temperature.

It should be noted that the susceptibility cannot be defined as $\chi = M/H$ in the ferromagnetic phase (below the Curie temperature) since in this phase a spontaneous magnetization can exist even without any externally applied field H . In principle, one could envision using a differential definition according to $\chi = \partial M / \partial H$. But even this proves problematic, because the magnetization M is not uniquely determined by the external field H due to magnetic hysteresis.

To characterize ferromagnets, one may instead use the relative permeability μ/μ_0 which is very large in the ferromagnetic phase due to the contribution from the magnetization $\mathbf{M}$:

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) = \mu\mathbf{H}. \quad (16.49)$$

16.6 Relation between exchange energy and magnetic field strength inside a ferromagnet

Since the Zeeman-energy of a magnetic dipole $\boldsymbol{\mu}$ in a magnetic field $\mathbf{B}$ is $h = -\boldsymbol{\mu} \cdot \mathbf{B}$, it might seem tempting to use such a relation to estimate what the magnitude of the magnetic field is inside a ferromagnet. For instance, it is known that transition metal ferromagnets may have exchange energies of 50-100 meV. However, it is important to realize that this exchange energy does *not* come from the Zeeman-effect of the magnetization coupling to the electron spin moments. Indeed, if we try to compute how large magnetic field $\mathbf{B}$ that is required to provide an electron spin with a Zeeman-energy of 100 meV, we would have obtained thousands of Tesla. This is not the field strength inside a ferromagnet.

So what is wrong with this reasoning? The point is that the exchange energy in a mean-field Hamiltonian describing the itinerant electrons in a ferromagnet can be *modelled* as a Zeeman-type interaction of the form $\mathbf{S} \cdot \mathbf{M}$ where $\mathbf{M}$ is the background field coupling to the electrons and $\mathbf{S}$ is the

electron spin. However, the actual physical origin of the exchange field is the Coulomb interaction in addition to the Pauli principle. Mathematically, it is obtained from overlap integrals between electron wavefunctions. In effect, $\mathbf{M}$ can be treated as an effective field which models the combined effect of the Coulomb interaction and the Pauli principle, but it is not the actual magnetization of the material - it is not a physical magnetic field. The actual magnetization inside the material corresponds to a much weaker field than thousands of Tesla: for a magnetization of $M \sim 10^5$ A/m, one obtains $B \sim 1$ T.

16.7 Demagnetization field

The demagnetization field is a magnetic field generated by the magnetization of a material. It is a field that therefore appears in ferromagnets, but also in superconductors due to the magnetization created by screening currents.

16.7.1 Demagnetization field in ferromagnets

The demagnetization field can be understood by considering the fundamental equations $\nabla \cdot \mathbf{B} = 0$ and $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$ which are combined into

$$\nabla \cdot \mathbf{H} = -\nabla \cdot \mathbf{M}. \quad (16.50)$$

In the simplest case where $\mathbf{M}$ is constant inside a magnet (homogeneous ferromagnet) and zero outside, the gradient is finite right at the edge of the material. Due to the minus sign in the above equation, the demagnetization field $\mathbf{H}$ has to provide a flux in the opposite direction as $\mathbf{M}$ and thus has to act as to partially cancel the total magnetic field inside the ferromagnet. The manner in which this is realized is illustrated in the figure below.

Let us show analytically why the demagnetization field (known as the *stray field* outside of the ferromagnet) points in the opposite direction of $\mathbf{M}$. The main point is that we can show from Maxwell's equations for the magnetic field that in the situation above $\mathbf{H}$ acts mathematically analogously to an electric field $\mathbf{E}$ created by a charge distribution. Therefore, we can think of $\mathbf{H}$ as created by fictitious magnetic monopoles just as an $\mathbf{E}$ -field can be created by electric monopoles. These magnetic monopoles are positioned at the N and S poles of the magnet, and give rise to an $\mathbf{H}$ -field which points either inward or outward as shown in Fig. 16.4.

Consider Maxwell's equation for the $\mathbf{H}$ -field in the absence of any macroscopic currents in the material and time-varying electric fields. This is the situation of a ferromagnet in thermodynamic equilibrium. Maxwell's equation then reads

$$\nabla \times \mathbf{H} = 0 \quad (16.51)$$

which means that we can write $\mathbf{H} = -\nabla U(\mathbf{r})$ where $U(\mathbf{r})$ is referred to as a magnetic potential. Furthermore, since $\nabla \cdot \mathbf{B} = \mu_0(\nabla \cdot \mathbf{B} + \nabla \cdot \mathbf{M})$, it follows that $\nabla^2 U(\mathbf{r}) = \nabla \cdot \mathbf{M}$. Outside of the material where $\mathbf{M} = 0$, we have $\nabla^2 U(\mathbf{r}) = 0$.

To solve the above equations, we need accompanying boundary conditions. The continuity conditions for $H_{\parallel}$ and $B_{\perp}$ at the surface of the material dictate that $U(\mathbf{r})$ has to be continuous at the surface and that

$$\left(\frac{\partial U}{\partial n}\right)_{\text{int}} - \left(\frac{\partial U}{\partial n}\right)_{\text{ext}} = \mathbf{M} \cdot \mathbf{n} \quad (16.52)$$

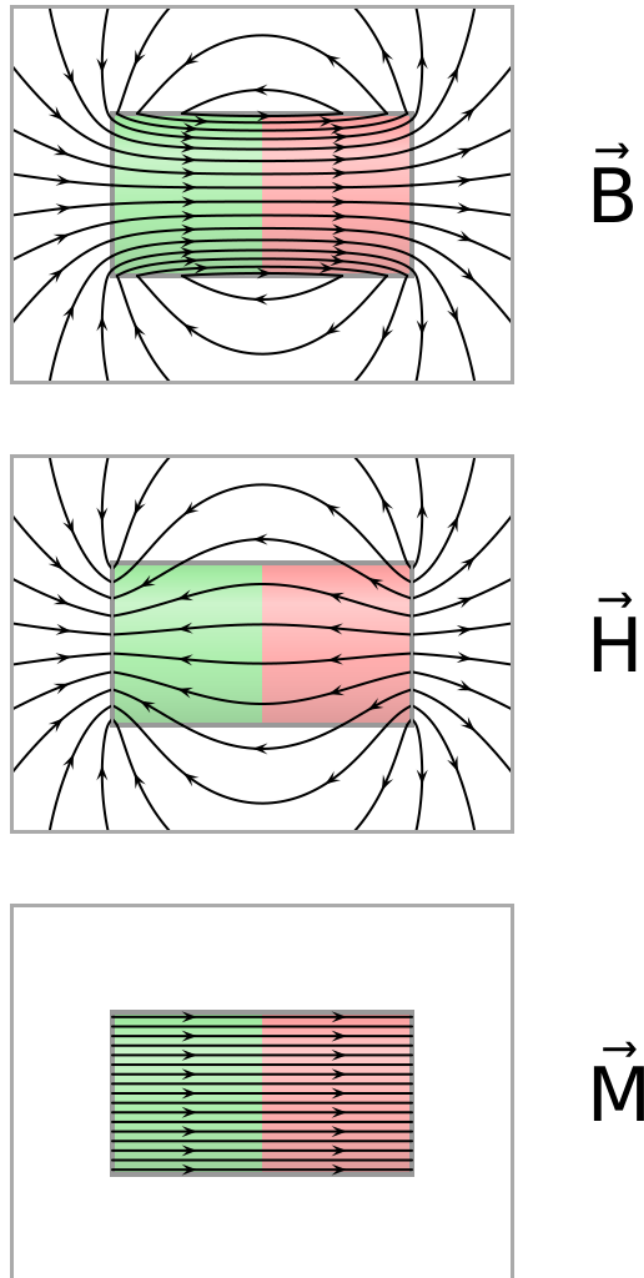


Figure 16.4: (Color online) Illustration of the magnetic field $\mathbf{B}$ and the corresponding $\mathbf{H}$ and $\mathbf{M}$ fields for a cylindrical bar magnet. The field $\mathbf{H}$ is referred to as the demagnetization field. The picture is taken from Wikipedia.

where $\mathbf{n}$ is the surface normal.

The above system of equations and boundary conditions is analogous to the problem of an electro-

static potential produced by charge distribution. The solution for $U(\mathbf{r})$ can be shown to be:

$$U(\mathbf{r}) = \frac{1}{4\pi} \left[- \int_V \frac{\nabla \cdot \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \int_S \frac{\mathbf{n} \cdot \mathbf{M}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dS' \right]. \quad (16.53)$$

The first term is zero in our case of a homogeneous ferromagnet since $\nabla \cdot \mathbf{M} = 0$ inside the material. The second term of the potential is the potential associated with the surface density of "magnetic poles" $\sigma \equiv \mathbf{M} \cdot \mathbf{n}$. These poles arise due to the discontinuity of the magnetization at the surface. The magnetic poles are positive at N, where the magnetization points out of the surface, whereas they are negative at S. Therefore, the belonging $\mathbf{H}$ -field points in opposite directions at the two poles, just as the $\mathbf{E}$ -field of two opposite charges.

The demagnetization field is thus created by the magnetization itself and acts to reduce the total $\mathbf{B}$ -field inside the magnet. If an external field is also present, we would write the total $\mathbf{H}$ -field as

$$\mathbf{H} = \mathbf{H}_a + \mathbf{H}_d \quad (16.54)$$

where $\mathbf{H}_a$ is the applied magnetic field and $\mathbf{H}_d = \mathbf{H}_d(\mathbf{M})$ in general has a complicated dependence on the magnetization $\mathbf{M}$, as shown by the analytical expressions above. For certain shapes of the magnet, the expression for the demagnetization field becomes more tractable. In particular, for an ellipsoidally shaped magnet the demagnetization field inside the material is uniform if the magnetization is uniform and takes the form

$$\mathbf{H}_d = -N\mathbf{M} \quad (16.55)$$

where N is a tensor.

We note that when solving the Maxwell equation in strictly 2D for a ferromagnet with OOP magnetization, there is no stray field. We can understand this by thinking of an infinite solenoid that has a finite field inside of it but zero field outside of it: the 2D ferromagnetic case is thus a slice of such as solenoid.

16.7.2 Energy of demagnetization field

The demagnetization energy, also called magnetostatic energy or stray-field energy, is the energy of the magnetization in the magnetic field created by the magnetization itself. This means that this energy contribution accounts for the dipole-dipole interaction of the elementary magnets.

In deriving an energy for the magnetostatic energy of a magnetized body, it is useful to first show that when there are no free currents or time-dependent electric fields,

$$\int_{\infty} \mathbf{B} \cdot \mathbf{H} d\mathbf{r} = 0 \quad (16.56)$$

where the integral is taken over all of space. This equation is valid for the magnetostatic field created entirely due to a localized distribution of permanent magnetization, in effect no free currents according to Maxwell's equations. To prove this, we know that $\nabla \times \mathbf{H} = 0$ in the absence of free currents and time-dependent electric fields. Since the magnetization is localized, all fields must vanish at infinity. First note that

$$\begin{aligned} \int_{\infty} \mathbf{B} \cdot \mathbf{H} d\mathbf{r} &= \int_{\infty} \mathbf{H} \cdot (\nabla \times \mathbf{A}) d\mathbf{r} \\ &= \int_{\infty} \nabla \cdot (\mathbf{A} \times \mathbf{H}) d\mathbf{r} + \int_{\infty} \mathbf{A} \cdot (\nabla \times \mathbf{H}) d\mathbf{r} \end{aligned} \quad (16.57)$$

by using a vector identity. The second integral is immediately zero since $\mathbf{J} = 0$, and thus we have

$$\int_{\infty} \mathbf{B} \cdot \mathbf{H} d\mathbf{r} = \int_{\infty} \nabla \cdot (\mathbf{A} \times \mathbf{H}) d\mathbf{r} = \int_S \mathbf{n} \cdot (\mathbf{A} \times \mathbf{H}) dS \quad (16.58)$$

where S is the surface of the volume at infinite distance. This integral has to be zero since all fields are zero at infinity, due to the sources being localized. This completes the proof that $\int_{\infty} \mathbf{B} \cdot \mathbf{H} d\mathbf{r} = 0$ generally.

We will now derive an expression for the magnetostatic energy of a magnetized body and also make use of the above result at the end. We will also compare how the final result matches the general expression for the total energy of magnetic field in a region V :

$$U_{\text{tot}} = \frac{1}{2\mu} \int_V \mathbf{B}^2 dV \quad (16.59)$$

in a region of space with permeability μ (for a linear magnetic material). First of all, consider the potential energy of a dipole $\mathbf{m}$ located in a region where a field $\mathbf{B}$ exists:

$$U = -\mathbf{m} \cdot \mathbf{B} \quad (16.60)$$

If we start with one dipole and then bring another one in from infinity, $\mathbf{B}$ is caused by the first dipole. Assembling a whole collection of dipoles means that we have to sum over the potential energy of every dipole due to the field of every other dipole, but also divide by 2 to account for double-counting:

$$U = -\frac{1}{2} \sum_{i \neq j} \mathbf{m}_i \cdot \mathbf{B}_{ij}. \quad (16.61)$$

Here, $\mathbf{B}_{ij}$ is the magnetic field caused by dipole j at the position of dipole i . This is the demagnetization energy (the energy due to the magnetization interacting with itself) and we refer to this as U_{demag} from now on for clarity. Now, a continuous distribution of magnetization can be thought of as a collection of magnetic dipoles in the limit that they become very small and so closely spaced that they are essentially continuous. The sum is then replaced by an integral:

$$U_{\text{demag}} = -\frac{1}{2} \int_V d\mathbf{m} \cdot \mathbf{B} dV \quad (16.62)$$

where the integral is taken over the volume of the magnetized body. But this can be rewritten as

$$\begin{aligned} U_{\text{demag}} &= -\frac{1}{2} \int_V dV \frac{d\mathbf{m}}{dV} \cdot \mathbf{B} \\ &= -\frac{1}{2} \int_V dV \mathbf{M} \cdot \mathbf{B} \end{aligned} \quad (16.63)$$

since dipole moment per volume is magnetization: $d\mathbf{m}/dV = \mathbf{M}$. If we now use the general definition that $\mathbf{B} = \mu_0(\mathbf{M} + \mathbf{H})$, we see that

$$U = -\frac{\mu_0}{2} \int \mathbf{M}^2 dV - \frac{\mu_0}{2} \int \mathbf{M} \cdot \mathbf{H} dV. \quad (16.64)$$

At this point it is useful to compare this expression against Eq. (16.59). We rewrite:

$$\begin{aligned}
 U_{\text{demag}} &= -\frac{1}{2} \int_V dV \mathbf{M} \cdot \mathbf{B} \\
 &= -\frac{1}{2} \int_V \frac{\mathbf{B}^2}{\mu_0} dV + \frac{1}{2} \int_V \mathbf{H} \cdot \mathbf{B} dV \\
 &= U_{\text{tot}} - \frac{1}{2} \int_V \frac{\mathbf{B}^2}{\mu_0} dV
 \end{aligned} \tag{16.65}$$

where we used that $\mathbf{B} = \mu \mathbf{H}$ for a linear magnetic material in the transition from the second last line to the last line. Therefore, we have shown that

$$\begin{aligned}
 U_{\text{tot}} &= U_{\text{demag}} + \frac{1}{2} \int_V \frac{\mathbf{B}^2}{\mu_0} dV \\
 &= U_{\text{demag}} + U_{\text{vac}},
 \end{aligned} \tag{16.66}$$

where we used that the last term is in fact the energy of a magnetic field in vacuum. This equation is reasonable physically: the total energy of a magnetic field in a region V is the energy that the field would have in vacuum (without any magnetic material) pluss the energy that any magnetic dipoles have in that volume due to their interaction with each other.

Of course, the magnetic field outside of the magnetized body also has an energy density associated with it and thus contribution has to be computed separately if one wishes to find the total energy of the field in all of space. The above calculation is thus only concerned with the magnetostatic energy of the magnetized body.

Let us now revert to Eq. (16.64), where we emphasize that no assumption has been made about the material being magnetically linear (i.e. that $\mathbf{B} = \mu \mathbf{H}$). Most ferromagnetic materials are not linear, and thus the following derivation is still valid for such materials. The first part of Eq. (16.64) only depends on the magnetization and can be thought of as an additive constant. The formation of magnetic domains does not alter this term, since the magnetization just changes direction in some parts (which does not alter $\mathbf{M}^2 = M^2$). However, the second term is *not* independent of the orientation or position of the various magnetic dipoles constituting the magnetized body. This is in fact then the final expression for the demagnetization energy since $\mathbf{H} = \mathbf{H}_d$ is the demagnetization field inside a ferromagnet:

$$U_{\text{demag}} = -\frac{\mu_0}{2} \int_V \mathbf{M} \cdot \mathbf{H}_d dV. \tag{16.67}$$

where we have emphasized that the integration takes place only over the magnetized body. By extending the integral to cover all of space (which we can do since $\mathbf{M} = 0$ outside the ferromagnet) and using that $\int_{\infty} \mathbf{H} \cdot \mathbf{B} = 0$, we obtain the alternative expression $U_{\text{demag}} = \frac{\mu_0}{2} \int_{\infty} \mathbf{H}^2 dV$ where the integration is now taken over all of space. We underline again that this is only the contribution to the magnetostatic energy from the magnetic field inside the magnetized body: to obtain the total energy including the stray field, we have to add that separately.

We finally note that, strictly speaking, the demagnetization field $\mathbf{H}$ entering U_{demag} should not take into account the contribution from a region centered near $\mathbf{r}$ when evaluating the integral $\int \mathbf{M}(\mathbf{r}) \cdot \mathbf{H}(\mathbf{r}) d\mathbf{r}$ since we are summing only over $i \neq j$ in the dipole-interactions. Otherwise, $H(\mathbf{r})$ would diverge.

16.7.3 Magnetic domains and shape anisotropy due to demagnetization field

The demagnetization field has several important consequences. Firstly, it leads to the formation of magnetic domains in large magnetic materials. This occurs as a consequence of the system trying to minimize its demagnetization energy. By dividing the system into smaller domains, one achieves a smaller demagnetization energy E_D inside the material, for instance by the domains taking the shape of an object that minimizes the demagnetization field. Moreover, one obtains a reduction of the stray field outside the ferromagnet by formation of domains, which in turn reduces the energy density of the total magnetic field outside the material.

The demagnetization field is also responsible for shape anisotropy in small magnetic materials which only have a single domain. To reduce the demagnetization field, it is desirable for the magnetization to point in a direction which minimizes the number of magnetic poles, since it is the latter that create the demagnetization field. If one imagines a thin film ferromagnet, it is clear that the surfaces will have a large number of poles if the magnetization points out of the film plane. On the other hand, if the magnetization lies in the plane of the film, the number of poles is minimized at the edges of the film and E_D is minimized. This is referred to as the pole-minimizing principle.

16.7.4 Demagnetization field in superconductors

In a superconductor, the magnetization that creates the demagnetization field exists due to the screening currents at the surface of the superconductor. Recall that for ellipsoidal shapes it is valid that $\mathbf{H}_d = -n\mathbf{M}$. In a superconductor, $\mathbf{B} = \mu_0(\mathbf{H}_i + \mathbf{M}) = 0$ in its interior which means that $\mathbf{H}_i = -\mathbf{M}$. Now, $\mathbf{H}_i = \mathbf{H}_a + \mathbf{H}_d$ so that inside the superconductor we obtain

$$\mathbf{H}_i = \mathbf{H}_a + n\mathbf{H}_i \quad (16.68)$$

which is rearranged to

$$\mathbf{H}_i = \frac{1}{1-n}\mathbf{H}_a. \quad (16.69)$$

In effect, the $\mathbf{H}$ -field inside the superconductor is larger than the externally applied $\mathbf{H}$ -field ($\mathbf{H}_a$). For a sphere, $n = 1/3$ while for an externally applied field applied along the axis of a long cylindrical rod, $n = 0$.

In contrast, in a paramagnetic material we would expect that the induced magnetization points in the same direction as the externally applied field, so that $\mathbf{M} = c\mathbf{H}_a$ where c is some constant. It then follows that

$$\mathbf{H}_i = \mathbf{H}_a - nc\mathbf{H}_a = (1 - nc)\mathbf{H}_a \quad (16.70)$$

Therefore, $\mathbf{H}_i$ inside a paramagnetic material is smaller than the externally applied field $\mathbf{H}_a$.

16.8 Heisenberg model

16.8.1 Exchange interaction

16.8.2 Anisotropy

16.8.3 Zeeman energy

16.8.4 Dipole-dipole interactions

16.8.5 Dzyaloshinskii-Moriya interactions

First postulated by I. Dzyaloshinskii on phenomenological grounds, the Hamiltonian for the anti-symmetric exchange interaction between two spins can be written as

$$H_{DM} = \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \quad (16.71)$$

Dzyaloshinskii-Moriya interaction (DMI) requires a superexchange mechanism in systems lacking inversion symmetry (i.e. with spin-orbit coupling). The superexchange mechanism is the interaction between two spins via a third (so-called ligand) non-magnetic spin and occurs via electron hopping between empty orbitals on the atoms. Note that superexchange is not enough to get DMI, we also need the spin-orbit coupling from inversion symmetry breaking as shown in Moriya's seminal paper. The form of H_{DM} arises precisely when considering an anisotropic superexchange mechanism, thus taking into account spin-orbit coupling.

The main effect of H_{DM} is that it favors a non-collinear arrangement of magnetic moments, in contrast to the exchange interaction we considered previously which favors a P or AP alignment of $\mathbf{S}_i$ and $\mathbf{S}_j$. Thus, H_{DM} can for instance act as a source of weakly ferromagnetic behavior in an antiferromagnetically ordered system. The antisymmetric exchange is also of importance for the understanding of magnetism induced electric polarization in some multiferroic systems. What transpires in these materials is that the formation of magnetic ordering provides a small shift of ligand ions, as the gain in magnetic interaction energy compensates the cost of additional lattice energy. When all the ligand ions are shifted in the same direction, the result is a net electric polarization which thus comes from the magnetically inhomogeneous ordering. This is also known as the inverse Dzyaloshinskii-Moriya effect.

The direction of the antisymmetric vector $\mathbf{D}_{ij} = -\mathbf{D}_{ji}$ is dictated by the symmetries present in the system or crystal lattice structure. The general rules for how $\mathbf{D}_{ij}$ is oriented were developed by Moriya as follows. Let the coupling between two ions in a crystal be considered first, located at points A and B, respectively. The point bisecting the straight line AB is called C. Then:

- When a center of inversion is located at C, $\mathbf{D}_{ij} = 0$.
- When a mirror plane perpendicular to AB passes through C, $\mathbf{D}_{ij} \parallel$ mirror plane or $\mathbf{D}_{ij} \perp$ AB.
- When there exists a mirror plane including A and B, $\mathbf{D}_{ij} \perp$ mirror plane.
- When a two-fold rotation axis perpendicular to AB passes through C, $\mathbf{D}_{ij} \perp$ two-fold axis.
- When there is an n -fold axis ($n \geq 2$) along AB, $\mathbf{D}_{ij} \parallel$ AB.

In general, the $\mathbf{D}_{ij}$ term is allowed when it does not violate the symmetry of the crystal structure. Let $\mathbf{S}_1$ and $\mathbf{S}_2$ be two spins and let C be the center point of the line connecting the two spins. Now, if C is an inversion center of the crystal, H_{DM} should be invariant under the inversion operation. Inversion interchanges the positions of the two spins and hence $\mathbf{S}_1 \times \mathbf{S}_2 \rightarrow \mathbf{S}_2 \times \mathbf{S}_1 = -\mathbf{S}_1 \times \mathbf{S}_2$. Thus, $\mathbf{D}_{12}$ must be zero to leave the Hamiltonian invariant. If inversion symmetry is not present, however, $\mathbf{D}_{12}$ can be nonzero. Keep the same two spins, but now consider the situation where the crystal lattice is such that there exists a two-fold rotation axis passing through C in a perpendicular direction to the line connecting the two spins (see figure below). The Hamiltonian should then be invariant under a C_2 rotation. Performing this rotation corresponds to the mapping

$$S_{1x} \rightarrow -S_{2x}, S_{1y} \rightarrow -S_{2y}, S_{1z} \rightarrow S_{2z}. \quad (16.72)$$

Now, the original Hamiltonian reads:

$$H_{DM} = D_{12,x}(S_{1y}S_{2z} - S_{1z}S_{2y}) + D_{12,y}(S_{1z}S_{2x} - S_{1x}S_{2z}) + D_{12,z}(S_{1x}S_{2y} - S_{1y}S_{2x}). \quad (16.73)$$

It is clear that performing the mapping in Eq. (16.72) on Eq. (16.73) leaves the two first terms invariant, but not the last one. Hence, the total Hamiltonian is only invariant if $D_{12,z} = 0$. As a result, $\mathbf{D}_{12}$ must be perpendicular to the two-fold symmetry axis, i.e. the z -axis shown in the figure. To find its precise orientation in the xy -plane, one would need to compute it for a given crystal structure and with specific interactions, but the general arguments put forward here still hold. Let us now consider some special cases in more detail.

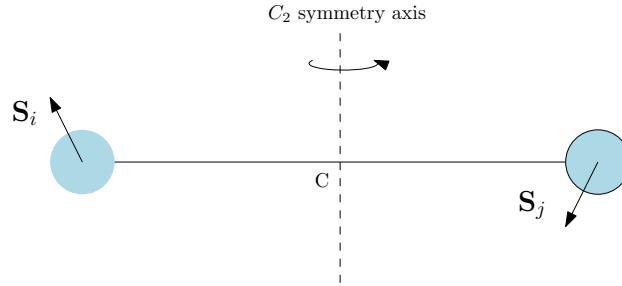


Figure 16.5: (Color online) C_2 symmetry axis between two spins $\mathbf{S}_1$ and $\mathbf{S}_2$.

Bulk DMI interaction

For a lattice of spins, we have

$$H_{DM} = \sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{M}_i \times \mathbf{M}_j), \quad (16.74)$$

where we have absorbed some constants into $\mathbf{D}_{ij}$ (as magnetic moments are proportional to spin) and the sum runs over nearest neighbors. To acquire the continuum form of this interaction, we Taylor expand the magnetization in the different nearest neighbor directions:

$$\mathbf{M}_{i+1} \simeq \mathbf{M}_i + a_i \frac{\partial \mathbf{M}_i}{\partial x} \quad (16.75)$$

where a_i is the distance between the nearest neighbors. Now, $\mathbf{D}_{ij} = -\mathbf{D}_{ji}$ changes sign upon interchanging i and j since the interaction energy between spin i and j has to be the same as the

interaction energy between spin j and i . Thus, we obtain in the continuum limit for the energy density $\mathcal{H}_{DM}$:

$$\mathcal{H}_{DM} = \mathbf{D}_{x_i} a_i \cdot (\mathbf{M} \times \frac{\partial \mathbf{M}}{\partial x_i}), \quad (16.76)$$

where $\mathbf{D}_{x_i}$ is the DM vector for the pairs connected in the x_i direction. For a cubic lattice, we have $x_i \in \{x, y, z\}$. As seen in the general rules, when there exists *e.g.* a 2-fold rotation axis along the line connecting the interacting spin pair, then $\mathbf{D}$ will be parallel to that axis. In this case, we can set $\mathbf{D}_{x_i} = -(D/a_i)\mathbf{x}_i$ and obtain from Eq. (16.76) that

$$\begin{aligned} \mathcal{H}_{DM} &= -D \left[\hat{x} \cdot (\mathbf{M} \times \partial \mathbf{M} / \partial x) + (x \rightarrow y) + (x \rightarrow z) \right] \\ &= D \left[M_x (\partial M_z / \partial y - \partial M_y / \partial z) + M_y (\partial M_x / \partial z - \partial M_z / \partial x) + M_z (\partial M_x / \partial y - \partial M_y / \partial x) \right] \\ &= D \mathbf{M} \cdot (\nabla \times \mathbf{M}). \end{aligned} \quad (16.77)$$

This is a commonly used form for bulk DMI, where we are thus considering similar DMI in all spatial directions.

Interaction between two ions mediated by a third ion (ligand)

Considering the case that the magnetic interaction between two neighboring ions is transferred via a single third ion (ligand) by the superexchange mechanism, the orientation of $\mathbf{D}_{ij}$ is obtained by

$$\mathbf{D}_{ij} \propto \mathbf{r}_i \times \mathbf{r}_j \quad (16.78)$$

so that $\mathbf{D}_{ij}$ is oriented perpendicular to the triangle spanned by the involved three ions. This is similar to the example above for the C_2 symmetry. If the three ions are in line, then $\mathbf{D} = 0$ since inversion symmetry is restored ($\mathbf{r}_i \parallel \mathbf{r}_j$). This mechanism for generating DMI is especially relevant for interfacial inversion symmetry breaking, *e.g.* in ultrathin ferromagnetic thin films in contact with some substrate or heavy normal metal layer.

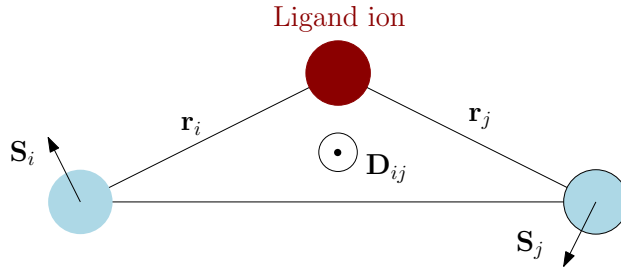


Figure 16.6: (Color online) Orientation of DM vector for interfacial symmetry breaking. $\mathbf{D}_{ij}$ can point both in and out of plane depending on its sign.

As an example, consider the case where $\mathbf{z}$ is normal to the interface. It follows that $\mathbf{D}_z$ must be zero. Writing $\mathbf{D}_x = (D/a_x)\mathbf{y}$ and $\mathbf{D}_y = -(D/a_y)\mathbf{x}$, we obtain:

$$\mathcal{H}_{DM} = D[M_z(\nabla \cdot \mathbf{M}) - (\mathbf{M} \cdot \nabla)M_z]. \quad (16.79)$$

which is a commonly used form for the interface DMI energy density. That this is related to inversion symmetry breaking along the $\mathbf{z}$ axis can be seen more explicitly by writing the above as:

$$\mathcal{H}_{DM} = D[(\mathbf{z} \cdot \mathbf{M})(\nabla \cdot \mathbf{M}) - (\mathbf{M} \cdot \nabla)(\mathbf{z} \cdot \mathbf{M})]. \quad (16.80)$$

16.8.6 Relation between spin-orbit coupling and DMI

When inversion symmetry is broken, either in a crystal structure or due to the geometry (interfaces or surfaces), Rashba spin-orbit coupling is in general present. The broken inversion symmetry means that the electric potential acquires a gradient as $V(\mathbf{r}) \neq V(-\mathbf{r})$, and thus electrons moving in this electric field see a net magnetic field (due to relativity) which couples to its spin. The Rashba Hamiltonian can be written as

$$H_R = \alpha_R(\boldsymbol{\sigma} \times \mathbf{k}) \cdot \mathbf{n} = \frac{\alpha_R}{\hbar} \boldsymbol{\sigma} \cdot (\mathbf{p} \times \mathbf{n}). \quad (16.81)$$

Here, $\mathbf{n}$ is the orientation along which inversion symmetry is broken. The total Hamiltonian describing electrons under the influence of a Rashba effect and an exchange interaction between their spins reads:

$$H = H_{\text{kinetic}} + H_R + H_{\text{exchange}} = \frac{\mathbf{p}^2}{2m} + \frac{\alpha_R}{\hbar} \boldsymbol{\sigma} \cdot (\mathbf{p} \times \mathbf{n}) + J\boldsymbol{\sigma} \cdot \mathbf{M}. \quad (16.82)$$

We now follow the idea of Kim *et al.* (PRL 2013). Performing a unitary transformation on the Hamiltonian so that $H' = U^\dagger H U$, H' is guaranteed to be hermitian and to have the same eigenvalues as H . In effect, the physics described by the two Hamiltonians should be the same. Let such a unitary matrix be given as

$$U = \exp\left[-ik_R \boldsymbol{\sigma} \cdot (\mathbf{r} \times \mathbf{n})/2\right], \quad k_R = 2\alpha_R m/\hbar^2. \quad (16.83)$$

This unitary transformation describes rotation of a spin around the axis $(\mathbf{r} \times \mathbf{n})$ by an angle $\phi = k_R |\mathbf{r}|$. The net effect of this transformation is that it removes the Rashba term from the Hamiltonian, but at the expense of making the magnetization spatially dependent $\mathbf{M} \rightarrow \mathbf{M}'$. Thus, the transformed Hamiltonian [up to $\mathcal{O}(\alpha_R^2)$ to be precise] reads:

$$H' = U^\dagger H U = \frac{\mathbf{p}^2}{2m} + J\boldsymbol{\sigma} \cdot \mathbf{M}'. \quad (16.84)$$

The relation between $\mathbf{M}'$ and $\mathbf{M}$ turns out to be $\mathbf{M}' = R^{-1}\mathbf{M}$ where R is 3×3 rotation matrix which performs the equivalent rotation (around the same axis and with the same angle) on the classical vector $\mathbf{M}$ as U performs on a spin. It follows that

$$\partial_i(R^{-1}\mathbf{M}) = R^{-1}[\partial_i \mathbf{M} + k_R(\mathbf{n} \times \mathbf{i}) \times \mathbf{M}], \quad (16.85)$$

where $\mathbf{i}$ is the unit vector in i -direction. The exchange energy density for the inhomogeneous field is then:

$$\begin{aligned} \mathcal{H}' &= A \partial_i \mathbf{M}' \partial_i \mathbf{M}' \\ &= A \partial_i \mathbf{M} \partial_i \mathbf{M} + 2k_R A (\partial_i \mathbf{M}) [(\mathbf{n} \times \mathbf{i}) \times \mathbf{M}] + \mathcal{O}(\alpha_R^2) \\ &= A \partial_i \mathbf{M} \partial_i \mathbf{M} + D(\mathbf{n} \times \mathbf{i}) \cdot (\mathbf{M} \times \partial_i \mathbf{M}) + \mathcal{O}(\alpha_R^2). \end{aligned} \quad (16.86)$$

We defined $D = 2k_R A$ and there is an explicit summation over the index i . By setting $\mathbf{n} = \mathbf{z}$, one obtains the previously derived interfacial form of the DMI for an interface normal to the $\mathbf{z}$ direction. We thus see that the DMI interaction arises due to the presence of *both* the exchange interaction between the spins and the spin-orbit coupling, which is consistent with our previous discussion.

The effect DMI can also be derived in a lattice model with fermion operators, see <https://arxiv.org/pdf/1205.6211.pdf> for a unitary transformation (S-W transformation).

16.9 Magnons and Holstein-Primakoff transformation

To discuss magnons, which are excitations above the magnetic ground-state of a Hamiltonian, we first discuss the actual ground-states themselves. The material from below is primarily from https://mpl.mpg.de/fileadmin/user_upload/Viola_Kusminskiy_RG/Lectures/QMSWL_Notes_1_.pdf.

16.9.1 Ground-state of the ferromagnetic Heisenberg Hamiltonian

Consider the Hamiltonian

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \quad (16.87)$$

where $J_{ij} = J_{ji} \geq 0$. This is a ferromagnetic interaction. If all spins were classical vectors, the ground-state (which has the lowest energy) would be the one where all N spins are aligned. In this quantum case, a natural expectation is thus that the ground state for $\hat{H}$ is a product state:

$$|0\rangle = |S, S\rangle_1 \dots |S, S\rangle_N \quad (16.88)$$

with $\hat{\mathbf{S}}_i^2 |S, m\rangle_i = S(S+1) |S, m\rangle_i$ and $\hat{S}_i^z |S, m\rangle_i = m |S, m\rangle_i$. This means that all spins take their maximum project along z . One verifies that the individual spins do not commute with $\hat{H}$, in effect $[\hat{\mathbf{S}}_i, \hat{H}] \neq 0$. This means that although a product state of the form

$$|\psi\rangle = |S, m_1\rangle |S, m_2\rangle \dots \quad (16.89)$$

form a basis for the Hilbert space, such states are not necessarily eigenstates of $\hat{H}$. However, the total spin operator $\mathbf{S}_{\text{tot}} = \sum_i \hat{\mathbf{S}}_i$ does commute with $\hat{H}$. Thus, we now prove that Eq. (16.88) is an eigenstate of $\hat{H}$ and that it is the ground-state.

To do so, we introduce the ladder operators

$$\begin{aligned} \hat{S}_i^\pm &= \hat{S}_i^x \pm i\hat{S}_i^y, \\ \hat{S}_i^\pm |S_i, m_i\rangle &= \sqrt{(S_i \mp m_i)(S_i + 1 \pm m_i)} |S_i, m_i \pm 1\rangle. \end{aligned} \quad (16.90)$$

We can then write $\hat{H}$ in terms of these operators

$$\hat{H} = -\frac{1}{2} \sum_{ij} J_{ij} \left[\frac{1}{2} (\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) + \hat{S}_i^z \hat{S}_j^z \right]. \quad (16.91)$$

Now we can straightforwardly show that $|0\rangle$ is an eigenstate of $\hat{H}$:

$$\hat{H} = -\frac{1}{2} \sum_{ij} J_{ij} \hat{S}_i^z \hat{S}_j^z |0\rangle = -\frac{S^2}{2} \sum_{ij} J_{ij} |0\rangle \quad (16.92)$$

as $\hat{S}_i^+ |0\rangle = 0$ for any i (the spin projection cannot be increased any further in $|0\rangle$) and we used that spin operators at different sites commute as well as $J_{ii} = 0$.

Thus, $\hat{H}|0\rangle = E_0|0\rangle$ and we need to prove that $E_0 = -\frac{S^2}{2} \sum_{ij} J_{ij}$ is the minimum possible energy. This is done by considering an arbitrary product state $|\psi\rangle$ for which

$$E'_0 = \langle \psi | \hat{H} | \psi \rangle = -\frac{1}{2} \sum_{ij} J_{ij} m_i m_j \quad (16.93)$$

where we used that $\langle \psi | \hat{S}_i^+ \hat{S}_j^- | \psi \rangle = 0$. If now $J_{ij} \geq 0$, as it is for a ferromagnet, we have

$$\sum_{ij} J_{ij} m_i m_j \leq \sum_{ij} J_{ij} S S \quad (16.94)$$

which means $E'_0 \geq E_0$. The fully polarized state $|0\rangle$ is thus the ground-state, but it is not unique: it is $2S_{\text{tot}} + 1$ degenerate in spin space where $S_{\text{tot}} = NS$. To understand this, consider the 2-spin case. We have $S_{\text{tot}} = 1$ and the triplet state has three possible projections of $\hat{S}_z$. This means that there are three possible degenerate ground-states. Same reasoning applies to a system with N spins. This model features spontaneous symmetry breaking since the ground-state is one specific realization out of the possible degenerate ground-states. All of this is generally valid at $T = 0$, whereas Mermin-Wagner tells us that in 1D and 2D we cannot have a spontaneously broken continuous symmetry. An external magnetic field adds a term $-g\mu_B BNS$ to E_0 and explicitly breaks the spin rotational symmetry.

16.9.2 Ground-state of the antiferromagnetic Heisenberg Hamiltonian

Consider a bipartite lattice with antiferromagnetic order. This means $J_{ij} \leq 0$ for any neighbors i, j and the entire lattice can be divided into two sublattices A and B . Simplest case to visualize is a square lattice with nearest neighbor interactions where all spins on A point in one direction and all on B point in the opposite direction.

The classical ground-state would be a Néel state: the two sublattices are fully polarized, but in opposite directions. The quantum version of this is

$$|\bar{0}\rangle = \prod_{i \in A} |S, S\rangle_i \prod_{j \in B} |S, -S\rangle_j. \quad (16.95)$$

Although a reasonable guess, this is in fact not the ground state of the quantum Heisenberg Hamiltonian. We can see this by writing H in terms of ladder operators, as in the ferromagnetic case, in which case we see that

$$\hat{H}|\bar{0}\rangle = -\frac{1}{2} \sum_{i \in A, j \in B} J_{ij} \left[\frac{1}{2} (\hat{S}_i^+ \hat{S}_j^- |\bar{0}\rangle + \hat{S}_i^- \hat{S}_j^+ |\bar{0}\rangle) + \hat{S}_i^z \hat{S}_j^z |\bar{0}\rangle \right]. \quad (16.96)$$

The first term is zero since the sublattices are fully polarized in the right way with respect to the operators. The last term is proportional to $|\bar{0}\rangle$. However, the second term becomes

$$\hat{S}_i^- \hat{S}_j^+ |\bar{0}\rangle \propto |S, -m_N\rangle \dots |S, -S+1\rangle_j \dots |S, S-1\rangle_i \dots |S, m_N\rangle. \quad (16.97)$$

This is not proportional to $|\bar{0}\rangle$, which therefore cannot be an eigenstate or ground-state. It is thus the lowering and raising spin operators, which can be thought of as quantum fluctuations, which play an important role in causing the antiferromagnetic quantum ground state to deviate from its classical version. This was not the case in the ferromagnetic case, where these fluctuation terms vanished. Quantum fluctuations thus play a much more important role in antiferromagnets than in ferromagnets.

Generally, one can instead prove that the true ground state $|0\rangle$ is non-degenerate and a singlet of total spin so that $\hat{S}_{\text{tot}}|0\rangle = 0$. This is called Marshall's theorem. As shown in John Ove FjÅrrestad's lecture notes, one can prove that the ground-state energy of the Heisenberg antiferromagnet (where there are no magnon excitations present) is lower than the classical ground-state energy. Thus, quantum fluctuations lower the energy of the system in the antiferromagnetic case, whereas there is no quantum fluctuation correction to the ferromagnetic ground state.

16.9.3 Classical Heisenberg model ground state

We comment briefly on the classical ground state. Replace the operators $\hat{S}$ with simple vectors with fixed length S . This becomes a better approximation the larger the spin is. For a translationally invariant system where $J_{ij} = J(\mathbf{R}_i - \mathbf{R}_j)$, one can find the ground-state, where $\mathbf{R}_i$ are the points on a Bravais lattice. In Fourier-space, we have

$$\begin{aligned} \mathbf{S}_i &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathbf{S}_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_i} \\ \mathbf{S}_{\mathbf{k}} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathbf{S}_i e^{-i\mathbf{k} \cdot \mathbf{R}_i} \end{aligned} \quad (16.98)$$

which inserted into the Heisenberg real-space Hamiltonian gives

$$H = -\frac{1}{2} \sum_{\mathbf{k}} J(\mathbf{k}) \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{-\mathbf{k}} \quad (16.99)$$

where $J(\mathbf{k}) = \sum_i J(\Delta \mathbf{R}) e^{i\mathbf{k} \cdot \Delta \mathbf{R}}$ and $\Delta \mathbf{R} = \mathbf{R}_i - \mathbf{R}_j$. With the constraint of fixed length of the spins, as mentioned initially, one can prove that the minimum energy of the above H is given by a real space spin configuration

$$\mathbf{S}_i = S[\cos(\mathbf{Q} \cdot \mathbf{R}_i), \sin(\mathbf{Q} \cdot \mathbf{R}_i), 0] \quad (16.100)$$

where $\mathbf{Q}$ is the wavevector which maximizes $J(\mathbf{Q})$. This is proven in D. H. Lyons and T. A. Kaplan, Phys. Rev. 120, 1580 (1960). The resulting spin order is not necessarily commensurate with the lattice. For $\mathbf{Q} = 0$ we get ferromagnetic order, and if $\mathbf{Q}$ takes a value at the edge of the 1st BZ, we get antiferromagnetic order.

16.9.4 Spin-waves and magnons

Having now covered the ground-state of the ferromagnetic and antiferromagnetic models, both the quantum and classical version, we look at excitations above the ground-state. At low temperatures, only the ground state is occupied. At low but finite temperatures, excitations above the ground state determine the behavior of the system. These turn out to be delocalized spin-flips called spin-waves in the classical case or magnons in the quantum case.

Excitations of the Heisenberg ferromagnet

At $T = 0$, the spins are aligned and the total magnetization is $M_s = g\mu_B NS/V$. At $T \neq 0$, some spins therefore have to flip in order to decrease the magnetization from its saturated value. An obvious candidate for an excited state is

$$|i\rangle = |S, S\rangle_1 \dots |S, S-1\rangle_i \dots |S, S\rangle_N. \quad (16.101)$$

Such a state can be obtained from the GS by

$$|i\rangle = \frac{1}{\sqrt{2S}} \hat{S}_i^- |0\rangle. \quad (16.102)$$

While $|i\rangle$ is an eigenstate of $\hat{S}_z$, it is not an eigenstate of the term $\hat{S}_j^- \hat{S}_i^+$ that appears in the Heisenberg Hamiltonian:

$$\hat{S}_j^- \quad (16.103)$$

In the HP transformation, one generally obtains linear terms in $a, a^\dagger$. However, these terms must vanish so long that we are expanding around the classical ground-state spin configuration. The reason is as follows. The classical ground-state yields the lowest energy. Thus, introducing any additional parameters in the model which change the spin configuration (which is what the HP transformation does) can only increase the energy. Considering then $a, a^\dagger$ as such additional parameters, it is clear that the ground-state of $H(a, a^\dagger)$ is obtained at $\partial H/\partial a = \partial H/\partial a^\dagger = 0$ since this minimizes H with respect to the additional parameters. Therefore, the coefficients associated with the linear terms must vanish, and thus the linear terms vanish all together.

In summary, the zeroth-order contribution gives the classical ground-state energy, the terms linear in the boson operators vanish when the classical ground-state is used to define the local spin frames, and the quadratic terms describe the spin-excitations.

16.9.5 Including dipolar interactions

The introduction below is taken (modified) from Phys. Rev. B **62**, 6545 (2000).

Ultrathin ferromagnetic films are of great interest due to their widespread technological applicability. This is because these films can have properties, both static and dynamic, that differ significantly from bulk samples of the same material. For example, it is well known theoretically that, in these quasi-two-dimensional systems, the short-range exchange interactions alone are not sufficient to establish a ferromagnetically ordered ground state, and it is necessary to take into account the anisotropy and long-range character of the dipolar interactions. Regarding the spin dynamics in ferromagnetic films, a macroscopic (or continuous medium) theory for the dipole-dominated regime was given by Damon and Eshbach in terms of magnetostatic modes. They identified a surface branch to the spectrum, now known as the Damon-Eshbach (DE) mode. Subsequently there has been extensive work to generalize the magnetostatic theory to include also the exchange effects, leading to dipole-exchange theory. In these theories the DE surface mode becomes modified and various quantization effects become evident for the bulk modes. In addition, Benson and Mills considered a microscopic formalism for the dipole interactions in a thin ferromagnetic film, obtaining a rapidly converging series for the dipole sums. More recently, their approach has been extended to a description of the dipole-exchange spin waves (SW) in various ferromagnetic and antiferromagnetic films.

All of the studies mentioned above neglected the higher-order effects that give rise to SW interactions. These occur because the SW are not exact eigenstates of the magnetic Hamiltonian and they are the source of several nonlinear effects, such as parallel pumping of SW, auto-oscillations and the transition to chaos, soliton formation, and energy renormalization and damping of the SW modes. Previous studies of the SW interactions in films were carried out from a macroscopic point of view, where the dipolar terms were introduced using Maxwell's equations. Again, this should be appropriate for small wave vectors and for moderate film thickness. In infinite ferromagnets, either with or without the inclusion of the dipolar interactions, the treatment of the interactions between the bulk SW modes is well established. The dominant contributions at $T \ll T_c$ come from three-magnon confluence and splitting processes and from four-magnon scattering processes. In the special case of a Heisenberg ferromagnet, where there are only exchange interactions, the three-magnon process is absent. However, for a finite ferromagnet, the presence of surfaces leads to a richer SW spectrum that may consist of one or more localized surface SW modes as well as the

bulk modes (which become quantized in a film geometry). The occurrence of surface and modified bulk modes in a finite ferromagnet will give rise to more complicated schemes or SW interactions, since the scattering processes may now involve both types of modes.

There has previously been a number of calculations for SW interactions in semi-infinite Heisenberg ferromagnets at low temperatures $T \ll T_c$ using a Hamiltonian approach. In particular, results for the damping and the energy renormalization of the surface SW were obtained in some special cases by Tarasenko and Kharitonov and Mazur and Mills. More detailed results, which were applicable to both surface and bulk (volume SWs and induced pinning through surface anisotropy and modified surface exchange, were derived by Kontos and Cottam using a diagrammatic perturbation method. In the above-mentioned studies for Heisenberg systems, the dipole-dipole interactions were ignored, leading to a description of SW interactions at $T \ll T_c$ only in terms of the leading-order four-magnon processes. When the dipolar terms are included there are also three-magnon processes involving the splitting of SW into two SW modes and the confluence of two SW modes into a single SW. For example, Rahman and Mills calculated the renormalized energies for the bulk and Damon-Eshbach surface SW in the dipolar-exchange regime. For ferromagnetic films in this regime of long wavelengths (or small wave vectors), there have been extensive calculations of the nonlinear SW properties using a macroscopic (or continuous-medium) type of theory. A nonlinear microscopic theory, based on a Hamiltonian approach, allows us to study the SW interactions and the renormalization of the discrete SW modes.

We consider a quite general Hamiltonian, disregarding the anisotropy term which gives a spin-wave gap since we here want to highlight the effect of the short-ranged strong exchange interaction and the long-ranged weak dipolar interaction. It reads

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - g\mu_B B_0 \sum_i S_i^z + \frac{1}{2} (g\mu_B)^2 \sum_{ij} D_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta, \quad (16.104)$$

where the two first terms are well-known and the dipole-dipole interaction between spins in different lattice sites is given by

$$D_{ij}^{\alpha\beta} = \frac{|\mathbf{r}_{ij}|^2 \delta_{\alpha\beta} - 3r_{ij}^\alpha r_{ij}^\beta}{|\mathbf{r}_{ij}|^5}, \quad (16.105)$$

where $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ and the term $i = j$ is excluded from the summations in the Hamiltonian.

In general, the dipolar interactions will have their most significant effect on the long-wavelength (small q) SW properties in each material, while the exchange effects dominate at shorter wavelengths (large q).

Performing a Holstein-Primakoff transformation, the part of the above Hamiltonian which is bilinear in the magnon operators takes the form

$$H = \sum_{\mathbf{q}, n, n'} A_{\mathbf{q}nn'} a_{\mathbf{q}n}^\dagger a_{\mathbf{q}n'} + B_{\mathbf{q}nn'} (a_{\mathbf{q}n} a_{-\mathbf{q}n'} + a_{\mathbf{q}n}^\dagger a_{-\mathbf{q}n'}^\dagger). \quad (16.106)$$

Here, $\mathbf{q} = (\mathbf{q}_x, \mathbf{q}_z)$ for a thin ferromagnet (along the z -direction) whereas $n, n' = 1, 2, \dots, N$ label atomic layers parallel to the film. In the absence of dipolar interactions, $B_{\mathbf{q}nn'} = 0$. The above Hamiltonian can now be diagonalized in a standard way to obtain the eigenstates of the system.

Higher order terms (with three or four magnon operators) describe SW interactions. They describe processes whereby energy from a given SW with wave vector $\mathbf{q}$ can be transferred to other SW modes

of the film. Thus they can be used to calculate the damping (or reciprocal lifetime) of any given SW, as well as the shift (or renormalization) in its energy dispersion. If dipolar interactions are neglected, there is no term with three magnon operators. This can be accomplished using a diagrammatic perturbation method with Green functions, treating the third and fourth order magnon operator terms as perturbations giving rise to a self-energy which enters the magnon propagator. This method is shown in the reference given initially in this section.

16.9.6 Relation between Curie temperature T_c and magnon gap

By performing a non-linear spin-wave expansion, one can show that the critical temperature for the ferromagnetic transition is determined by the spin-wave gap Δ in the magnon dispersion $E = \Delta + \rho k^2$ where ρJ is a constant proportional to the exchange interaction J between the spins. As the magnon gap increases, so does T_c . This can be understood intuitively by noting that the magnetization is reduced with the generation of magnons. If the number of magnons increases, the fluctuations in the magnetization become stronger and ultimately the magnetization goes to zero. Now, the spin-wave Δ_0 makes it harder to excite magnons thermally. Thus, it is natural that the critical temperature T_c becomes larger when the spin-wave gap increases since magnon generation is thwarted.

16.10 Magnetization dynamics: LLG equation

16.10.1 Effective field B_{eff}

As derived in Gilbert's IEEE 2004 paper, the effective magnetic field is the functional derivative of the magnetic potential energy with respect to the magnetization:

$$\mathbf{B}_{\text{eff}} = \frac{-\delta U}{\delta \mathbf{M}}. \quad (16.107)$$

A trivial case is when an external field $\mathbf{B}$ is present so that $U = -\mathbf{B} \cdot \mathbf{M}$, which creates a torque on $\mathbf{M}$ whenever they are not collinear. If we now want to include the effect of itinerant electrons coupled to the magnetization $\mathbf{M}$ set up by localized electron magnetic moments, we have to include a term

$$U_{\text{sd}} = \langle \mathbf{S} \rangle \cdot \mathbf{M} \quad (16.108)$$

where $\mathbf{S} = \sum_{\mathbf{k}\alpha\beta} c_{\mathbf{k}\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}\beta}$ is the itinerant electron spin operator. The LLG equation then gives the dynamics of $\mathbf{M}$ in the presence of a coupling to itinerant spins. Should we like to describe the dynamics of $\mathbf{S}$ as well, due to the dynamics of $\mathbf{M}$, we have derive an equation of motion for $\mathbf{S}$ using the Heisenberg equations. The two coupled, time-dependent equations for $\mathbf{S}$ and $\mathbf{M}$ can then in principle be solved.

So how do we compute $\langle \mathbf{S} \rangle$? There are two approaches one can take. In both cases, we neglect the dynamics of the itinerant electrons and consider them to be in equilibrium, feeling a background field $\mathbf{M}$.

(1) We can use the thermal density matrix to evaluate the expectation value $\langle \mathbf{S} \rangle$ through

$$\langle \mathbf{S} \rangle = \text{Tr}\{\rho \mathbf{S}\}. \quad (16.109)$$

As derived earlier in these notes, the density matrix ρ has elements $\rho_{nn'} = \langle n | \hat{\rho} | n' \rangle$ obtained from the density operator $\hat{\rho} = e^{-\beta \hat{H}} / Z$. Assume the background magnetization points along the z -axis

for concreteness, in which case one obtains using the above formulae that

$$\langle \mathbf{S} \rangle = \sum_{\mathbf{k}\sigma} \sigma f(\varepsilon_{\mathbf{k}\sigma}), \quad (16.110)$$

where f is the Fermi-Dirac distribution function and $\varepsilon_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} - \sigma M$. This is a reasonable expression physically: the polarization of the electrons is given by the difference in distribution functions for spin-up and spin-down. However, consider now instead the free energy $F = -\frac{1}{\beta} \ln(Z)$ of the system. We obtain exactly the same expression from $-dF/d\mathbf{M}$ in the case of a free electron gas, since

$$F = -\frac{1}{\beta} \sum_{\mathbf{k}\sigma} \ln(1 + e^{-\beta \varepsilon_{\mathbf{k}\sigma}}). \quad (16.111)$$

So it looks like can get $\mathbf{B}_{\text{eff}}$ both from $\text{Tr}\{\rho \mathbf{S}\}$ or from $dF/d\mathbf{M}$: both give the same result. It is nevertheless presently not clear if this is only valid for the free electron gas case or if is a more general result. One way to check could be to compare the two expressions for a spin-split superconductor.

Actually, in hindsight we can prove it generally right away by using Eq. (6.81). Consider a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 - \mathbf{h} \cdot \hat{\mathbf{S}} \quad (16.112)$$

where $\hat{H}$ and $\hat{\mathbf{S}}$ are operators. This proof extends beyond spin systems, but let us first consider the case of a magnetic field along the z -axis for concreteness. We get:

$$\hat{H} = \hat{H}_0 + h \cdot \hat{S}_z. \quad (16.113)$$

It is clear that $\partial \hat{H} / \partial h = \hat{S}_z$. Using Eq. (6.81), it follows immediately that:

$$\langle \hat{S}_z \rangle = \frac{\partial F}{\partial h}. \quad (16.114)$$

(2) This is a more qualitative argument, which is not required in light of the above general proof, but let us mention it anyway. In thermodynamics, the polarization of a system can be obtained from the free energy as

$$\mathbf{M}_{\text{pol}} = -\frac{dF}{d\mathbf{B}} \quad (16.115)$$

where $\mathbf{B}$ is an external field. As far as the itinerant electrons are concerned, the background magnetization $\mathbf{M}$ set up by the localized spins acts as an effective external magnetic field. Therefore, we can obtain the polarization created by the itinerant electrons as:

$$\mathbf{M}_{\text{pol}} = \langle \mathbf{S} \rangle = -\frac{dF}{d\mathbf{M}}. \quad (16.116)$$

16.10.2 Spin-transfer torque

Homogeneous $\mathbf{M}$: Magnetization switching

Inhomogeneous $\mathbf{M}$: Domain wall motion

Spin-orbit torque vs. spin-Hall torque

Thin-film structures comprised of ferromagnets and heavy normal metals are known to give rise to spin-orbit torques and spin-Hall torques. Both of these effects can be described in the LLG

framework. The presence of Rashba spin-orbit interactions influences how angular momentum is transferred between the conduction electrons and the local magnetic moments described by $\mathbf{M}$. Assume that we have a thin-film in the xy -plane and that the axis of inversion asymmetry is $\hat{\mathbf{z}}$. In that case, the Rashba spin-orbit torques are accounted for [33] via a term $\mathbf{H}_{\text{so}}$:

$$\mathbf{H}_{\text{so}} = \frac{\alpha_R m_e P_{\text{current}}}{\hbar e M_0 (1 + \beta^2)} \hat{\mathbf{z}} \times \mathbf{j}, \quad (16.117)$$

α_R characterizes the strength of the spin-orbit coupling. P_{current} and $\mathbf{j}$ are the polarization and density of the injected current, whereas m_e and M_0 are the electron mass and magnitude of the magnetization, respectively. The parameter β is known as the nonadiabaticity parameter in the literature.

Before demonstrating the precise manner in which $\mathbf{H}_{\text{so}}$ is included in the LLG equation, we also explain the physics of the spin Hall torque. When a charge current is injected into a heavy normal metal layer connected to a ferromagnet, the spin Hall effect causes a transverse spin current to flow into the magnetic layer which then deposits its transversely polarized component to $\mathbf{M}$ as a spin-transfer torque. Therefore, the spin Hall torque may be described in the same manner as one would describe the spin-transfer torque from a spin polarized current incident on a magnetization $\mathbf{M}$ (see the above subsection).

We may take into account all of these terms, as well as the usual STT and Gilbert damping

$$\begin{aligned} \partial_t \mathbf{M} &= -\gamma \mathbf{M} \times \left(\mathbf{H}_{\text{eff}} + \mathbf{H}_{\text{so}} - \frac{\beta}{M_0} \mathbf{M} \times \mathbf{H}_{\text{so}} + a_J (\mathbf{M} \times \hat{\mathbf{p}}) + b_J \hat{\mathbf{p}} \right) \\ &= \frac{\alpha}{M_0} \mathbf{M} \times \partial_t \mathbf{M} + \Gamma \partial_x \mathbf{M} - \frac{\beta \Gamma}{M_0} \mathbf{M} \times \partial_x \mathbf{M}, \end{aligned} \quad (16.118)$$

where $\hat{\mathbf{p}}$ is a unit vector representing the spin direction of the electrons impinging on the magnetic layer via SHE, a_J and b_J are proportional to the spin Hall angle θ_{SH} in the normal metal layer, and

$$\Gamma = \frac{\mu_B P_{\text{current}}}{e M_0 (1 + \beta^2)}. \quad (16.119)$$

16.11 Skyrmions

Skyrmions can form both in the presence DMI and due to long-range dipole-dipole interactions.

16.12 The role of magnetism in the four fundamental interactions

The four known fundamental interactions are:

- Gravitational force (acting on objects with mass)
- Electromagnetic force (acting on objects with charge)
- Weak force (acting on objects with flavor)
- Strong force (acting on objects with color)

Magnetic forces act on charged particles that are moving. But even the Lorentz force originates from the Coulomb interaction between charges. The point is that in order to describe the Coulomb interaction between two charges that are moving relative each other, it is not sufficient to just use the electrostatic Coulomb interaction equation: we must make a Lorentz-transformation to find out what the electric field looks like in the moving frame of one of the electron. As known, it will have a form of the type $\mathbf{E}' = \mathbf{E} + \mathbf{v} \times \mathbf{B}$ for non-relativistic velocities. Therefore, it is clear that the force coming from the electric field $\mathbf{E}'$ in the moving frame is equivalent to the force from the electric field $\mathbf{E}$ in the stationary frame *and* the magnetic force $\mathbf{v} \times \mathbf{B}$. It is just much more convenient to work with magnetic forces when charged particles are moving rather than applying the Coulomb interaction between them in moving frames.

The Zeeman-effect, which is the interaction between a magnetic moment and an external field, can be understood from this framework by noting that a magnetic (dipole) moment is equivalent to a circulating charge loop where $r \rightarrow 0$ and $q \rightarrow \infty$ in such a manner that the magnetic moment remains constant. But what about the *intrinsic magnetic moment* of particles known as spin? Particles without charge can also have spin, such as neutrinos. The point is then that a magnetic moment is equal to the *charge* of the particle times its spin, and it is the magnetic moment which interacts with *e.g.* external fields or other magnetic moments via a dipole-dipole interaction. A neutrino, despite having spin, thus does not experience a Zeeman effect since it is neutral. There exists proposals to provide neutrinos with a net magnetic moment from higher-order loop diagrams in QED. Summarizing so far, the magnetic dipole-dipole interaction thus also requires charge and can then be traced back to the electromagnetic force. Electrons, charged particles with spin $1/2$, thus experience both Zeeman effect and dipole-dipole interactions because they have $q \neq 0$.

It is also worth remarking that according to the above reasoning, the neutron should not have a magnetic moment and thus experience no Zeeman effect. However, this is incorrect, because it is experimentally known that the neutron does have a magnetic moment (which by the way surprisingly has the sign equivalent to that of a negatively charged particle!). The fact that this happens is a strong indication of the neutron not being an elementary particles. We know today that neutrons consist of quarks, which are charged spin $1/2$ particles, and it is because of the magnetic moments of these quarks that the neutron also acquires a net moment. This is then in contrast to a *fundamental neutral* particle with spin, such as the neutrino, which has no measurable magnetic moment.

16.13 Magnetism in Hubbard model: FM, AFM, and nesting

Consider the Hubbard model on a square lattice. At half-filling, it is straight-forward to show that $\mu = U/2$.

We focus to begin with on the $U = 0$ case where the Fermi surface has a nesting vector $\mathbf{Q} = (\pm\pi, \pm\pi)$ which means that if $\mathbf{k}$ is on the Fermi surface, then so is $\mathbf{k} + \mathbf{Q}$. The Fermi-surface is defined by

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) = 0 \quad (16.120)$$

since $\mu = 0$ at half-filling in this model. Since $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}} = 0$ when $\mathbf{k}$ lies on the Fermi surface for the above $\mathbf{Q}$, the vector $\mathbf{Q}$ maps one part of the Fermi surface onto a different part of the Fermi surface. The density of states

$$D(\epsilon) = \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) \quad (16.121)$$

in this model diverges at $\epsilon = 0$ since one can show that $D(\epsilon) \sim \ln(\epsilon/4t)$ for small energies. Without interactions ($U = 0$), the spin susceptibility per spin can be computed via the Kubo formula [52]. The result is [52, 53]:

$$\chi_0(\mathbf{q}) = -\frac{1}{N} \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}+\mathbf{q}}) - f(\epsilon_{\mathbf{k}})}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}. \quad (16.122)$$

A diverging spin susceptibility is indicative of the onset of magnetic ordering and we see that the above susceptibility can diverge both at $\mathbf{q} = 0$ and at $\mathbf{q} = \mathbf{Q}$, the latter due to the property $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$. The divergences as $T \rightarrow 0$ are [53]

$$\begin{aligned} \chi_0(\mathbf{q} = 0) &\sim -\ln \frac{T}{t}, \\ \chi_0(\mathbf{q} = \mathbf{Q}) &\sim \left(\ln \frac{T}{t} \right)^2. \end{aligned} \quad (16.123)$$

Thus, the $\mathbf{q} = \mathbf{Q}$ divergence is stronger for low temperatures, indicating the special role of the nesting wavevector $\mathbf{Q}$.

It remains to be clarified which types of magnetic instabilities the wavevectors $\mathbf{q} = 0$ and $\mathbf{q} = \mathbf{Q}$ correspond to. To understand this, consider the following order parameter for magnetism:

$$M_{\mathbf{i}} = \sum_{\sigma} \sigma \langle c_{i\sigma}^{\dagger} c_{i\sigma} \rangle = \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle \quad (16.124)$$

where $\mathbf{i} = (i_x, i_y)$. The Fourier-expansion of this order parameter is

$$M_{\mathbf{i}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} M_{\mathbf{q}} e^{-i\mathbf{q}\mathbf{i}}, \quad (16.125)$$

and the inverse transformation

$$M_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{i}} M_{\mathbf{i}} e^{i\mathbf{q}\mathbf{i}} = \sum_{\mathbf{k}, \sigma} \langle c_{\mathbf{k}+\mathbf{q}, \sigma}^{\dagger} c_{\mathbf{k}, \sigma} \rangle. \quad (16.126)$$

For ferromagnetic order, $M_{\mathbf{i}} = M$ and we see that $M_{\mathbf{q}} = M\sqrt{N}\delta_{\mathbf{q},0}$. In effect, the magnetic order parameter $M_{\mathbf{q}}$ is maximal at the FM ordering vector $\mathbf{q} = 0$ and in fact zero for all other $\mathbf{q}$.

In the AFM case, the spin-polarization alternates between neighboring lattice points and for a square lattice we may write $M_{\mathbf{i}} = M \times (-1)^{i_x+i_y}$. But we can also write the alternating sign factor as

$$(-1)^{i_x+i_y} = e^{-i\mathbf{Q}\mathbf{i}} \quad (16.127)$$

where $\mathbf{Q} = (\pm\pi, \pm\pi)$ (the lattice constant a is set to unity). Therefore, in momentum space the magnetic order parameter becomes

$$\begin{aligned} M_{\mathbf{q}} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{i}} M_{\mathbf{i}} e^{i\mathbf{q}\mathbf{i}} \\ &= \frac{1}{\sqrt{N}} \sum_{\mathbf{i}} M e^{-i\mathbf{Q}\mathbf{i}} e^{i\mathbf{q}\mathbf{i}} \\ &= M\sqrt{N}\delta_{\mathbf{q},\mathbf{Q}}. \end{aligned} \quad (16.128)$$

In effect, the magnetic order parameter $M_{\mathbf{q}}$ in the antiferromagnetic case is maximal at the AFM ordering vector $\mathbf{q} = \mathbf{Q} = (\pm\pi, \pm\pi)$ and in fact zero for all other $\mathbf{q}$.

We conclude that the $\mathbf{q} = 0$ divergence in the spin susceptibility corresponds to a ferromagnetic instability whereas the $\mathbf{q} = \mathbf{Q}$ divergence corresponds to an antiferromagnetic instability. This instability then occurs as a band-structure effect (even for $U = 0$) since the nesting vector for the Fermi surface is identical to the antiferromagnetic ordering vector.

In the presence of finite interactions U , can one do a RPA calculation [52] to show that the onset of FM order requires a critical value of U whereas the onset of AFM order will always occur at sufficiently low temperatures regardless of the value of U .

16.14 Antiferromagnetism

Antiferromagnetism can be modelled using mean-field theory on a lattice as an exchange field alternating for each subsequent lattice site:

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + M \sum_i (-1)^i (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}). \quad (16.129)$$

If we assume translational invariance in all directions, so that the Hamiltonian is written in $\mathbf{k}$ -space, it takes the following form for a square lattice

$$H = \frac{1}{2} \sum_{\mathbf{k} \in \diamond, \sigma} (c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q},\sigma}^\dagger) \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & \sigma M \\ \sigma M & \epsilon_{\mathbf{k}+\mathbf{Q}} - \mu \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ c_{\mathbf{k}+\mathbf{Q},\sigma} \end{pmatrix} \quad (16.130)$$

where $\mathbf{Q} = (\pi, \pi)$ and $\epsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)]$ is the normal-state dispersion. Here, $\diamond$ denotes the reduced BZ. One obtains the expression above by first Fourier-transforming the c -operators:

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \square} e^{i\mathbf{k} \cdot \mathbf{r}_i} c_{\mathbf{k}\sigma}, \quad (16.131)$$

where N is the number of lattice points. Here, $\square$ denotes the full square lattice BC. Below, we will explain why the $\mathbf{k}$ -values that one performs a summation over take different values.

The summation over $\mathbf{k}$ in the Fourier-transformed operators is then over the full lattice Brillouin zone $-\pi < k_i < \pi$. However, we can rewrite the resulting Hamiltonian by using that

$$\begin{aligned} H &= \sum_{\mathbf{k} \in \square, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + M c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q},\sigma} \\ &= \frac{1}{2} \sum_{\mathbf{k} \in \diamond, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \epsilon_{\mathbf{k}+\mathbf{Q}} c_{\mathbf{k}+\mathbf{Q},\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q},\sigma} + M c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q},\sigma} + M c_{\mathbf{k}+\mathbf{Q},\sigma}^\dagger c_{\mathbf{k}\sigma}, \end{aligned} \quad (16.132)$$

where we used if $\mathbf{k} \in \diamond$, then $\mathbf{k} + \mathbf{Q}$ lies in the region of $\square$ that is not part of $\diamond$. In effect, adding $\mathbf{Q}$ to a value $\mathbf{k} \in \diamond$ brings you to a point in the square lattice BZ $\square$ which lies outside of the reduced BZ. We get in general

$$\sum_{\mathbf{k} \in \square} F(\mathbf{k}) = \sum_{\mathbf{k} \in \diamond} [F(\mathbf{k}) + F(\mathbf{k} + \mathbf{G})], \quad (16.133)$$

if the quantity $F(\mathbf{k})$ has a $2\pi/a$ -periodicity in each k_i -component.

Therefore, the full sum over the BZ can be written as the sum over the reduced BZ for the original term plus a term where $\mathbf{Q}$ has been added to the momentum. This shifts the momentum values into the regions $\pi/2 < k_i < \pi$ and $-\pi < k_i < -\pi/2$, which is precisely the region omitted when going from the full BZ $\square$ to reduced BZ $\diamond$.

In 2D, we have a magnetic Brillouin zone (or the BZ of the individual sublattices) which is rotated by $\pi/4$ and has half the size of the original BZ. This can be seen by considering Fig. 16.7(a). Let us put a label A and B on the fermion operators on each sublattice so that

$$c_{i\sigma}^{A,B} = \frac{1}{\sqrt{N_{A,B}}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} c_{\mathbf{k}\sigma}^{A,B}. \quad (16.134)$$

Since the A sublattice is rotated by $\pi/4$ compared to the original lattice, we also have a distance $\sqrt{2}a$ between each A sublattice point. Above, N_A is the number of A sublattice atoms. Let there be $N_{A,y'}$ atoms along the y' -direction and $N_{A,x'}$ atoms along the x' -direction. Translational invariance along both x' and y' then requires that

$$c_{i\sigma}^A = c_{i+N_{A,x'}\hat{x}',\sigma}^A \quad (16.135)$$

which gives the condition

$$k_{x'}\sqrt{2}aN_{A,x'} = 2\pi n_{x'}, \quad (16.136)$$

where $n_{x'}$ is an integer. Therefore, the allowed values of $k_{x'}$ are:

$$k_{x'} = \frac{\sqrt{2}\pi n_{x'}}{N_{A,x'}}. \quad (16.137)$$

There has to be as many $c_{\mathbf{k}}$ operators as there c_i operators. Since there are $N_{A,x'}$ possible c_i -operators along a string in the x' direction, there also has to be $N_{A,x'}$ possible $k_{x'}$ values. It is customary to take $-N_{A,x'}/2 < n_{x'} < N_{A,x'}/2$ to allow for both positive and negative momenta, and thus

$$-\pi/\sqrt{2} < k_{x'} < \pi/\sqrt{2}. \quad (16.138)$$

Similarly for $k_{y'}$. The reduced, or magnetic Brillouin zone, is thus rotated $\pi/4$ compared to the original one and its size is $(\sqrt{2}\pi)^2 = 2\pi^2 = A_{\text{full BZ}}/2$.

Notice how the same reduced BZ is obtained for the lattice of unit cells if we choose unit cells as shown in Fig. 16.7(b). As noted above, it is possible to rewrite a summation over $\mathbf{k}$ in the full crystal lattice BZ ($\mathbf{k} \in \square$) as a summation over $\mathbf{k}$ in the reduced BZ ($\mathbf{k} \in \diamond$) by using a reciprocal lattice vector $\mathbf{G} = \frac{\pi}{a}(\hat{x} + \hat{y})$. We get in general

$$\sum_{\mathbf{k} \in \square} F(\mathbf{k}) = \sum_{\mathbf{k} \in \diamond} [F(\mathbf{k}) + F(\mathbf{k} + \mathbf{G})], \quad (16.139)$$

so long that $F(\mathbf{k})$ has a $2\pi/a$ -periodicity in each k_i -component. For instance, we could have $F(\mathbf{k}) = \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$. This can be verified by inspecting Fig. 16.7(c), since the $\mathbf{k}$ -values accessed in the full BZ of the crystal lattice when considering the quantity $\mathbf{k} + \mathbf{G}$ with $\mathbf{k} \in \diamond$ are precisely the

$\mathbf{k}$ -values outside the reduced BZ.

On the other hand, we note that $c_{\mathbf{k}\pm\mathbf{G}}^A = c_{\mathbf{k}}^A$ and $c_{\mathbf{k}\pm\mathbf{G}}^B = -c_{\mathbf{k}}^B$ since these objects are not $2\pi/a$ -periodic in momentum, as the fermion operators for a square lattice without antiferromagnetic ordering, but rather $\mathbf{G}$ -periodic. We will see why the minus sign appears for the B sublattices below.

Finally, we note that it might not be obvious at first glance that the allowed $\mathbf{k}$ -values in $\diamond$ are also allowed in $\square$. This property is required if Eq. (16.139) is to be valid. Let us therefore prove that this holds. First, consider the $\mathbf{k}$ -values in $\square$:

$$\begin{aligned} k_x &= \frac{2\pi n_x}{N_x a}, \quad n_x = -N_x/2, \dots, N_x/2 - 1, \\ k_y &= \frac{2\pi n_y}{N_y a}, \quad n_y = -N_y/2, \dots, N_y/2 - 1. \end{aligned} \quad (16.140)$$

For simplicity, we assumed N_x (the total number of lattice sites in the x -direction) and N_y to be even. Assume then that n_x, n_y is allowed to take values so that $\mathbf{k} \in \diamond$. If we add $\mathbf{G} = (\pi, \pi)/a$ to such a $\mathbf{k}$ -value, we obtain

$$\begin{aligned} k_x \rightarrow k_x &= \frac{2\pi n_x}{N_x a} + \frac{\pi}{a} \\ &= \frac{2\pi(n_x + N_x/2)}{N_x a} \\ &= \frac{2\pi n'}{N_x a} \end{aligned} \quad (16.141)$$

where $n' = n_x + N_x/2$ is a new integer, and thus it is a permitted $\mathbf{k}$ -value.

Finally, it is instructive to consider a few properties of what an electron-magnon interaction looks like in an antiferromagnet when Fourier-transforming to reciprocal space. Consider for instance the appendix of <https://arxiv.org/pdf/1903.01470.pdf>. One of the interaction terms is

$$H_{\text{int}} = J \sum_{i \in A} c_{i\alpha}^\dagger \sigma_{i,\alpha\beta} c_{i\beta} \mathbf{S}_i. \quad (16.142)$$

Let us consider how the z -component of this interaction would be written out in momentum-space. We have $\mathbf{S}_{i,z} = s - a_i^\dagger a_i$. It is sufficient to consider the constant contribution s in order to illustrate some important points. After inserting

$$\begin{aligned} c_{i\sigma} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \square} c_{\mathbf{k}\sigma} e^{-i\mathbf{k} \cdot \mathbf{r}_i} \\ &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \diamond} \left(c_{\mathbf{k}\sigma} e^{-i\mathbf{k} \cdot \mathbf{r}_i} + c_{\mathbf{k}+\mathbf{G},\sigma} e^{-i(\mathbf{k}+\mathbf{G}) \cdot \mathbf{r}_i} \right) \end{aligned} \quad (16.143)$$

with $\mathbf{G} = (\pi/a)(\hat{x} + \hat{y})$, we obtain (keeping only the z -component of the interaction)

$$\begin{aligned} H_{\text{int}} &= J \sum_{i \in A} i \in A \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}' \in \diamond} \sigma \left(c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_i} + c_{\mathbf{k}+\mathbf{G},\sigma}^\dagger c_{\mathbf{k}'+\mathbf{G},\sigma} e^{i(\mathbf{k}+\mathbf{G}-\mathbf{k}') \cdot \mathbf{r}_i} \right. \\ &\quad \left. + c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'+\mathbf{G},\sigma} e^{i(\mathbf{k}-\mathbf{k}'-\mathbf{G}) \cdot \mathbf{r}_i} + c_{\mathbf{k}+\mathbf{G},\sigma}^\dagger c_{\mathbf{k}'+\mathbf{G},\sigma} e^{i(\mathbf{k}+\mathbf{G}-\mathbf{k}') \cdot \mathbf{r}_i} \right). \end{aligned} \quad (16.144)$$

Since $\mathbf{k} \in \diamond$ are the allowed momenta in the reduced BZ, corresponding to a single real-space sublattice, we have that for $\mathbf{k}, \mathbf{k}' \in \diamond$:

$$\frac{1}{N_A} \sum_{i \in A} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_i} = \delta_{\mathbf{k}, \mathbf{k}'} \quad (16.145)$$

Note that adding a vector $\mathbf{G}$ in the exponent does not change anything: $\mathbf{G} \cdot \mathbf{r}_i = 2n\pi$ since $\mathbf{r}_i = 2n_x a \hat{\mathbf{x}} + 2n_y a \hat{\mathbf{y}}$ for sublattice points A. The same equation as above holds also if we replace $i \in A$ with $i \in B$. However, adding $\mathbf{G}$ now has an effect. Since the B sublattice is shifted compared to A with a vector $a\mathbf{x}$, we get

$$\frac{1}{N_B} \sum_{i \in B} e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{G}) \cdot \mathbf{r}_i} = \frac{1}{N_B} \sum_{i \in A} e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{G}) \cdot (\mathbf{r}_i + a\mathbf{x})} = -\delta_{\mathbf{k}, \mathbf{k}'} \quad (16.146)$$

due to $\mathbf{G} \cdot a\mathbf{x} = \pi$. This is because In this way, performing the summation over i in Eq. (16.144) to produce Kronecker delta-functions, and then performing the summation over $\mathbf{k}'$ to get rid of the Kronecker delta-functions, we are left with

$$H_{\text{int}} = J \sum_{\mathbf{k} \in \diamond} \sigma (c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}+\mathbf{G},\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{G},\sigma} + c_{\mathbf{k}+\mathbf{G},\sigma}^\dagger c_{\mathbf{k}+\mathbf{G},\sigma}). \quad (16.147)$$

Finally, we can convert the summation back to being over the full crystal BZ $\square$ by using Eq. (16.139) with $F(\mathbf{k}) = c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}+\mathbf{G},\sigma}^\dagger c_{\mathbf{k}\sigma}$:

$$H_{\text{int}} = J \sum_{\mathbf{k} \in \square} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}+\mathbf{G},\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (16.148)$$

where we used that $c_{\mathbf{k}+2\mathbf{G}} = c_{\mathbf{k}}$.

Coming back to the Fourier-transformed Hamiltonian we wrote down, diagonalization of the matrix yields two bands:

$$E_{\mathbf{k}} = \pm \sqrt{\epsilon_{\mathbf{k}}^2 + M^2} - \mu. \quad (16.149)$$

Consider the case $\mu = 0$. It is clear that the system is fully gapped and looks essentially like the quasiparticle spectrum of a superconductor. This is an antiferromagnetic insulator. However, letting μ be finite, we can now have an antiferromagnetic metal since it is possible to find a $\mathbf{k}$ which makes $E_{\mathbf{k}} = 0$. Note how μ enters in a different way than the superconducting excitation spectrum.

A self-consistent solution of the mean-field square lattice Hubbard model for antiferromagnetism provides precisely an antiferromagnetic insulator if μ is close to zero. The self-consistent solution does not give an antiferromagnetic metal for $\mu \neq 0$, but we can nevertheless *model* such a scenario by using the non-selfconsistent model above.

16.14.1 Details on how to derive Fourier-transform of sublattice operators

We provide some additional details of results that were used in the above section.

Consider a 1D lattice with alternating A and B atoms separated by a distance a . Let the first lattice point be an A atom and let origo be defined on this first lattice point. This means that we can write

the position vector of all A sublattice points as $r_i = (2i - 2)a$. In effect, the position vector of the first lattice point $i = 1$ in the A sublattice is $r_1 = 0$ (since it is the origo), while the second A sublattice point is $r_2 = 2a$, and so on. For the B sublattice, we have $r_i = (2i - 1)a$. Set $a = 1$ from now on.

If we did not distinguish between A and B sublattices, we would have written

$$c_i = \frac{1}{\sqrt{N}} \sum_{k \in \square} e^{ikr_i} c_k. \quad (16.150)$$

Now we have that

$$\begin{aligned} c_i^A &= \frac{1}{\sqrt{N}} \sum_{k \in \square} e^{ikr_i} c_k \\ &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} e^{ikr_i} (c_k + e^{i\pi r_i} c_{k+\pi}). \end{aligned} \quad (16.151)$$

Since $r_i = (2i - 2)$ for the A sublattice, the exponential factor inside the paranthesis is unity. Defining

$$c_k^A \equiv \frac{c_k + c_{k+\pi}}{\sqrt{2}} \quad (16.152)$$

we obtain the formula we used in the previous subsection

$$c_i^A = \frac{1}{\sqrt{N_A}} \sum_{k \in \diamond} e^{ikr_i} c_k^A \quad (16.153)$$

where we used that $N_A = N/2$.

For the B sublattice, the procedure is the same, but one difference is that $e^{i\pi r_i} = -1$ since $r_i = (2i - 1)$. Therefore, we get

$$c_i^B = \frac{1}{\sqrt{N_B}} \sum_{k \in \diamond} e^{ikr_i} c_k^B \quad (16.154)$$

where

$$c_k^B \equiv \frac{c_k - c_{k+\pi}}{\sqrt{2}}. \quad (16.155)$$

We then see that while $c_{k+\pi}^A = c_k^A$, we have $c_{k+\pi}^B = -c_k^B$, as commented on in the previous subsection. The extra minus sign thus comes from the fact that the B sublattice is shifted by a single lattice constant compared to the A sublattice.

Let us also briefly comment on how this can be used to express Fourier-transformed operators using a unit cell index notation, as in the paper on interface-induced magnetization in altermagnets with Erik and Pavlo. There, the Fourier-tarnsformation

$$c_{I,\alpha} = \frac{1}{\sqrt{N_{\text{uc}}}} \sum_k c_{k,\alpha} e^{ikr_I} \quad (16.156)$$

was used where N_{uc} is the number of unit cells, r_I is the coordinate to the I 'th unit cell. Let us prove this relation. We use the same 1D lattice as above. Here, α is the index labelling the atoms in the unit cell. Therefore, $\alpha = 1$ is the A sublattice and $\alpha = 2$ is the B sublattice. We put the origo of the coordinate system on the A atom in the first unit cell $I = 1$. We then have

$$c_{I,\alpha=1} = c_{i=2I-1} \text{ and } r_{i=2I-1} = (2I - 2). \quad (16.157)$$

Keep in mind we set $a = 1$. We get

$$c_{I,1} = \frac{1}{\sqrt{N}} \sum_{k \in \square} e^{ikr_{2I-1}} c_k. \quad (16.158)$$

All terms inside the summation are invariant under $k \rightarrow k + 2\pi$, hence we may write

$$\begin{aligned} c_{I,1} &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} (e^{ikr_{2I-1}} c_k + e^{i(k+\pi)r_{2I-1}} c_{k+\pi}) \\ &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} e^{ikr_{2I-1}} (c_k + e^{i\pi r_{2I-1}} c_{k+\pi}). \end{aligned} \quad (16.159)$$

But

$$e^{i\pi r_{2I-1}} = e^{i\pi(2I-2)} = 1. \quad (16.160)$$

Therefore,

$$\begin{aligned} c_{I,1} &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} e^{ikr_{2I-1}} (c_k + c_{k+\pi}) \\ &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} e^{ikR_I} (c_k + c_{k+\pi}) \\ &= \frac{1}{\sqrt{N_{\text{uc}}}} \sum_{k \in \diamond} e^{ikR_I} c_{k,1}. \end{aligned} \quad (16.161)$$

In the last line we defined the following quantities:

$$R_I \equiv r_{2I-1} \text{ (position of unit cell } I, \text{ defined as the position of atom A in unit cell } I). \quad (16.162)$$

and

$$c_{k,1} = (c_k + c_{k+\pi})/\sqrt{2}. \quad (16.163)$$

Let us now repeat this for the $c_{I,\alpha=2}$ operators. We have

$$c_{I,\alpha=2} = c_{i=2I} \text{ and } r_{i=2I} = (2I - 1). \quad (16.164)$$

One difference from the procedure for $\alpha = 1$ is that now

$$e^{i\pi r_{2I}} = e^{i\pi(2I-1)} = -1. \quad (16.165)$$

Therefore, we obtain (using that $r_{2I} = R_I + a$)

$$\begin{aligned}
 c_{I,2} &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} e^{ikr_{2I}} (c_k - c_{k+\pi}) \\
 &= \frac{1}{\sqrt{N}} \sum_{k \in \diamond} e^{ikR_I} e^{ika} (c_k - c_{k+\pi}) \\
 &= \frac{1}{\sqrt{N_{\text{uc}}}} \sum_{k \in \diamond} e^{ikR_I} c_{k,2}.
 \end{aligned} \tag{16.166}$$

In the last line we defined:

$$c_{k,2} = e^{ika} (c_k - c_{k+\pi}) / \sqrt{2}. \tag{16.167}$$

We have now derived that in general

$$c_{I,\alpha} = \frac{1}{\sqrt{N_{\text{uc}}}} \sum_{k \in \diamond} e^{ikR_I} c_{k,\alpha}. \tag{16.168}$$

16.14.2 AFM heterostructures and Fourier-transformation

Consider an compensated AFM interface as shown in Fig. 16.7(d). We now only have translational invariance in the y -direction and assume there are N_y lattice points in total along y . Therefore, we can only Fourier-transform in that direction and if we write fermion operators on each lattice point (without distinguishing between A and B sublattices), then we need $c_{i_x, i_y} = c_{i_x, i_y + N_y}$, which gives the usual condition

$$-\pi/a < k_y < \pi/a. \tag{16.169}$$

16.14.3 Continuum model and wavefunctions for eigenstates in AFM

This gives

$$H = \begin{pmatrix} -J - \mu & \gamma(\mathbf{k}) & 0 & 0 \\ \gamma(\mathbf{k}) & J - \mu & 0 & 0 \\ 0 & 0 & J - \mu & \gamma(\mathbf{k}) \\ 0 & 0 & \gamma(\mathbf{k}) & -J - \mu \end{pmatrix}, \quad \psi = \begin{pmatrix} \psi_{A\uparrow} \\ \psi_{B\uparrow} \\ \psi_{A\downarrow} \\ \psi_{B\downarrow} \end{pmatrix}. \tag{16.170}$$

For $\sigma = \uparrow$, we have the following eigenstates and eigenvalues:

$$\begin{aligned}
 E &= \sqrt{\gamma^2 + \mu^2} - \mu, \quad \psi = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \\ \sqrt{1 - \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \end{pmatrix}, \\
 E &= -\sqrt{\gamma^2 + \mu^2} - \mu, \quad \psi = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 - \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \\ -\sqrt{1 + \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \end{pmatrix}.
 \end{aligned} \tag{16.171}$$

For $\sigma = \downarrow$, we have the following eigenstates and eigenvalues:

$$\begin{aligned}
 E &= \sqrt{\gamma^2 + \mu^2} - \mu, \quad \psi = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 - \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \\ \sqrt{1 + \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \end{pmatrix}, \\
 E &= -\sqrt{\gamma^2 + \mu^2} - \mu, \quad \psi = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 + \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \\ -\sqrt{1 - \frac{J}{\gamma_{\mathbf{k}}^2 + J^2}} \end{pmatrix}.
 \end{aligned} \tag{16.172}$$

16.14.4 Superconducting proximity effect in antiferromagnets

A unique feature of the textbook AF/S bilayer (with a 2D G -type AF) is so-called Neel triplet pairing. This is a triplet pairing correlation that oscillates on an atomic scale, changing sign every time it advances one lattice site. This can be understood as follows.

The SC proximity effect induces correlations between k and $-k$ electrons in the AF conduction band. The presence of AF order allows for scattering between k and $k + Q$ with $Q = (\pi, \pi)/a$. Therefore, new correlations are formed between for instance k and $-k + Q$ electrons. Transforming a correlation function of the type $\sum_k \langle c_{k\uparrow} c_{-k+Q,\downarrow} \rangle$ to real space gives $\sum_i \langle c_{i\uparrow} c_{i\downarrow} (-1)^i \rangle$. This shows that the superconducting correlations change sign every other lattice site.

Now, does this happen for both singlet and triplet pairing? To answer this, let us first consider the following symmetry analysis. Singlet pairing must be even in M since it has no spin. Triplet pairing must be odd in the Neel order parameter M since it vanishes for $M = 0$ and inverting M is the same as flipping all spins. But flipping the sign of M is the same as interchanging sublattices A and B . Therefore, any singlet correlation (even- ω even-parity and odd- ω odd-parity) must be even in sublattice indices, hence of the type AA+BB or AB+BA, corresponding to pairing of the type ρ_0 or ρ_x in sublattice space. Similarly, any triplet correlation must be odd in sublattice index, hence of the type AB-BA or AA-BB, corresponding to ρ_y and ρ_z in sublattice space.

This means that any pairing that changes sign as we interchange sublattice, precisely such as the pairing between k and $-k + Q$, must be triplet. This is Neel triplet pairing. This can be viewed as interband pairing due to the band folding into the reduced BZ of the AF, see *e.g.* Fig. 2 in <https://arxiv.org/pdf/2408.11883>.

16.14.5 Decay of superconducting correlations in antiferromagnets and Q -scattering at antiferromagnetic interfaces

What about the decaying behavior of singlet and triplet correlations into an AFM that is in contact with a SC through an interface? In diffusive systems, both decay monotonically, as shown in the work by Fyhn *et al.* PRL 2023 and PRB 2023. In clean systems, only the singlets decay monotonically whereas the Neel triplets decay in an oscillatory fashion. Note that this oscillatory decay is of different origin than the atomic-scale oscillations of the Neel triplets: monitoring correlations on a single sublattice gives a homogeneous amplitude for the Neel triplets if translational symmetry is not broken by an interface.

The oscillatory decay of the triplets in an AFM/SC structure can be understood as follows. Consider Fig. 16.8. It shows the Brillouin zone for a unit cell in an antiferromagnet chosen as two lattice sites in the y -direction, since we are breaking translational invariance in the x -direction due to the SC interface. Due to the doubling of the unit cell in the y -direction (interface direction) compared to a square lattice, additional branches of the Fermi surface appear in the BZ. Now, although singlet pairing occurs for electrons at opposite sides of the Fermi-surface, we know that Neel triplet pairing occurs for electrons with a total momentum of (π, π) . This corresponds to 2-3 pairing in Fig. 16.8.

A few comments are in order to understand this. First of all, pairing between $-k$ and $k + Q$ with a single band existing in the full BZ (not the reduced) turns into pairing between $-k$ and k in the reduced BZ between states in two separate bands. This occurs due to the band-folding back

into the BZ for the reduced case. The point is then that the band-folding back into the BZ can give rise to an extra momentum shift δp between a state at k in one band and a state in the other band which corresponds to the state at $-k + Q$ which was folded back into the reduced BZ (and giving rise to an extra band). Whether or not this happens depends on if we confine our attention to electron forming pairs at exactly the same energy (as in Fig. 16.8) or if electrons at different energies are allowed to form pairs (as in Fig. 2 in Bobkova's review). If we only consider pairing between electrons at the same energy, an extra small momentum δp arises for such Neel triplet pairs, which in turn gives rise to an oscillatory decay since such a pair has finite momentum (like in a ferromagnet). We proceed to analyze this quantitatively below.

Interfaces with AFMs enable a new type of scattering at interfaces called Q -scattering. Consider an incident electron (p_{x1}, p_y) incoming toward the interface from the AF side. This is marked 1 in Fig. 16.8. For any scattering event, p_y is conserved. Due to the additional branches of the Fermi surface that appears in the reduced BZ, electron 1 can be reflected as electron 3. This is Q -reflection which is really a type of Umklapp scattering. It is present also without any superconductivity, i.e. AF/N interface.

Now, if proximity-induced pairing correlations exist between 1 and 2, then pairing is also established between 2 and 3. The finite momentum δp of this pair is obtained from the normal-state electron dispersion in the AF

$$E = \sqrt{M^2 + 4t^2(\cos p_x a + \cos p_y a + \cos p_z a)^2} - \mu \quad (16.173)$$

which gives

$$\delta p = \sqrt{\mu^2 - M^2} / (ta \sin p_x a) \quad (16.174)$$

The denominator is essentially the electron Fermi velocity at $\mu = M = 0$. In effect, this type of pairing correlation (2-3) will oscillate with a length $l_{\text{osc}} \propto 1/\sqrt{\mu^2 - M^2}$. The 2-3 pairing correlation has to be a Neel triplet, because it originates from pairing between a state at $-k$ and a state at $k + Q$ which when folded back into the reduced BZ looks like interband pairing with a momentum δp . In other words, transforming an interband Cooper pair with finite momentum δp (which is much smaller than Q) to real space should produce the atomic-scale sign-changing oscillation for this type of correlation. The Q -part of the momentum difference, which is not seen in the momentum indices of fermion operators in different bands that make up the Neel triplet correlator, should lie hidden in the way that these fermion-operators transform back into real space differently for different bands. The singlet correlations, on the other hand, simply decays monotonically. Hence, triplet and singlet correlations have different decay behavior inside an AF, in contrast to in a ferromagnet.

16.15 Umklapp scattering

Umklapp scattering in a crystal is a scattering process which results in a wavevector $\mathbf{k}$ that falls outside of the 1st BZ.

The basic distinction between normal (N) and Umklapp (U) scattering processes can be described as follows. In an N-process involving an electron with crystal momentum $\mathbf{k}_1$ scattering on a phonon $\mathbf{q}$ into a new electron state $\mathbf{k}_2$, one has crystal momentum conservation

$$\mathbf{k}_1 + \mathbf{q} = \mathbf{k}_2 \quad (16.175)$$

On the other hand, in an Umklapp scattering process, crystal momentum is not conserved and there is an additional non-zero reciprocal lattice vector $\mathbf{G}$ on the right-hand side

$$\mathbf{k}_1 + \mathbf{q} = \mathbf{k}_2 + \mathbf{G}. \quad (16.176)$$

As a result, the U process results in a scattered electron that has a momentum different than $\mathbf{k}_1 + \mathbf{q}$. The word "Umklapp" is a German term meaning "flip over". However, we note that $\mathbf{G}$ does not necessarily have to be collinear with $\mathbf{k}_1 + \mathbf{q}$. The "Umklapp" description of a scattering process is required for large momentum transfers if we want to operate solely within the 1st BZ.

Also, note that regardless of whether one has an N or U process, energy has to be conserved:

$$E(\mathbf{k}_1) + E_{\text{ph}}(\mathbf{q}) = E(\mathbf{k}_2), \quad (16.177)$$

since $E(\mathbf{k}) = E(\mathbf{k} + \mathbf{G})$ by definition.

Since wavevectors are only defined up to a reciprocal lattice vector $\mathbf{G}$ anyway, there is nothing unphysical about this. This is true both for electrons and phonons. The net mechanical momentum of a phonon is in fact zero, since a lattice vibration does not involve mass transfer to the lattice. This is especially transparent for a transverse phonon where the motion of the phonon is perpendicular to the wavevector.

What *is*, on the other hand, conserved only in the N process, and not the U process, is the reduced momentum which is defined within the primitive cell of the reciprocal lattice. Note that the definition of this primitive cell is usually chosen as the 1st BZ, but it does not have to be: even for the square lattice, there are many possible choices for the primitive reciprocal space unit cell. It is important to note that a different choice of the primitive cell can turn an N process into an U process and vice versa.

To look at a practical example of an Umklapp scattering process, consider a square lattice with an electron with $k_1 = 4\pi/5a$ scattering out of the 1st BZ $[-\pi/a, \pi/a)$ via a phonon with $q = 2\pi/5a$ to a state $k_2 = 6\pi/5a$. However, k_2 can now be folded back to the 1st BZ by writing

$$k_1 + q = k_2 + G \quad (16.178)$$

with a new $k_2 = -4\pi/5a$ and $G = 2\pi/a$ a reciprocal lattice vector on the square lattice. Note that since $E = -2t \cos(ka)$, we have (as announced) $E(6\pi/5a) = E(-4\pi/5a)$.

It should be noted that the distinction of N and U processes depends on which basic cell that is chosen of the reciprocal lattice: there is not one unique choice. The first BZ is one choice of primitive cell in reciprocal space, but it is not the only one. In effect, some N processes with one basic cell may be U processes if choosing a different basic cell. Therefore, one should not assign special physical meaning to N vs. U processes since their characterization depends on which choice we make for basic cell.

16.16 Altermagnetism

It is useful to start by considering the effect of PT symmetry (parity and time-reversal) on the band-structure $\epsilon(\mathbf{k}, \sigma)$ of a material. If we have spin-degeneracy, then $\epsilon(\mathbf{k}, \sigma) = \epsilon(\mathbf{k}, -\sigma)$. Since

$T\epsilon(\mathbf{k}, \sigma) = \epsilon(-\mathbf{k}, -\sigma)$ and $P\epsilon(\mathbf{k}, \sigma) = \epsilon(-\mathbf{k}, \sigma)$, we see that $PT\epsilon(\mathbf{k}, \sigma) = \epsilon(\mathbf{k}, -\sigma)$. Therefore, a system (crystal structure and belonging spin order) that has PT symmetry must be spin degenerate.

It is important to note that broken PT symmetry is a necessary but not sufficient requirement for lifting spin degeneracy. For instance, there might exist another type of operation O which when taken in combination with PT is a symmetry, so that PTO is a symmetry. If then O is such that $PTO = \epsilon(\mathbf{k}, -\sigma)$ (for instance if O is a lattice translation τ which does nothing with $\mathbf{k}$ or σ), then spin degeneracy is preserved.

Consider a square lattice with all spins pointing in the same direction. This is a ferromagnetic system. To perform the P operation (inversion), we have to choose a point in the crystal structure. The point is then that if we can find at least *one* point where the crystal structure and spin order has PT symmetry, the band structure must be spin degenerate. For the ferromagnetic case, T changes the direction of all spins. There is no point on the lattice we can choose to perform a P operation about which will turn the spins back to their original position. Thus, PT symmetry is broken and the band structure is non-degenerate: $\epsilon(\mathbf{k}, \uparrow) \neq \epsilon(\mathbf{k}, \downarrow)$.

Consider next a square lattice with alternating spins in every direction, in effect a conventional antiferromagnet. Time-reversal again inverts the direction of all spins. The effect of P is now different depending on point one chooses. If we choose a lattice site to perform inversion around, the system does not have PT symmetry and seemingly should not have a spin degenerate band structure. However, it is known that the bands in such an antiferromagnet are spin degenerate. This is because we *can* find a point where P cancels the effect of T , namely a point in between two lattice sites. Performing P around such a point swaps the two spins and thus cancels the effect of time-reversal. The system thus has PT symmetry, which explains why the bands are spin degenerate.

A point which might cause confusion is that a square lattice antiferromagnet could also be said to have inversion symmetry, since the P operation applied around any lattice point leaves the system invariant. So the system is said to be inversion symmetric if we can find at least one point where P is a symmetry.

Now consider an altermagnet. We examine two models for this, shown in Fig. 16.10. In the left figure, the hopping constant in x and y direction is different for spin- $\uparrow$ and $\downarrow$ particles. Performing time-reversal interchanges spin- $\uparrow$ and spin- $\downarrow$ particles, or equivalently lets $m \rightarrow (-m)$. Coming now to the P operation, we see that it is impossible to choose a point around which to apply P that causes the spin-dependent hoppings to be swapped back to their original position. Therefore, PT symmetry is broken in this model. To visualize this more clearly in real space, one can think of the spin-dependent hoppings as wavy lines with a certain color between the atoms and then apply P symmetry.

In the right figure, we see that it is the extra non-magnetic atom which causes PT symmetry to be broken. Applying T inverts all spins. Applying P around any lattice point is a symmetry operation. Thus, PT symmetry is broken if one chooses any lattice point. Now, if we choose an arbitrary point (in empty space, such as the middle of the unit cell), then P symmetry is lost. Since one then neither has P or T symmetry, one could in principle still have PT symmetry. However, actually applying these operations when choosing any point in the lattice is seen to not restore the starting point. Thus, PT symmetry is broken, and spin degeneracy is lifted.

Note that whenever spin-orbit coupling (SOC) is disregarded, we also have spin rotational symmetry. This means that for any magnet with collinear spin ordering, spin rotation R can always cancel the effect of time-reversal T , by rotating the spins back. Thus, for collinear magnets, RT is a symmetry. This means that $RT\epsilon(\mathbf{k}, \sigma) = \epsilon(-\mathbf{k}, \sigma)$ must equal $\epsilon(\mathbf{k}, \sigma)$. Thus, collinear magnets without SOC have RT symmetry, but they can still lack PT symmetry. In such a case, the spin-splitting must be symmetric according to $\epsilon(\mathbf{k}, \sigma) = \epsilon(-\mathbf{k}, \sigma)$. This is the case in inversion-symmetric altermagnets, meaning that the band structure must therefore be even in $\mathbf{k}$.

Note that τ can also be part of a symmetry operation, for instance in a magnon altermagnet paper stating that $PT\tau$ -broken symmetry lifts spin degeneracy in the eigenstates where τ is half-unit cell lattice translation. Depending on the direction in which τ is applied, this could exchange sublattices of the localized spin moments in the lattice.

16.17 p -wave magnetism

Antisymmetric-in-momentum spin polarization for itinerant electrons due to magnetism is closely related to helimagnetism, and in fact occurs for any rotation period (see results by Erik Hodt). It was also discussed in more general grounds for $T\tau$ symmetric systems by Hellenes et al. in 2023. The simplest effective model describing such a polarization is a Rashba-like model with a term $\alpha k_x \sigma_z$ in addition to kinetic energy and chemical potential. However, such a model would yield fully spin polarized bands and neglect spin-flip scattering between the bands. However, in the actual magnetic lattice system hosting a p -wave spin polarization the localized spins will be non-collinear and spin-flip processes will thus be inevitable. The Rashba-like model does not account for this, whereas our model does.

Other differences:

- Our model was motivated by magnets with noncollinear spin texture (see v2 of Hellenes paper). There, there is a single Fermi surface with a nontrivial spin texture. The Rashba-like model gives a two-band fully spin-polarized model - however, it could make sense as an effective low-energy model for our model with strong inter-sectoral hopping. This still has to be proven.
- As for differences in transport, the two-band model (aka Tanaka model) does not allow for spin filtering in the longitudinal direction. In the bulk, there is no anisotropy of the electric current (first-order response) and the second-order response vanishes. This model seems to have additional (accidental) symmetries that preclude several effects.
- The underlying physics providing our effective model, including the $T\tau$ -symmetry, is very evident from our case. It demonstrates how our model is tailored to p -wave magnets.
- The partial spin-polarization reflects the non-collinearity of p -wave magnets.
- The Rashba model, in contrast to our model, is already thoroughly studied. This makes it more difficult to write high-impact papers. This point was important to us.

One could ask: is it possible to get p -wave magnetism from collinear magnetism? A p -wave magnet has a band-structure that satisfies:

$$\epsilon(\mathbf{k}, \sigma) = \epsilon(-\mathbf{k}, -\sigma) \quad (16.179)$$

while simultaneously having broken PT -symmetry so that spin states at a fixed $\mathbf{k}$ are not degenerate. However, as we remarked above, collinear magnets always have RT symmetry. Here, R is specifically $C_{2,\perp}$ where the $\perp$ axis is perpendicular to the collinear direction of the spins. Note that the $SU(2)$ representation of a C_2 operation would be a matrix providing a rotation angle of 360 degrees, in order to flip the spin. Due to the RT -symmetry, it follows that $E(\mathbf{k}, \sigma) = E(\mathbf{k}, -\sigma)$. But if the magnet is to be p -wave, then combining this relation with the p -wave relation gives $E(\mathbf{k}, \sigma) = E(\mathbf{k}, -\sigma)$, thus contradicting spin degeneracy. Hence, p -wave magnets must be non-collinear.

16.18 Spin glass, spin ice, spin liquid

Paramagnetic phase:

$$\langle \mathbf{S}_i \rangle = 0, \quad M \equiv \frac{1}{N} \sum_i \langle \mathbf{S}_i \rangle = 0. \quad (16.180)$$

Spin-glass phase:

$$\langle \mathbf{S}_i \rangle \neq 0, \quad M \equiv \frac{1}{N} \sum_i \langle \mathbf{S}_i \rangle = 0. \quad (16.181)$$

The order parameter for the spin-glass phase is, since the spin on each site is finite:

$$q \equiv \frac{1}{N} \sum_i \langle \mathbf{S}_i \rangle^2 \neq 0. \quad (16.182)$$

In the spin glass, the spins freeze in random orientations on each site. This can be quantified using the temporal autocorrelation function

$$C(t) \equiv \frac{1}{N} \sum_i \langle \mathbf{S}_i(t) \mathbf{S}_i(0) \rangle. \quad (16.183)$$

For a spin glass, one then has

$$C(t) \Big|_{t \rightarrow \infty} = \frac{1}{N} \sum_i \langle \mathbf{S}_i \rangle^2 = q. \quad (16.184)$$

In contrast, in a spin liquid, the spins do not freeze but continue to change as t increases. Thus, the spin liquid still has strong quantum fluctuations whereas the spin glass does not. Neither spin glass or spin liquid has long range order at $T = 0$. The spin liquid is not a paramagnet, however, since it develops short-range spin-spin correlations.

The simplest model which shows a spin glass transition is an Ising model with random couplings J_{ij} . The actual ground state will be difficult to determine as there are many metastable states - just like in regular glass.

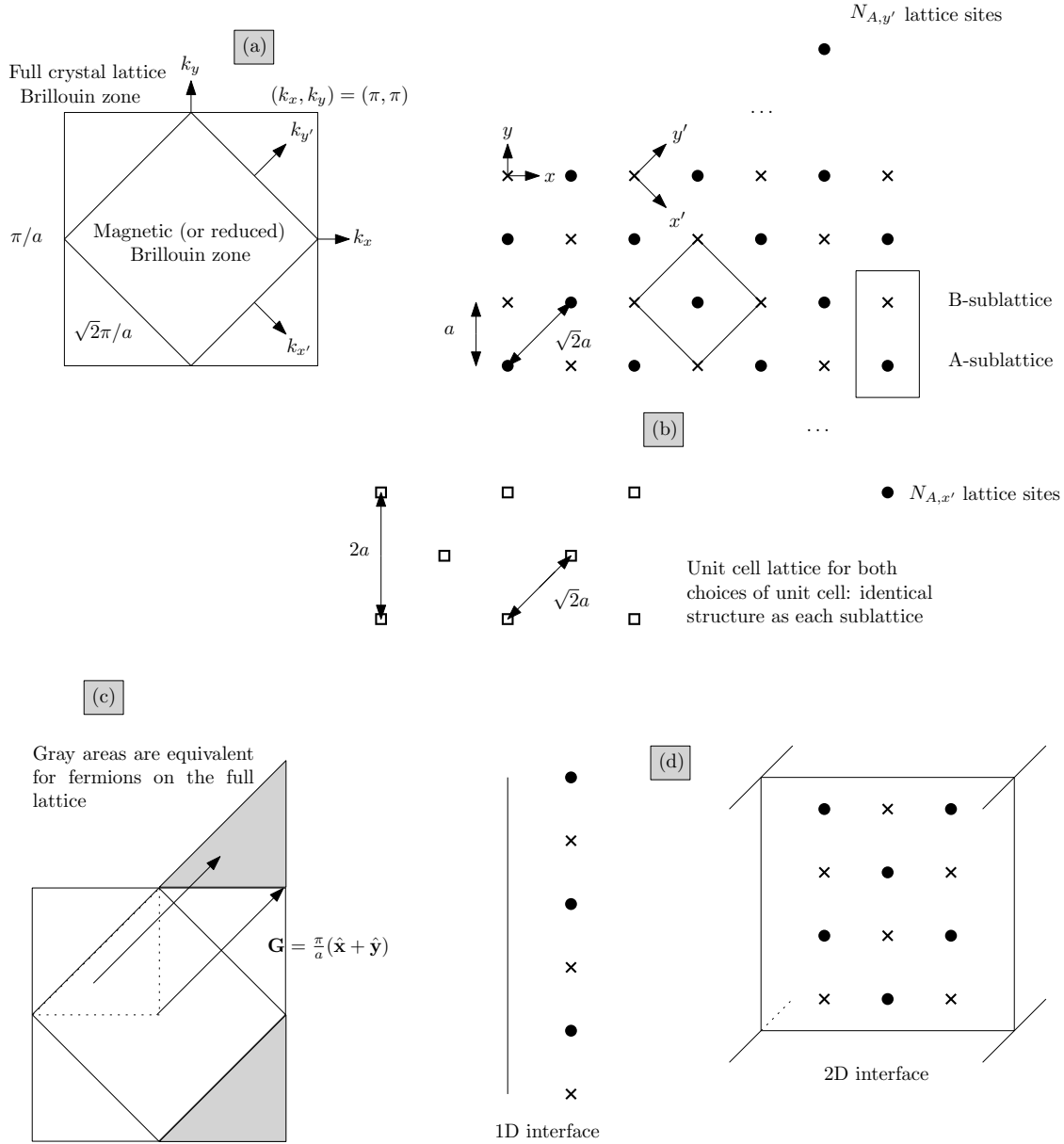


Figure 16.7: (Color online) (a) Brillouin zone for the full crystal lattice (including both A and B sublattices) and the magnetic (or reduced) Brillouin zone for each sublattice. These are the allowed, independent $\mathbf{k}$ -values operators on the corresponding lattices can take. (b) The real-space square lattice comprised of an A and B sublattice. Periodic boundary conditions along the y' and x' directions gives a different set of k -values (and thus different BZ) than for a regular square lattice. Two different choices for unit cell are shown, but both choices have the same unit cell lattice structure: in fact, it is the same as the sublattice structures. (c) For a square lattice BZ, the momenta are periodic with periodicity given by the reciprocal lattice vector $2\pi/a$ in $\pm\hat{x}$ or $\pm\hat{y}$ direction. For the sublattice BZ, the momenta are periodic with periodicity given by the reciprocal lattice vector $2\pi/\sqrt{2}a$ in the $\pm(\hat{x} + \hat{y})/2$ and $\pm(\hat{x} - \hat{y})/2$ directions. This allows us to map out the entire BZ of the full crystal lattice by using the BZ of the sublattice structure *and* a $\mathbf{G}$ -vector. (d) Two possible types of interfaces for AFM/X heterostructures: the 1D case has translational invariance along the y -direction, whereas the 2D case has translational invariance in the yz -plane. The direction normal to the interface is x in both cases.

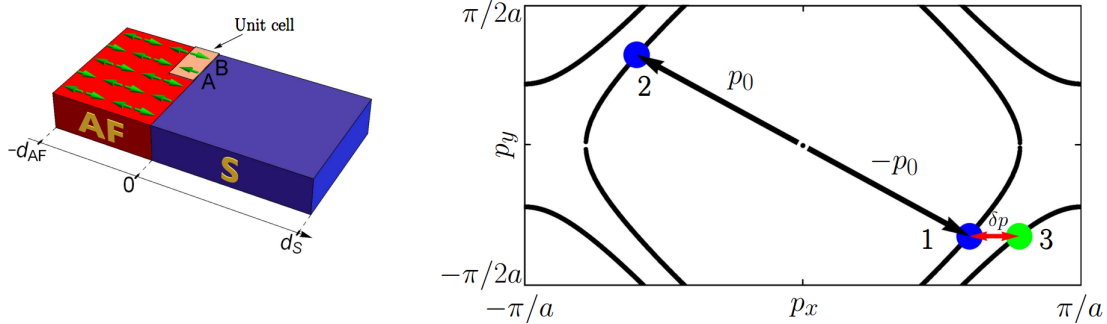


Figure 16.8: Left: S/AF interface and choice of unit cell. Right: BZ and Fermi surface (black curves) of the AF layer. Zero-momentum Cooper pair between electrons 1 and 2 is schematically shown by black arrows. There is also Neel-type finite-momentum triplet pairing between electrons 2 and 3, which is produced from electron 1 due to the Umklapp reflection process from the AF/S interface, see text for details. The total momentum of the pair (2,3) δp is shown by the red arrow.

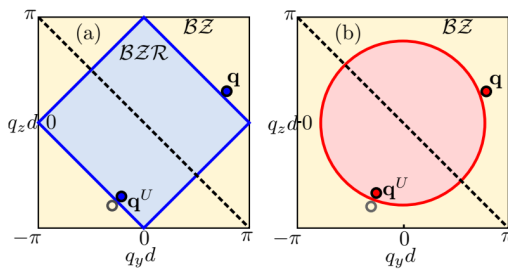


FIG. 3. (Color online) Fermi surfaces for (a) the tight-binding model (blue) and (b) the quadratic model (red). The Brillouin zone of the conduction electrons ($\mathcal{BZ}$) is shown in yellow. The reduced (magnon) Brillouin zone ($\mathcal{BZR}$) corresponds to the interior of the Fermi surface of the tight-binding model (light blue). The Umklapp momentum $\mathbf{q}^U$ is related to $\mathbf{q}$ by a reflection across the diagonal of the $\mathcal{BZ}$ (dashed line) and a subsequent reflection in the Fermi surface.

The momenta ($\mathbf{q}$) of the conduction electrons reside in the Brillouin zone, $\mathcal{BZ}$, of the lattice of the NM. By contrast, the magnon momenta ($\mathbf{k}$) are defined in the reduced Brillouin zone of the sublattices, $\mathcal{BZR}$; see Fig. 3 (a). At half-filling, the $\mathcal{BZR}$ matches the interior of the Fermi surface of the tight-binding model.

$$\mathbf{q}^U = \mathbf{q} + \mathbf{q}_{AF} \text{ with } \mathbf{q}_{AF} = (\hat{y} + \hat{z})\pi/d$$

In the electronic tight-binding model at half-filling, the Umklapp process $\mathbf{q} \rightarrow \mathbf{q}^U$ can be split into two steps; see Fig. 3 (a). First, there is a reflection across one of the diagonals of the full Brillouin zone ($\mathcal{BZ}$). Second, there is a reflection across the Fermi surface. The second reflection occurs at the surface parallel to the diagonal of the first reflection. For initial states on the Fermi surface, an Umklapp process takes a state $\mathbf{k}$ to another state $\mathbf{k}^U$ that is also on the Fermi surface.

Figure 16.9: (Color online) Illustration of Umklapp scattering in a square antiferromagnet.

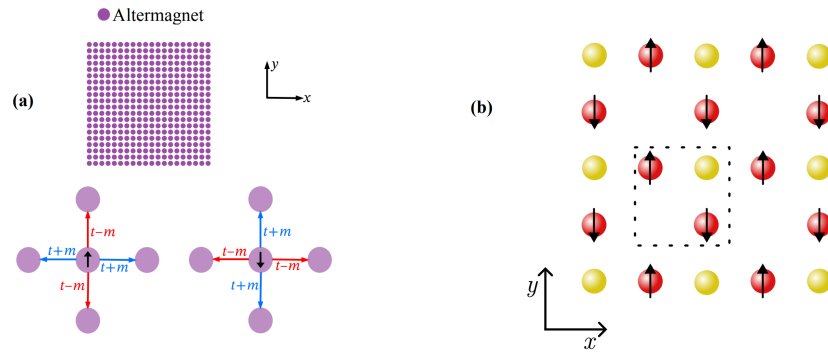


Figure 16.10: (Color online) (a) Simplified lattice structure with spin-dependent hopping reproducing the altermagnetic band structure. (b) More realistic lattice structure for altermagnet where the correct band structure emerges from considering isotropic hopping and local exchange interaction. Each lattice site in (a) can be considered as a unit cell in (b): it is seen that in (b), it will be easier for a $\uparrow$ electron to jump left or right since such spins are favored on the left and right parts of the unit cell, whereas $\downarrow$ electrons have an easier time jumping up or down from the non-magnetic atom at the top or bottom of the unit cell since such spins are favored at the atom they are jumping to.

Chapter 17

Ferroelectric and multiferroic materials

17.1 Ferroelectricity

It is important to emphasize that the magnetic dipole-dipole interaction is too weak to provide an appreciable Curie-temperature in the ferromagnet case. As we saw in the previous chapter, the underlying physical mechanism for spontaneous magnetization is the exchange interaction resulting from an interplay between Coulomb repulsion and the Pauli principle with respect to the spins of the electrons.

In contrast, the electric dipole-dipole interaction can in some cases be responsible for ferroelectricity [2]: the spontaneous electric polarization that may arise in certain types of materials (typical examples include BaTiO_3 , PbTiO_3). This phenomenon was discovered in 1920 and it is interesting to note that the word "ferro" is included due to its formal resemblance to the phenomenon of ferromagnetism despite the fact that ferroelectric materials rarely actually contain iron. Another key mechanism for establishing ferroelectric order is a structural phase transition where the lattice rearranges itself in a way that produces a spontaneous electric polarization. In the 1960s, the soft-mode concept was introduced to describe the mechanism of the ferroelectric structural phase transition. This idea was based on the assumption that the crystal is rendered unstable against a particular normal vibration of the lattice: a soft phonon-mode. This soft-mode exists in the disordered high-temperature phase, and its frequency goes down as the temperature approaches T_c (the phonon "softens"), becoming zero at $T = T_c$. When this happens, the corresponding vibration (or the atomic positions) become "frozen" at this temperature and produce a structure with another symmetry hosting a finite dipole moment.

17.2 Multiferroic materials

We follow here the exposition given in Ref. [8]. Let us address how it is possible that magnetic ordering can induce ferroelectricity. We focus here on multiferroic materials that have a centrosymmetric crystal structure. This means that the free energy describing the system must have both time-reversal and inversion symmetry. As we will explain more detail below, what happens is that time-reversal symmetry is spontaneously broken due to the formation of (inhomogeneous) magnetic order at some temperature T_m . At a lower temperature, inversion symmetry is also *spontaneously* (not explicitly) broken at lower temperature $T_p < T_m$ due to the formation of an electric polarization

resulting from a lattice distortion. The manner in which electric polarization and magnetization are allowed to couple to each other is determined by the symmetries of these order parameters. The electric polarization $\mathbf{P}$ and electric field $\mathbf{E}$ both change sign upon inversion, $\mathbf{r} \rightarrow -\mathbf{r}$, but are invariant upon time reversal $t \rightarrow -t$. The magnetization $\mathbf{M}$ and magnetic field $\mathbf{H}$ behave in the opposite manner: time reversal causes them to change sign, but spatial inversion leaves them unchanged. If the system (Hamiltonian) under consideration does not break either of these symmetries explicitly, any coupling between $(\mathbf{P}, \mathbf{E})$ and $(\mathbf{M}, \mathbf{H})$ must respect these symmetries. Note that the linear coupling between these quantities as described in Maxwell's equations is only possible when they vary both in space and in time. For instance, spatial derivatives of $\mathbf{E}$ are proportional to the time derivative of $\mathbf{H}$ and vice versa.

Static $\mathbf{P}$ and $\mathbf{M}$ can thus only be coupled nonlinearly. This can occur physically due to an interplay of charge, spin, orbital, and lattice degrees of freedom and is generically present in solids, albeit weak. Whether or not it can actually induce an electric polarization in a magnetically ordered state depends on its specific form. A small energy gain of the form $-P^2 M^2$ does not induce ferroelectricity since it is overcompensated by the energy cost associated with a polar lattice distortion which goes like $+P^2$. The fourth-order term nevertheless accounts for small changes in the dielectric constant below magnetic transitions in *e.g.* YMnO_3 and BiMnO_3 .

If the magnetic ordering is inhomogeneous, $\mathbf{M} = \mathbf{M}(\mathbf{r})$, the situation becomes more interesting. Now, third-order coupling terms of the type $P\mathbf{M}\partial\mathbf{M}$ are allowed since such a term is invariant both under time-reversal and parity. Since this is linear in P , it is sufficient with an arbitrarily weak interaction of this type to generate electric polarization as soon as the proper magnetic ordering $\mathbf{M}(\mathbf{r})$ is established. For cubic crystals, one obtains the following allowed form of the magnetically induced electric polarization:

$$\mathbf{P} \propto (\mathbf{M} \cdot \nabla)\mathbf{M} - \mathbf{M}(\nabla \cdot \mathbf{M}). \quad (17.1)$$

Frustration can play a key role in terms of creating spatial variations of the magnetization that, in turn, generate $\mathbf{P}$. For example, a spin chain with a ferromagnetic interaction $J < 0$ between n.n. has a uniform ground-state with all spins being parallel. However, if one introduces an antiferromagnetic next-n.n. interaction $J' > 0$, this simple ordering becomes frustrated and, when sufficiently strong, stabilizes a spiral magnetic state of the type

$$\mathbf{M} = M_0[\mathbf{e}_1 \cos(Qx) + \mathbf{e}_2 \sin(Qx)]. \quad (17.2)$$

Here, $\mathbf{e}_i$ are two orthogonal unit vectors and the wavevector Q is given by

$$\cos(Q/2) = -J'/(4J). \quad (17.3)$$

Magnetic ordering spontaneously breaks time-reversal symmetry. However, a magnetic spiral (with proper spatial profile) also breaks inversion symmetry since the change of the sign of all coordinates also inverts the direction of the rotation of the spins in the spiral. This fact allows for the presence of an electric polarization, which also is inversion symmetry breaking, and which sign is coupled to the direction of spin rotation.

Note that whether or not an electric polarization appears depends both on the dimensionality of the system and on the exact form of the inhomogeneous magnetic texture. For instance, cycloidal textures where the magnetization has a component along the texture give different results from helical textures that rotate in a plane perpendicular to the direction along which the texture varies. It

is for instance possible to have a metallic state in the xy -plane if the magnetic texture has a spatial dependence that produces an electric polarization out-of-plane, as has been experimentally verified in certain ferroelectric materials like WTe_2 (these are without any magnetic ordering, though). More details regarding which polarization that specific textures produce can be found in an email exchange with Pavlo from November 2024. For instance, a set of N copies (along the y -direction) of helical chains extending in the x -direction produce no electric polarization.

But what is the microscopic mechanism behind the appearance of ferroelectricity in a magnetically inhomogeneous environment? A plausible mechanism inducing ferroelectricity in a magnetic spiral was discussed in Refs. [9] and [10]. The basic ingredient is the *inverse DM mechanism*. Let us define what this is:

- **DM mechanism:** in a system where inversion symmetry is explicitly broken in its ground-state, DM-interactions exist which in general tend to create inhomogeneous magnetic order.
- **Inverse DM mechanism:** in a system with inhomogeneous magnetic order, inversion symmetry can become spontaneously broken in the ground-state via a lattice distortion if the resulting DM-interaction energy gain is larger than the energy loss associated with distorting the lattice.

Going back to the above discussion about T_m and T_p , the inhomogeneous magnetic ordering is responsible for inducing a distortion in the lattice and thus spontaneously breaking inversion symmetry in the following way. For $T < T_p$, the energy loss of distorting the lattice by pushing a ligand atom in some direction is compensated by the energy gain of having a superexchange between two spins mediated by this ligand atom via the DM interaction. Now, the direction this ligand atom is pushed in is not unique: it might as well have been pushed in another direction. The free energy describing the system must remain invariant under inversion symmetry, but the ground-state that is realized spontaneously breaks this symmetry. The origin of the spontaneous inversion symmetry breaking is thus the presence of inhomogeneous magnetic order and the DM interaction. Note that not any type of magnetic inhomogeneous texture is sufficient to create the polarization: it must have a specific form.

The antisymmetric DM interaction is $\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$ where $\mathbf{D}$ is the Dzyaloshinskii-vector. This is a relativistic correction to the usual superexchange which arises when spin-orbit coupling is present. The DM interaction generally favors non-collinear spin ordering. Now, ferroelectricity induced by spiral magnetic ordering results from lattice relaxation in a magnetically ordered state and can be understood as follows. The exchange between spins of transition metal ions are usually mediated by ligands, for instance oxygen ions, which form bonds between pairs of ions (see our previous treatment of DM-interaction for a picture: the ions typically form a triangle). The energy of the DM interaction increases with the separation distance $\mathbf{x}$ between the oxygen ion and the line connecting the pairs of spins. This can also be thought of as a measure of the degree of inversion symmetry breaking at the oxygen site.

Assume now that a spiral magnetic state exists. Since in a spiral state the vector product $\mathbf{S}_i \times \mathbf{S}_j$ has the same sign for all pairs of neighboring spins, the DM interaction thus effectively tries to push the negative oxygen ions in one direction perpendicular to the spin chain formed by positive magnetic ions (along $\mathbf{x}$). The system gains energy through the DM interaction $\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$ by displacing the ions. This corresponds to a net distortion of the charge polarization (since the negative oxygen ions are pushed into the same direction) and thus induces an electric polarization.

Note that this argument depends on the *spiral* pattern (since we need $\mathbf{S}_i \times \mathbf{S}_j$ to be in the same direction for all $\{i,j\}$): other types of inhomogeneous magnetic ordering, such as certain types of domain walls, do not induce ferroelectricity.

17.3 Scattering of magnons

There are two particular scattering processes involving magnons that are of importance when it comes to transport in magnetic structures.

Magnon-electron scattering: this coupling occurs via the spin degree of freedom of these particles. Itinerant electrons couple to localized moments via the $s - d$ interaction (typical $\mathbf{J} \mathbf{s} \cdot \mathbf{S}$ Hamiltonian), so that when magnons are created, which perturb the spin moments $\mathbf{S}$ of the localized d electrons, this couples to the spin $\mathbf{s}$ of the itinerant electrons.

Magnon-phonon scattering: while magnons carry spin, longitudinal phonons are spinless. There can nevertheless exist an effective interaction between them in the following manner. A displacement of the ions via phonons alters the magnetic landscape that magnons propagate through, since the distribution of the localized ion spins $\mathbf{S}$ becomes different. A perturbation of these spins $\mathbf{S}$, in effect a magnon excitation, will thus change since *e.g.* the distance between the spins is altered. Formally, the *spin-orbit interaction* can cause a coupling between magnons and phonons. A magnon spin couples to a localized atom with net spin due to spin-orbit interaction: the magnon sees a circulating non-zero effective charge if it passes close enough by (sufficiently far away, the magnon sees no net charge on the atom since the atom is neutral), which in turn creates a magnetic field that couples to its spin. In that way, the magnon also acts with a force on the atom which in turn provides phonons.

Note that transverse phonons carry spin 1 because they are polarized unlike a longitudinal phonon which has no polarization (it oscillates in the same direction as it moves). Even if the phonon dispersion is linear in some part of the BZ, its effective mass being zero is not a Lorentz-invariant property and thus one would expect a transverse phonon to have three spin polarization projections (unlike the two projections of the massless photon).

Chapter 18

Spin-orbit interactions

18.1 Classification

Spin-orbit interactions come from the coupling between the spin and the orbital motion of electrons around the atoms (or impurity atoms) in a material. Broadly, one may distinguish between intrinsic and extrinsic spin-orbit interactions. First, we briefly review some basic considerations on atomic SOC.

18.1.1 Intrinsic spin-orbit coupling

At the interface between two different materials or at the surface of a material terminated by vacuum (thin films), inversion symmetry is broken locally for the few atomic layers closest to the interface/surface. This is clear since the electric potential energy satisfies $V(\mathbf{r}) \neq V(-\mathbf{r})$ there. In effect, the *structure* itself breaks inversion symmetry. The inversion asymmetry may be characterized to lowest order by an effective constant electric field $\mathbf{E}$ by Taylor-expanding the potential:

$$V(\mathbf{r}) = V_0 + \partial V / \partial r \cdot \mathbf{r} + \dots = V_0 - q\mathbf{E} \cdot \mathbf{r} + \dots \quad (18.1)$$

where q is the charge of the particle feeling the potential. Such a term $\mathbf{E}$ is for instance not present in a centrosymmetric lattice (such as a square lattice) where $V(\mathbf{r}) = V(-\mathbf{r})$ assuming $\mathbf{r} = 0$ is at the center of a unit cell. As soon as such an $\mathbf{E}$ field exists, it is clear that spin-orbit interactions come into play and this ultimately gives rise to the Rashba model. Note that gradients in the crystal potential exists even in a centrosymmetric lattice, but since such a potential has even parity there can be no effective electric field term in its Taylor-expansion, as above.

This is the intuitive picture, albeit highly simplified. Although it is clear that the electric potential must be locally inversion asymmetric and thus have a gradient near interfaces/surfaces, the expectation value $\langle \mathbf{E} \rangle$ of the electric field in the direction of broken inversion symmetry should vanish for bound states. For instance, $\langle \mathbf{E}_z \rangle$ experienced by a state bound to the xy -plane of a 2DEG should be vanishing by virtue of Ehrenfest's theorem since there is no net force or motion in the z -direction. Moreover, we certainly cannot be dealing with a constant macroscopic electric field which gives rise to a net current in equilibrium. A very detailed calculation (see Winkler, 2003) shows that the spin-orbit coupling in the band structure arising from structural inversion asymmetry does not come from the average electric field $\langle \mathbf{E} \rangle$ near the interface, but that it still exists because of the locally inversion asymmetric potential and the existence of atomic spin-orbit interaction. In effect, it is not the average electric field near the interface which provides the (dominant) contribution to Rashba spin-orbit coupling. For instance, in semiconductors it can be shown that the effective

electric field giving rise to a Rashba-type spin-orbit coupling in the conduction band is the electric field coming from the valence band because of a hybridization that exists between the conduction and valence band (tunneling between them). Such a detailed treatment is given in the textbook by Winkler from 2003.

Asymmetric spin-orbit interactions such as Rashba-coupling exists because of *both* inversion asymmetry in the potential and atomic spin-orbit interactions. A simple picture accounting for this is that the inversion asymmetric potential produces an effective local electric field which allows the electron spins to couple to it, but it should be kept in mind that the expectation value of the total field may well vanish despite that Rashba interactions survive - only a detailed microscopic calculation clearly demonstrates the reason for this, including the asymmetry of the resulting electron wavefunction near the interface.

There are two commonly used ways to derive the Rashba interaction in the literature. One way is to use $\mathbf{k} \cdot \mathbf{p}$ theory for semiconductors, including atomic spin-orbit interactions for a model with multiple orbitals, and then including an additional inversion-symmetry breaking potential $V = Ez$. By a Löwdin partition of the Hamiltonian (similar to a Schrieffer-Wolff transformation), one can derive an effective Hamiltonian for the conduction band in the semiconductor (so-called downfolding of a large 8×8 matrix describing the Hamiltonian in an original orbital basis $[s_{\uparrow}, s_{\downarrow}, p_{z,\uparrow}, p_{z,\downarrow}, p_{y,\uparrow}, \dots]$). This effective Hamiltonian then has a Rashba term with a coefficient that is proportional to both the strength of the atomic spin-orbit coupling ($\alpha \mathbf{L} \cdot \mathbf{S}$) and the symmetry breaking potential parameter E . This is a quite lengthy calculation.

The other way is to use a tight-binding model [63, 64] on a lattice which includes nearest neighbor hopping, atomic spin-orbit coupling, and a symmetry breaking term Ez that enables couplings between orbitals that otherwise have vanishing matrix elements, such as $\langle p_z | H | p_{x,y} \rangle$ if H does not contain the inversion symmetry breaking term. By writing down the full Hamiltonian and then performing a unitary transformation of it (which does not change its eigenvalues) so that it becomes block-diagonal, one obtains an effective theory for one of the bands to any desired order in the off-diagonal part (which includes the atomic spin-orbit coupling). An example of how this can be done in practice is shown in Appendix B in Ref. [68]. We also give a concrete example below.

Model calculation for Löwdin partitioning

Consider the surface states of Au(111) in Ref. [64] which are described by a Hamiltonian

$$H_0 = \sum_{\alpha\beta\sigma\sigma'ij} t_{\alpha\beta ij} \delta_{\sigma\sigma'} c_{\alpha\sigma i}^\dagger c_{\beta\sigma' j} \quad (18.2)$$

in a basis

$$\phi_i = \begin{pmatrix} c_{p_x \uparrow i} \\ c_{p_x \downarrow i} \\ c_{p_y \uparrow i} \\ c_{p_y \downarrow i} \\ c_{p_z \uparrow i} \\ c_{p_z \downarrow i} \end{pmatrix}, \quad (18.3)$$

which may be compactly written as

$$H = \sum_{ij} \phi_j^\dagger M \phi_i, \quad M = \begin{pmatrix} WX_{ij} + \delta Y_{ij} & 0 & 0 & 0 & \gamma\delta_{ij} & 0 \\ 0 & WX_{ij} + \delta Y_{ij} & 0 & 0 & 0 & \gamma\delta_{ij} \\ 0 & 0 & WY_{ij} - \delta X_{ij} & 0 & \gamma\delta_{ij} & 0 \\ 0 & 0 & 0 & WY_{ij} - \delta X_{ij} & 0 & \gamma\delta_{ij} \\ \gamma\delta_{ij} & 0 & \gamma\delta_{ij} & 0 - \delta(X_{ij} + Y_{ij}) & 0 & 0 \\ 0 & \gamma\delta_{ij} & 0 & \gamma\delta_{ij} & 0 & -\delta(X_{ij} + Y_{ij}) \end{pmatrix}. \quad (18.4)$$

Here, we omitted nearest-neighbor hybridization matrix elements induced by Ez for simplicity: the onsite contribution is sufficient to show a spin-flip type of interaction in the effective Hamiltonian for the conduction band, albeit it does not have precisely a Rashba form. Moreover, we used the following overlap matrix elements for nearest neighbor sites (i, j) on a square lattice:

$$t_{\alpha\beta ij} = \begin{cases} w \cos^2(\theta_{ij} + \delta \sin^2(\theta_{ij})) \text{ for } (\alpha, \beta) = (x, x) \\ (w + \delta) \cos(\theta_{ij}) \sin(\theta_{ij}) \text{ for } (\alpha, \beta) = (x, y) \text{ or } (y, x) \\ w \sin^2(\theta_{ij}) - \delta \cos^2(\theta_{ij}) \text{ for } (\alpha, \beta) = (y, y) \\ \gamma \cos(\theta_{ij}) \text{ for } (\alpha, \beta) = (x, z) \text{ or } (z, x) \\ \gamma \sin(\theta_{ij}) \text{ for } (\alpha, \beta) = (y, z) \text{ or } (z, y) \\ -\delta \text{ for } (\alpha, \beta) = (z, z) \end{cases} \quad (18.5)$$

and defined

$$X_{ij} = \delta_{i,i+1_x} + \delta_{i,i-1_x}, \quad Y_{ij} = \delta_{i,i+1_y} + \delta_{i,i-1_y}. \quad (18.6)$$

The angle θ_{ij} is the angle that the vector $\mathbf{R}_i - \mathbf{R}_j$ forms with the x -axis.

In addition to H_0 , we have atomic SOC coupling the orbitals. We will treat this term as a perturbation. Written in the orbital basis ϕ , we have

$$H_{\text{atom-SOC}} = \sum_{\alpha\beta ij} \alpha \langle \mathbf{L} \cdot \mathbf{S} \rangle_{\alpha\beta\sigma\sigma'} \delta_{ij} c_{\alpha\sigma i}^\dagger c_{\beta\sigma' j} \quad (18.7)$$

The corresponding ΔM matrix reads

$$\Delta M = \frac{\alpha}{2} \begin{pmatrix} 0 & -i & 0 & 0 & 0 & 1 \\ i & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & i & 0 \\ 0 & 0 & -1 & 0 & i & 0 \\ 0 & 0 & -i & -i & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (18.8)$$

We will now apply the following steps to do the Löwdin partitioning of this Hamiltonian, i.e. obtaining an effective low-energy description.

- Diagonalize M and identify the high and low-energy sectors after first Fourier-transforming to $\mathbf{k}$ -space.
- Write the perturbation $H_{\text{atom-SOC}}$ in the new basis which is the eigenstate of M .

- Perform a unitary transformation of the total Hamiltonian $M + \Delta M$ in such a way that its matrix elements between high- and low-energy sectors are zero.
- Set up the resulting H_{eff} by projecting out the high-energy sector. This may now be diagonalized to obtain the low-energy bands including the effect of the perturbation.

A point worth mentioning in the tight-binding approach is how to second quantize the orbital angular momentum operator. In other words, what is the second quantized version of the atomic spin-orbit coupling $\alpha \mathbf{L} \cdot \mathbf{S}$? This can be worked out by considering a specific basis for the fermion operators, such as (for a given lattice site)

$$[c_{p_x, \uparrow, i}, c_{p_x, \downarrow, i}, c_{p_y, \uparrow, i}, \dots, c_{p_z, \downarrow, i}] \quad (18.9)$$

where the c -operators annihilate an electron at a given site, orbital, and spin. Next, one uses that the matrix elements determining the coefficients in the second-quantized Hamiltonian are of the type

$$\langle l'm' | \hat{L}_j | lm \rangle \quad (18.10)$$

where $\hat{L}_j$ is the j 'th component of the angular momentum operator while $|lm\rangle$ are quantum states with angular momentum l and m . In the position representation, they are described by the spherical harmonics Y_l^m which are complex. Here, the spin part of the matrix elements is separated out as a direct product $|lms\rangle = |lm\rangle \otimes |s\rangle$, so that $\mathbf{L}$ and $\mathbf{S}$ in the spin-orbit Hamiltonian act on separate kets. Finally, one notes that the various orbitals are expressed in terms of spherical harmonics Y_l^m as

$$s = Y_0^0, p_x = \sqrt{12}(Y_1^{-1} - Y_1^1), p_y = i\sqrt{12}(Y_1^{-1} + Y_1^1), p_z = Y_1^0. \quad (18.11)$$

We can then simply evaluate $\langle l'm' | \hat{L}_j | lm \rangle$ for the various orbitals by using results like

$$\langle l'm' | \hat{L}_x | lm \rangle = \frac{\hbar}{2} [\delta_{ll'} \delta_{m', m+1} \sqrt{(j-m)(j+m+1)} + \delta_{ll'} \delta_{m', m-1} \sqrt{(j+m)(j-m+1)}]. \quad (18.12)$$

This procedure is described in section 3.3 in Ref. [65]. In the end, one ends up with a matrix containing the matrix elements with the various orbitals.

To show how an effective spin-orbit interaction arises in the conduction band, it is sufficient to proceed with just the p_x and p_z orbitals to illustrate the principle. Dropping p_y and Fourier-transforming H_0 to momentum space, so that we are now using a basis $[c_{p_x \uparrow \mathbf{k}}, c_{p_x \downarrow \mathbf{k}}, c_{p_z \uparrow \mathbf{k}}, c_{p_z \downarrow \mathbf{k}}]$ then gives the M - and ΔM matrices

$$M = \begin{pmatrix} K & 0 & \gamma & 0 \\ 0 & K & 0 & \gamma \\ \gamma & 0 & -K_\delta & 0 \\ 0 & \gamma & 0 & -K_\delta \end{pmatrix}, \quad \Delta M = \frac{\alpha}{2} \begin{pmatrix} 0 & -i & 0 & 1 \\ i & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}. \quad (18.13)$$

Here, we defined $K = -2(W \cos k_x + \delta \cos k_y)$ and $K_\delta = -2\delta(\cos k_x + \cos k_y)$. We see that M in fact consists of two independent 2×2 matrices. We now want to diagonalize M and then reexpress ΔM in the eigenbasis of M . The diagonalization of M yields a diagonalization matrix P satisfying $PDP^\dagger = M$ (after normalizing the eigenvectors entering P):

$$P = \begin{pmatrix} \frac{N_+ \gamma}{E_+ - K} & 0 & \frac{N_- \gamma}{E_- - K} & 0 \\ 0 & \frac{N_+ \gamma}{E_+ - K} & 0 & \frac{N_- \gamma}{E_- - K} \\ N_+ & 0 & N_- & 0 \\ 0 & N_+ & 0 & N_- \end{pmatrix}, \quad D = \text{diag}(E_+, E_+, E_-, E_-). \quad (18.14)$$

where $N_{\pm}$ are normalization coefficients (their value can be read out from the above matrix) whereas the eigenvalues are

$$E_{\pm} = \frac{1}{2}[K - K_{\delta} \pm \sqrt{(K - K_{\delta})^2 + 4(K_{\delta} + \gamma^2)}]. \quad (18.15)$$

If we now assume that $\gamma \gg K, K_{\delta}$, we have a clear splitting between the high- and low-energy sectors E_{+} and E_{-} of the H_0 -Hamiltonian. This is what we need to do the partitioning. The lower 2×2 block is now the part of the Hamilton-operator we are interested in (low-energy). The remaining step is to express ΔM (atomic SOC) in the eigenbasis of H_0 (turning it into $\tilde{\Delta M}$), add it to the matrix D , and then perform a unitary transformation $e^{iS}(D + \tilde{\Delta M})e^{-iS}$ with S chosen so that the off-diagonal parts of $\tilde{\Delta M}$ are zero. Then, the lower 2×2 block of the resulting matrix will be our effective Hamiltonian. The prescription for how to choose S is standard. In this particular case, we get the spin-orbit interaction in the effective Hamiltonian straight from the diagonal part of $\tilde{\Delta M}$, i.e. to first order in α . This is because the choice of S matrix eliminating the off-diagonal part of $\tilde{\Delta M}$ still allows for a contribution to H_{eff} from the diagonal part of $\tilde{\Delta M}$, as remarked previously. We get:

$$H_{\text{eff}} = \begin{pmatrix} E_{-} + 0 + \mathcal{O}(\alpha^2) & 0 + \frac{N_{-}^2 \gamma \alpha}{E_{-} - K} \left(1 - \frac{iN_{-} \gamma}{E_{-} - K}\right) \\ 0 + \frac{N_{-}^2 \gamma \alpha}{E_{-} - K} \left(1 + \frac{iN_{-} \gamma}{E_{-} - K}\right) & E_{-} + 0 + \mathcal{O}(\alpha^2) \end{pmatrix}. \quad (18.16)$$

This is now in a basis $[c_{\text{low-energy band}, \uparrow, \mathbf{k}}, c_{\text{low-energy band}, \downarrow, \mathbf{k}}]$ which can be diagonalized to obtain the effective excitation bands in the low-energy sector. Note how we have obtained a coupling between the spins of the low-energy bands: it doesn't look exactly like a Rashba-term, but is somewhat reminiscent of it. Taking into account the p_y orbital as well would have given a Rashba-like coupling, just like in Petersen *et al.* 2000.

In this way, one ends up with an effective model for a conduction band that is separated from other bands by a gap induced by the inversion-symmetry breaking term and which has an effective spin-orbit coupling. The magnitude of this SOC term is typically orders of magnitude larger than the coefficient for a free electron model ($\alpha_R = g\mu_B E/2mc^2$), and is given by

$$\alpha_R \propto E\alpha/t \quad (18.17)$$

In the absence of either the symmetry-breaking potential or the atomic SOC (α), the Rashba-term thus vanishes: both are required.

Note that a simple truncation of the Hamiltonian to the desired subspace (p_z) will give no spin-orbit splitting. We must therefore include virtual transitions to the other orbitals to second order in the coupling, which is a good approximation when there is a sufficiently large band gap separating the p_z band from the p_x, p_y bands.

The physical picture behind the Rashba effect can be understood in the tight-binding framework, following the explanation on the Wikipedia-site. The symmetry-breaking term $H_E = Ez$ (in first-quantized form) induces a gap in the band spectrum, and also hybridizes the p_x, p_y, p_z orbitals (meaning it induces matrix elements between them that were previously zero). For instance, it enables hopping from a p_z -state at site i with a given spin to a p_x state at a different site j with the same spin. This is not possible for $E = 0$ due to symmetry. The Rashba effect can then be understood as a second order perturbation theory effect describing virtual hopping from a p_z orbital

to a p_x orbital and then back to p_z again. Namely, an electron can jump from a $|p_z, i, \uparrow\rangle$ state to a $|p_x, i+1, \uparrow\rangle$ state with amplitude $\propto E$. Then, it uses the atomic spin-orbit coupling to flip its spin and go back to a $|p_z, i+1, \downarrow\rangle$ state. This transition has amplitude α . Overall, the effect is that the electron hopped one site and flipped its spin. This is exactly what the Rashba-term accomplishes. The effect is then $\mathcal{O}(\alpha E)$.

18.1.2 Does Rashba SOC cause momentum scattering?

When writing down the Hamilton operator for Rashba SOC, one will in general have terms like $c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}$ which look like spin-flip terms. Then, one might ask: why does Rashba SOC only cause electron spins to change and not their momentum? In other words, why aren't there terms like $c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow}$ present?

The reason is that Rashba SOC expresses the modification in energy of a particle moving in a direction $\mathbf{k}$ and with a given spin $\mathbf{S}$. To express this modification, we have to check if there are spins pointing in the $\mathbf{S}$ -direction in our system, which is done precisely via the spin operator $c_{\mathbf{k}\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}\beta}$. However, translational symmetry is still preserved and there is nothing that can change the momentum of the electron. On the other hand, a spin-flip Hamilton operator includes some potential $V_{\text{sf}}(\mathbf{r})$ which *breaks* translational symmetry. In this case, the Fourier-transformation produces a Hamiltonian of the type

$$\sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow} \quad (18.18)$$

where $V_{\mathbf{k}\mathbf{k}'} \propto \int d\mathbf{r} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} V_{\text{sf}}(\mathbf{r})$ and thus causes momentum scattering as well. I

Write more:

present without external fields or impurities, thus inherent to the material itself. - noncentrosymmetric lattice - interfaces

can be both of rashba and dresselhaus type. structural inversion asymmetry (interfaces) typically of rashba type. SOC is of course also present even with inversion symmetry in general, and is then even-in-k.

18.1.3 Extrinsic spin-orbit coupling

present due to external electric fields or impurities. thus induced via external agents. - impurities - external electric field

does not necessarily have to break inversion symmetry. external field can cause Rashba SOC in InAs, InSb nanowires or 2DEGs.

Chapter 19

Spintronics

19.1 Spin currents and continuity equations

There are two fundamentally different types of spin currents: equilibrium spin currents and non-equilibrium spin currents. There is a nice discussion about the distinction between them in Waintal and Brouwer, PRB 2002.

Equilibrium spin currents can exist in the absence of any voltage or temperature drive, i.e. even when the electrons are described by the Fermi-Dirac distribution. There are two prominent cases where equilibrium spin currents arise. One is in spin-valves, like FNF. The F's interact via the conduction electrons in N and exert a torque on each other if they are misaligned. What happens is that a spin current arises in N if the F's are misaligned and this spin current becomes absorbed as it enters each F. Since the angular momentum of the spin current is lost in the ferromagnet, it means that a torque has been exerted on the magnetization. Hence, the F's try to establish a collinear configuration.

The equilibrium spin current here only exists in a non-collinear state. This means that one must apply an external magnetic field to force such a state, as it is not the ground-state of the system. If one removes the magnetic field, time-dynamics ensue due to the torque exerted by the spin current and equilibrium ceases to exist since we now have time-dependence. An observable consequence of the equilibrium spin current, also called exchange spin current, is therefore its torque which gives rise to magnetization dynamics in the absence of an external field.

The other prominent case where such an equilibrium spin current exists is in Rashba spin-orbit coupled systems. This can be seen by writing down the continuity equation for spin in such a system. In this case, if one uses the conventional definition of a spin current tensor:

$$\mathbf{J} \propto \frac{\hbar}{2} \frac{1}{2} \langle \psi | \{ \boldsymbol{\sigma}, \mathbf{v} \} | \psi \rangle, \quad (19.1)$$

then the continuity equation takes the form

$$\frac{\partial S_z}{\partial t} + \nabla \cdot \mathbf{J} = T \quad (19.2)$$

where $T \propto \langle \psi | [\boldsymbol{\sigma}, H] | \psi \rangle$ is a torque term. Due to the Rashba spin-orbit coupling, $T \neq 0$. It is possible to redefine the spin current in such a way that it absorbs T , in which case such a spin current is conserved even in the presence of spin-orbit coupling. Since spin current cannot be directly in

any case, there is an ambiguity in how one chooses to define a spin current. Therefore, as discussed in D. Go *et al.*, Phys. Rev. Research 2, 033401 (2020), it is only experimentally meaningful to discuss signatures of measurable quantities like spin accumulation or torques on magnetizations.

The other type of spin current is a non-equilibrium one that appears only when driving the system out of equilibrium with *e.g.* a voltage or temperature gradient. This induces spin flow due to a gradient in the chemical potential: more precisely, a gradient in the difference between chemical potential for spin up and spin down. The easiest way to make this happen is to drive a charge current through a ferromagnet, which polarizes it. As this spin current enters a normal metal, it generates a spin accumulation. This can also exert torques on magnetizations as long as the spin current polarization is non-collinear with the magnetization.

An electric current can also generate a non-equilibrium torque in homogeneous (collinear) ferromagnets. For instance, the torque induced on the magnetization of local magnetic moments $\mathbf{M}$ in a homogeneous ferromagnet with spin-orbit coupling acquires a contribution from a spin-orbit torque when one applies an electric current to such a material. Since this happens even for a homogeneous ferromagnet, it is not due to the conventional effect of spin-transfer torque, which requires non-collinearity. Instead, this happens because the Rashba spin-orbit coupling induces a non-equilibrium spin accumulation $\mathbf{m}_{\text{non-eq}}$ as one applies electric current, and this spin accumulation of the conduction electrons can exert a torque on $\mathbf{M}$ which is $\propto \mathbf{m}_{\text{non-eq}} \times \mathbf{M}$ (see Manchon and Zhang, PRB 2009).

19.2 GMR

GMR can be qualitatively understood using the Mott model, which was introduced as early as 1936 to explain the sudden increase in resistivity of ferromagnetic metals as they are heated above the Curie temperature.²⁹ There are two main points proposed by Mott. First, the electrical conductivity in metals can be described in terms of two largely independent conducting channels, corresponding to the up-spin and down-spin electrons, which are distinguished according to the projection of their spins along the quantization axis. The probability of spin-flip scattering processes in metals is normally small as compared to the probability of the scattering processes in which the spin is conserved. This means that the up-spin and down-spin electrons do not mix over long distances and, therefore, the electrical conduction occurs in parallel for the two spin channels. Second, in ferromagnetic metals the scattering rates of the up-spin and down-spin electrons are quite different, whatever the nature of the scattering centers is.

In a transition metal ferromagnet, the electric current is primarily carried by *s*-electrons due to their low effective mass and high mobility. The *d* bands play an important role in providing final states for the scattering of the *s* electrons. In ferromagnets the *d* bands are exchange-split, so that the density of states is not the same for the $\uparrow$ and $\downarrow$ electrons at the Fermi energy (see Fig. 19.1). The probability of scattering into these states is proportional to their density, so that the scattering rates are spin-dependent, i.e. are different for the two conduction channels. More precisely, the $\downarrow$ electron have more empty states to scatter to, so the resistivity will be higher for these electrons. This picture is simplified since there can be hybridization between the *s* and *d*-states, but it nevertheless forms a useful basis for a qualitative understanding of the spin-dependent conduction in transition metals.

But is not the conductivity of a metal proportional to the density of states at the Fermi level? Above, we said that higher density of states at Fermi level gives more states to scatter to and thus

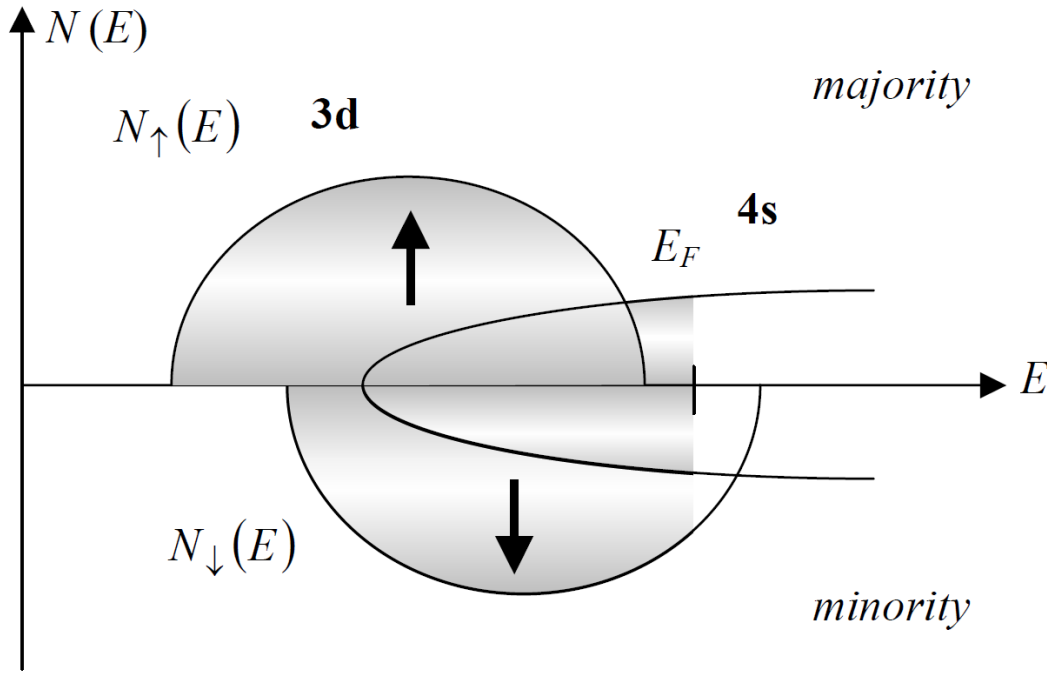


Figure 19.1: (Color online) ...

lower conductivity. The Drude formula for conductivity $\sigma = \sigma_{\uparrow} + \sigma_{\downarrow}$ is given by

$$\sigma_{\sigma} = \frac{e^2 k_F^2}{\pi \hbar 6\pi} \lambda \quad (19.3)$$

where k_F^2 is proportional to the cross sectional area of the Fermi surface (and thus the density of states squared for free electrons since $N_0 \propto k_F$ for 3D free electrons). Spin indices are implicitly assumed on all relevant quantities on the right hand side. The point is that $\lambda = v_F \tau$ is the mean free path, and this quantity diminishes with the density of states N_0 since Fermi's golden rule gives a scattering rate

$$\tau^{-1} = \frac{2\pi}{\hbar} \langle V_{\text{scatt}}^2 \rangle N_0. \quad (19.4)$$

Now, the conductivity σ_{σ} in total therefore goes like N_0 and increases with density of states. But in the GMR effect, it is the DOS for the d -electrons which enters τ^{-1} , whereas the DOS for the s -electrons is the one determining the cross-sectional area of the Fermi surface (k_F^2). Thus, we are dealing with two different density of states. Increasing the DOS in the d -band electrons increases scattering and thus resistivity, and the d -electrons are the ones that are spin-split.

19.3 Basic concepts in spin transport

In a diffusive conductor, charge carriers experience a mean free path, l_{mfp} which is the average distance they can travel before their initial momentum is randomized, that is much smaller than the dimensions of the conductor. When such a conductor is driven away from equilibrium, for

instance by applying a voltage, a local linear relationship should hold between the current density j and the chemical potential μ so long as the non-equilibrium conditions are not extreme:

$$j_x = \frac{\sigma}{e} \frac{\partial \mu}{\partial x}. \quad (19.5)$$

Here, σ is the conductivity which can be treated as a phenomenological parameter where all properties originating from the conductor band structure and scattering mechanisms are taken into account. We emphasize that linear regime non-equilibrium transport, as considered here, involves electrons at the Fermi energy only. In the particular case of a metallic system, in the linear regime, the Einstein relation gives us a microscopic expression for σ :

$$\sigma = \nu_D e^2 D \quad (19.6)$$

where $\nu_D = \nu_D(E_F)$ is the density of states at the Fermi energy and D is the diffusion constant. The latter is expressed as $D = v_F l_{\text{mfp}}/3$ in a three-dimensional system where v_F is the Fermi velocity. This means that if L is the size of the metal, the electrons will need on average a time $\tau_D = L^2/D$ to traverse the whole system. This is the Thouless dwell time and $E_T = D/L^2$ is the associated Thouless energy.

We now wish to generalize this to spin-dependent transport, which was done in work by van Son *et al.* (1987), Johnson and Silsbee (1988), and Valet and Fert (1993). A review was given by Gijs and Bauer (1996). We make the assumption that the spin lifetime τ_{sf} (which is finite since electron spins interact with the host metal, such as magnetic impurities) is longer than the momentum relaxation time τ_{el} caused by elastic scattering. In this case, two chemical potentials $\mu_{\uparrow}$ and $\mu_{\downarrow}$ where $\uparrow / \downarrow$ are defined as parallel and antiparallel to a spin quantization axis. Ohm's law now applies separately to each spin channel:

$$\begin{aligned} j_{\uparrow} &= \frac{\sigma_{\uparrow}}{e} \frac{\partial \mu_{\uparrow}}{\partial x}, \\ j_{\downarrow} &= \frac{\sigma_{\downarrow}}{e} \frac{\partial \mu_{\downarrow}}{\partial x}. \end{aligned} \quad (19.7)$$

We dropped the subscript 'x' here. The conductivities are thus in general different for the two spin species, $\sigma_{\uparrow/\downarrow} = \nu_D^{\uparrow/\downarrow} e^2 D^{\uparrow/\downarrow}$. We emphasize that these expressions change for very strong spin relaxation $\tau_{\text{el}} \simeq \tau_{\text{sf}}$. The bulk polarization of a ferromagnet, where $\mu_{\uparrow} = \mu_{\downarrow}$, can be defined as β_F where

$$\beta_F = \frac{\sigma_{\uparrow} - \sigma_{\downarrow}}{\sigma_{\uparrow} + \sigma_{\downarrow}} = \frac{j_{\uparrow} - j_{\downarrow}}{j_{\uparrow} + j_{\downarrow}}. \quad (19.8)$$

Inside a metal, whether it is ferromagnetic or non-magnetic, a spin polarized in a certain direction will lose its original orientation due to interactions with *e.g.* magnetic impurities after the spin relaxation time τ_{sf} . A spin imbalance $\Delta\mu \equiv (\mu_{\uparrow} - \mu_{\downarrow})/2$ thus decays on a length scale given by the spin relaxation length

$$\lambda_{\text{sf}} = \sqrt{D\tau_{\text{sf}}}. \quad (19.9)$$

The physical mechanism for spin relaxation are spin-spin interactions, including magnetic impurities, and spin-orbit coupling. The latter is usually the dominant one.

19.4 Transport equations for charge and spin

Whereas spin-up and spin-down currents are given by Eq. (19.7), spin relaxation processes cause them to not be conserved separately. Their sum (charge current) is nevertheless conserved, so that $\nabla \cdot \mathbf{j} = 0$ where

$$\mathbf{j} = \mathbf{j}_\uparrow + \mathbf{j}_\downarrow = \partial_x(\sigma_\uparrow \mu_\uparrow + \sigma_\downarrow \mu_\downarrow). \quad (19.10)$$

We define $\mu = (\mu_\uparrow + \mu_\downarrow)/2$ and $\mu_z = (\mu_\uparrow - \mu_\downarrow)/2$. It is clear that $\nabla(\mu_\uparrow + \mu_\downarrow)$ is not a conserved quantity in general.

To describe spin relaxation processes, we follow van Son *et al.* (1987) who used the equation

$$D_s \nabla^2 \mu_z = \frac{\mu_z}{\tau_{\text{sf}}} \quad (19.11)$$

where we defined

$$D_s = \frac{\sigma_\downarrow D_\uparrow + \sigma_\uparrow D_\downarrow}{\sigma} = \frac{(\nu^\uparrow + \nu^\downarrow) D_\uparrow D_\downarrow e^2}{\sigma}. \quad (19.12)$$

In the non-magnetic (spin-independent case), we see that $D_s \rightarrow D$, i.e. the charge diffusion constant. To understand where Eq. (19.11) comes from, we consider the arguments of Filip (2002) and Jedema (2002). Conservation of charge current means that one spin population can change only by spin-flip processes. For instance, the number of spin- $\uparrow$ electrons decreases via $\uparrow \rightarrow \downarrow$ spin-flips, whereas the number of spin- $\downarrow$ electrons increase by the reverse process. We can then write down the equations:

$$\begin{aligned} \nabla \cdot \mathbf{j}_\uparrow &= \partial_x j_\uparrow = \frac{\rho_\downarrow}{\tau_{\downarrow\uparrow}} - \frac{\rho_\uparrow}{\tau_{\uparrow\downarrow}}, \\ \nabla \cdot \mathbf{j}_\downarrow &= \partial_x j_\downarrow = \frac{\rho_\uparrow}{\tau_{\uparrow\downarrow}} - \frac{\rho_\downarrow}{\tau_{\downarrow\uparrow}}, \end{aligned} \quad (19.13)$$

where $\rho_{\uparrow/\downarrow} = e\nu_{\uparrow/\downarrow}\mu_{\uparrow/\downarrow}$ are the non-equilibrium charge densities for the spin- $\uparrow / \downarrow$ electrons while $\tau_{\uparrow\downarrow}^{-1}$ is the spin-flip rate from up to down electrons and conversely for $\tau_{\downarrow\uparrow}^{-1}$. Using Ohm's law for each spin, we see that

$$\partial_x(\partial_x \mu_\uparrow - \partial_x \mu_\downarrow)/2 = e\partial_x(j_\uparrow/\sigma_\uparrow - \partial_x j_\downarrow/\sigma_\downarrow)/2. \quad (19.14)$$

Note that according to the principle of detailed balance between up and down spin populations, there should be no spin-flips occurring at equilibrium $\mu_\uparrow = \mu_\downarrow$. Looking at the right-hand side of Eq. (19.13), we see that this means that we must have

$$\tau_{\uparrow\downarrow}^{-1} \nu_\uparrow(E_F) = \tau_{\downarrow\uparrow}^{-1} \nu_\downarrow(E_F). \quad (19.15)$$

Using this result and inserting the expressions for the derivatives of $j_{\uparrow/\downarrow}$ from Eq. (19.13), we arrive at Eq. (19.11) when defining the spin relaxation rate as:

$$\tau_{\text{sf}}^{-1} = \tau_{\uparrow\downarrow}^{-1} + \tau_{\downarrow\uparrow}^{-1}. \quad (19.16)$$

The spin relaxation length λ_{sf} defined previously defines the length scale over which a spin imbalance relaxes. In a ferromagnet, it is typically in the range 5 – 50 nm. For a non-magnetic metal, it can be hundreds of nm. A typical value for the spin accumulation in a non-magnetic metal is about $\mu_z = 10\mu\text{eV}$.

19.5 Spin accumulation

In the quest toward designing spintronics transport experiments and devices, one has to consider the following sequence of phenomena: spin accumulation, spin transport, and how to detect spin accumulation. We begin by considering spin accumulation in the simplest possible structure where it occurs, namely a F/N bilayer.

Electrical spin injection refers to the generation of a non-equilibrium spin density in a normal metal (N). This happens by applying an electric bias voltage across the interface of a F/N bilayer. The charge current becomes spin polarized as it flows through the F region. The inverse phenomenon, spin extraction, takes place if one reverses the current flow so that the current flows from N to F - a spin accumulation still occurs in N near the interface.

The concept of a spin accumulation is shown in Fig. 19.3. The spin-dependent band structure in the F region leads to different electrical resistivities for the two spin orientations $\uparrow$ and $\downarrow$. In general, a larger DOS leads to a larger resistivity since there are more states to scatter into. This means that the total current $j = j_{\uparrow} + j_{\downarrow}$ is polarized, since $j_{\uparrow} > j_{\downarrow}$. When the spin current reaches the N metal, it enters and causes an accumulation of spins near the interface.

Why does this happen? The reason can be understood by considering the behavior of the current far away from the interfaces: it is polarized in F but unpolarized in N. Therefore, in the region near the interface *there must be a transfer of current from one spin channel to the other*. As the spin-polarized current enters the normal metal, the only way that it can remain spin-polarized right after passing through the interface is if there is a spin accumulation since the density of states and resistivities are *spin-independent* in the normal metal. Therefore, a non-equilibrium spin density builds up in N near the interface, as shown in Fig. 19.2. This spin accumulation must then decay as one moves into the normal metal in order for the current to become unpolarized. This physically takes place via scattering on magnetic impurities and spin-orbit impurities, i.e. spin-flip scattering which destroys the spin accumulation $\Delta\mu(x) = \mu_{\uparrow}(x) - \mu_{\downarrow}(x)$ so that $\Delta\mu(x \rightarrow \infty) \rightarrow 0$.

Fig. 19.2 also shows (top figure) the case of tunneling between two non-magnetic metals for comparison. In that case, the chemical potential simply drops linearly (except possibly at the interface) throughout the regions which in turn drives a constant electric current from left to right as a voltage $eV = \mu_L - \mu_R$ is applied. Note how the density of states curves are shifted along with the drop in chemical potential μ all the way - otherwise, we would have had a fewer and fewer electrons in the system since fewer and fewer levels would have been occupied, i.e. charge accumulation, which is not the case.

In the lower panel, an applied voltage at the left side raises the chemical potential for both spin species compared to deep inside the N bulk. They are still equal, $\mu_{\uparrow} = \mu_{\downarrow}$, since the applied voltage acts equally on both bands and the current is still spin-polarized due to the difference in Fermi level density of states. On the normal metal side, both spin bands (which are degenerate due to the absence of an exchange field in N) continue to be lowered as one moves into N due to the voltage drop (the reduction in μ). However, the chemical potentials are not the same in each band due to spin accumulation. Therefore, it is important to realize that spin accumulation means that there exists a true non-equilibrium spin density, i.e. more spin- $\uparrow$ particles in N than spin- $\downarrow$ in N. Each spin band in N cannot be shifted to follow μ_{σ} individually because then there would be no spin-density. The current injected from the ferromagnet is pumping more spin- $\uparrow$ particles than spin- $\downarrow$ particles

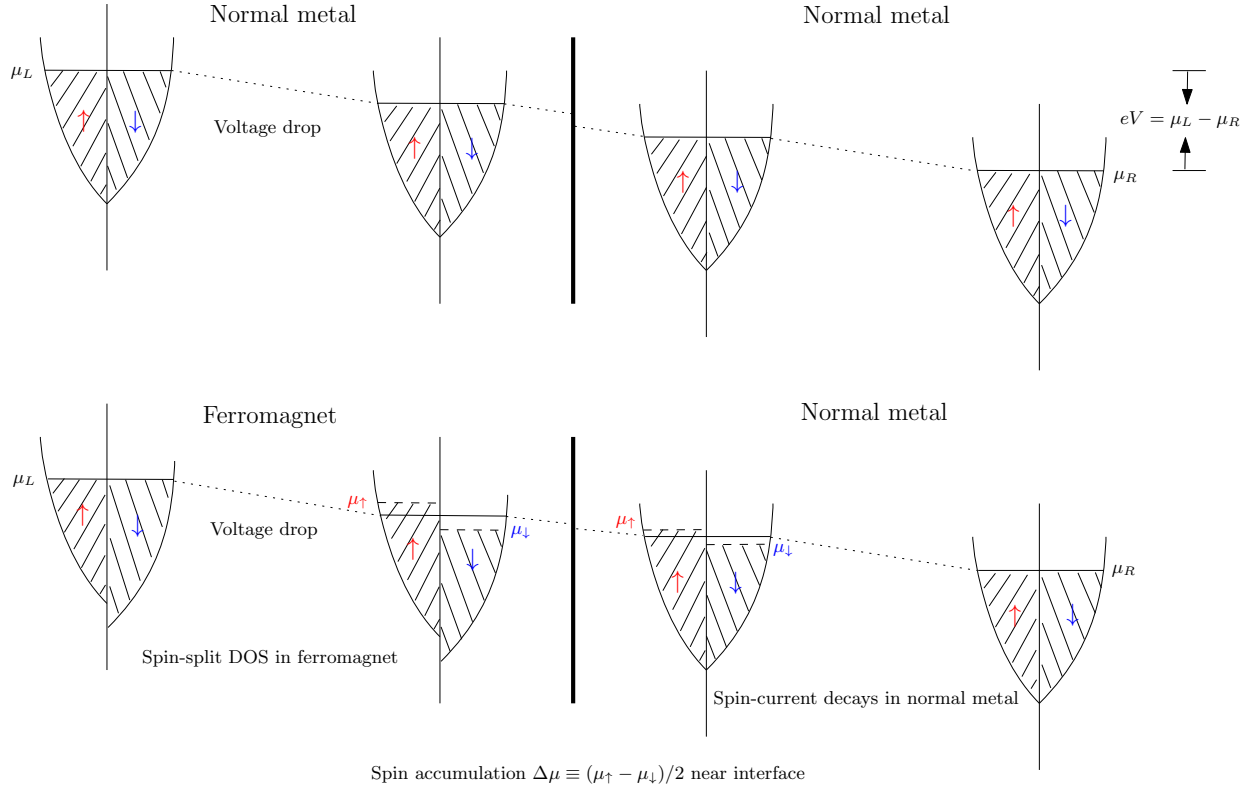


Figure 19.2: (Color online) *Top figure:* density of states and local chemical potential profile in a voltage-biased N/N junction. *Bottom figure:* spin-split DOS in a ferromagnet and spin-degenerate DOS in a normal metal in a voltage-biased F/N junction. A spin accumulation exists near the interface which decays due to spin-flip scattering as one moves either into F or N. In both the bulk of F and N, $\mu_\uparrow = \mu_\downarrow$. At the same time, a gradient in the average chemical potential $\mu = (\mu_\uparrow + \mu_\downarrow)/2$ exists throughout the structure in order to give an electric current.

into the normal metal.

If one, hypothetically, were able to apply a *pure spin-voltage* in an N/N junction, the spin-up band DOS would have shifted up and the spin-down band DOS would have shifted down so that a pure spin current would flow, but that is a different scenario: there is not any spatially varying spin density in that case.

The spin accumulation decay length on the F and N sides of the interface is different, λ_S^F and λ_S^N respectively. The spin-dependent chemical potentials μ_σ are continuous at the interface if one neglects interface resistance (as in Fig. 19.3) - otherwise, there is a voltage drop across the interface as well. Because of the boundary condition, there must exist a spin accumulation on the F side near the interface as well which also relaxes due to spin-flip processes as one moves into the bulk of F so that $\mu_\uparrow(x \rightarrow -\infty) = \mu_\downarrow(x \rightarrow -\infty)$. Note that inside the bulk of F, the chemical potentials for both spins are equal despite the fact that an electric voltage is applied: there is no reason for why the voltage should act differently on electrons of one spin compared to the other type. As we have seen previously, in the bulk of F we have $\mu_\uparrow = \mu_\downarrow$ so that spin-current for each spin species is conserved.

Importance of interface resistance. It is instructive to distinguish between spin injection into

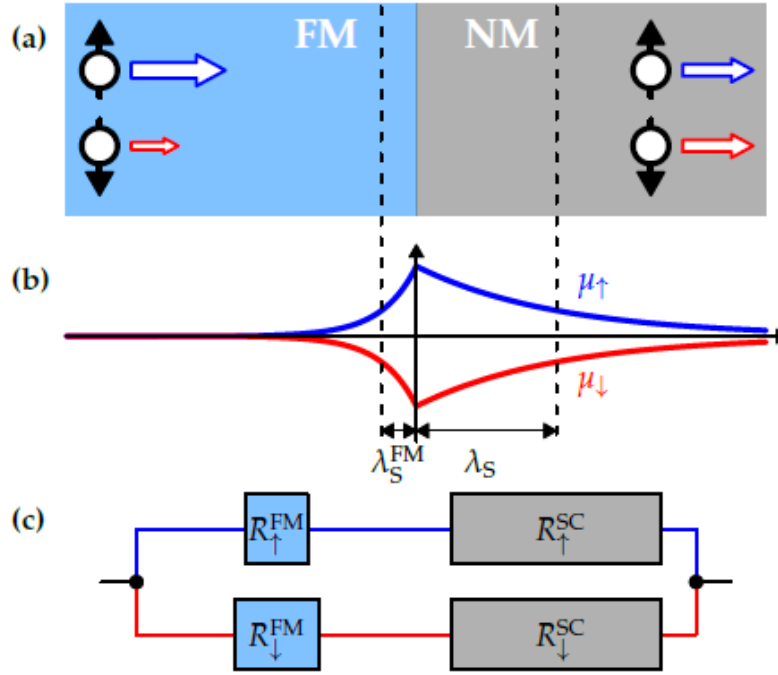


Figure 19.3: (Color online) (a) Schematic representation of a ferromagnetic metal/normal metal contact. The current injected into the F is spin-polarized, but is unpolarized deep into the N. (b) Profile of the electrochemical potential close to the interface for spin-up ($\mu_{\uparrow}$) and spin-down ($\mu_{\downarrow}$) electrons. Note that we have not shown the overall potential drop occurring for the net chemical potential, which has to be present when a current flows. The spin diffusion length is λ_S^{F} in the F region and λ_S^{N} in the N region. (c) Two-current resistor model with the resistances of spin-up and spin-down electrons in each region. Figure taken from Ph.D dissertation of Y. Manzke "Non-local, local, and extraction spin-valves based on ferromagnetic metal/GaAs hybrid structures".

semiconducting and normal metal regions. The reason for this is that *conductance mismatch* is an obstacle for injection of spin-currents into a non-magnetic material from a metallic ferromagnet. As we shall see in a more detailed treatment below, this occurs when the resistance in the non-magnetic material $R_{\sigma}^{\text{N}} \equiv R^{\text{N}}$ is much greater than the spin-dependent resistances in the magnetic region, $R^{\text{N}} \gg R_{\uparrow/\downarrow}^{\text{FM}}$. This causes the total currents to be approximately equal for both spin channels meaning that the spin injection is inefficient.

19.5.1 Relation between spin-accumulation and induced magnetization

The spin-accumulation gives rise to a magnetization in a normal metal which can be computed in the same way as one would compute the paramagnetic response of a normal metal in the presence of a Zeeman-splitting magnetic field. The spin accumulation $\mu_S = \mu_{\uparrow} - \mu_{\downarrow}$ takes the same role as the Zeeman-splitting $\mu_B B$, at least in the limit of a weak spin accumulation or Zeeman-splitting. The derivation can be found here http://www.phys.lsu.edu/~jarrell/COURSES/ADV_SOLID_HTML/Other_online_texts/Valenti/chapter3_twoside.pdf and the spin-accumulation case can be obtained in the same way simply by letting the arguments of the distribution functions for $\langle c_{\sigma}^{\dagger} c_{\sigma} \rangle$ be shifted with $\pm \mu_S/2$ compared to each other.

19.6 Spin pumping

19.6.1 Ferromagnetic metal/normal metal

In an FN bilayer, setting the magnetization $\mathbf{M}$ into a precession via an external field causes spin-pumping: a transfer of angular momentum into the normal region. In other words, a spin-current is generated and sent into the N part. Part of this spin-current is sent back into F via a backflow mechanism which differs depending on whether it is a metallic or insulating F. In the metallic case, if spin is injected into N faster than the spin relaxation time, a spin accumulation will build up close to the interface. This will, in turn, cause a spin-flow back into the F region and thus counteracting the pumped spin-current. A stationary situation is reached when the backflow is sufficiently large to cause the spin accumulation to stop changing so that the net injection rate equals the relaxation rate.

The loss of angular momentum from the ferromagnet can be described as a torque in the LLG equation. From the form of the spin-current, one can identify what the corresponding physical consequence is. For instance, one finds that the spin-current can be written

$$\mathbf{J}_S \propto \text{Re}\{g_{\text{mix}}\}\mathbf{m} \times d\mathbf{m}/dt + \text{Im}\{g_{\text{mix}}\}d\mathbf{m}/dt. \quad (19.17)$$

The real part of the mixing conductance thus renormalizes the Gilbert damping coefficient in the ferromagnet, while the imaginary part of the mixing conductance renormalizes the gyromagnetic ratio γ . The corresponding physical consequences is that the linewidth is changed and the FMR resonance frequency is changed, correspondingly. Thus, by identifying how the spin-current depends on $\mathbf{m}$ and $d\mathbf{m}/dt$, one can make predictions about how experimentally measurable quantities will change.

In the Usadel framework, the interface parameters describing the real and imaginary part of the mixing conductance for an insulating F are G_2^ϕ and G^ϕ in Eschrig NJP 2015. We have (ignoring channel-dependence for simplicity):

$$\begin{aligned} G^\phi &\propto \Delta\phi, \\ G_2^\phi &\propto (\Delta\phi)^2. \end{aligned} \quad (19.18)$$

Here, $\Delta\phi = \phi_\uparrow - \phi_\downarrow$ where $r_\sigma = |r_\sigma|e^{i\phi_\sigma}$ is the reflection coefficient at the interface for spin σ .

Derivation of spin-pumping spin current using quasiclassical theory

We here show how one can study spin-pumping using quasiclassical Keldysh-Usadel theory. There are two approaches. The first approach is to solve a time-dependent problem with a time-dependent magnetization $\mathbf{m}(t)$ that precesses and compute the spin currents. The second approach is simpler: it consists of changing coordinate system to a frame which rotates with the magnetization vector. In this frame, the problem has no time-dependence but instead becomes a non-equilibrium, stationary problem. We will use the second approach.

The mapping from a time-dependent to stationary, non-equilibrium problem requires the magnetization to be written in a specific way:

$$\mathbf{m}(t) = m[\sin\theta \cos\Omega t, \sin\theta \sin\Omega t, \cos\theta]. \quad (19.19)$$

There is not much loss of experimental relevance in considering this form for magnetization. The tilt angle θ and angular frequency Ω are independent of time. In writing the magnetization like

this, we are considering a situation where the magnetization is kept in precession despite Gilbert damping by applying an ac magnetic field H_t . The tilt angle θ can be estimated from the LLG equation as

$$\theta \simeq \mu H_t / \alpha \hbar \Omega_0 \quad (19.20)$$

where Ω_0 is the resonance frequency.

In the original lab-frame where the magnetization is precessing, the magnetization is described by the above $\mathbf{m}(t)$. We want to change coordinate system to a frame which is rotating together with the magnetization so that the magnetization in that frame becomes time-independent. Mathematically, we seek a unitary matrix $U(t)$ so that

$$U(t)\mathbf{m}(t) \cdot \hat{\boldsymbol{\sigma}} U^\dagger(t) = \mathbf{m}(0) \cdot \hat{\boldsymbol{\sigma}}, \quad (19.21)$$

where

$$\hat{\boldsymbol{\sigma}} = \begin{pmatrix} \hat{\sigma}_x & 0 \\ 0 & \hat{\sigma}^* \end{pmatrix}. \quad (19.22)$$

The solution is that

$$U(t) = e^{i\Omega t \hat{\rho}_3 \hat{\sigma}_3} \quad (19.23)$$

as can be verified by using the identity

$$e^{i\theta \hat{\rho}_3 \hat{\sigma}_3} = \cos \theta + i \sin \theta \hat{\rho}_3 \hat{\sigma}_3. \quad (19.24)$$

The goal is to make this transformation to the total Usadel equation to see what it looks like in the rotating frame. To do so, we start with the Gorkov equation

$$\begin{aligned} i \frac{\partial}{\partial t_1} \rho_3 \check{G}(1, 2) + i \frac{\partial}{\partial t_2} \check{G}(1, 2) \rho_3 = & \begin{pmatrix} \xi(1) + \lambda(1) & -\Delta(1) \\ -\Delta^*(1) & \xi(1) + \lambda^*(1) \end{pmatrix} \check{G}(1, 2) \\ & - \check{G}(1, 2) \begin{pmatrix} \xi(2) + \lambda^\dagger(2) & -\Delta(2) \\ -\Delta^*(2) & \xi(2) + \lambda^T(2) \end{pmatrix}. \end{aligned} \quad (19.25)$$

We have defined

$$\Delta(1) = i\sigma_2 \Delta(1), \quad (19.26)$$

$$\xi(1) = e\phi(1) - \mu + V_{\text{imp}}(1) \quad (19.27)$$

$$\lambda(1) = -\frac{1}{2m} \nabla^2 - \mathbf{m}(1) \cdot \boldsymbol{\sigma}. \quad (19.28)$$

To make the transition to a rotating coordinate frame, described by primed coordinates, we define

$$\check{G}'(\mathbf{r}, \mathbf{R}, t) = \hat{U}(t_1) \check{G}(\mathbf{r}, \mathbf{R}, t, T) \hat{U}^\dagger(t_2). \quad (19.29)$$

The center-of-mass time dependence via T is transformed away by $\hat{U}$, as we shall see. We want to find the Gor'kov equation for $\check{G}'$. To this end, we insert $\check{G}(1, 2) = \hat{U}^\dagger(t_2) \check{G}' \hat{U}(t_1)$ into Eq. (19.25) and see that the part including the magnetization becomes

$$\begin{aligned} & -\mathbf{m}(t_1) \cdot \hat{\boldsymbol{\sigma}} U^\dagger(t_1) \check{G}'(1, 2) U(t_2) + U^\dagger(t_1) \check{G}'(1, 2) U(t_2) \mathbf{m}(t_2) \cdot \hat{\boldsymbol{\sigma}} \\ & = U^\dagger(t_1) [-\mathbf{m}(0) \cdot \hat{\boldsymbol{\sigma}}, \check{G}'(1, 2)]_- U(t_2). \end{aligned} \quad (19.30)$$

We used that $U(t)\mathbf{m}(t) \cdot \hat{\boldsymbol{\sigma}} U^\dagger(t) = \mathbf{m}(0) \cdot \hat{\boldsymbol{\sigma}}$. It is clear that the transformation of the Green function yields a stationary magnetization. We also need to do the transformation on the other terms and the left hand side of the Gor'kov equation. The left hand side becomes

$$\begin{aligned} i \frac{\partial}{\partial t_1} \rho_3 U^\dagger(t_1) \check{G}'(1, 2) U(t_2) + i \frac{\partial}{\partial t_2} U^\dagger(t_1) \check{G}'(1, 2) U(t_2) \rho_3 &= U^\dagger(t_1) \left(\frac{\Omega}{2} \hat{\sigma}_3 + \frac{\partial}{\partial t_1} \right) \check{G}'(1, 2) U(t_2) + U^\dagger(t_1) \\ &= U^\dagger(t_1) \left(\left[\frac{\Omega}{2} \hat{\sigma}_3, \check{G}'(1, 2) \right]_- + i \rho_3 \frac{\partial}{\partial t_1} \check{G}'(1, 2) + i \frac{\partial}{\partial t_2} \check{G}'(1, 2) \rho_3 \right) U(t_2). \end{aligned} \quad (19.31)$$

We used that $\rho_3, \hat{\sigma}_3, U^\dagger(t_1), U(t_2)$ all commute with each other and that $(\rho_3)^2 = 1$. Note how the left term in the last line of the above equation looks exactly like a new magnetization in the z -direction, which thus can be combined with the transformed, time-independent magnetization terms in Eq. (19.30) to give:

$$U^\dagger(t_1) \left[-\mathbf{m}(0) \cdot \hat{\boldsymbol{\sigma}} - \frac{\Omega}{2} \hat{\sigma}_3, \check{G}'(1, 2) \right]_- U(t_2). \quad (19.32)$$

We see that we are left with a new, effective magnetization in the rotating frame which gains an additional contribution to its z -component proportional to Ω . The transformation with $U^\dagger(t_1) \dots U(t_2)$ leaves all other terms in the Gor'kov equation invariant, such as $\hat{\Delta}(1)$.

If we now multiply our new Gor'kov equation with $U(t_1)$ from the left and $U^\dagger(t_2)$ from the right, we are left with the Gor'kov equation in the rotating frame for the Green function $\check{G}'$:

$$\begin{aligned} i \frac{\partial}{\partial t_1} \rho_3 \check{G}'(1, 2) + i \frac{\partial}{\partial t_2} \check{G}'(1, 2) \rho_3 &= \begin{pmatrix} \xi(1) + \lambda(1) & -\Delta(1) \\ -\Delta^*(1) & \xi(1) + \lambda^*(1) \end{pmatrix} \check{G}'(1, 2) \\ &\quad - \check{G}'(1, 2) \begin{pmatrix} \xi(2) + \lambda^\dagger(2) & -\Delta(2) \\ -\Delta^*(2) & \xi(2) + \lambda^T(2) \end{pmatrix}. \end{aligned} \quad (19.33)$$

The magnetization is now time-independent and has an extra term in the z -direction compared to the original, laboratory frame:

$$\lambda(1) = -\frac{1}{2m} \nabla^2 - \mathbf{m}' \cdot \boldsymbol{\sigma}, \quad \mathbf{m}' = \mathbf{m}(0) + \frac{\Omega}{2} \hat{\mathbf{z}}. \quad (19.34)$$

Note how the extra term Ω appears just due to the coordinate frame change even if there is no magnetization to start with ($\mathbf{m} = 0$).

We can now proceed and perform the standard quasiclassical treatment and derive an Usadel equation which will be stationary without any time-dependent magnetization. After solving the Usadel equation in the rotating frame, we can then easily transform back to the Green function solution in the laboratory frame and compute physical quantities such as spin currents and spin accumulations.

Although the Usadel equation in the rotating frame has no center-of-mass time dependence, attaching the ferromagnet to a normal metal will now turn into a non-equilibrium problem. The reason is that we should not only transform the Usadel equation, but also the boundary conditions to adjacent materials. As we will see below, this results in non-equilibrium boundary conditions where the normal metal (as seen from the rotating frame) is seen to have a spin accumulation.

Transformation of boundary conditions in rotating frame The quasiclassical Keldysh Green function may be parametrized as follows in general:

$$g^K = g^R \circ h - h \circ g^A. \quad (19.35)$$

Here, h is the distribution function matrix and the $\circ$ -product is defined via

$$(f \circ g)(t_1, t_2) = \int dt_3 f(t_1, t_3) g(t_3, t_2). \quad (19.36)$$

Fourier-transforming the relative time-coordinate $t_1 - t_2$, we get

$$(f \circ g)(T, E) = \int dt (f \circ g)(T, t) e^{iEt}. \quad (19.37)$$

The relation between the lab-frame quasiclassical Green function $\hat{g}$ and the rotating frame Green function $\hat{g}'$ is (as can be seen by applying the quasiclassical approximation to the Gor'kov Green function):

$$\hat{g}(t, T) = U^\dagger(t_1) g'(t) U(t_2). \quad (19.38)$$

Thus, we have

$$\begin{aligned} \hat{g}(E, T) &= \int dt e^{iEt} \hat{g}(t, T) \\ &= \frac{1}{2\pi} \int \int dE' dt e^{i(E-E')t} U^\dagger(t_1) \hat{g}'(E) U(t_2). \end{aligned} \quad (19.39)$$

This transformation means that the lab-frame Green function matrix can be expressed using the rotating Green function matrix, but where the elements of the latter will have shifted energy-arguments or additional exponential terms of the type $e^{\pm i\Omega T}$. To see this, we first note that

$$U^\dagger(t_1) \hat{g}'(E) U(t_2) = \begin{pmatrix} g'_{11} e^{-i\Omega t/2} & g'_{12} e^{-i\Omega T} & g'_{13} e^{-i\Omega T} & g'_{14} e^{-i\Omega t/2} \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

Inserting this into Eq. (19.39) then gives

$$\hat{g}(E, T) = \begin{pmatrix} g'_{11}(E - \Omega/2) & g'_{12}(E) e^{-i\Omega T} & g'_{13}(E) e^{-i\Omega T} & g'_{14}(E - \Omega/2) \\ \dots & \dots & \dots & \dots \end{pmatrix}.$$

Thus, every element of the lab Green function either gains a center-of-mass dependence T or experiences an energy shift relative the rotating frame Green function.

Let us now apply this to the boundary condition to see what it looks like in the stationary frame. It reads

$$2\zeta L \hat{g} \circ \nabla \hat{g} = [\hat{g}_L(E, T) \circ, \hat{g}_R(E, T)]. \quad (19.40)$$

The circle-product on the rhs looks troublesome. However, the following identity makes the evaluation of the circle product easier. If $f(E, T) = e^{i\omega_1 T} f(E)$ and $g(E, T) = e^{i\omega_2 T}$, then

$$(f \circ g)(E, T) = e^{i(\omega_1 + \omega_2)T} f(E - \omega_2/2) g(E + \omega_1/2). \quad (19.41)$$

Using this relation, we find that if one has an energy-dependent matrix A' in the rotating frame (for instance the distribution function matrix h), then in the laboratory frame this matrix has the form

$$\hat{A}(E, T) = \begin{pmatrix} A'_{11}(E - \Omega/2) & A'_{12}(E) e^{-i\Omega T} & A'_{13} e^{-i\Omega T} & A'_{14}(E - \Omega/2) \\ A'_{21}(E) e^{i\Omega T} & A'_{22}(E + \Omega/2) & A'_{23}(E + \Omega/2) & A'_{24}(E) e^{i\Omega T} \\ \dots & \dots & \dots & \dots \end{pmatrix} \quad (19.42)$$

The final identity we will need to evaluate the KL boundary conditions is the following. Let $C' = A'B'$ be an energy-dependent Green function or distribution function matrix in the rotating frame. Then the ring product of the matrices in the lab frame is

$$C(E, T) = A(E, T) \circ B(E, T) = \begin{pmatrix} C'_{11}(E - \Omega/2) & C'_{12}(E)e^{-i\Omega T} & C'_{13}(E)e^{-i\Omega T} & C'_{14}(E - \Omega/2) \\ C'_{21}(E)e^{i\Omega T} & C'_{22}(E + \Omega/2) & C'_{23}(E + \Omega/2) & C'_{24}(E)e^{i\Omega T} \\ \dots & \dots & \dots & \dots \end{pmatrix}. \quad (19.43)$$

This can be verified using

$$\begin{aligned} (A(E, T) \circ B(E, T))_{11} &= A'_{11}(E - \Omega/2) \circ B'_{11}(E - \Omega/2) + A'_{12}(E)e^{-i\Omega T} \circ B'_{21}(E)e^{i\Omega T} + \dots \\ &= A'_{11}(E - \Omega/2)B'_{11}(E - \Omega/2) + A'_{12}(E - \Omega/2)B'_{21}(E - \Omega/2) + \dots \\ &= C'_{11}(E - \Omega/2). \end{aligned} \quad (19.44)$$

Now we have everything we need to evaluate the KL boundary conditions. Denote the (i, j) component of $\hat{g}'(E)\nabla\hat{g}'(E)$ as $\Gamma'_{ij}(E)$ and use the above identifies to write

$$2\zeta L\hat{g} \circ \nabla\hat{g} = 2\zeta L \begin{pmatrix} \Gamma'_{11}(E - \Omega/2) & \Gamma'_{12}(E)e^{-i\Omega T} & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}. \quad (19.45)$$

For the rhs of the KL boundary condition, denoting the (i, j) component of $[\hat{g}'_L(E), \hat{g}'_R(E)]$ as $\Pi'_{ij}(E)$, we get

$$[\hat{g}'_L(E, T) \circ, \hat{g}'_R(E, T)] = \begin{pmatrix} \Pi'_{11}(E - \Omega/2) & \Pi'_{12}(E)e^{-i\Omega T} & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}. \quad (19.46)$$

An important observation is that the center-of-mass dependence and exponentials cancel for each individual element when comparing the lhs and rhs of the KL boundary condition. Therefore, we can make an energy substitution for each individual element so that for every element we have

$$\Gamma'_{ij}(E) = \Pi'_{ij}(E) \quad (19.47)$$

which can be written simply as a stationary KL boundary condition for the rotating frame Green function $\hat{g}'$:

$$2\zeta L\hat{g}'(E)\nabla\hat{g}'(E) = [\hat{g}'_L(E), \hat{g}'_R(E)]. \quad (19.48)$$

We can now solve for the rotating frame Green function using the above boundary condition and the Usadel equation in the rotating frame, which has no time-dependence, and then transform back to the Green function in the stationary frame. Note that the Usadel problem in the rotating frame becomes a non-equilibrium one since if, say, the $\hat{g}'_R$ in Eq. (19.48) corresponds to a stationary BCS superconductor in the lab frame, it will have a non-equilibrium form in the rotating frame. For instance, if the distribution function $\hat{h}$ is equilibrium in the lab frame:

$$\hat{h} = \text{diag}[\tanh(\beta E/2)], \quad (19.49)$$

then in the rotating frame one finds [according to Eq. (19.42)]

$$\hat{h} = \begin{pmatrix} \tanh[\beta(E + \Omega/2)/2] & 0 & 0 & 0 \\ \tanh[\beta(E - \Omega/2)/2] & 0 & 0 & 0 \\ \tanh[\beta(E - \Omega/2)/2] & 0 & 0 & 0 \\ \tanh[\beta(E + \Omega/2)/2] & 0 & 0 & 0 \end{pmatrix}. \quad (19.50)$$

Parametrizing the distribution function matrix as

$$\hat{h} = \sum_n \hat{\rho}_n h_n \quad (19.51)$$

where

$$\begin{aligned} \hat{\rho}_1 &= \tau_0 \sigma_0, \quad \rho_2 = \tau_0 \sigma_1, \dots \\ \hat{\rho}_5 &= \tau_3 \rho_0, \quad \hat{\rho}_6 = \tau_3 \rho_1, \dots, \end{aligned} \quad (19.52)$$

one finds that the spin-current polarized in the z -direction evaluated in the lab frame equals

$$I_s^z = \frac{N_0 D}{2} \int dE \left[\frac{dh_8(E + \Omega/2)}{dx} + \frac{dh_8(E - \Omega/2)}{dx} \right] \quad (19.53)$$

which when inserting the solution for h_8 (obtained by first solving the equations for $\hat{h}'$ in the rotating frame and then transforming these to the lab frame) gives

$$I_s^z = N_0 D \frac{M_x^2}{(M')^2} \Omega \kappa [C_1 \sinh(\kappa x) + C_2 \sin(\kappa x)], \quad (19.54)$$

where C_1, C_2 are two constants and $M' = |\mathbf{M}'|$ is the magnitude of the effective exchange field in the rotating frame, $\mathbf{M}' = (M \sin \theta, 0, M \cos \theta + \Omega/2)$. As expected, the spin current vanishes both if $\Omega = 0$ or if $M = 0$.

The spin accumulation should also vanish in the limit $M = 0$. However, note that the spin accumulation (in the z -direction) computed in the rotating frame does not vanish. This is because the spin accumulation is given quasiclassically by

$$\boldsymbol{\mu} = \int dE \text{Tr} \{ \boldsymbol{\sigma} \hat{g}^K \} \quad (19.55)$$

and due to the fact that $\hat{g}^R$ equals unity for a quasiclassical ferromagnet, i.e. the different DOS for spins is not taken into account. However, if one instead uses the full Green function in order to compute the *total* magnetization:

$$\mathbf{m} = \int dE \text{Tr} \{ \boldsymbol{\sigma} \hat{G}^K \} \quad (19.56)$$

one would find that the total magnetization in the z -direction vanishes also in the rotating frame since the shift in distribution functions would be cancelled by the different DOS for spins due to the extra $\Omega/2$ exchange field appearing in the Usadel equation. Recall that the retarded Green function matrix (nonquasiclassical) is obtained from

$$G^R = (E + i\delta - \xi_{\mathbf{k}} - \mathbf{h} \cdot \boldsymbol{\sigma})^{-1} \quad (19.57)$$

which thus takes into account the exchange field in the Usadel equation.

Another point that is worth to note is that if $\theta = \pi/2$, so that the magnetization $\mathbf{M}$ is precessing in the xy -plane without any z -component, there is still a spin accumulation induced in the z -direction and hence a spin-current flows polarized to the z -axis. This can again be seen by using the full expression for G^R with $\mathbf{h} = (M, 0, \Omega/2)$ which enters the Usadel equation. The total magnetization

m_z in the ferromagnet is obtained using $G_{\sigma\sigma}^R$ and these are now dependent on M as can be seen by evaluating Eq. (19.57).

More intuitive physical explanation using torques

The fact that the rotating magnetization in the xy -plane can induce a spin accumulation in the z -direction can be understood by considering some basic equations. The localized magnetization is $\mathbf{M} = -\gamma\hbar\langle\hat{\mathbf{S}}(\mathbf{r}, t)\rangle$ and the magnetization of the conduction electrons is $\mathbf{m} = -\gamma_e\hbar\langle\hat{\mathbf{s}}(\mathbf{r}, t)\rangle$. The Hamiltonian describing the $s-d$ coupling between the localized and conduction electrons is:

$$H_{sd} = -J_{sd} \int d\mathbf{r} \hat{\mathbf{S}} \cdot \hat{\mathbf{s}}, \quad (19.58)$$

whereas the Zeeman-coupling to the external field is

$$H_Z = \gamma\hbar \int d\mathbf{r} \hat{\mathbf{S}} \cdot \mathbf{B}_{\text{eff}} + \gamma_e\hbar \int d\mathbf{r} \hat{\mathbf{s}} \cdot \mathbf{B} \quad (19.59)$$

Here, $\mathbf{B}_{\text{eff}}$ is the effective field acting on the localized spins, including the external applied field $\mathbf{B}$, demagnetization field, magnetocrystalline anisotropy, et.c. The spin operators are

$$\begin{aligned} \hat{\mathbf{S}}(\mathbf{r}, t) &= \sum_i \hat{\mathbf{S}}_i(t) \delta(\mathbf{r} - \mathbf{r}_i), \\ \hat{\mathbf{s}}(\mathbf{r}, t) &= \sum_{\sigma\sigma'} \psi_{\sigma'}^\dagger(\mathbf{r}, t) \boldsymbol{\sigma}_{\sigma'\sigma} \psi_{\sigma}(\mathbf{r}, t). \end{aligned} \quad (19.60)$$

Equations of motion are obtained via $d\hat{\mathbf{S}}/dt = i\hbar^{-1}[H, \hat{\mathbf{S}}]$ and then taking the expectation value:

$$\partial_t \mathbf{M} = -\gamma \mathbf{M} \times \mathbf{B}_{\text{eff}} - \gamma J_{sd} \mathbf{M} \times \mathbf{m} + \alpha \mathbf{M} \times \partial_T \mathbf{M}, \quad (19.61)$$

where $J_{\text{ex}} \propto J_{sd}$. Similarly, $d\hat{\mathbf{s}}/dt = i\hbar^{-1}[H, \hat{\mathbf{s}}]$ and taking expectation value:

$$\partial_t \mathbf{m} = -\gamma_e \mathbf{m} \times \mathbf{B} - \gamma_e J_{\text{ex}} \mathbf{m} \times \mathbf{M} - \frac{\delta \mathbf{m}}{\tau_{\text{sf}}} + \nabla \mathbf{j}_m. \quad (19.62)$$

Here, the spin current density is the expectation value of the operator

$$\hat{\mathbf{j}}_m(\mathbf{r}, t) = -\gamma_e \hbar \sum_{\sigma\sigma'} \text{Re} \left\{ \psi_{\sigma'}^\dagger(\mathbf{r}, t) \boldsymbol{\sigma}_{\sigma'\sigma} \left(\frac{\hbar \nabla}{im_e} \right) \psi_{\sigma}(\mathbf{r}, t) \right\}. \quad (19.63)$$

Phenomenologically, we also added a damping term $\alpha \mathbf{M} \times \partial_t \mathbf{M}$ to the equation of motion for the localized spins. Similarly, we added a spin relaxation term $\propto 1/\tau_{\text{sf}}$ on phenomenological grounds where $\delta \mathbf{m} \equiv \mathbf{m} - \mathbf{m}_0$ and $\mathbf{m}_0 = m_0 \mathbf{M}/M$ is the instantaneous value of the localized spin which is the equilibrium local value. Finally, the spin current will be treated in the diffusive limit so that $\mathbf{j}_m = -D \nabla \mathbf{m}$ where D is the diffusion constant.

In what follows, we neglect the applied field (dc as well as ac, in addition to any contribution from demagnetization/demagnetization fields, et.c.) effect on $\mathbf{m}$ for simplicity, because it is not necessary to explain the spin pumping effect. Including it does not change anything qualitatively so long that the dynamics of $\mathbf{M}$ and $\mathbf{m}$ occurs at different time-scales so that they can become misaligned, which is reasonable. Moreover, the localized spin magnitude is typically much larger than

$\hbar/2$, causing the coupling of the the $\mathbf{B}$ field to $\mathbf{M}$ to be quantitatively larger than its coupling to $\mathbf{m}$.

The two coupled equations of motions for $\mathbf{m}$ and $\mathbf{M}$ can be solved, as shown in chapter 35 of Ref. XX. To make the transition from eq. (12) to (13) in that reference, perform a Fourier-transformation first, to obtain an equation of the type $(k^2 + c)\delta\mathbf{m}(k, t) = d$ where c, d are constants. This gives $\delta\mathbf{m}(k, t) = d/(k^2 + c)$. Now perform an inverse Fourier-transformation to obtain $\delta\mathbf{m}(x, t)$ and the result is precisely eq. (13). Namely, the result is (for a 1D model with the ferromagnet localized at $x = 0$)

$$\delta\mathbf{m}(x, t) = -\frac{\chi_e}{\gamma_e} \left[\frac{1}{1 + \Gamma_a^2} (\mathbf{M} \times \partial_t \mathbf{M}) + \frac{\Gamma_a}{1 + \Gamma_a^2} \partial_t \mathbf{M} \right] e^{-|x|/\lambda_s}. \quad (19.64)$$

The meaning of the symbols are given in detail in Ref. XX, but the important point to note is that $\mathbf{M} \times \partial_t \mathbf{M}$ points along the direction of the $\mathbf{B}$.

What we see is that the above equations show that the localized magnetization $\mathbf{M}$ will act with a torque on the conduction electron spins $\mathbf{m}$, since the spins of the conduction electrons will try to follow the exchange field $\mathbf{M}$ as it rotates. When the conduction electron spins and exchange field $\mathbf{M}$ become misaligned due to the rotating magnetization, a torque appears which points in the z -direction. This results in a small z -component of $\delta\mathbf{m}$, the deviation of the conduction spin magnetization from the instantaneous value of $\mathbf{M}$, i.e. along the applied field $\mathbf{B}$. This non-equilibrium magnetization $\delta\mathbf{m}$ polarized along $\mathbf{B}$ manifests itself precisely through the effective magnetic field and non-equilibrium distribution functions in the quasiclassical theory given above. Finally, we can then understand why a spin accumulation is induced in N: it is because of the $\delta\mathbf{m}$ which will leak into N (like a proximity effect) and then establish a stationary situation when the spin backflow is equally large as the in-flow of spin (due to the diffusion current $\mathbf{j} \propto \nabla \mathbf{m}$). The amount of spin-flip scattering in N will also influence how much spin accumulation that is built up close to the interface. The spin accumulation induced in N represents a loss of angular momentum from F, which is manifested as an increased Gilbert damping coefficient for the localized spins $\mathbf{M}$. This can be seen by inserting the solution for $\delta\mathbf{m}$ into the equation of motion for $\mathbf{M}$: it renormalizes the Gilbert damping coefficient. Physically, this means that the spin-pumped current provides an additional outlet for magnetization loss besides the usual Gilbert damping processes, causing relaxation of $\mathbf{M}$ to occur faster. This should be related to $\mathbf{m}$ relaxing faster toward the direction of $\mathbf{B}$ when spin-current polarized along $\mathbf{B}$ flows out of F (in order to conserve angular momentum in the z -direction), thus dragging $\mathbf{M}$ along with it.

Thus, the quasiclassical expression is useful to compute the spin current across the junction, but not the total magnetization in either the N or F region in the rotating frame, since the quasiclassical expression ignores the difference in DOS for the different spins. For instance, one can compute spin-pumping in a reservoir/N/F/reservoir system with F precessing and then compute the spin accumulation and spin current flowing in the N region. Both of these expressions, evaluated quasiclassically in the lab-frame, should then be entirely accurate since there is no magnetization in the N region.

19.6.2 Ferromagnetic insulator/normal metal

A precessing magnetization generates magnon excitations. This can be seen by writing down the H-P transformed Hamiltonian of a Heisenberg model with a dc field along the quantization axis (for instance z) and an ac field along a transverse axis (for instance x). Coupling the FI to a normal

metal allows for spin-dependent reflection of electrons that scatter at the interface. The electrons can absorb or emit a magnon into the FI and flip their spins in the process. This causes a spin current being transferred into the normal metal. I am not aware of any simple way to see that the magnon-electron scattering at the interface leads to up and down spins moving in opposite directions, but a calculation of the tunneling spin current via Keldysh Green functions and using Langreth's theorem shows that it is finite. This demonstrates that the spin-flip at the interface is preferential in the sense that it gives rise to a finite spin current flowing into N.

It is worth to remark that the perturbative calculation of the tunneling spin current gives a finite result even if we set the dc magnetic field to zero, so that only the transverse field is required. However, if the dc magnetic field is set to zero, the spin current diverges when the frequency of the ac field goes to zero. This is not physically reasonable since a static transverse field should not induce a magnon spin current. Moreover, it breaks the assumption of a tunneling perturbation. Therefore, a dc field is required in the calculation.

We can compute the spin-pumping in this kind of structure using the Schrödinger equation and scattering wavefunctions as shown in *Physics of the Solid State* **61**, No. 9, pp. 1583–1589 (2019). Some comments are in order due to typos in that manuscript. First, we find the general eigenstates in ferromagnet. There are two of these: $\psi_{\pm}^F$ given in eq 4. As we discussed, the Ω in the $e^{\pm i\Omega t}$ factor should be $\Omega/2$ in eq 4.

The, we find the general eigenstates in the normal metal. There are two of these: $\psi_{\pm}^N$ given in eqs 8 and 9.

Now, we want to match these eigenstates using the continuity of the wavefunction and its derivative. Consider the boundary condition involving continuity of the wavefunction. We are considering an incident electron from the N side toward the F side. Therefore, the general wavefunction on the N side will consist of an incoming electron and reflected electrons: there are two possible reflections (up and down) since we can have spin-flip at the interface due to the precessing magnetization. This gives us the total wavefunction eq. 11.

In eq. 11, the energies epsilon depend on the wavevector according to eq 10. Therefore, the epsilon in the first two terms of eq. 11 is really $\epsilon = \epsilon(k)$. The epsilon the last term of eq 11 is really $\epsilon = \epsilon(k')$. We have allowed k to be different from k' in general. We will see that this is required when we examine the boundary conditions more carefully. Note that if we define

$$\epsilon' = \epsilon(k') \quad (19.65)$$

then the epsilon in the last term of eq 11 should be ϵ' . But if we understand the epsilon in the last term of eq 11 as $\epsilon(k')$, then it is correct as it stands.

Now, we need the general wavefunction on the F side. It will be a superposition of the two possible eigenstates given in eq 4 that are moving away from the interface (since they are produced from an incoming electron). The author uses the notation $\epsilon_{1,2}$, but this is unnecessary. We can just use the notation $\epsilon_{\pm}$ to compare more easily with eq. 4. With this notation, the wavefunction on the F side is (eq 12):

$$\psi_L = \zeta_+ [C\psi_+^F(\epsilon_+, k_+) + D\psi_-^F(\epsilon_-, k_-)] \quad (19.66)$$

Note that we are writing this in a general way: both the energies ($\epsilon_{\pm}$) and the momenta ($k_{\pm}$) can be different from each other.

Finally, let us now use the boundary conditions to derive the same relations that the author has done. We consider continuity of the wavefunction. This means that the upper line of

$$\psi_{L+} = \zeta_+[C\psi_+^F(\epsilon_+, k_+) + D\psi_-^F(\epsilon_-, k_-)] \quad (19.67)$$

should equal the upper line of eq. 11 in the paper at $x = 0$ for any time t . The only way to achieve this, is to make sure the time-dependence on all terms are identical. This gives us the condition

$$-\epsilon_+(k_+) - \Omega/2 = -\epsilon(k) = -\epsilon_-(k_-) - \Omega/2 [EQ1] \quad (19.68)$$

Similarly, the continuity of the second line of the wavefunctions gives us the condition

$$-\epsilon_+(k_+) + \Omega/2 = -\epsilon(k') = -\epsilon_-(k_-) + \Omega/2 [EQ2]. \quad (19.69)$$

We can now draw several conclusions mathematically. One conclusion is that $\epsilon_+(k_+) = \epsilon_-(k_-)$ which in the notation of the author means $\epsilon_1 = \epsilon_2$. This is consistent with his definitions of ϵ_1 and ϵ_2 . It also follows that

$$\epsilon_+(k_+) = \epsilon(k) - \Omega/2\epsilon_-(k_-) = \epsilon(k) - \Omega/2 \quad (19.70)$$

Since we are using the notation $\epsilon_{\pm}(k_{\pm}) = \epsilon_{1,2}$, this is entirely consistent with the paper. By solving the two above equations for $k_{\pm}$, we get eq. 13.

Now, we can also see how he obtains eq 14. Combine the second equality sign in [EQ 1] and the second equality sign in [EQ 2] above to get:

$$\epsilon(k') = \epsilon(k) - \Omega. \quad (19.71)$$

This is consistent with eq. 14. Note again that this is correct since the author uses the notation $\epsilon' = \epsilon(k')$.

19.6.3 Spin-to-charge conversion via spin pumping

There are two important mechanisms for spin-to-charge conversion that depend on spin-orbit interactions. One is the inverse spin Hall effect. The other one is the inverse Rashba-Edelstein effect (also known as spin-galvanic effect). The spin-to-charge conversion can be probed by pumping a spin current from a ferromagnet into a layer with spin-orbit coupling where it is converted into a transverse charge current which gives rise to a measurable voltage.

The quantitative measure of the spin-to-charge conversion efficiency is slightly different for these two mechanisms. Consider first the inverse spin Hall effect. A spin current induces a charge current in a bulk material, and this is not a surface effect in general: it can arise from extrinsic impurities in the material. Therefore, one defines the spin Hall angle θ as

$$\theta_{\text{SH}} = \frac{\hbar}{2e} \frac{j_c}{j_{s,\text{physical}}}. \quad (19.72)$$

The subscript physical is meant to emphasize that a physical charge current density has units A/m², whereas a physical spin current density has different dimension since a spin current carries units of $\hbar/2$ (spin angular momentum) rather than charge e . However, it is common in the literature to define a normalized spin current j_s which has the same dimension as the charge current:

$$j_s = \frac{2e}{\hbar} j_{s,\text{physical}} \quad (19.73)$$

so that the dimensions of j_s and j_c are the same. In this case, the spin Hall angle simply reads:

$$\theta_{\text{SH}} = \frac{j_c}{j_s} \quad (19.74)$$

and both current densities have units A/m².

Now let us consider the inverse Rashba-Edelstein effect. This is a surface effect, which means that the induced charge current flows in a 2D plane. Note that a current density in 2D has dimension A/m, in contrast to a current density in 3D which has dimension A/m². This is because a density in 3D is current per cross sectional area whereas a density in 2D is current per width. Therefore, the measure λ_{REE} of the spin-to-charge conversion efficiency in the case of the inverse Rashba-Edelstein effect has dimension length:

$$\lambda_{\text{REE}} = \frac{j_c^{2\text{D}}}{j_s}. \quad (19.75)$$

In order to compare this conversion efficiency with the spin Hall mechanism, one can multiply θ_{SH} with the thickness t of the region in which the charge current flows. In other words, if one experimentally measures a spin Hall angle in a sample of thickness $t \ll l_{\text{sf}}$ where l_{sf} is the spin diffusion length and wants to compare that spin-to-charge conversion efficiency with the inverse Rashba-Edelstein effect at an interface layer, we can compute an effective "spin Hall" angle θ_{REE} corresponding to the Rashba-Edelstein effect as follows:

$$\theta_{\text{REE}} = \lambda_{\text{REE}}/(t/2). \quad (19.76)$$

The factor 1/2 is there because of theoretical details which are not important here. Typically, θ_{REE} would be much larger than θ_{SH} , indicating the the inverse Rashba-Edelstein effect is much more efficient than the inverse spin Hall effect in converting spin to charge.

Returning now to the pumped spin current, an expression was derived for this spin current density in J. Appl. Phys. **109**, 103913 (2011):

$$j_s = \frac{g_r^{\uparrow\downarrow} \gamma^2 \hbar (\mu_0 h_{\text{rf}})^2 [\mu_0 M \gamma + \sqrt{(\mu_0 M \gamma)^2 + 4\omega^2}]}{8\pi\alpha^2 [(\mu_0 M \gamma)^2 + 4\omega^2]} \frac{2e}{\hbar}. \quad (19.77)$$

Since the units of $g_{\uparrow\downarrow}^r$ is nm⁻² and $\mu_0 h_{\text{rf}}$ is T, the units of the above spin current density is A/m².

Let us now consider the work by Lesne *et al.* in Nature Materials 2016, where they study spin-to-charge conversion at oxide interfaces. The first odd thing is that despite using the same expression in their Eq. (3) as our expression for j_s above, they end up with a unit for j_s which is not A/m², but A/(m² G²) where G is Gauss. This is not consistent with their Eq. (3). To understand what is going on, we can consider their definition of a charge current density in 2D which is given in the text

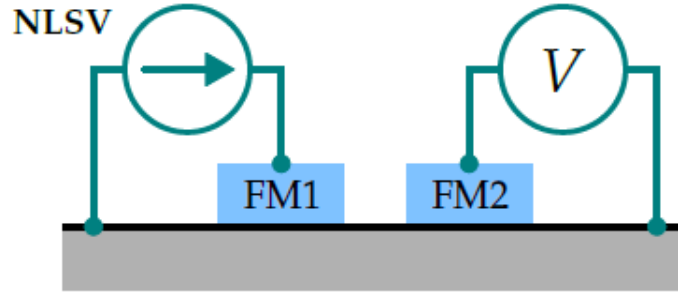


Figure 19.4: (Color online) Non-local spin-valve setup for measuring non-local electrical resistance.

above Eq. (3). There, they have an extra factor h_{rf}^2 in the denominator, which is not standard. A 2D current density should, as explained above, have units A/m. However, since they have an extra factor h_{rf}^2 their $j_c^{2\text{D}}$ has dimension A/(m G²). Because of this, I suspect that when they cite their value of $j_s = 8.4 \times 10^6 \text{ A m}^{-2} \text{ G}^{-2}$ in the text below Eq. (3) [which is not dimensionally consistent with Eq. (3)], they have divided on an extra factor of h_{rf}^2 without writing this in the text. This is rather confusing, since they both use a non-standard definition of a charge current density *and* their analytical expression for j_s and obtained numerical value for j_s are not consistent.

19.7 Non-local spin-valve resistance

In a non-local geometry shown in the figure, the spin and charge currents become separated. The left ferromagnet F1 injects a current into N which causes a spin accumulation as explained previously. On the left-hand side of the structure, where the charge current I flows, the spin accumulation is subject to both drift and diffusion. To the right, however, the spin transport occurs only via diffusion meaning that $\Delta\mu$ decays exponentially with distance from the spin generating contact. In order to detect this spin accumulation, one uses an open circuit as shown on the right-hand side where a potential drop develops between F2 and N. This detection scheme was initially used in all-metallic spin valves and later used to study transport in ferromagnet/semiconductor systems.

We illustrate the concept of non-local resistance by using fully polarized ferromagnets F1 and F2 for simplicity as shown in Fig. XX. Applying a voltage V_i across the F1/N interface leads to a spin-current and induces a spin accumulation $\Delta\mu$ in the non-magnetic channel which is shown in the figure. After diffusing toward F2, the spin accumulation forces the chemical potential in F2 to adjust so that no charge current I can flow into F since the circuit is open in the right end. This mechanism results in the appearance of a spin-induced non-local voltage, measurable via a standard voltmeter.

Background signals such as non-local resistances can appear due to other effects, but the spin-dependent signal can be identified explicitly by switching the relative magnetization orientation of F1 and F2. When F1 is kept fixed and F2 switched between a P and AP configuration relative F1, the non-local voltage changes by $\Delta V = \Delta\mu$ (assuming that F2 is fully spin-polarized) as shown in Fig. 19.5. If it is not fully polarized, a spin detection efficiency less than unity has to be taken into account. Spin transport can also be studied using the manipulation of spin accumulation through an external field via the Hanle effect.

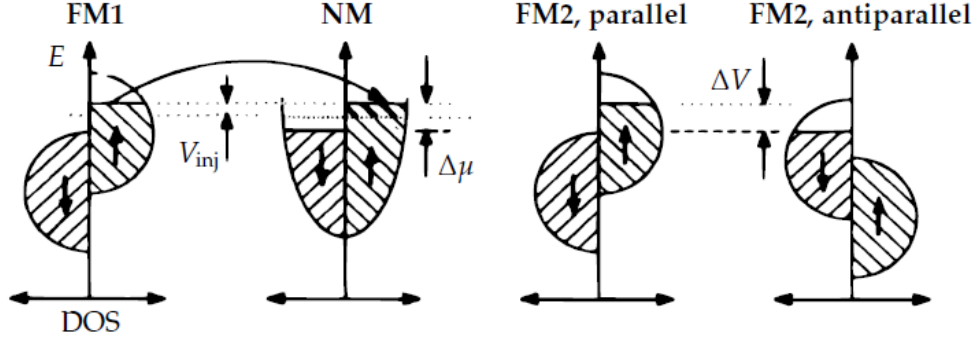


Figure 19.5: (Color online) Schematic representation of the density of states as a function of energy E for the ferromagnetic injector F1, the normal metal N, and the ferromagnetic detector F2 in the non-local spin-valve geometry. The applied voltage V_{inj} causes spin accumulation $\Delta\mu$ to build up in N (it does not in general have to be equal to $\Delta\mu$ as shown in this particular figure). This spin accumulation is detected in F2 and results in a voltage change ΔV upon magnetization reversal. Above, we neglected spin relaxation in N since $\Delta\mu$ is seen to be equally large at the injector and detector electrode.

The change in non-local voltage upon reversing the magnetization configuration can be shown to equal

$$\Delta V = P \Delta\mu \quad (19.78)$$

by using that no electric current flows ($I = 0$). Here, P is the spin polarization of the detector tunnel conductance:

$$P = \frac{G_{\uparrow} - G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}} \quad (19.79)$$

where $\Delta\mu$ is the spin accumulation in the normal metal at the detector site. The derivation of the above formula goes as follows. At the F2/N detector point, the currents are given by

$$\begin{aligned} I_{\uparrow} &= G_{\uparrow}(V_{\uparrow} - \mu_{\uparrow}), \\ I_{\downarrow} &= G_{\downarrow}(V_{\downarrow} - \mu_{\downarrow}). \end{aligned} \quad (19.80)$$

Here, V_{σ} is the electrochemical potential for spin σ in the detector electrode whereas μ_{σ} is the electrochemical potential for spin σ in the normal metal where the spin accumulation has diffused from the injector site. The detector part of the circuit is open, meaning no electric current can flow. Therefore, $I_{\uparrow} + I_{\downarrow} = 0$. This gives

$$G_{\uparrow}(V_{\uparrow} - \mu_{\uparrow}) + G_{\downarrow}(V_{\downarrow} - \mu_{\downarrow}) = 0. \quad (19.81)$$

The electric voltage in the detector is $V = (V_{\uparrow} + V_{\downarrow})/2$ whereas the spin accumulation in the detector is $\Delta\mu^{\text{det}} = V_{\uparrow} - V_{\downarrow}$. Similarly, in the normal metal we have $\mu_{\sigma} = \mu_0 + \sigma\Delta\mu/2$ so that the voltage is μ_0 and the spin accumulation is $\Delta\mu$. Finally, the voltage *difference* between the detector and normal metal (which is what is measured experimentally for either the P or AP alignment) is

$$\delta V = V - \mu_0. \quad (19.82)$$

Note that the voltage μ_0 is constant throughout the normal metal since there is no charge accumulation. Inserting these relations into the condition that the total current is zero gives

$$G_{\uparrow}(\delta V - \Delta\mu/2 + \Delta\mu^{\text{det}}/2) + G_{\downarrow}(\delta V + \Delta\mu/2 - \Delta\mu^{\text{det}}/2) = 0, \quad (19.83)$$

which is rearranged to

$$\delta V = P \left(\frac{\Delta\mu}{2} - \frac{\Delta\mu^{\text{det}}}{2} \right). \quad (19.84)$$

Assuming that we can neglect the spin accumulation in the detector electrode, which is accomplished by assuming a very short spin-relaxation length there satisfying $\lambda_S^{\text{det}}/L^{\text{det}} \ll 1$, we get $\delta V = P\Delta\mu/2$. So the difference in voltage between the P and AP alignment of the detector and injector electrode is then

$$\Delta V = \delta V|_{\text{P alignment}} - \delta V|_{\text{AP alignment}}. \quad (19.85)$$

This gives

$$\Delta V = P\Delta\mu. \quad (19.86)$$

We can also express this in terms of the spin accumulation in the normal metal at the *injector site* as follows:

$$\Delta V = P\Delta\mu^{\text{inj}} e^{-d/\lambda_S^N} \quad (19.87)$$

where d is the distance from the injector electrode to the detector electrode, λ_S^N is the spin relaxation length in the normal metal.

19.7.1 Using spin-dependent tunnel barrier for efficient spin injection

Allowing the tunnel barrier to be explicitly spin-dependent (using *e.g.* a ferromagnetic insulator as the interface) enhances spin injection. To see this, consider for simplicity an interface without spin-flip processes. The current in each channel is then conserved upon tunneling through the interface and we let g^{σ} be the tunneling conductance for spin σ .

19.8 Key effects coupling spin, heat, and charge flow

We here list some important physical effects that describe the coupling between spin, heat, and charge currents in non-equilibrium situations.

19.8.1 Edelstein effect

Steady charge current driven by electric field produces a steady non-equilibrium spin-polarization [3].

Inverse: production of a steady charge current due to an induced non-equilibrium spin-polarization (the latter produced *e.g.* via external field). This is also known as the spin-galvanic effect.

The mechanism responsible for the conversion is spin-orbit coupling in both cases.

The Edelstein-effect (also known as Rashba-Edelstein effect) is an intrinsic mechanism, meaning that it relies on Rashba spin-orbit interactions due to inversion asymmetry in the structure. Consider a 2D material with Rashba interactions. The Edelstein-effect produces a spin accumulation that lies in the same plane as the material, and diffusion of this spin current into a different layer can thus cause a spin current that is polarized in the plane of the material. This is different from the spin current produced by the spin Hall effect, which is polarized out-of-plane (perpendicular to both the injected charge current and the flow of the resulting spin current).

Besides the polarization direction of the spin current produced by an Edelstein-effect and a spin Hall-effect being different, another difference is that the Edelstein effect is an intrinsic mechanism whereas the spin Hall effect can have both an intrinsic and extrinsic (impurities) contribution.

The appearance of a non-equilibrium spin accumulation in the Edelstein effect can be understood as follows. In equilibrium, the Fermi surfaces in the presence of Rashba SOC are two concentric circles where the spin expectation value rotates as one moves around the circle. The spin expectation value is opposite on the two surfaces and in both cases perpendicular to the momentum direction. When applying a current, the distribution function shifts the Fermi surfaces horizontally since the relevant distribution function becomes $f(E_{\mathbf{k}}) \rightarrow f(E_{\mathbf{k}+c\mathbf{E}\tau})$ where c is a constant. This can be understood physically from there will now be more electrons moving in a certain direction than the other in the presence of a current. Therefore, the Fermi surfaces maintain their spin rotation pattern but are shifted horizontally. Importantly, the spin expectation value of the rotating spin on each surface is no longer equal in magnitude on the opposite side of each surface. Therefore, a net spin accumulation arises in the direction perpendicular to the current flow, as can be seen by computing the total spin expectation value for the system $\langle \mathbf{S} \rangle = \int \mathbf{S}_{\mathbf{k}} f_{\mathbf{k}} d\mathbf{k}$.

The appearance of an out-of-plane (z) polarized spin current flowing in the y -direction for a current applied in the x -direction in the spin Hall case can be understood from the following argument. The current shifts the Fermi surfaces according to the argument above. Therefore, a net spin torque will act on the spins from the spin-orbit field $\mathbf{B}_{\mathbf{k}} = \alpha(k_y, -k_x, 0)$, since this field is no longer $\perp \mathbf{k}$ (as it is in the case without current). The result of this torque is that a small z -component of the spin develops, which is positive for $k_y > 0$ and negative for $k_y < 0$. Therefore, a net spin current polarized in the z -direction will flow in the y -direction giving rise to an out-of-plane spin accumulation at the edges of the sample. Therefore, applying a current to a 2DEG with Rashba SOC should give rise to both a spin Hall effect and an Edelstein effect, i.e. spin polarization both out-of-plane and in-plane, respectively.

19.8.2 Seebeck effect

The conversion of a temperature gradient into an electric current. One can describe $E_{\text{Seebeck}} = -S\nabla T$ where S is the Seebeck coefficient (or thermopower) which depends on temperature and varies from materials to materials.

19.8.3 Peltier effect

The presence of heat transfer (heating or cooling) in a junction where an electric current flows. Note that there can be other sources of heat generation such as Joule heating, but this is not related to heat transfer between the conductors.

19.8.4 Spin Hall effect

An electric current driven by electric field produces a transverse spin accumulation due to spin-orbit interactions.

The spin-orbit interactions deflect the charge-carriers in a spin-dependent manner and thus cause a transverse spin current to flow. The spins therefore start to accumulate at the transverse edges of the material and consequently induce a diffusion spin-flow which partially counteracts the original spin-current. The spin accumulation builds up until a steady state is reached, meaning that the accumulation stays constant. This happens when a balance has been created between the drift spin current (from the injected charge current), diffusion spin current, and spin relaxation. It is important to note that a spatially dependent transverse spin current flow can exist even in steady state since the spin current is *not conserved* (unlike charge current): all that is required is that the spin current right at the edges must vanish.

Inverse: spin current produces a net charge accumulation due to spin-orbit coupling.

19.9 Zeeman spin Hall effect in graphene

Whereas the spin Hall effect usually requires spin-orbit interactions, an interesting exception is a spin Hall effect in graphene that can be induced by a Zeeman interaction.

Applying a $\mathbf{B}$ field to graphene Zeeman splits the Dirac cone dispersion with an amount $2\hbar$, similarly to what occurs in a normal metal with quadratic dispersion. If the graphene layer is charge neutral, meaning that the Fermi level is at the Dirac point $E_F = 0$ prior to the exchange splitting, the Fermi level will cross the spin-down band in the conduction band and the spin-up band in the valence band as shown in the figure.

If we now inject a charge current between two terminals 1 and 2 as shown in the figure, the current is carried by conduction band electrons and valence band electrons. Both have group velocity in the same direction, since both are electrons with negative charge which respond in the same way to an applied voltage. However, the valence band electrons have opposite group velocity $\mathbf{v} = \nabla_{\mathbf{k}} E / \hbar$ compared to their crystal momentum $\mathbf{k}$. This is an important observation with regard to how the valence band electrons respond to an out-of-plane magnetic field $\mathbf{B}$. The reason for this is that the electron dynamics are governed by the equation

$$\hbar \partial_t \mathbf{k} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \quad (19.88)$$

which is the analogue of Newton's second law for charge carriers in a crystal. Now, $q = -|e|$ is the same for both conduction and valence band electrons, so the Lorentz force acts on them in the same direction. However, they will *physically move* in opposite directions since $\partial_t \mathbf{k}$ is oppositely directed to $\mathbf{v}$ for the two types of electrons.

The net result of this is that a *pure spin current* is generated transversely to the charge flow. In turn, this spin current flow can be detected electrically using non-local probes in a Hall bar geometry via the *inverse Zeeman spin Hall effect* which causes the spin current to generate a transverse charge current (and thus voltage drop) as shown in the figure.

There are two additional equivalent ways of looking at the ZSHE. The first viewpoint is as follows. The valence band electrons have a *negative effective mass*, meaning that they will accelerate oppositely to the force. One can capture this statement by writing that

$$\mathbf{F} = m^* \mathbf{a} \quad (19.89)$$

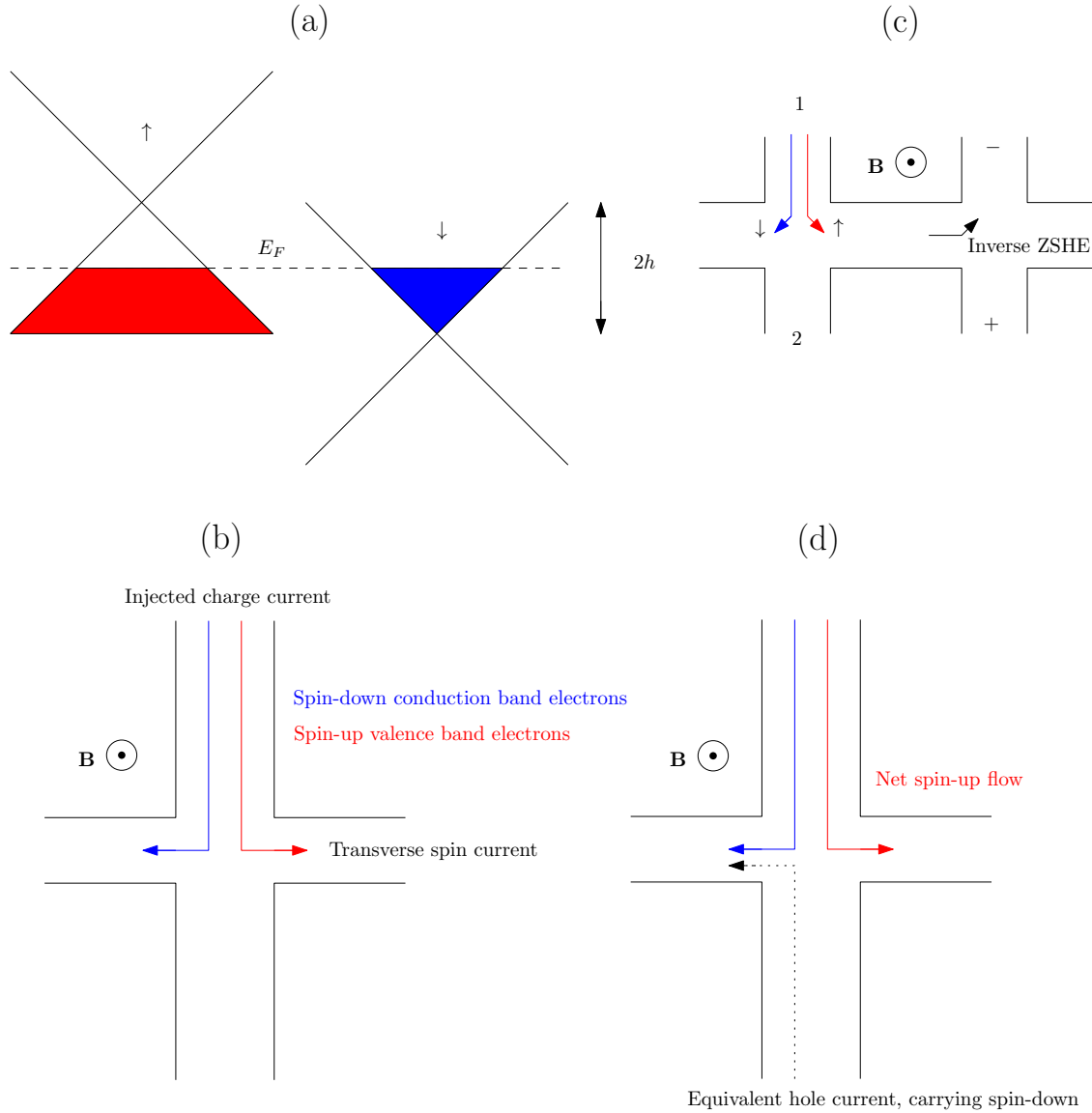


Figure 19.6: (Color online) Illustration of the ZSHE. (a) The Dirac cone is Zeeman split in the presence of an out-of-plane magnetic field. (b) Upon current injection, this gives rise to a transverse spin current which can be (c) detected as a non-local electric voltage. (d) Considering a hole current is an equivalent physical picture.

where F is the force acting on the electrons, m^* is their effective mass, and a is the acceleration in the direction of their physical motion. Eqs. (19.88) and (19.89) are consistent with each other. The second viewpoint is that instead of considering spin-up valence band electrons, we can model the contribution to the electric current from them as spin-down holes which move in the opposite direction. Keep in mind that a missing spin-up electron is a hole with spin-down, so that spin-down holes formally come from missing spin-up electrons. This is the standard viewpoint taken when treating charge transport in semiconductors: instead of considering the movement of all valence band electrons, one models the absent valence band electrons at the top of the band as excited holes with positive charge. Now, these holes have a *positive effective mass* and a positive charge. Therefore, the Lorentz force acts oppositely on them compared to the conduction band electrons, as

shown in the figure. Note also that the momentum of valence-band holes is aligned with the group velocity. As a result, the movement of the holes is shown with black arrows and is accompanied by a spin-down current. Therefore, the spin-down current flowing along the black dashed line is equivalent to a spin-up current flowing in the opposite direction [red arrows in (d)]. The physical outcome in all these three considerations is the same: a transverse spin current.

19.10 Hidden spin polarization in centrosymmetric materials

Relevant experiment <https://www.nature.com/articles/nphys3105>, relevant theory <https://www.nature.com/articles/nphys2933>.

The situation is somewhat different from altermagnets.

The hidden spin polarization originates from SOC, and not localized magnetic moments. Moreover, the material is inversion and time-reversal symmetric. The bulk bands are still doubly spin-degenerate, as required by Kramer's theorem, but the bands can originate from spatially separate parts of the unit cell: in this way, if one is able to probe just a particular spatial part of the unit cell, it is possible to see a spin-polarized band.

However, unlike altermagnets, we cannot have a $k_x k_y \sigma_z$ type of band structure. This breaks TRS. Instead, we must have a combination of even power of k and even power of σ , such as $k\sigma$, $k^2\sigma^2$, $k^3\sigma^3$, to preserve time-reversal symmetry. This also seems consistent figs 2e,2f in Zunger's paper, where the OOP spin component changes sign when $k \rightarrow (-k)$.

So I guess two important differences from altermagnets is that (1) we can only access the spin-polarized band if one is able to probe just a particular, localized part of the unit cell and (2) the spin-polarized band is not even-in- k times odd-in- σ .

Chapter 20

Orbitronics

20.1 Quenching of orbital angular momentum: role of P and T symmetry.

The orbital angular momentum (OAM) in the ground-state of a system is restricted by time-reversal and parity symmetry. If the system has T symmetry, then ¹

$$\langle \mathbf{L} \rangle_{\mathbf{k}} = -\langle \mathbf{L} \rangle_{-\mathbf{k}}. \quad (20.1)$$

If the system has P symmetry, then

$$\langle \mathbf{L} \rangle_{\mathbf{k}} = \langle \mathbf{L} \rangle_{-\mathbf{k}}. \quad (20.2)$$

It follows that if the system has PT symmetry, as in a non-magnetic centrosymmetric crystal, both of these equations are valid. Combining them leads to $\langle \mathbf{L} \rangle_{\mathbf{k}} = 0$ for every single $\mathbf{k}$. This is strong orbital quenching. However, an electric field can lift this condition due to orbital hybridization. This is achieved via current injection, in effect out of equilibrium. The electric field lifts the parity symmetry, and now allows for a finite $\mathbf{k}$ -resolved orbital angular momentum.

On the other hand, in noncentrosymmetric crystals, OAM may already be present in equilibrium at each $\mathbf{k}$ -point although the total OAM vanishes in the presence of timereversal symmetry. This is called weak orbital quenching).

20.2 Contributions to orbital current

There are in general two contributions to currents transporting orbital angular momentum. One is the flow of the orbital angular momentum defined around atoms at each lattice point. For instance, hopping of one electron in a d -wave orbital to another atomic site to a d -wave or p -wave orbital: in both cases is angular momentum transferred. The other contribution to a flow of orbital angular momentum comes from the itinerant circulation. This stems from an internal rotation of the wavepacket describing itinerant electrons moving through a lattice. This contribution is particularly important in noncentrosymmetric systems: see section 2.1.1 and Fig. 1 in

¹Note that T symmetry is broken in a ferromagnet if one treats the exchange field that the electrons feel as external. In effect, if only considering the itinerant electrons, then T symmetry is broken, but T symmetry is not broken for the system as a whole (including the source of the exchange field). Instead, T symmetry is spontaneously broken (not explicitly) in a ferromagnet if one considers the whole system.

<https://www.tandfonline.com/doi/full/10.1080/23746149.2024.2371972#d1e619>. The origin of the angular momentum being transferred in the case of this internal rotation is thus the center of the wavepacket.

The latter is quite analogous to spin transport in fact: the electrons carry an intrinsic orbital angular momentum which corresponds to an actual physical rotation of the center of the wavepacket describing the particles.

20.3 Continuity equation for orbital current

When a spin current is injected into a ferromagnet with a misaligned polarization axis, the angular momentum from the spin current is transferred to the magnetization via a spin-transfer torque. This sets the magnetization into a precessional motion.

Imagine that we now inject an orbitally polarized current into a metal which has a coupling between orbital angular momentum and the momentum of the electrons in the Hamiltonian. This term will then act as a source term in the continuity equation for the orbitally polarized current.

The absorption of the orbital moment by the lattice, mediated by the crystal field, induces a mechanical torque. The first step to evaluate the orbital torque is to establish a continuity equation for the angular momentum for the itinerant electrons. Let's say that we are interested in L_z . Then:

$$\frac{dL_z}{dt} = i[H, L_z]. \quad (20.3)$$

Now, H can contain in general both $\mathbf{k}$ -dependent and independent terms. The question is then which part of $i[H, L_z]$ that should be interpreted as divergence of a current and which part that should be interpreted as torque exerted on the lattice. The conventional choice in the spin case is discussed in <https://arxiv.org/pdf/2509.18363>, and consists of writing

$$\frac{dS_z}{dt} = \nabla \cdot \mathbf{J}_s + \tau_z \quad (20.4)$$

where $S_z = \langle \psi | \sigma_z | \psi \rangle$ and

$$\mathbf{J}_s = \frac{1}{2} \langle \psi | \{\hat{\mathbf{v}}, \sigma_z\} | \psi \rangle \quad (20.5)$$

with $\hat{\mathbf{v}} = \frac{1}{\hbar} \frac{\partial H}{\partial \mathbf{k}}$ being the velocity operator, and finally

$$\tau_z = \langle \psi | \frac{i}{\hbar} [H, \sigma_z] | \psi \rangle \quad (20.6)$$

is the expectation value of the spin-torque operator. A similar definition thus seems reasonable in the orbital angular momentum case.

Chapter 21

Quantum technology

The three main areas are:

- Quantum computing
- Quantum communication
- Quantum sensing

21.1 Quantum computing

This field studies the use of intrinsic quantum phenomena, like superposition and entanglement, to perform calculations that are impossible or impractical for classical computers. Quantum computers could have a major impact in fields such as drug discovery, materials science, and weather or financial modeling by solving complex problems much faster than current technology.

21.1.1 Fundamentals and comparison to classical computing

The fundamental building block in a quantum computer is a qubit. Qubits can be likened to vectors, $\mathbf{v} = a\mathbf{x} + b\mathbf{y} + c\mathbf{z}$ that exist in a vector space. The difference is that qubits live in a complex vector space, where the coefficients can be complex. The α and β of a state $\alpha|0\rangle + \beta|1\rangle$ are complex numbers. This suggests four degrees of freedom, which for a single, normalized qubit is reduced to two degrees of freedom due to normalization and arbitrary phase.

The gist of a quantum computer is now to manipulate α and β as a function of time, so that a new state is obtained. Measurements in a basis comprised of precisely $|0\rangle$ and $|1\rangle$ will then give results with a probability determined by the absolute value squared of these coefficients. The modulus of the amplitudes can be estimated by varying out multiple measurements of the state.

A key concept with regard to the potential of a quantum computer comes from when one entangles qubits together. One important point is what this means with regard to the scaling of the information contained in multiple qubits. For instance, the Hilbert state of a two-qubit systems can be written

$$|\Psi\rangle = \gamma_1|00\rangle + \gamma_2|01\rangle + \gamma_3|10\rangle + \gamma_4|11\rangle \quad (21.1)$$

In a multiqubit state such as this, the goal is also to manipulate the coefficients. There are now four basis states: a two-qubit state is described by four complex amplitudes (minus two if one insists on

normalization and a global phase).

We can generalize this to n qubits. We get that an n -qubit state has 2^n complex numbers, or 2^{n+1} real numbers. For instance, a particular 3-qubit state is described by 8 complex numbers. Compare this now to a classical computer working with bits, states which are deterministically either 0 or 1. A particular 3-bit state is described by 3 real numbers, for instance 010. A particular 4-bit state is described by 4 real numbers, and so on: the scaling is linear. This is in stark contrast to the exponential scaling of the qubits.

A classical computer would need a number of bits equal to 2^n to represent a state with the same information as an n -qubit state. A quantum computer with 50 qubits thus holds a quadrillion numbers of information in a given multi-qubit state, which is impossible for any classical computer. This capability makes quantum computers potentially powerful tools for simulating complex systems. The property of entanglement is leveraged in quantum computers to break certain types of encryption. In particular, quantum computers should be much better than classical computers to model physical systems, since these are governed by quantum states.

Let us give a concrete example of how qubits and superpositions of states can be used to solve a problem much faster than a classical computer using bits. This is not a very useful problem to solve in practice, but it gives a quite understandable example of a quantum algorithm. It is called the Deutsch algorithm and we will illustrate it for a case with two qubits.

Imagine that you have a particular function f on a configuration of n classical bits, $C = \{0, 1\}^n$. The function takes each of the 2^n possible configurations to a single bit. This can be thought of as a black box that implements a function from n -bit strings, such as 11010, to either 0 or 1. Expressed in symbols:

$$f : \{0, 1\}^n \rightarrow \{0, 1\} \quad (21.2)$$

We are to begin with given the information that this function is either

1. Constant – all configurations are mapped to the same value.
2. Balanced – exactly half of the configurations map to 1, the other half to 0.

The task is to find out if f is either constant or balanced. Let us first do this in a classical way. The worst case scenario is that we have to evaluate half of the possible configurations plus one to determine with certainty the nature of the function f . There are 2^n possible configurations. For n bits, the worst case scenario therefore amounts to $2^{n-1} + 1$ evaluations of the function f .

Let us see how well we can do using a quantum computer instead. A common misconception is that a quantum computer using qubits perform multiple computations in parallel since the qubit is in a superposition of multiple states. However, the difference between quantum computation and classical parallel computing can be likened to the difference between randomized computation (e.g. using coin-flips, or some other form of random number generation) and parallelism. In randomized computation, depending on the outcome of the coin-flips, you explore one out of many possible computational possibilities. If the vast majority of those paths give quickly rise to a particular answer, then that is the answer. By contrast, in a truly parallel computation, each parallel process is obviously and independently present for querying and inspection. Anything "parallel" about quantum computing attributed to operations performed on the superposition of states of qubits can

only be addressed statistically via a large amount of measurements, and is conceptually different from classical parallel computing (which involves breaking down a large problem into smaller, independent parts that can be executed concurrently by multiple processors or cores).

But we disgress: back to the example. The Deutsch- quantum algorithm will produce an answer that is entirely correct with only a single evaluation of f . We will use $n = 2$ qubits to achieve this. The algorithm can be executed with many more qubits, and that's where it is actually much faster than the classical method explained above (i.e. requires far less evaluations and operations). But we here want to illustrate how a quantum algorithm, so we keep it simple.

To show how the Deutsch algorithm is superior to the classical one, relying only on a single evaluation of f , we will make use of the following two properties:

- **Superposition:** We're putting a qubit in superposition, and then apply $f(x)$ on it. This allows us to evaluate $f(x)$ for both inputs at the same time.
- **Phase Kickback:** The effect where the phase of a qubit is "kicked back" onto another qubit during a controlled quantum operation.

We will use so-called quantum gates to perform operations on our 2-qubit state. The classical black box we had before, which lets f act on a n -bit string and then spit out 0 or 1, is now a quantum black box. It acts similarly to the classical black box we had before: it takes qubits and spits the result. We define the quantum black box via the following transformation:

$$|a\rangle|b\rangle \rightarrow |a\rangle|b \oplus f(a)\rangle. \quad (21.3)$$

The $\oplus$ signifies addition modulo 2, and keep in mind that a, b are equal to 0 or 1. One concern that might come now: is it even fair to compare a quantum black box to a classical black box? The boxes do different things since they act on a string of numbers and a qubit, respectively, even if the definition of f is the same in both cases. The answer is: it is reasonable. Even with a quantum black box, classical computers still need 2 queries because they cannot exploit superpositions, hence it is reasonable to compare. So in the classical case, the function f acts on the state of 2 bits whereas in the quantum case the function f acts on the state of a qubit.

It might seem unfair that the black box does different things in the classical and quantum case, even if f works in the same way. The goal is to figure out what f is in both cases. The point is nevertheless that in a classical black box, even if it was different from how we described that it works above, there is no way to design a black box differently that will allow us to determine what f is with a single evaluation of f on some object. We make this statement without proof, but you can try to think up some classical black box which when acting on a state with n bits can figure out what f is with a single evaluation. In contrast, we now show that a quantum black box acting on a state with n qubits can figure out what f is with a single evaluation.

We also have at our disposal a Hadamard gate which takes a single qubit and places it in a superposition:

$$\begin{aligned} |1\rangle &\rightarrow (|0\rangle - |1\rangle)/\sqrt{2}, \\ |0\rangle &\rightarrow (|0\rangle + |1\rangle)/\sqrt{2}. \end{aligned} \quad (21.4)$$

The first step of the algorithm is to prepare our 2-qubit system in the state $|0\rangle|1\rangle$. This is our initial state, denoted $|\phi\rangle_0$:

$$|\phi\rangle_0 = |0\rangle|1\rangle. \quad (21.5)$$

Then apply the above Hadamard gate to obtain the state

$$\begin{aligned} |\phi\rangle_1 &= H^{\otimes 2} |\phi\rangle_0 \\ &= (|0\rangle - |1\rangle)(|0\rangle + |1\rangle)/2. \end{aligned} \quad (21.6)$$

Now apply the black box quantum gate U_f involving f , so that we obtain

$$\begin{aligned} |\phi\rangle_2 &= U_f |\phi\rangle_1 \\ &= \frac{1}{2} |0\rangle (|0\rangle + \oplus f(0)\rangle - |1 \oplus f(0)\rangle) + \frac{1}{2} (|0 \oplus f(1)\rangle - |1 \oplus f(1)\rangle). \end{aligned} \quad (21.7)$$

We can simplify this, since

$$|0 \oplus a\rangle - |1 \oplus a\rangle = (-1)^a (|0\rangle - |1\rangle), \quad (21.8)$$

where a is either $f(0)$ or $f(1)$. Therefore, a is either 0 or 1. Note how the application of U_f thus produces an extra phase $(-1)^a$ on the second qubit. Rewriting, we now get:

$$\begin{aligned} |\phi\rangle_2 &= \frac{1}{2} (-1)^{f(0)} |0\rangle (|0\rangle - |1\rangle) + \frac{1}{2} (-1)^{f(1)} |1\rangle (|0\rangle - |1\rangle) \\ &= \frac{1}{\sqrt{2}} \left((-1)^{f(0)} |0\rangle + (-1)^{f(1)} |1\rangle \right) (|0\rangle - |1\rangle). \end{aligned} \quad (21.9)$$

Notice how we have now witnessed phase kickback in action: U_f acted on the second qubit, which resulted in kicking back a phase factor $(-1)^{f(x)}$ in front of the first qubit while leaving the second qubit unchanged.

Now, pull out a common factor $(-1)^{f(0)}$ and omit the second qubit, $(|0\rangle - |1\rangle)$, from the notation since it has served its purpose. We get:

$$|\phi\rangle_2 = \frac{1}{\sqrt{2}} (-1)^{f(0)} \left(|0\rangle + (-1)^{f(0) \oplus f(1)} |1\rangle \right) \quad (21.10)$$

where we used the fact that $(-1)^{f(1)-f(0)} = (-1)^{f(0) \oplus f(1)}$. This is because $f(0)$ and $f(1)$ are either 0 or 1, so the difference between them is 0, 1 or -1. If the difference is zero, then we get $(-1)^0 = 1$. If the difference is 1 or -1, we get $(-1)^1 = (-1)^{-1} = -1$. The overall phase factor can be discarded since it is unobservable, but we're left with a relative phase between the $|0\rangle$ and $|1\rangle$ inside the paranthesis.

Let us then examine the term $|0\rangle + (-1)^{f(0) \oplus f(1)} |1\rangle$ more carefully. Since $f(0) \oplus f(1)$ is either 0 or 1, we get that the term is either $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ if $f(0) \oplus f(1) = 0$ or it is $|-\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$ if $f(0) \oplus f(1) = 1$. This means that we either have

$$|\phi\rangle_2 = \begin{cases} |+\rangle & \text{if } f(0) \oplus f(1) = 0 \text{ } f \text{ is constant} \\ |-\rangle & \text{if } f(0) \oplus f(1) = 1 \text{ } f \text{ is balanced} \end{cases} \quad (21.11)$$

Thus, by measuring the first qubit in a $|\pm\rangle$ basis, we can say with a single measurement whether the function f is constant or balanced!

1

We can see from this example that an important part of quantum computation is the task of finding ways to implement manipulations of entangled qubit states. Manipulations of qubits are represented with unitary matrices mathematically. Note that entangled states are always in a superposition of states.

A more useful algorithm in quantum computing is Grover's algorithm, also known as the quantum search algorithm. This is a quantum algorithm for searching an unsorted database to find a particular piece of information. Grover's algorithm provides a quadratic speedup compared to a classical search algorithm. However, there exists other quantum algorithms, based on Grover, which provide an exponential speedup. Grover's algorithm also relies on entanglement, but it is too complicated to present here.

Possible applications of quantum computers include development of drugs (simulation of behavior of molecules), optimization problems, and prime factorization of large numbers. The latter is achieved via Shor's algorithm.

21.2 Quantum communication

Quantum communication takes on the task of how to establish secure and efficient ways to transmit information using intrinsic quantum properties. This includes generating encryption keys that are secure, making it impossible for a third party to obtain the information since measuring the quantum state will alter it and thus immediately exposing the eavesdropping so that one can abort the communication.

21.3 Quantum sensing

Quantum sensing deals with the use of quantum systems to make extremely accurate measurements, which can be used to detect minute variations in physical quantities such as magnetic fields, temperature gradients, and gravitational waves. This has applications in fields like medical imaging, navigation, and fundamental physics research.

¹A quick word on notation in the n -qubit generalized case: there, one applies first a Hadamard gate on an n -qubit state with $|0\rangle$ tensor products:

$$H^{\otimes n}|0\rangle^{\otimes n} = \left(\frac{1}{\sqrt{2}}\right)^n (|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle) \otimes \dots \otimes (|0\rangle + |1\rangle). \quad (21.12)$$

Expanding out the tensor products, this can be rewritten as

$$H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle. \quad (21.13)$$

This is a common and useful way of abbreviating the notation. What it means is: the n -qubit Hadamard gate acting on the n -qubit state of all zeros gives a superposition of all n -qubit basis states called an equally weighted superposition. In other words, it is a sum over every possible tensor product combination of zeros and ones that can be made with n states.

21.4 Quantum decoherence

Macroscopic, classical objects do not display quantum mechanical properties such as being in a superposition of states. Why? The answer is given by quantum decoherence.

Quantum states are either pure or mixed. For a pure state $|\psi\rangle$, there is full certainty about the outcome of some measurement on that system which probes a particular state contained in the superposition of states that makes up $|\psi\rangle$. Put differently, there exists a measurement for which one of the possible outcomes will occur with unit probability. When isolated, a pure quantum state remains pure due to unitarity of the time-evolution operator.

However, if the system interacts with an environment, then coherence can be thought of as shared with the environment. Recall that coherence is a measure of the extent to which two waves can interfere with each other. It tells us how well-defined the relative phase of the two waves is. Therefore, coherence within the system itself is lost over time: this is the essence of quantum decoherence. Quantum decoherence can therefore be viewed as the loss of information from a system into the environment. The total system (isolated system + environment) nevertheless evolves with time in a unitary fashion, even though the isolated system has a non-unitary time-evolution. The isolated system can in this way evolve from a pure state to a mixed state where no measurement can be done to yield an outcome with absolute certainty.

Let us start by giving a qualitative understanding of quantum decoherence and then provide a mathematical derivation.

21.4.1 Qualitative argument

Consider a quantum mechanical system that is coupled to an environment. If the system and environment are decoupled, their state vectors occupy different Hilbert spaces. The macroscopic environment Hilbert space is going to have a very large dimensionality due to the large number of degrees of freedom. When the system and environment start to interact, their state vectors are no longer confined to being in their respective subspaces. Instead, the combined state vector evolves through time in a Hilbert space whose dimensionality is the product of the dimensions of the two subspaces.

At this point, the extent to which two vectors describing the joint system plus environment system can interfere depends on how "close" they are to each other in the Hilbert space. Since the available phase space volume increases enormously once the system and environment couple to each other, two vectors evolving in time will very rapidly become lost from each other and have zero overlap. Therefore, a system that is initially in a superposition of states will be described by a state vector in the combined system plus environment Hilbert space that almost immediately loses the property of being in a superposition of states and instead becomes a mixed state, corresponding to a classical statistical mixture of states. Put in other words, the original states comprising the superposition of states rapidly decohere from each other and can no longer exhibit quantum interference, such as in the double-slit experiment.

21.4.2 Quantitative derivation

The destruction of a superposition of states in a system via interaction with an environment, i.e. decoherence, is closely related to entanglement. This can be illustrated as follows. Consider an electron spin and an environment consisting of an observer. The observer is initially in a state $|\rangle$ where he does not know the spin of the electron, thus he is blank. However, he is such inclined that he becomes happy $|\rangle$ when he measures a spin $\uparrow$ particle and sad $|\rangle$ if he measures a spin $\downarrow$ particle. Assume that the electron initially is in a superposition of states $|\uparrow\rangle + |\downarrow\rangle$. The total Hilbert space is given by

$$H = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\} \otimes \text{span}\{|\rangle, |\rangle, |\rangle\} \quad (21.14)$$

The initial state of the combined system is then

$$|\psi\rangle = (|\uparrow\rangle + |\downarrow\rangle) \otimes |\rangle. \quad (21.15)$$

This is not an entangled state: it is pure. Now, let the act of measurement (the interaction between the system and observer) be represented by a unitary operator U which according to the above inclinations of the observer is defined as follows:

$$\begin{aligned} U(|\uparrow\rangle \otimes |\rangle) &= (|\uparrow\rangle \otimes |\rangle), \\ U(|\downarrow\rangle \otimes |\rangle) &= (|\downarrow\rangle \otimes |\rangle). \end{aligned} \quad (21.16)$$

Hence, it follows that when the system and observer interact, the resulting state is

$$U(|\uparrow\rangle + |\downarrow\rangle) \otimes |\rangle = |\uparrow\rangle \otimes |\rangle + (|\downarrow\rangle \otimes |\rangle) \quad (21.17)$$

The interaction with the environment has thus produced an *entangled* state between the system and environment. We see that the initial superposition of states is lost: decoherence has taken place. Any subsequent measurement on the system alone will not be able to detect the superposition present in the initial state of the system.

Let us now provide a more general derivation of how we go from a superposition of states to a mixed state without quantum mechanical interference terms, typical for superposition of states, contributing to the probability distribution. Let the system initially be in a state

$$|\psi\rangle = \sum_i |i\rangle \langle i|\psi\rangle \quad (21.18)$$

where $|i\rangle$ are a complete, orthonormal set of states (basis) and let the environment be in state $|\epsilon\rangle$. Before the system and environment interact, the joint before-state $|B\rangle$ is therefore

$$|B\rangle = \sum_i |i\rangle \otimes |\epsilon\rangle \langle i|\psi\rangle. \quad (21.19)$$

It is instructive to compare two limiting cases of how the system and environment can interact.

The system becomes totally absorbed by the environment

This means that each element in the system's basis interacts with the environment in a way so that

$$|i\rangle |\epsilon\rangle \rightarrow |\epsilon_i\rangle \quad (21.20)$$

where $|\epsilon_i\rangle$ is the state representing how the environment has been disturbed by the environment. Thus, the before state $|B\rangle$ evolves into an after-state $|A\rangle$

$$|B\rangle \rightarrow |A\rangle = \sum_i |\epsilon_i\rangle \langle i|\psi\rangle. \quad (21.21)$$

The time evolution has to be unitary, so that the norm of the time-evolving state is preserved. It follows that the total state basis $\{|\epsilon_i\rangle\}$ has to remain orthonormal after the system has been absorbed by the environment. Mathematically, this is seen since $\langle i|j\rangle = \delta_{ij}$, we must also have $\langle \epsilon_i|\epsilon_j\rangle = \delta_{ij}$. This is proven as follows. Since the initial state is assumed normalized $\langle \psi|\psi\rangle = 1$, it follows from $\langle B|B\rangle = 1$ that $\sum_i |\langle \psi|j\rangle|^2 = 1$. Now consider $\langle A|A\rangle$ which yields $\sum_{ij} \langle \epsilon_i|\epsilon_j\rangle \langle i|\psi\rangle \langle \psi|j\rangle$. To ensure this is unity for any orthonormal basis states $\{|i\rangle\}$, we must therefore have $\langle \epsilon_i|\epsilon_j\rangle = \delta_{ij}$.

This condition expresses that the system states $|i\rangle$ have been coupled to the environment in such a way that there is no overlap between two such states. There was no overlap between them initially either since $\langle i|j\rangle = \delta_{ij}$. We keep this in mind, as this will be used in our next limiting case.

The system remains undisturbed by the environment

We now assume that we are performing an idealized measurement where the system disturbs the environment (our measurement apparatus), but the system itself remains undisturbed by the environment. This means that $|i\rangle |\epsilon\rangle$ evolves into $|i\rangle |\epsilon_i\rangle \equiv |i, \epsilon_i\rangle$. Now the before state evolves into

$$|B\rangle \rightarrow |A\rangle = \sum_i |i, \epsilon_i\rangle \langle i|\psi\rangle. \quad (21.22)$$

Applying the unitarity requirement on the after-state $|A\rangle$ yields the condition

$$\langle i, \epsilon_i | j, \epsilon_j \rangle = \langle i | j \rangle \langle \epsilon_i | \epsilon_j \rangle = \delta_{ij} \langle \epsilon_i | \epsilon_j \rangle = \delta_{ij} \langle \epsilon_i | \epsilon_i \rangle \quad (21.23)$$

Note that we have no criterion for what $\langle \epsilon_i | \epsilon_j \rangle$ has to equal this time. We can nevertheless impose such a condition on physical grounds. After the environment with its huge number of degrees of freedom has interacted with the system, it is reasonable to expect that the different environmental states $|\epsilon_i\rangle$ have no chance to interfere with each other as they evolve along very different paths in Hilbert space. This condition does not follow strictly mathematically from unitarity of time-evolution in the case where the system remains undisturbed, unlike the previous case where the system was absorbed fully by the environment. However, due to the argument above (large number of degrees of freedom) it should nevertheless be a very good approximation to set

$$\langle \epsilon_i | \epsilon_j \rangle \simeq 1. \quad (21.24)$$

As we will now proceed to show, this condition is precisely the reason for why decoherence in the system sets in and quantum effects are lost when the system makes transitions between states. When this condition is fulfilled, one says that einselection (environmentally-induced superselection) has taken place where the environment has in effect selected out the decompositions (basis vectors) of the original system state that lose phase coherence with each other.

A general interaction between system and environment is comprised of a mixture of the two limiting cases considered above.

Loss of interference in systems interacting with environment

To illustrate how the interaction with the environment leads to quantum decoherence, we pose the

question: what is the probability of the system making a transition from $\psi \rightarrow \phi$? We calculate this both before and after the system has interacted with the environment. We assume that the environment is affected by the system, but not vice versa (ideal measurement) and will see how this still leads to quantum decoherence.

Before the interaction, we know that the probability is computed as

$$|\langle \psi | \phi \rangle|^2 = \left| \sum_i \psi_i^* \phi_i \right|^2 = \sum_i |\psi_i^* \phi_i|^2 + \sum_{ij, i \neq j} \psi_i^* \psi_j \phi_j^* \phi_i. \quad (21.25)$$

There exists terms where $i \neq j$ which represent interference between different basis elements, which is precisely a quantum mechanical effect occurring for a pure state which is in a superposition of states.

Compare this with the probability for the same transition after the system has interacted with the environment. The state after the interaction was given earlier as $|A\rangle = \sum_i |i, \epsilon_i\rangle \langle i | \psi \rangle$, given that the system was initially in state $|\psi\rangle$. The transition probability is given as the overlap between this state and any possible state where the system is in $|\phi\rangle$, irrespective of the state of the environment. Thus, we get:

$$\begin{aligned} |\langle \psi | \phi \rangle|^2 &= \sum_j |\langle A | \phi, \epsilon_j \rangle|^2 \\ &= \sum_j \left| \sum_i \psi_i^* \langle i, \epsilon_i | \phi, \epsilon_j \rangle \right|^2 \\ &= \sum_j \left| \sum_i \psi_i^* \phi_i \langle \epsilon_i | \epsilon_j \rangle \right|^2. \end{aligned} \quad (21.26)$$

The internal summation inside the absolute value signs vanishes if we apply the decoherence criterion Eq. (21.24), simplifying the probability expression to

$$|\langle \psi | \phi \rangle|^2 \simeq \sum_i |\psi_i^* \phi_i|^2. \quad (21.27)$$

Comparing this to the probability before the interaction with the environment, Eq. (21.25), we see that all cross-terms describing quantum interference between the projections of $|\psi\rangle$ and $|\phi\rangle$ onto different basis states i and j are gone. We instead have exclusively additive probability amplitudes in the same way as in classical physics.

Density-matrix approach

Decoherence is seen in density matrices through a decay of the off-diagonal elements² of the reduced density matrix of the system alone. The reduced density matrix is obtained from a partial trace of the total density matrix with respect to the environment. The interaction with the environment described above causes a transition from a pure state in the system to a mixed state, as can be verified from the reduced density matrix. In effect, this is what supporters of the many-worlds interpretation of quantum mechanics would say is the reason for the appearance of a wavefunction

²The off-diagonal elements of a density matrix ρ quantifies to what extent the system contains a quantum superposition between the elements of the basis chosen to represent ρ . For instance, for a pure state $|\psi\rangle = \cos \theta |0\rangle + e^{i\phi} \sin \theta |1\rangle$, one would obtain $\rho = |\psi\rangle \langle \psi|$ with $\rho_{01} = e^{-i\phi} \cos \theta \sin \theta$ which contains the relative phase between the states.

collapse.

Using the density matrix before the transition

$$\rho = |B\rangle \langle B| = |\psi\rangle \langle \psi| \otimes |\epsilon\rangle \langle \epsilon| \quad (21.28)$$

tracing out the environment to obtain the reduced density matrix describing the system alone

$$\rho_{\text{sys}} = \text{Tr}_{\text{env}}(\rho) = |\psi\rangle \langle \psi| = |\psi\rangle \langle \psi| \quad (21.29)$$

and then computing the transition probability for $\psi \rightarrow \phi$ using this density matrix as

$$\langle \phi | \rho_{\text{sys}} | \phi \rangle \quad (21.30)$$

The above equation (transition probability) expresses the probability of finding the system in state ϕ given a certain density matrix ρ . This procedure yields exactly the same probability as in the section above.

We can repeat this calculation using the density matrix after the interaction between system and environment has taken place:

$$\rho = |A\rangle \langle A| = \sum_{ij} \psi_i \psi_j^* |i, \epsilon_i\rangle \langle j, \epsilon_j|, \quad (21.31)$$

tracing over the system environment

$$\rho_{\text{sys}} = \sum_i |\psi_i|^2 |i\rangle \langle i|, \quad (21.32)$$

and then computing the transition probability

$$\langle \phi | \rho_{\text{sys}} | \phi \rangle \quad (21.33)$$

also produces the same result as in the above section: in effect, without interference terms.

21.5 Quantum circuit diagrams

In quantum computing, a quantum logic gate (or simply quantum gate) is a quantum circuit operating on a small number of qubits. Unlike many classical logic gates, quantum logic gates are reversible. Quantum gates are described mathematically by unitary operators, and can be represented as unitary matrices relative to some orthonormal basis. Fig. 21.1 shows common quantum logic gates by name, including abbreviation, circuit form(s), and the corresponding unitary matrices. The way to understand these gates can be shown with an example. Consider Fig. 21.2 which is a two-qubit circuit diagram. The top line denotes the qubit labelled q_1 , and the bottom lines denotes the qubit labelled q_2 . In this example, both qubits have been initialized to $|0\rangle$. Quantum circuits represent these gates with labeled boxes and solid circles, as in the figure, each representing a special gate. So in this example the gate X is applied to q_1 , and the gates H and Y are applied to q_1 and q_2 afterwards. These are single qubit gates that affect each qubit independently. Finally, we conclude the circuit by performing measurements on different qubits.

Operator	Gate(s)	Matrix
Pauli-X (X)	 	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

Figure 21.1: (Color online)

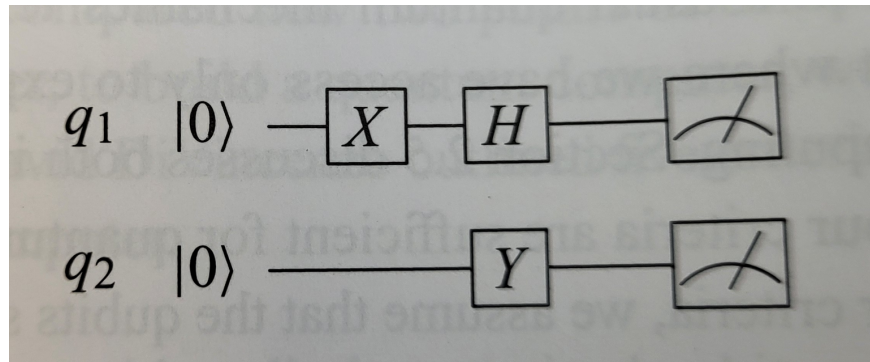


Figure 21.2: (Color online)

We will also need multi-qubit gates, as shown in Fig. 21.3, to achieve universal quantum computation. To depict a multi-qubit gate, draw a box over the qubits the gate acts on. In the figure, the first gate is a three-qubit gate U . Some multi-qubit gates consist of a control qubit and a target qubit. These are known as control gates. A control gate can be understood as being implemented on the target qubit if the control qubit is in state 1. The second gate in the figure is a controlled X gate, better known as CNOT. The state of q_2 is modified by the CNOT in a way that depends on the state of q_1 . A control gate can have multiple targets or controls, as depicted by the third and fourth gates in the figure. When multiple controls are present, all of them need to be in state 1 to activate the gate.

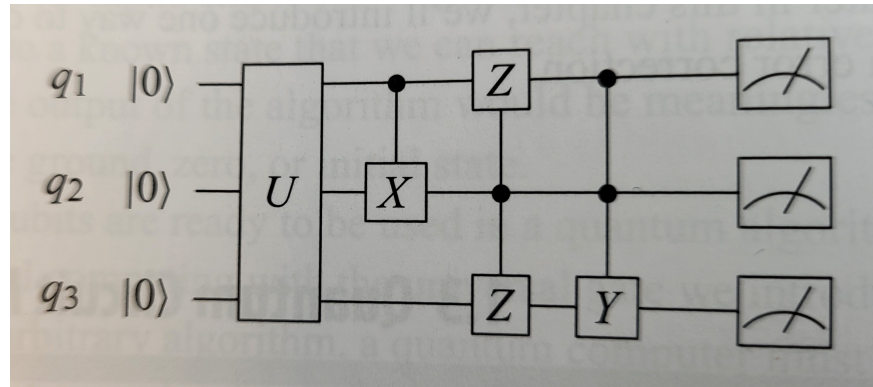


Figure 21.3: (Color online)

Complete universal control over a two-qubit system is obtained if you have gates that can do any single-qubit rotation on the Bloch sphere and an entangling gate, such as the CNOT. An arbitrary single-qubit rotation can be achieved by two single qubit-gates corresponding to rotation around two different axes.

21.6 Fundamental theorems in quantum technology

21.6.1 No-cloning theorem

The no-cloning theorem states that it is impossible to create an independent and identical copy of an arbitrary unknown quantum state. Developed in 1970s and 80s.

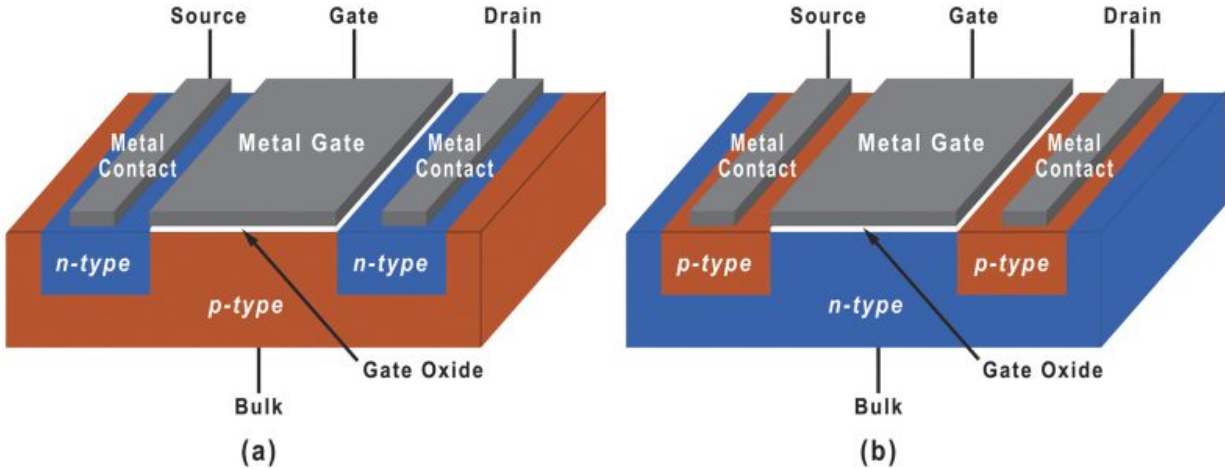


Figure 22.1: (Color online)

Chapter 22

Low-dimensional Systems

22.1 Tuning the Fermi level in a 2DEG by gate voltage

One often speaks of controlling the Fermi level in a 2DEG or nanowire using a gate voltage. However, what is actually meant here is a bending of the energy-bands, called band bending. What happens is that the density of states at the Fermi level is changed as the band is lowered or raised relative to the existing Fermi level. The Fermi level itself actually remains unchanged.

This is done in *e.g.* MOSFET structures. In such structures, a metallic gate lies on top of an insulating oxide which in turn is connected to a semiconducting layer. A voltage ΔV is applied between the metal and the semiconductor. Due to the oxide, no current is flowing, but an electric field exists. This is analogous to a capacitor with the oxide being the dielectric. Thus, a charging effect exists just like in a capacitor. The interfaces of the oxide layer are polarized and this polarization attracts charge of a certain sign (+ or -), depending on the polarity of the gate voltage, on the semiconducting side of the interface as well. The MOSFET can use either a *p*-type or *n*-type semiconductor, as shown in Fig. 22.1.

This causes a build-up or reduction of electron density on the semiconducting side depending on

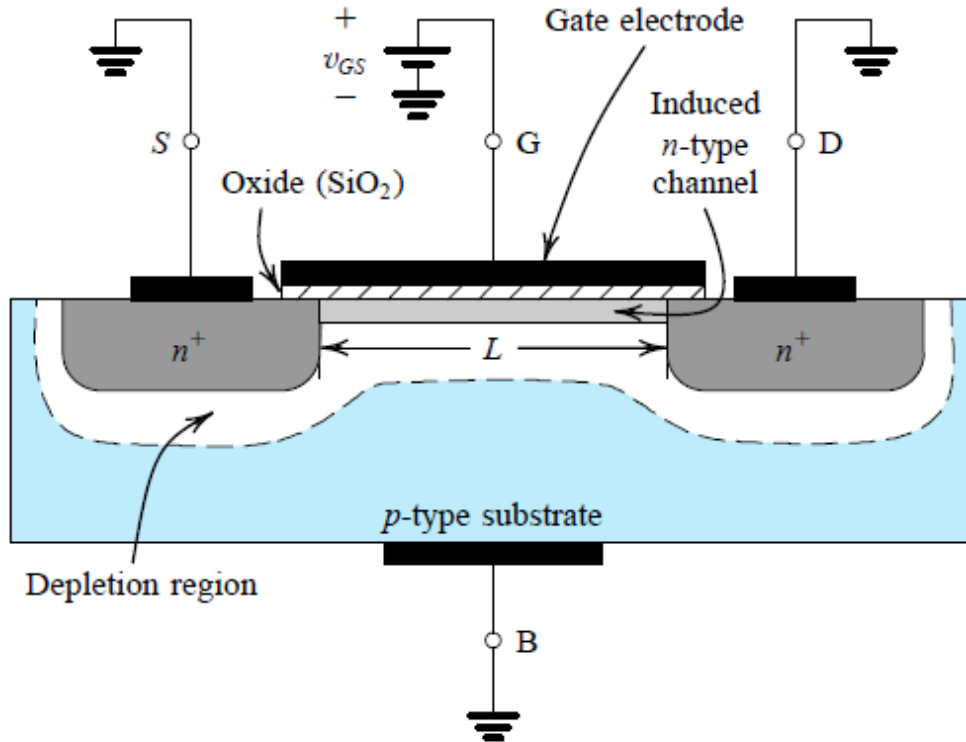


Figure 22.2: (Color online)

if the voltage is positive or negative on the metal side. The change in electron density on the semiconducting side $\Delta n \propto \Delta V$, resulting in so-called band-bending near the interface. This means that the energy of the bands is modified in a way (lowered or raised) that the Fermi level now effectively lies *e.g.* higher in the conduction band or lower in the valence band. The reason for why one usually refers to this as "tuning the Fermi level" is that, although it is more correct to say that the band-structure itself is changed due to the induced charge density whereas the Fermi level remains invariant, this may be viewed as an effective change of the Fermi level (raised or lowered) in terms of the density of states changing at the Fermi level.

The physical situation which has been realized is now that a two-dimensional electron gas has formed at the interface of the oxide and the semiconductor. This is also referred to as an inversion layer. If the semiconductor is *p*-doped, applying a positive gate voltage across the structure (top voltage minus bottom) results in electrons being attracted to the oxide-interface from the semiconducting side. If sufficiently many such electrons are attracted, a thin conducting layer with electrons is formed, as shown in Fig. 22.2.

If the channel is *p*-type (*n*-type), then under a positive (negative) gate bias the semiconductor bands near the surface will bend downwards (upwards), assuming the Fermi level is kept horizontal. The surface area will start being depleted from free majority carriers, referred to as depletion. Once the Fermi level makes it way through the bandgap and moves towards one of the bands, minority carriers start to be thermally generated and form a conducting inversion layer.

22.1.1 Physical mechanism for band bending

Now, what is the physics behind the bending of the bands? The bands are a simple representation of energy states where electrons are allowed. This is in contrast to a band gap, where electron states are forbidden. However, when voltage is applied to the gate, an electric field is formed. We know that this leads to a charge accumulation at the surface of the oxide/semiconductor (seen from the semiconducting side). It is important to note that the Fermi level in the substrate remains invariant even under an applied bias since no current can flow through the device due to the presence of an insulator. Note that the Fermi level is determined by the electrochemical potential μ_{ec} which includes both the electrostatic potential and the particle chemical potential. In the absence of current, there can be no gradient in μ_{ec} .

Since there now is an increased concentration of *e.g.* electrons at the interface, the DOS at the Fermi level has to be higher there. In the electron band picture, this means that the Fermi level remains constant and horizontal whereas the band bends to give the resulting change in DOS at the Fermi level.

It is important to note that there exists an electric field perpendicular to the 2DEG, yet no current flows in this direction. This is because there is a balancing **diffusion force** from the varying charge concentration close to the interface. This is the same physics as for electric field screening in a conventional metal. When an external electric field is applied and there is no charge transfer, mobile electrons move to the surfaces of the metal until the electric field inside the metal is cancelled. This is of course only true if the metal is not part of an electric circuit, in which case the electrons can travel down the circuit as a result of the field. However, in the present case the $\mathbf{E}$ -field is screened. However, it is not screened instantly. There is a decay length of the electric field determined by *e.g.* how many mobile electrons that are available. In metals, this decay length is very short ($\sim$ nm. But in semiconductors, it is much larger due to the lower concentration of mobile carriers (depending on doping level), say tens of nm.

The diffusion current is a result of the electrons having mass and the temperature being finite. The electrons move due to the energy supplied by heat, i.e. their thermal energy. Instead, the drift current is a result of electrons having charge. The electrons then move due to the energy supplied by an electric field, i.e. their electric energy.

22.1.2 Estimating the electric field screening length

This explanation follows https://www.tf.uni-kiel.de/matwis/amat/elmat_en/kap_2/backbone/r2_4_2.html.

How do charged and mobile particles in a material redistribute themselves when an electric field is applied?

This is an important question which governs the physical behavior of many physical systems, including semiconducting *n*-junctions, batteries, fuel cells, or gas sensors, and, if you like, simply all junctions. Let us consider a material that essentially contains mobile carriers of only one kind, i.e. a metal (electrons), a (doped) semiconductor (electrons or holes, depending on doping), or a suitable ionic conductor (one kind of mobile ion). We imagine that we hold a positively charged plate at some (small) distance to the surface of a material having mobile negative charges (a metal, a suitable ionic conductor, a *n*-doped semiconductor). In other words, the positively charged plate

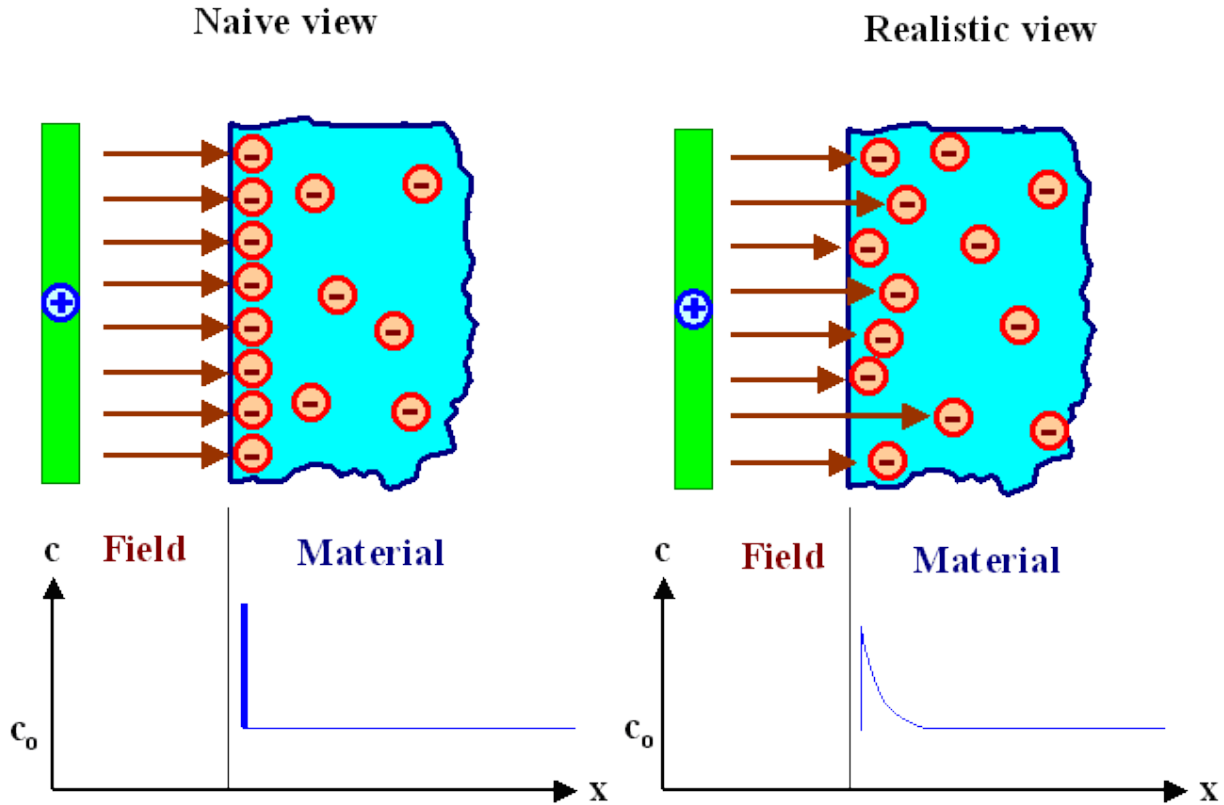


Figure 22.3: (Color online)

and the material are insulated, and no currents of any kind can flow between the two. However, there will be an electrical field, with field lines starting at the positive charges on the plate and ending on the negative charges inside the material. We have the situation shown in Fig. 22.3.

In a naive (and wrong) view, enough negatively charged carriers in the material would move to the surface to screen the field completely, i.e. prevent its penetration into the material. "Enough", to be more precise, means just the right number so that every field line originating from some charge in the positively charged plate ends on a negatively charged carrier inside the material.

But that would mean that the concentration of carriers at the surface would be pretty much a δ -function, or at least a function with a very steep slope. That does not seem to be physically sensible. We certainly would expect that the concentration varies smoothly within a certain distance, and this distance we call Debye length right away.

The Debye length is a crucial material parameter not only in all questions concerning ionic conductivity (the field of "Ionics"), but whenever the carrier concentration is not extremely large (i.e. comparable to the concentration of atoms, i.e. in metals).

We will now derive a simple formula for the Debye length. If all (necessarily mobile) carriers would pile up at the interface, we would have a large concentration gradient and Ficks law would induce a very large particle current away from the interface, and, since the particles are charged, an

electrical current at the same time! Since this electrical diffusion current j_d is proportional to the concentration gradient $-\nabla n(x)$, we have:

$$j_d(x) = -qD\nabla n(x) \quad (22.1)$$

where D is the diffusion coefficient, $n(x)$ is the concentration (density), and q is the charge of the carriers. Be clear about the fact that whenever you have a concentration gradient of mobile carriers, you will always have an electrical current by necessity. You may not notice that current because it might be cancelled by some other current, but it exists nevertheless.

The electrical field $E(x)$, that caused the concentration gradient in the first place, however, will also induce an electrical field current (also called drift current) j_E , obeying Ohms law in the most simple case, which flows in the opposite direction of the electrical diffusion current. We have:

$$j_E(x) = qn\zeta E(x) \quad (22.2)$$

where ζ is the mobility of the carriers, and $qn\zeta = \sigma$ is the conductivity.

The total electrical current will then be the sum of the electrical field and diffusion current. In equilibrium, both electrical currents obviously must be identical in magnitude and opposite in sign for every x , leading for one dimension to

$$qn(x)\mu E(x) = qD \frac{dn(x)}{dx}. \quad (22.3)$$

We can simplify this equation bit by using a relation between the diffusion coefficient and the mobility (Einstein-Smoluchowski relation):

$$\mu = eD/kT. \quad (22.4)$$

Moreover, the electric field can be substituted by $-d\phi/dx$ where ϕ is the electric potential of the system. We then obtain

$$-e \frac{d\phi}{dx} = kT \frac{d[\ln n(x)]}{dx}. \quad (22.5)$$

This is a kind of basic property of ionic devices. It results from the difference of the driving forces for the two opposing currents as noted before: The diffusion current is proportional to the gradient of the concentration whereas the field current is directly proportional to the concentration. Integrating this simple differential equation once gives

$$\phi(x) + \frac{kT}{e} \ln n(x) = \text{constant}. \quad (22.6)$$

Quite interesting: the sum of two functions of x must be constant for any x and for any functions conceivable; the above sum is obviously a kind of conserved quantity. That's why we give it a name and call it the electrochemical potential μ_{ec} (after multiplying with e so we have energy dimensions). While its two factors will be functions of the coordinates, its total value for any spatial coordinate in equilibrium is a constant (the three dimensional generalization is trivial). In other words we have

$$\mu_{ec} = V(x) + kT \ln n(x) \quad (22.7)$$

where μ_{ec} is the electrochemical potential and $V(x) = e\phi(x)$ is the electrostatic potential energy.

Obviously, in equilibrium (which means that nowhere in the material do we have a net current flow) the electrochemical potential must have the same value anywhere in the material. This reminds us of the Fermi energy. In fact, the electrochemical potential is nothing but the Fermi energy and the Fermi distribution in disguise.

However, since we are considering classical particles here, we get the classical approximation to the Fermi distribution which is, of course, the Boltzmann distribution for EF or Vec, respectively, defining the zero point of the energy scale. This is easy to see: Just rewriting the equation from above for $n(x)$ yields

$$n(x) = \exp([V(x) - \mu_{ec}]/kT). \quad (22.8)$$

What we have is the simple Boltzmann distribution for classical particles with the energy $V(x) - \mu_{ec}$.

Now we are ready to compute the Debye length. First we realize that the voltage or potential distribution (voltage times e) in the interior of a material in equilibrium can only be caused by concentration distributions of carriers that obey equilibrium statistics, i.e. the Boltzmann or the Fermi distribution. This is simply what the equation above tells us. What we still need in order to calculate the Debye length is a linkage between potentials $V(x)$ and concentration $n(x)$. This is of course what the Poisson equation, the main equation for electrostatics, is all about. We will only look at the one-dimensional case here. The Poisson equation then states

$$-\frac{d^2\phi}{dx^2} = \frac{dE}{dx} = \frac{en(x)}{\epsilon_0} \quad (22.9)$$

where we used Gauss law in differential form in the last step, $dE/dx = \rho/\epsilon_0$, where $\rho = en(x)$. We note in passing that for good conductors, for good conductors $n \sim 10^{22} \text{ cm}^3$, only a few of the carriers (a very small percentage) are needed to screen any reasonable electrical field. We may thus assume within a very good approximation that the carrier density at any point is given by the constant volume density n_0 of the field free material, plus a rather small space dependent addition $n_1(x)$:

$$n(x) = n_0 + n_1(x). \quad (22.10)$$

From Boltzmanns distribution, we know that

$$\frac{n(x)}{n_0} = 1 + n_1(x)/n_0 = e^{-[V(x)-V_0]/kT} \quad (22.11)$$

where V_0 is the potential energy in the case without electric field, in which case the distribution reads $n_0 = \exp([V_0 - \mu_{ec}]/kT)$. Let us for simplicity set the constant V_0 to zero. Since we assumed $n_1 \ll n_0$, we may express the exponential function as a Taylor series where we only retain the first term:

$$n_1(x) = n_0 V(x)/kT. \quad (22.12)$$

Plugging this back into Poisson's equation gives

$$\frac{d^2 n_1(x)}{dx^2} = \frac{e^2 n_0 n_1(x)}{\epsilon^0 kT} \quad (22.13)$$

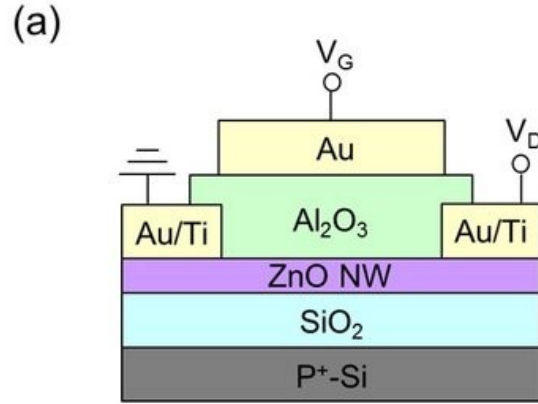


Figure 22.4: (Color online)

The general solution is of the form

$$n_1(x) = Ae^{x/d} + Be^{-x/d} \quad (22.14)$$

where

$$d \equiv \sqrt{\frac{\epsilon_0 kT}{e^2 n_0}} \quad (22.15)$$

With a bulk material for $x \rightarrow \infty$, so that $n_1(x \rightarrow \infty) \rightarrow 0$, and a surface at $x = 0$, we obtain $B = 0$, $A = n_1(0)$.

The quantity d is the Debye length we have been searching for. It also gives the length-scale over which the electrostatic potential returns to its equilibrium value. We see that the higher the electron concentration n_0 , the smaller the screening length.

22.2 Tuning Rashba strength in nanowires

The nanowire case is similar to the 2DEG case described above. Consider a geometry as shown in Fig. 22.4. There is no current injection into the nanowire, but there is an electric field. The nanowire thus acts as a poor metallic plate in a capacitor setup. Since it is a poor metal, the screening length of the electric field will be much longer than a nm or two.

Again, it is important to note that although there exists an electric field perpendicular to the nanowire, yet no current flows in this direction due to the diffusion force from the varying charge concentration close to the interface. So the electrochemical potential remains constant as one moves across the diameter of the nanowire, there is no current, but there is an electric field and a gradient in electron concentration.

Therefore, one can have an electric field across the entire diameter of a nanowire (typically d is some tens of nm) without any accompanying current. This field then gives rise to the Rashba effect

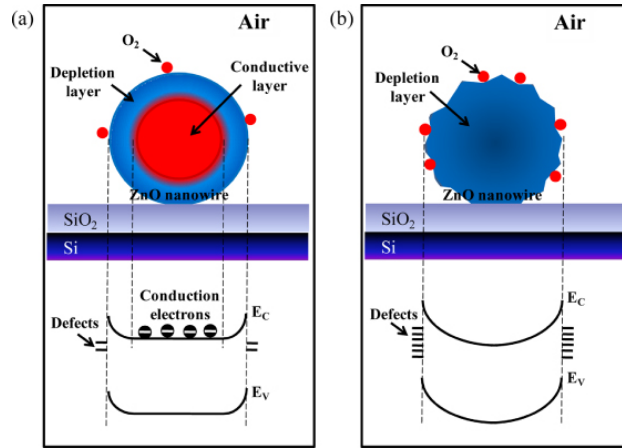


Figure 22.5: (Color online)

throughout the nanowire. Note that connecting a source and drain at the ends of the nanowire still permits a current to run along the wire length (rather than across its diameter) since there are mobile carriers present.

One can thus view the situation in the nanowire as being a screening region for electric field. This means that the electric field is strictly speaking not constant in the nanowire, but decaying. However, this non-uniformness of the Rashba effect is usually ignored when modelling the effect analytically in simple theoretical models. Moreover, there should also be band bending in the nanowire, so that the effective Fermi level is also tuned. The band bending should be in the opposite direction at the two surfaces of the nanowire since the accumulated charge has opposite polarity. The band bending could thus be such that one band is bent up and crosses the Fermi level at one interface, whereas it bends away from the Fermi level at the other interface. Then, one has effectively obtained free charge carriers at one interface of the nanowire, even if the average band bending is zero.

However, for a different geometry where the entire nanowire is encapsulated by the gate and oxide (see Fig. ??), the band bending should be equal at all interfaces and thus favorable to tuning the Fermi level (the Rashba tuning should be less efficient here since the electric field points radially relative the middle of the nanowire).

The explanation given here is qualitatively the same for why Rashba in 2DEGs can be tuned by a gate voltage. In that case one also tunes the Fermi level simultaneously, strictly speaking.

22.3 Quantum dots

Very pedagogical intro to quantum dots: https://www.fkf.mpg.de/5694184/Tutorial_SET2003.pdf

22.3.1 What is a quantum dot

It is useful to get acquainted with typical energy and length scales for quantum dots.

22.3.2 Hamiltonian for quantum dot

The Coulomb interaction U is essentially the electrostatic charging energy: the amount of energy we have to pay to bring an extra electron from lead to capacitor, moving against the established electric field.

The energy level parameter ϵ_i can be tuned via the gate voltage. This is because the

22.3.3 Coulomb blockade

Coulomb blockade is a classical phenomenon.

22.3.4 Kondo effect

Kondo effect can cause both increase and decrease of resistance, depending on whether we are dealing with metal or quantum dot.

22.3.5 Single-electron transistor

22.3.6 Qubits using quantum dots

There are different ways one can make a qubit state using quantum dots. The state of the qubit is typically read out via charge measurements.

Spin qubit

In this case, a single quantum dot can be used. The spin state of a single electron is the qubit state.

- Initialization: magnetic field to set the state of the spin.
- Read-out: convert the spin state to a charge signal.
- Advantage: Long coherence time, less sensitive to noise than charge-qubits, can operate at higher temperatures.
- Disadvantage: slower operation speed, need magnetic fields for manipulation.

The conversion is typically done via spin blockade. This is a mechanism where the spin state of a quantum dot system determines whether or not a charge transition between two quantum dots is permitted. For instance, if two electrons in a DQD are in a spin-singlet state, charge can move freely between the dots. If they are in an equal spin-triplet state, Pauli exclusion forbids charge moving and thus current to flow between the dots.

In practice, one would use gate voltages to rapidly attempt to change the system configuration from a (1,1) to (2,0) charge configuration. If the qubit was in a singlet state, the transition can occur as movement is not blocked. If it was in a triplet state, the transition is blocked. By using a nearby charge sensor, such as a quantum point contact, one can detect the change in the charge state of the DQD and thus read out indirectly the initial spin state.

There also exists methods using light to convert the spin state into a charge signal. For example, spin-dependent absorption of a circularly polarized light pulse can be used to excite the dot differently depending on the spin, and which state it was in is then read out using photoluminescence (emission of light after the dot has absorbed the photon and emits it).

Charge qubit

In this case, a double quantum dot system is utilized. The qubit state is $|0\rangle$ if the electron is position in the left quantum dot and $|1\rangle$ if it is in the right dot. In general, the electron can be in a superposition of these states.

- Initialization: gate voltages tunes the energy levels and thus the occupation of the dots.
- Read-out: a charge sensor of some sort, for instance conductance to a QPC for each quantum dot.
- Advantage: fast operation speed and manipulation, can use electric fields, compatible with existing infrastructure (silicon-based semiconductor technology), compact.
- Disadvantage: highly sensitive to noise due to use of charge degree of freedom.

A 2-qubit based on this principle can be constructed by making a capacitive coupling between pairs of double qubits.

Chapter 23

Quantum transport in mesoscopic structures

23.1 The most important length scales

We first give a quick overview over typical values for the sizes of the most important length-scales in mesoscopic condensed matter physics. Then, we proceed to treat the various processes in more detail below, explaining their physical meaning and physical origin.

Length scale	Typical size (metals)	Typical size (2DEGs)
Lattice constant a	A few Å	A few Å
Fermi wavelength λ_F	0.1-1 nm	10-100 nm (depends on doping level)
Elastic mean free path l_{mfp}	5-100 nm	100 nm - 100 μm
System size L	1 nm - 1 μm	1 nm - 1 μm
Phase coherence length l_ϕ	0.1 μm - 10 μm	0.1 μm - 10 μm
Electron-electron scattering $l_{\text{e-e}}$	0.1 μm - 10 μm	1 μm - 10 μm
Electron-phonon scattering $l_{\text{e-ph}}$	1 μm - 10 μm	1 μm - 10 μm
Inelastic relaxation length l_{in}	$\min\{l_{\text{e-e}}, l_{\text{e-ph}}\}$	$\min\{l_{\text{e-e}}, l_{\text{e-ph}}\}$
Spin-flip scattering l_{sf}	1 nm - 1 μm	1 nm - 1 μm

In metals, the typical order of some of these length-scales at low temperatures is [?]

$$\lambda_F \ll l_{\text{mfp}} \ll l_{\text{e-e}}, l_{\text{e-ph}}. \quad (23.1)$$

Down to ~ 1 K, $l_{\text{e-ph}} < l_{\text{e-e}}$, whereas for even for even lower temperatures we have $l_{\text{e-e}} < l_{\text{e-ph}}$. This is because of the strong temperature dependence of the electron-phonon scattering rate.

We can also set up a table which classifies various regimes of quantum transport and which quantity that is conserved in each case [?]. In the clean limit, the electron trajectories are ballistic as the system size L is too small for them to encounter any scattering. In the diffusive limit, elastic scattering on impurities is sufficiently frequent to randomize the momentum direction, so that momentum is no longer a good quantum number. If L is still smaller than electron-electron and electron-phonon scattering, the current for each energy is still conserved as energy relaxation does not occur. This means that the environment (phonons) and electrons are out-of-equilibrium. If the e-e scattering

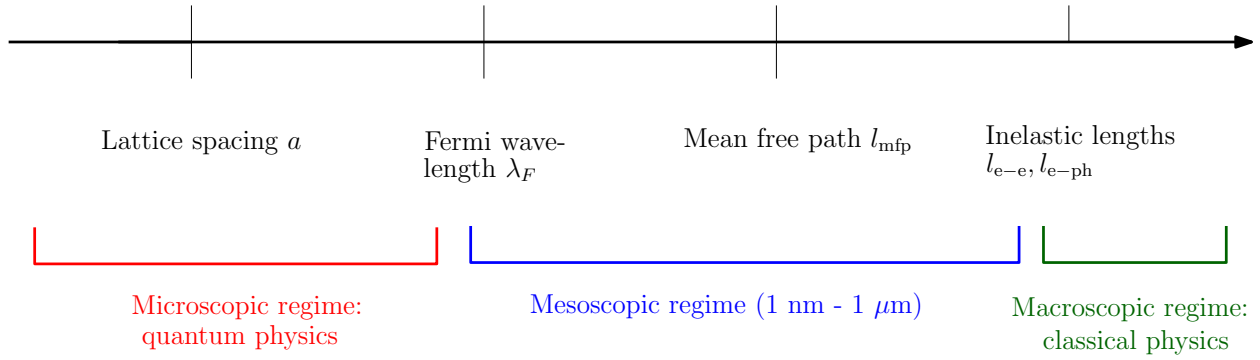


Figure 23.1: (Color online) Length scales determining the physics of a condensed matter system shown in their typical order.

becomes stronger, it mixes different energies so that only the total energy current is now conserved instead of the current carried by each energy mode. If in addition e-ph scattering becomes strong, we have an energy exchange between the electrons and the environment, so that local equilibrium is established between the electrons and the environment and only the charge current is conserved.

Regime of transport	Length hierarchy	Conserved quantity
Ballistic	$L \ll \text{all length scales}$	Current for each momentum state
Diffusive: non-equilibrium	$l_{\text{mfp}} \ll L \ll l_{\text{e-e}}, l_{\text{e-ph}}$	Current for each energy
Diffusive: quasi-equilibrium	$l_{\text{mfp}}, l_{\text{e-e}} \ll L \ll l_{\text{e-ph}}$	Charge and total energy current
Diffusive: local equilibrium	$l_{\text{mfp}}, l_{\text{e-e}}, l_{\text{e-ph}} \ll L$	Charge current

23.1.1 Bohr radius a_0

The Bohr radius $a_0 \simeq 0.5 \text{ \AA}$ is also often used as a reference length scale, and is equal to the most probable distance between the proton and electron in the hydrogen atom. It is thus smaller than a typical lattice constant.

23.1.2 Lattice constant a

23.1.3 Fermi wavelength λ_F

Length-scale of oscillations of electron plane waves

23.1.4 Elastic mean free path l_{mfp}

Distance between scattering events caused by impurities

23.1.5 Inelastic impurity scattering length l_{in}

Scattering length between events causing scattering that decreases the energy of the electrons. Typically much longer than elastic scattering length l_{mfp} and determined by processes that do not conserve energy, such as e-e and e-ph scattering.

23.1.6 System size L

Physical extent of the system

23.1.7 Phase coherence length l_ϕ

Distance travelled by electron before the planewave describing it can no longer be viewed as a coherent wavepackage, i.e. its QM distinction from the classical view of a point particle ceases to be important for e.g. quantum mechanical interference properties.

Scattering mechanisms that give rise to a random phase-shift of the electron wavefunction lead to dephasing. The dephasing length is thus effectively determined by the shortest length-scale of scattering which causes such a random phase-shift. Processes that break time-reversal symmetry *e.g.* by not conserving energy contribute to phase-relaxation, such as inelastic e-e and e-ph scattering and also spin-flip scattering.

23.1.8 Relaxation length/time of electrons

The following description is from [27]. The characteristic time for a distribution of electrons in a solid to approach or 'relax' to equilibrium after a disturbance is removed. A familiar example is the property of electrical conductivity, in which an applied electric field generates an electron current which relaxes to an equilibrium zero current after the field is turned off. The conductivity of a material is directly proportional to this relaxation time; highly conductive materials have relatively long relaxation times. The closely related concept of a lifetime is the mean time that an electron will reside in a given quantum state before changing state as a result of collision with another particle or intrinsic excitation. This lifetime is related to equilibrium properties of the material, whereas the relaxation time relates to the thermal and electrical transport properties. The average distance that an electron travels before a collision is called the mean free path. Although typical collision times in metals are quite short (on the order of 10^{-14} s at room temperature), mean free paths range from about 100 atomic distances at room temperature to 10^6 atomic distances in pure metals near absolute zero temperature. Considering the very dense packing of atoms in a solid, these surprisingly long electron path lengths are analogous to the unlikely event that a rifle bullet might travel for miles through a dense forest without hitting a tree. The detailed explanation of the electron mean free path in metals is a major success of the modern theory of solids.

A relaxation time τ appears in the simplest expression for the transport property of electrical conductivity, which states that the electrical conductivity equals the product of the relaxation time, the density of conduction electrons, and the square of the electron charge, divided by the electron effective mass in the solid.

The conduction process is a steady-state balance between the accelerating force of an electric field and the decelerating friction of electron collisions which occur on the time scale of the relaxation time. This process may be described in terms of the probability distribution function for the electrons, which depends on the electron momentum (proportional to the wave vector, $\mathbf{k}$, which labels the quantum state of the electrons), the position, and the time. Viewed in $\mathbf{k}$ -space, the entire distribution will shift from an equilibrium state under the influence of a perturbation such as an electric field (see illustration). For example, in the ground state, the collection of occupied electron states in $\mathbf{k}$ -space is bounded by the Fermi surface centered at the origin, while in an electric field this region is shifted. Because of electron collisions with impurities, lattice imperfections, and vibrations (also called phonons), the displaced surface may be maintained in a steady state in an electric field. These collisions also restore the equilibrium distribution after the field is turned off, and the relaxation time is determined by the rate at which the shifted distribution returns to equilibrium. Specifically, the contribution of collisions to the rate of change of the shifted distribution after the field is turned off equals the difference between the shifted and equilibrium distributions divided by

the relaxation time. This statement is referred to as the relaxation-time approximation, and is a simple way of expressing the role of collisions in the maintenance of thermodynamic equilibrium. The details of the various collision mechanisms are lumped into the parameter of the relaxation time. For example, in the case of mixed scattering by impurities and phonons, the inverse $1/\tau$ of the relaxation time can be determined from the sum of collision rates as the sum of the inverses of the electron-impurity and electron-phonon scattering times:

$$\frac{1}{\tau} = \frac{1}{\tau_{\text{imp}}} + \frac{1}{\tau_{\text{e-ph}}}. \quad (23.2)$$

Note that since we have defined relaxation time to be the time-scale associated with bringing the distribution function back to equilibrium (Fermi-Dirac) when the external force is turned off, we are by definition talking about *inelastic scattering*. Elastic scattering can isotropize the distribution function, but not bring it back to equilibrium since energy is conserved. On the other hand, inelastic scattering can bring the distribution function back to equilibrium and causes Joule heating since now the energy of the electrons is transferred to the lattice (which in turn can cause heat transfer). So in the above equation, τ_{imp} cannot be elastic scattering. In the above equation, we could also add other contributions such as electron-electron scattering $\tau_{\text{e-e}}^{-1}$. Although we will discuss the Boltzmann equation in more detail in the next subsection, let us note for now that the difference mathematically between elastic and inelastic scattering in the Boltzmann equation should be accounted for by writing the source-term in different ways. In the elastic case:

$$\frac{f(\mathbf{k}) - f_s(\mathbf{k})}{\tau_{\text{elastic}}} \quad (23.3)$$

where f_s is an isotropic in momentum space distribution function (s for s -wave), but which is not necessarily Fermi-Dirac. In the inelastic case:

$$\frac{f(\mathbf{k}) - f_0(\mathbf{k})}{\tau_{\text{inelastic}}} \quad (23.4)$$

where f_0 is now Fermi-Dirac. It is also isotropic, but not equal to f_s out of equilibrium. In general, we should have both source terms present when both elastic and inelastic scattering is present. See section 3.1.2 and 3.1.3 in <https://www.osti.gov/servlets/purl/1048505> for more details.

Below, we will consider what happens in the relaxation time approximation both for inelastic scattering and for elastic scattering. Both scenarios produce Ohm's law and Joule heating, but no stationary (time-independent) solution can be found in the elastic case. This is because inelastic processes are needed to remove the Joule heating caused by collisions with impurities.

In pure metals at low temperatures, the long mean free path of conduction electrons results from their large velocity (on the order of 10^6 m/s near the Fermi surface) and relatively long relaxation time, on the order of 10^{-9} s. From a practical standpoint, this is what makes metals useful as electrical conductors even at room temperature, where a relaxation time on the order of 10^{-14} s and a mean free path (equal to the product of the velocity and the relaxation time) on the order of 10^{-8} m (or about 100 atomic distances) is typical. As compared to poorly conducting solids or insulators, an excess of so-called free electrons in a metal contributes to the long mean free paths. From a quantum mechanical standpoint, the free-electron wave function readjusts in a perfectly periodic atomic lattice to avoid the atomic ion cores and spend most of the time in the spaces between. In the analogy of the rifle fired into a forest, the bullet will not travel far, but the sound

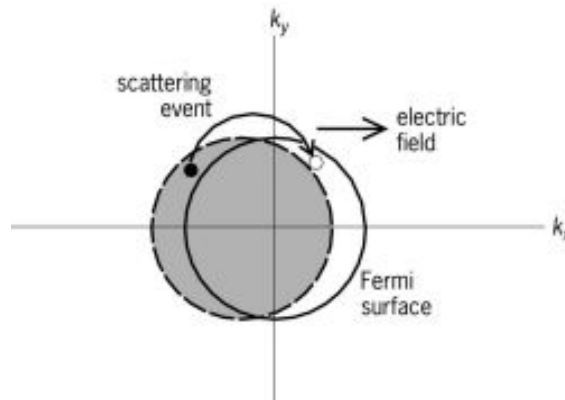


Figure 23.2: (Color online) Effect of the electric field on electron distribution in a solid, viewed in $\mathbf{k}$ -space, where $\mathbf{k}$ is the electron wave vector. The Fermi surface itself shifts when the electric field is applied due to a momentum-shift in the electrons originating from the component of the electric field which in the figure is applied in the x -direction. Recall that the concept of a Fermi surface is defined from the distribution function (the energy of electrons with 50% probability of occupancy). Figure from [27].

of the gunshot can, because the sound waves bend around the trees in a constructive manner. In a perfectly periodic lattice, the electron waves scatter constructively from the atomic ion cores, resulting in screening of the cores and coherent transmission of the waves over large distances. Any disturbance to the lattice periodicity tends to destroy this wave phenomenon, resulting in lower transmission or energy loss. At room temperature, the conductivity is usually limited by scattering from lattice vibrations (phonons). At lower temperatures, vibrations are greatly reduced, but the conductivity is still limited by scattering from impurities and imperfections.

In the superconductive state, observed in many metals and certain complex compounds at sufficiently low temperatures, impurities, imperfections, and lattice vibrations become completely ineffective in retarding current flow, leading to persistent electric currents even after the driving electric field is removed. This state of resistanceless conduction is described as an ordered quantum state of pairs of electrons resulting from lattice vibrations which deform the ion core potential in such a way as to provide an attractive electron-electron interaction. The relaxation time thus becomes infinite (as nearly as can be measured), a rare macroscopic manifestation of a quantum effect.

23.1.9 Boltzmann equation: semiclassical theory of transport

Let us now use the relaxation time approximation quantitatively by developing a kinetic equation that describes the spatial and temporal evolution of the distribution function in a quantum system driven out of equilibrium. The equation is obtained by using a mixture of classical and quantum arguments, thus earning its name as a *semiclassical* theory. We follow here closely the lecture notes of Carsten Timm.

If one wishes to determine how the current in a system depends on an applied electric field, there are different routes that can be taken. For a small perturbation (the electric field), one can use linear-response theory. In many-particle quantum theory, this results in the Kubo formula. If one additionally can assume that the external perturbation changes slowly in time and space (compared to atomic scales), we can approximate the current-response by using a semiclassical description.

The following derivation can be derived as a limit of many-particle quantum theory.

Consider the so-called phase space distribution function $\rho(\mathbf{r}, \mathbf{k}, t)$ of the system. It determines the probability $\rho d\mathbf{r} d\mathbf{k}$ that the system at time t will be found in the infinitesimal phase space volume $d\mathbf{r} d\mathbf{k}$. According to Liouville's theorem, the classical function ρ should satisfy

$$\frac{d\rho}{dt} = 0 \quad (23.5)$$

under a classical time evolution of the system. In quantum mechanics, we know that position and momentum are subject to the uncertainty principle $\Delta r \Delta p \geq \hbar/2$. Therefore, so long as we consider a distribution function ρ that is not localized in a phase-space volume $d\mathbf{r} d\mathbf{k}$ that is smaller than $\hbar^3$, quantum effects should be negligible. We can write out the total time-derivative as

$$\frac{\partial \rho}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial \rho}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial \rho}{\partial \mathbf{k}} = 0. \quad (23.6)$$

For a free particle, we have for the canonical Hamilton equations that

$$\begin{aligned} \dot{\mathbf{r}} &= \frac{\partial H}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m} = \frac{\hbar \mathbf{k}}{m}, \\ \dot{\mathbf{k}} &= \frac{1}{\hbar} \cdot \mathbf{p} = -\frac{1}{\hbar} \frac{\partial H}{\partial \mathbf{r}} = -\frac{1}{\hbar} \nabla V = \frac{1}{\hbar} \mathbf{F} \end{aligned} \quad (23.7)$$

where H is the Hamiltonian and $\mathbf{F}$ is the force. Therefore, we can write

$$\left(\partial_t + \frac{\hbar \mathbf{k}}{m} \cdot \partial_{\mathbf{r}} + \frac{\mathbf{F}}{\hbar} \cdot \partial_{\mathbf{k}} \right) \rho = 0. \quad (23.8)$$

For electrons in a uniform and time-independent electric field, $\mathbf{F} = -e\mathbf{E}$ (we use the convention $e > 0$). The above equation is suitable to describe ρ in the absence of any scattering. It can be directly verified that

$$\rho(\mathbf{r}, \mathbf{k}, t) = f(\mathbf{k} + e\mathbf{E}t/\hbar) \quad (23.9)$$

solves Eq. (23.8) for any differentiable function f . This particular solution is uniform in real space, so that $\partial_{\mathbf{r}} \rho = 0$, and describes the free acceleration of electrons in an electric field. This cannot be a realistic description of a normal metal. The reason is that we have neglected all forms for scattering.

We now remedy this by including an extra term in Eq. (23.8). Scattering will change ρ as a function of time beyond what is already included there without scattering. The presence of scattering is taken into account by setting $d\rho/dt$ equal to a *scattering term* $S = S[\rho(\mathbf{r}, \mathbf{k}, t)] \equiv -\frac{\partial f}{\partial t}|_{\text{coll}}$ so that

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t} \right) \Big|_{\text{coll}} = -S[\rho]. \quad (23.10)$$

We thus have.

$$\left(\partial_t + \frac{\hbar \mathbf{k}}{m} \cdot \partial_{\mathbf{r}} + \frac{\mathbf{F}}{\hbar} \cdot \partial_{\mathbf{k}} \right) \rho = -S[\rho]. \quad (23.11)$$

This is the *Boltzmann equation*. The scattering term is seen to generally be a functional of ρ and can depend on ρ at all positions and times, to the extent that such a dependence is consistent with causality. We note that the collision term thus causes the phase-space distribution function to not be constant in time. More generally, from a classical physics perspective, Liouville's theorem is violated by

- Any source or sink of particles, causing nonconservation of particle number.
- Any collisional/dissipative forces.

In a classical physics treatment, the collision term is zero if the equations of motion for the system can be generated from a Hamiltonian. This holds even in the presence of external fields, such as $\mathbf{E}$, which drives the system away from equilibrium. The existence of a Hamiltonian is classically a sufficient, but not necessary, condition for $\partial f / \partial t|_{\text{coll}} = 0$. We can then understand why any dissipative forces, arising *e.g.* from collisions between particles, violate Liouville's theorem since such forces satisfy $\nabla_{\mathbf{v}} \cdot \mathbf{F} \neq 0$ and cannot be directly included in a Hamiltonian (but rather as a Rayleigh dissipation-function).

Inelastic scattering

Different expressions for $S[\rho]$ can be derived for different physical systems, but here we discuss the common and simple relaxation-time approximation. The underlying assumption for this approximation is that $\rho(\mathbf{r}, \mathbf{k}, t)$ has to relax to thermal equilibrium (thermalize) at large times when no force is applied, even if scattering is present. For fermions, one has $\rho = \rho_0(\mathbf{k}) \propto n_F(\epsilon_{\mathbf{k}})$ in equilibrium. We can ensure this behavior by making the ansatz

$$S[\rho] = \frac{\rho(\mathbf{r}, \mathbf{k}, t) - \rho_0(\mathbf{k})}{\tau}. \quad (23.12)$$

The quantity τ is the relaxation time which determines how fast ρ relaxes to ρ_0 . Note that we are here talking about inelastic scattering since the collision term causes relaxation back to equilibrium, and *not elastic scattering*.

Qualitatively, by setting the time-derivative of ρ equal to minus the difference between ρ and its equilibrium value, we ensure that ρ mathematically changes with time in such a way as to minimize this difference. Let us show this explicitly. In the absence of forces and for a uniform distribution of electrons in space, $\partial_{\mathbf{r}}\rho = 0$, the Boltzmann equation takes the form:

$$\partial_t \rho(\mathbf{k}, t) = \frac{\rho_0(\mathbf{k}) - \rho(\mathbf{k}, t)}{\tau} \quad (23.13)$$

which is solved by

$$\rho(\mathbf{k}, t) = [\rho(\mathbf{k}, t=0) - \rho_0(\mathbf{k})]e^{-t/\tau} + \rho_0(\mathbf{k}). \quad (23.14)$$

This time-evolution of the phase-space distribution describes a system that starts with some initial non-equilibrium probability density function $\rho(\mathbf{k}, t=0)$ and then returns to equilibrium over a relaxation time τ . Note that τ is allowed to depend on $\mathbf{k}$, $\tau = \tau(\mathbf{k})$.

When different scattering mechanisms are present which act independently, the total scattering term $S[\rho]$ is simply a sum of the contributions of these mechanisms

$$S[\rho] = S_1[\rho] + S_2[\rho] + \dots \quad (23.15)$$

This is known as Matthiessen's rule. Therefore, the relaxation rate $1/\tau$ can in total be written as

$$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \dots \quad (23.16)$$

Three important scattering mechanisms are:

- Scattering of electrons by disorder/impurities. This contribution does not have a strong dependence on temperature.
- Electron-phonon scattering. This mechanism does depend strongly on temperature, because the number of available phonons decreases drastically at low temperatures. For a conventional metal, one finds $\tau_{\text{e-ph}}^{-1} \propto T^3$.
- Electron-electron scattering. The temperature-dependence is typically $\tau_{\text{e-e}}^{-1} \propto T^2$.

We now come back to the issue of how an applied electric field modifies the distribution function. Consider the force $\mathbf{F} = -e\mathbf{E}$ and apply the relaxation-time approximation, so that the Boltzmann equation takes the form:

$$\left(\partial_t + \frac{\hbar \mathbf{k}}{m} \cdot \partial_{\mathbf{r}} - \frac{e\mathbf{E}}{\hbar} \cdot \partial_{\mathbf{k}} \right) \rho = -\frac{(\rho - \rho_0)}{\tau}. \quad (23.17)$$

In a stationary scenario $\partial\rho/\partial t = 0$ and for a spatially uniform field, which we assume allows for $\partial\rho/\partial\mathbf{r} = 0$, we obtain the differential equation

$$-\frac{e\mathbf{E}}{\hbar} \cdot \partial_{\mathbf{k}} \rho(\mathbf{k}) = \frac{\rho_0(\mathbf{k}) - \rho(\mathbf{k})}{\tau}. \quad (23.18)$$

Rearranging terms produces

$$\rho(\mathbf{k}) = \rho_0(\mathbf{k}) + \frac{e\mathbf{E}\tau}{\hbar} \cdot \partial_{\mathbf{k}} \rho(\mathbf{k}). \quad (23.19)$$

We iterate this equation by inserting the lhs into the second term on the rhs and find

$$\rho(\mathbf{k}) = \rho_0(\mathbf{k}) + \frac{e\mathbf{E}\tau}{\hbar} \cdot \partial_{\mathbf{k}} \rho_0(\mathbf{k}) + \mathcal{O}(\mathbf{E}^2). \quad (23.20)$$

In linear-response, we thus truncate the expansion after the linear term so that

$$\rho(\mathbf{k}) = \rho_0(\mathbf{k}) + \frac{e\mathbf{E}\tau}{\hbar} \cdot \partial_{\mathbf{k}} \rho_0(\mathbf{k}) \quad (23.21)$$

But it is easy to verify that this is precisely the Taylor expansion of $\rho(\mathbf{k} + e\mathbf{E}\tau/\hbar)$. Therefore, to linear order in $\mathbf{E}$, the solution to the Boltzmann equation for a spatially and temporally homogeneous system is:

$$\rho(\mathbf{k}) = \rho_0(\mathbf{k} + e\mathbf{E}\tau/\hbar) \propto n_F(\epsilon_{\mathbf{k} + e\mathbf{E}\tau/\hbar}). \quad (23.22)$$

We see that the effect of the electric field is to shift the distribution function in $\mathbf{k}$ -space by $-e\mathbf{E}\tau/\hbar$. The distribution is thus shifted in the direction opposite to the applied electric field.

We can also evaluate the current if desirable, namely

$$\mathbf{j} = -e \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\hbar \mathbf{k}}{m} \rho_0(\mathbf{k} + e\mathbf{E}\tau/\hbar) \quad (23.23)$$

which upon insertion of our solution gives

$$\mathbf{j} = \frac{e^2 n \tau}{m} \mathbf{E} \equiv \sigma \mathbf{E}. \quad (23.24)$$

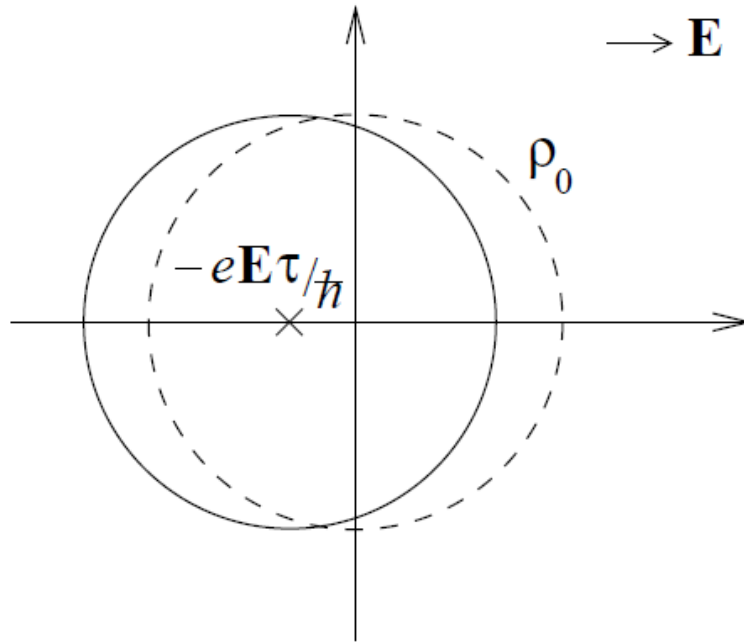


Figure 23.3: (Color online) Shift in the distribution function for electrons with negative charge upon applying an electric field $\mathbf{E}$.

Here, $n = N/V$ is the concentration of electrons in real space and σ is the conductivity. This is the *Drude formula*, which is independent on which particular equilibrium distribution function one uses (classical or quantum) and thus gives the same result in both cases. Basically, it gives Ohm's law. The resistivity indeed becomes

$$\rho = \frac{1}{\sigma} = \frac{m}{e^2 n \tau} = \frac{m}{e^2 n} \left(\frac{1}{\tau_{\text{imp}}} + \frac{1}{\tau_{\text{e-ph}}} + \frac{1}{\tau_{\text{e-e}}} \right). \quad (23.25)$$

There is also a *quantum Boltzmann equation* in which case the drift term $\mathbf{F} \cdot \partial_{\mathbf{k}} \rho$ and the diffusion term $\mathbf{k} \cdot \partial_{\mathbf{r}} \rho$ are omitted and the time-derivative of ρ is fully computed by a collision integral which is evaluated using quantum theory.

Elastic scattering: Ohm's law, Joule heating, but absence of steady state limit

It is instructive to solve the Boltzmann equation if we include elastic scattering in the relaxation time approximation instead of inelastic scattering. We will see that the elastic scattering leads to an isotropization of the distribution function, causing electrical resistance and Joule heating (in the form of an linearly increasing system energy with time), but does not give a stationary solution (unlike the inelastic case).

With elastic scattering only and a spatially homogeneous situation, the Boltzmann equation reads:

$$\left(\partial_t - \frac{e\mathbf{E}}{\hbar} \cdot \partial_{\mathbf{k}} \right) \rho = -\frac{(\rho - \bar{\rho})}{\tau}. \quad (23.26)$$

Here, τ is the elastic scattering time and $\bar{\rho} = \langle \rho \rangle$ is the momentum-direction averaged distribution

function. Assume that the solution can be expanded in powers of the applied field:

$$\rho = \rho^{(0)} + \rho^{(1)} + \rho^{(2)} + \dots \quad (23.27)$$

where

$$\rho^{(n)} \ll \rho^{(n-1)}. \quad (23.28)$$

To zeroth order, we know that $\rho^{(0)}$ is the Fermi-Dirac function

$$\rho^{(0)} = \frac{1}{e^{\beta[E(\mathbf{k}) - \mu]} + 1}. \quad (23.29)$$

We seek a stationary solution and thus see if we can solve the equation with $\partial\rho^{(1)}/\partial t = 0$. We get to first order in $\mathbf{E}$:

$$-e\mathbf{E} \cdot (\nabla_{\mathbf{k}}\rho^{(0)}) = -\frac{\rho^{(1)} - \bar{\rho}^{(1)}}{\tau}. \quad (23.30)$$

This equation is solved by

$$\rho^{(1)} = \tau\mathbf{E} \cdot (\nabla_{\mathbf{k}}\rho^{(0)}) \quad (23.31)$$

since then $\bar{\rho}^{(1)} = 0$. The first order term produces the current response to the electric field (to first order in $\mathbf{E}$) and thus the resistivity, just like for the inelastic scattering case. Note how the solution up to first order in $\mathbf{E}$ is thus completely time-independent.

However, when we go to second order in $\mathbf{E}$, considering $\rho^{(2)}$, we see why a stationary solution cannot be obtained for purely elastic scattering. The second order terms in $\mathbf{E}$ in the Boltzmann equation take the form:

$$\frac{\partial\rho^{(2)}}{\partial t} = \tau(e\mathbf{E} \cdot \nabla_{\mathbf{k}})^2\rho^{(0)} - \frac{\rho^{(2)} - \bar{\rho}^{(2)}}{\tau}. \quad (23.32)$$

Taking the angular average $\int d\Omega_{\mathbf{k}}/2\pi$ of the entire equation gives

$$\frac{\partial\bar{\rho}^{(2)}}{\partial t} = \tau \int \frac{\Omega_{\mathbf{k}}}{2\pi} (e\mathbf{E} \cdot \nabla_{\mathbf{k}})^2\rho^{(0)}. \quad (23.33)$$

It is clear that $\rho^{(2)}$ cannot be time-independent. Instead, we find the solution after integrating with respect to time:

$$\bar{\rho}^{(2)} = t\tau \int \frac{\Omega_{\mathbf{k}}}{2\pi} (e\mathbf{E} \cdot \nabla_{\mathbf{k}})^2\rho^{(0)}. \quad (23.34)$$

Thus, no stationary solution can be found for elastic scattering only. A consequence of the linearly increasing $\bar{\rho}^{(2)}$ is that the energy density grows linearly in time, and in fact produces Joule heating. The energy density is given by

$$\epsilon_{\text{tot}} = \int \frac{d\Omega_{\mathbf{k}}}{2\pi} \int d\epsilon \epsilon N(\epsilon) \rho \quad (23.35)$$

where $N(\epsilon)$ is the density of states. The first-order contribution vanishes since $\rho^{(1)}$ is odd in $\mathbf{k}$. The second-order contribution to the energy density is

$$\begin{aligned}\delta\epsilon &= t\tau \int N(\epsilon)\epsilon \int \frac{\Omega_{\mathbf{k}}}{2\pi} (e\mathbf{E} \cdot \nabla_{\mathbf{k}})^2 \rho^{(0)} \\ &= \frac{V^2}{R} t\end{aligned}\tag{23.36}$$

after using the expression for the current and Ohm's law. This is clearly the Joule heating contribution, giving a power V^2/R .

One might ask: how can elastic scattering, which preserves energy, lead to a system energy that increases linearly with time? It can be understood as the part of the kinetic energy provided by acceleration of the electric field that does not lead to an ever-increasing current, but rather isotropization of the electron motion and thus an effective higher temperature. Or think of the electric field applying a constant force on the electrons without any outlet for the energy via inelastic scattering: even though the elastic impurity scattering causes resistance which prevents free acceleration, the energy of the system still increases due to the continuously applied force which injects momentum/energy into the system.

In summary, both Ohm's law (to first order in $\mathbf{E}$) and Joule heating (to second order in $\mathbf{E}$) are recovered if we include only elastic scattering, but f has no steady-state solution.

23.2 Landauer-Büttiker formalism

This formalism provides a general approach to understanding the conduction properties of small, non-interacting quantum coherent systems which are connected to classical (decohering) reservoirs. The reservoirs effectively take the role of current sources/sinks and have well-defined chemical potentials with an equilibrium distribution function for the electrons. The leads serve as idealized, resistanceless contacts which connect the reservoirs to the sample (scattering region). The Landauer-Büttiker formalism makes several predictions that are independent of the microscopic details of the system or the measurements, which have been confirmed by experiments.

To set the stage, consider first transport between two reservoirs with chemical potentials μ_L and μ_R , corresponding to a voltage difference $eV = \mu_L - \mu_R$, connected via a ballistic wire free from any impurities or scattering. This is shown in Fig. 23.4(a). Landauer examined this system in 1959 and posted the question: is the conductance of this object infinite due to the absence of scattering? Experimentally, one finds that the conductance remains finite even if W and L are much smaller than the mean free path l_{mfp} . If the transmittance through the junction is 100%, how can there exist a resistance? As we shall see, the 2-terminal conductance is limited by a *contact resistance*.

At a given energy E , there exists a number $M(E)$ of transverse modes characterized by their transverse momentum $k_{\perp}$. Each mode is given a channel number n and the modes in general have different probabilities T_n of transmitting through a scattering region. In the present system, $T_n = 1$ since there are no impurities. The group velocity for a given mode with momentum k in the direction of the wire is

$$v_g(E) = \frac{1}{\hbar} \frac{\partial E}{\partial k}.\tag{23.37}$$

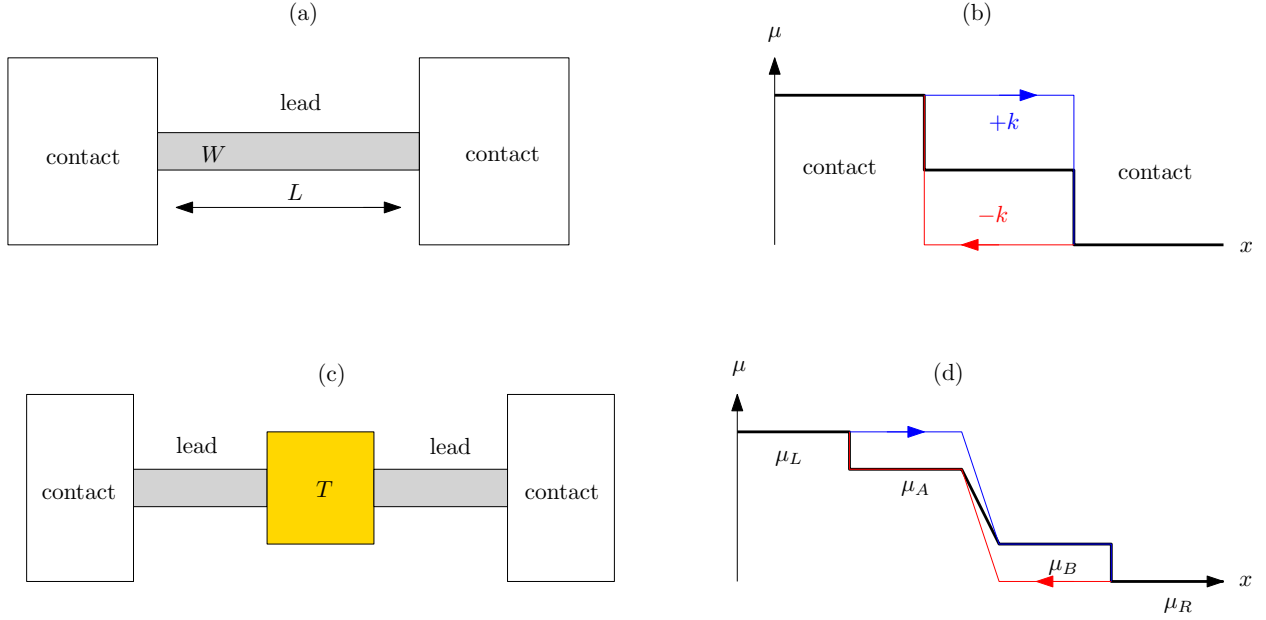


Figure 23.4: (Color online) ...

The resulting current carried from left to right is then

$$I_L = \frac{e}{L} \sum_{k_x, \sigma} v_g(E) f_L(E) M(E) \quad (23.38)$$

where $f_L(E)$ is the Fermi-Dirac distribution function in the left reservoir. Since there is no scattering, we are assuming that all right-moving particles originate from the left reservoir and thus their occupation is described by the corresponding distribution function $f_L(E)$. Note that $E = E_k$ depends on the momentum. For a small spacing $2\pi/L$ between the allowed k values, where L is the length of the ballistic wire, we can convert

$$\sum_{k, \sigma} g(k_x) \rightarrow 2 \times \frac{L}{2\pi} \int g(k) dk. \quad (23.39)$$

In this way, the current takes the form:

$$I_L = \frac{2e}{h} \int_{-\infty}^{\infty} f_L(E) M(E) dE \quad (23.40)$$

after converting it from an integral over momentum to energy over integral. Note how the group velocity has vanished due to the density of states factor $dk/dE = N(E) = 1/v_g$. This is a special feature of a 1D setup: in 2D, the two do not cancel in general. In other words, the current carried per mode per unit energy is $2e/h$.

Moreover, it is useful to comment specifically on the inclusion of the group velocity and how this depends on whether the wavefunctions are normalized by $1/\sqrt{v}$ so that the corresponding particle currents in each material carry the same particle flux. For instance, BTK do not include normalization factors, so the quantum mechanical particle current computed from an incoming wavefunctions on the N and S side of the interface, respectively, does not carry the same particle flux. Therefore,

the group velocity factor does *not* have to be included in the equation for the current: the transmission coefficient $M(E)$ derived by using probability current conservation already includes the effect of different group velocities.

On the other hand, if one includes in the wavefunctions the normalization factor $1/\sqrt{v}$, which can be dramatically different for quasiparticles in a normal metal and in a superconductor, then the probability amplitudes for transmission do not include the effect of different group velocities (since this has been normalized out). Then, v_g *must* be included in the formula for the total energy-integrated current.

Note that there is no blocking factor of the type $1 - f$ which usually is taken into account in the tunnel Hamiltonian framework. The reason is that in this derivation it is assumed that the scattering states are eigenmodes of the leads and since they are delocalized plane-waves an eigenmode E present in the left lead automatically means that an eigenmode with energy E is also present in the right lead. This is different from considering scattering directly between two reservoirs without any leads, where it is natural to include a blocking factor $1 - f$ when evaluating the current (such as in the tunnel Hamiltonian). This is a heuristic argument, but the final Landauer-Buttiker formula can also be derived microscopically from the Kubo formula and so this justifies the absence of the blocking factor due to the above argument.

Following exactly the same procedure, we can construct the current going from right to left. To find the net current flowing through the system, we must subtract the left-going from the right-going current:

$$I = I_L - I_R = \frac{2e}{h} \int_{-\infty}^{\infty} [f_L(E) - f_R(E)] M(E) dE. \quad (23.41)$$

In the zero-temperature limit, where the distribution functions become Heaviside step-functions, one obtains

$$I = \frac{2e}{h} M(\mu_L - \mu_R). \quad (23.42)$$

It is clear that the conductance of an M -channel ballistic wire is then

$$G = \frac{I}{V} = \frac{2e^2}{h} M. \quad (23.43)$$

At first glance, this might seem strange. There is no scattering in the system. How can there be a finite resistance? Since the conducting wire is ballistic, the resistance $R = G^{-1}$ must be associated with the reservoirs themselves. In fact, it is a *contact resistance* which physical origin is thermalization of the injected electrons into the reservoirs: in order for an electron coming from the left reservoir into the right reservoir to become part of the equilibrium Fermi gas in the right reservoir, it has to deposit its energy through scattering. This results in a voltage drop and energy loss, as illustrated in Fig. 23.4(b). The reservoirs thus account for the dissipation of energy. In order for us to assume that the reservoirs remain in equilibrium despite the fact that they absorb a current of electrons which thermalize, the reservoirs have to be sufficiently large.

The same type of resistance is also present when the lead (conducting wire) is diffusive, although in that case there is also an intrinsic resistance in the lead itself due to impurity scattering. In a diffusive wire, scattering cause the distribution function to change with position x and one has to

solve a kinetic equation to determine what it looks like. There is a voltage drop occurring continuously throughout the wire. In general, the resulting local distribution function will be non-thermal (in effect, deviate from a Fermi-Dirac distribution form).

The voltage drop in the structure of Fig. 23.4(a) is shown in (b). Right-moving carriers remain at the chemical potential μ_L until they reach the right contact, in which case they have to thermalize and a voltage drop occurs. Left-moving carriers behave in the corresponding way, staying at μ_R until they reach the left reservoir. The bold curve represents the average chemical potential $\mu_{\text{average}} = (\mu_L + \mu_R)/2$ in the conducting lead.

A more general and realistic setup can be obtained by considering Fig. 23.4(c). In this case, we add a scattering region characterized by the transmittance T which in turn is connected to ballistic leads and contacts (reservoirs). The Landauer formula now takes the form:

$$G = \frac{2e^2}{h} \times M \times T, \quad (23.44)$$

so that the resistance is

$$R = G^{-1} = \frac{h}{2e^2 M T}. \quad (23.45)$$

What does this resistance consist of? The contact resistance should be the same, so it should be contained within this R . To see this, note that we can rewrite:

$$R = \frac{h}{2e^2 M} + \frac{h}{2e^2 M} \frac{1-T}{T}. \quad (23.46)$$

The first term is the contact resistance while the second term is the resistance coming from the scattering region. As it should, the second term vanishes if $T = 1$ and diverges if $T = 0$.

For the present setup, the chemical potential in the various regions is shown in Fig. 23.4(d). Consider for instance the right-moving particles in lead A, which are described by the equilibrium distribution function from the left reservoir. They maintain their chemical potential μ_L until they reach right reservoir, but the chemical potential in lead B is now comprised of the contribution from both transmitted right-going particles coming from the left reservoir *and* reflected particles that originated from the right reservoir. The chemical potential for $+k$ states in lead B is thus determined by the value of T : for $T = 1$, it is equal to μ_L since such particles only come from the left reservoir, while for $T = 0$ it is equal to μ_R since $+k$ states can only come from reflected particles originating from the right reservoir. Same argument goes for the left-moving particles, and the chemical potential for the $-k$ states in lead A is now determined by the value of $1 - T$.

Thus, if we are interested in only the conductance of the actual device (lead/scattering region/lead), we must omit the contact resistance part and thus obtain

$$R_{\text{device}} = G_{\text{device}}^{-1} = \frac{h}{2e^2 M} \frac{1-T}{T} = \frac{\mu_A - \mu_B}{I}. \quad (23.47)$$

To probe this resistance alone, which should be zero for a truly ballistic device, one could use a 4-terminal measurement with a voltage probe on each lead. Complications that can arise in such a scenario include that the voltage probes can perturb the currents in the device and that they may not couple equally to $+k$ and $-k$ modes.

23.2.1 Derivation of Blonder-Tinkham-Klapwijk formula

23.2.2 Conductance quantization

An important consequence of the Landauer formula is that if we can deform the ballistic conductor in such a way as to controllably vary the number of modes M , one at the time, the conductance should display steps of $2e/h$. Such a scenario can be achieved by using 2DEGs such as GaAs/AlGaAs where a gate voltage controls the number of available transverse modes as the voltage changes the band structure. This was observed by Van Wees *et al.* in PRL **60**, 848 (1988).

23.3 Quantum fluctuations in a RC-circuit

To illustrate some important principles regarding quantum fluctuation effects on electron tunneling and how such fluctuations stem from the Heisenberg uncertainty principle, consider a circuit consisting of a capacitor C and a resistance R in a closed circuit.

If you place a charge Q_0 on the capacitor, so that there is $+Q_0$ charge on one side of it and $-Q_0$ on the other side, then we can find the time-evolution of the charge $Q(t)$ as follows. The total voltage across the capacitor and the resistance must vanish according to Kirchhoff's law. Therefore, we have

$$Q/C + \frac{dQ}{dt}R = 0 \quad (23.48)$$

which has the solution $Q(t) = Q_0 e^{-t/\tau}$ where $\tau = RC$. We used the initial condition $Q(0) = Q_0$. The charge on the capacitor will thus decay over time.

Now, the Heisenberg uncertainty principle for time and energy states that (see section 3.1.2 for a more detailed discussion), given that the system has an uncertainty in the energy ΔE , the time Δt required for the system to evolve in such a way that a physical observable A changes significantly (as defined by its rate of change relative its expectation value), satisfies:

$$\Delta E \Delta t \geq \hbar/2. \quad (23.49)$$

If the system is in an time-independent eigenstate of the Hamiltonian so that the energy is conserved, $\Delta E = 0$, and $\Delta t \rightarrow \infty$ as expected. In the present system, the significant change occurs after the lifetime, so that $\Delta t = \tau$. The corresponding uncertainty in energy of the system becomes $\Delta E \geq \hbar/(2RC)$.

Imagine that we want to use our RC-circuit to observe single-electron tunneling effects. This can in principle be done by detecting the charging energy associated with a single electron tunneling event, which equals $E_c = e^2/(2C)$. It is clear that if one is to be able to experimentally detect this charging energy of the capacitor, it must be much larger than the uncertainty in of the system's energy ΔE . It is precisely this ΔE which may be regarded as a quantum fluctuation. The condition to be able to observe single-electron tunneling clearly, so that quantum fluctuation effects are small, thus becomes:

$$E_c \gg \Delta E \quad (23.50)$$

which gives

$$G \ll \frac{2e^2}{h}\pi \quad (23.51)$$

where $G = 1/R$ is the conductance of the resistor. The tunneling resistance must thus be large.

23.4 Localization effects due to quantum interference

23.4.1 Weak localization

In electronic systems with disorder, a positive correction to the resistivity of a metal or semiconductor is obtained at low temperatures. This is known as *weak localization*.

The origin of this effect is quantum mechanical and comes from the fact that electron motion in such a system is diffusive rather than ballistic: electrons experience multiple random scatterings off impurities rather than moving in straight trajectories. Resistivity is related to the probability that an electron is backscattered. In a quantum mechanical treatment, we have to sum all paths between the points before computing the probability rather than performing a summation over all probabilities for individual paths as one would do classically. As a result, the QM treatment gives rise to interference terms: products of amplitudes corresponding to different paths.

The net result of these interference terms is that an electron is more likely to be backscattered as disorder increases and thus causes an increase in resistivity. The classical contribution (sum of probabilities of each path) to the conductivity of a metal is known as the Drude formula, whereas the weak localization correction corresponds to the quantum interference terms averaged over possible disorder configurations.

More specifically, the constructive interference between paths causing weak localization comes mainly from self-crossing paths where an electron propagates in a clock-wise and counter-clockwise direction around a loop before being backscattered in the same direction it came from. Since the loops have identical lengths, the quantum phases will enhance each other and increase the net amplitude for an electron being backscattered. The weak localization effect is most prominently manifested in low-dimensional systems (films and wires) since self-crossing trajectories are more likely to occur in low dimensions.

To be more quantitative, let A_+ be the amplitude for the electron path going clock-wise in the figure and A_- be the amplitude for the electron path going counter-clockwise. For a diffusive normal metal without spin-orbit coupling, we have $A_+ = A_-^*$. This no longer holds in the presence of a magnetic field. The total amplitude for scattering the electron back to where it came from classically would be

$$P_{\text{classical}} = |A_+|^2 + |A_-|^2 \equiv 2A^2 \quad (23.52)$$

whereas quantum mechanically we have

$$P_{\text{QM}} = |A_+ + A_-|^2 = 4A^2 = 2P_{\text{classical}} \quad (23.53)$$

thus enhancing the resistivity.

It is notable that the presence of a magnetic field $\mathbf{B}$ destroys weak localization, as the phases picked up upon transvering the loop clock-wise or counter-clockwise no longer interfere constructively (the magnetic field causes them to be different). For a textbook treatment, see *e.g.* [25]. To observe weak localization, the system needs to be shorter than the *dephasing length* l_ϕ . The dephasing length describes at which length scale the electrons cease to have a well-defined phase so that their quantum mechanical nature, giving rise to *e.g.* interference effects, is gradually lost. The physical origin of

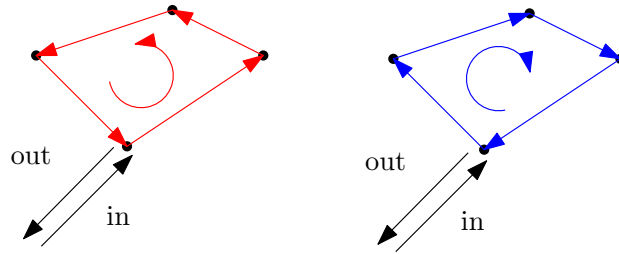


Figure 23.5: (Color online) Self-crossing scattering paths, causing a net increase in the resistivity at low temperatures.

dephasing is due to the interaction between the electron and an inevitably fluctuating environment. One physical origin for dephasing is voltage fluctuations due to electron-electron interactions: different electrons passing through a conductor will observe slightly different potentials, meaning that their acquired phases will also be randomized after a certain length l_ϕ . Another contributor to the dephasing is inelastic scattering, causing the electron to lose its energy, such as electron-phonon scattering or spin-flip scattering. These different mechanisms dominate in various temperature and size regimes of metals and semiconductors. The dephasing time is also temperature dependent due to *e.g.* the temperature dependence of voltage fluctuations (fluctuations in the electron densities at points in the system). Loosely speaking, it thus seems reasonable to state that the dephasing length should be the shortest length-scale associated with the mechanisms above, since that particular mechanism will dominate the dephasing process (such as inelastic electron-phonon scattering). *Weak localization is then caused by elastic impurity scattering (since the phase of the electron wavefunction must be well-defined), whereas dephasing is caused by mechanism causing a randomizing of this phase, such as e-e, e-ph, and spin-flip scattering.*

Weak localization is a precursor to strong localization (or Anderson localization) which occurs as the disorder increases even further. We treat this phenomenon in the next subsection.

23.4.2 Strong (Anderson) localization

Similarly to weak localization, Anderson localization stems from wave interference between multiple-scattering paths. In the presence of very strong disorder (and thus scattering), the interference effects can cause a complete cease of transport in the medium and thus insulating behavior. The strong localization effect increases with the length of the system, as trajectories which return to the same point twice or several times (which can be neglected in weak localization) become increasingly probable. The constructive interference between these trajectories means that the electron becomes more and more localized around a given point, thus ultimately giving rise to insulating behavior. More specifically, localization can occur when $L \simeq lN$ where l is the mean free path and N is the number of channels. This expression is equivalent to stating that $\delta G \simeq G$ where G is the conductance of the diffusive system and δG is the weak localization correction.

23.4.3 Weak anti-localization

In a system with spin-orbit coupling the spin of a carrier is coupled to its momentum. The spin of the carrier rotates as it goes around a self-crossing path shown in the figure, and the direction of this rotation is opposite for the two directions about the loop. Because of this, the two paths along any loop now interfere *destructively* which leads to a lower net resistivity since the probability

for backscattering is reduced. For more info, see *e.g.* [26]. A magnetic field also destroys weak anti-localization.

23.5 Universal conductance fluctuations

Text from Bruus and Flensberg.

As the temperature is lowered we expect quantum mechanical coherence to become more important because the phase coherence length l_ϕ increases with decreasing temperature. When the coherence length l_ϕ exceeds the mean free path l_{imp} for impurity scattering, scattering on different impurities can interfere. Here the coherence length means the scale on which the electrons preserve their quantum mechanical phase, i.e. the scale on which the wave function evolves according to the one-particle Schrodinger equation. If an electron interacts with another electron or with a phonon through an inelastic scattering event its energy changes, and hence the evolution of its phase. Due to these processes the phase of the electron wave acquires some randomization or dephasing, and its coherence length becomes finite. At low temperatures the dominant dephasing mechanism is electron-electron scattering, and the scattering rate for these processes is proportional to T^2 . Hence $l_\phi \propto 1/T^2$ can become very large at sufficiently low temperatures.

If the coherence length l_ϕ is longer than the mean free path l_{imp} , but still smaller than the sample size L , most of the interference effects disappear. This is because the limit $l_\phi \ll L$ effectively corresponds to averaging over many small independent segments, the so-called self-averaging. However, around 1980 it was found through the observation of the so-called weak localization that even in the case of large samples, $l_{\text{imp}} \ll l_\phi \ll L$, one very important class of interference processes survive the self-averaging. Naturally, as discovered around 1985, much more dramatic quantum effects appear in small samples in the so-called mesoscopic regime given by $L \ll l_{\text{phi}}$. In this regime all kinds of quantum interference processes become important, and most notably cause the appearance of the universal conductance fluctuations shown in the figure.

Mesoscopic normal-metal wires and rings exhibit random, reproducible fluctuations in the conductance as external parameters such as magnetic field or voltage are varied even slightly. This occurs due to quantum interference of electron waves. These fluctuations are called universal conductance fluctuations because at zero temperature their magnitude is of order of e^2/h , regardless of the degree of disorder and the sample size (so long as the size is larger than l_ϕ). The fluctuation pattern is sensitive to the microscopic distribution of elastic scatterers for electrons and therefore the fluctuations vary from sample to sample, although they are perfectly reproducible as *e.g.* voltage is swept up and down for a given sample. At finite temperature the size of the sample usually exceeds the inelastic diffusion length l_ϕ in of the electrons, and due to classical self-averaging the magnitude of the fluctuations is reduced.

Chapter 24

Hall effects & Quantum Hall effects

24.1 Landau levels in 2D

A point concerning how the localization of the Landau levels in a 2DEG is related to the choice of gauge is worth commenting on. In textbook treatments, a so called Landau gauge is often chosen in which case the electrons are free in one direction of the xy -plane whereas they are localized by harmonic oscillator wavefunctions in the other direction, for instance described by the wavefunction

$$\psi(x, y) = e^{ik_y y} u(x - x_0). \quad (24.1)$$

But we know that the Landau levels should be localized electron orbits around points in the xy -plane, analogously to the orbits of classical charged particles in a magnetic field. How is this consistent with the above wavefunction which has a probability density $|\psi|^2$ that is independent on y ? Moreover, if we chose a different gauge (but still producing the same magnetic field) such as $\mathbf{A} = \frac{1}{2}(-By, Bx, 0)$, we would have obtained a wavefunction $\psi(x, y)$ that was localized both in the x and y directions. Shouldn't the physics be the same regardless of gauge choice?

Indeed it should, and the resolution to this problem is that in the Landau gauge where one obtains a wavefunction that is localized only in the x direction, the resulting harmonic energy levels are strongly degenerate due to their dependence on k_y through the center position $x_0 \propto k_y$ (which does not influence the energy and hence causes degeneracy). A superposition of plane waves along y can produce a wavefunction that is localized in the y direction due to interference between the plane waves. Thus, a harmonic oscillator wavefunction in the y direction can always be represented as a plane wave superposition. In this way, we obtain the same physics as with the symmetric gauge choice $\mathbf{A}$ indicated above, with the degeneracy in that case being supplied by the angular momentum of the system along the z axis.

The key reason for choosing the Landau gauge is that the derivation of the wavefunction and energies is much simpler than in the symmetric gauge choice case. The resulting physics is nevertheless the same in the end.

We follow here several review articles, such as Refs. [15, 16].

24.2 Hall effects

Hall effect

The Hall effect, discovered by Hall in 1879, provides a voltage drop across a conductor transverse to the direction of the applied electrical current when there is a perpendicular magnetic field present (see left panel in Fig. 24.1). The physical origin of this effect is the deflection of electrons due to the Lorentz-force. The Hall voltage is thus proportional to the applied magnetic field and is widely used in industries as a direct measurement of a magnetic field. Note that although the Lorentz force scatters electrons to one side, this means that an electric potential difference is built up between the two sides. When the accumulated charge on one side is large enough to balance the Lorentz force, the injected current flows straight ahead (thus, the net transverse current is zero), but there now exists a transverse voltage difference.

Anomalous Hall effect

Shortly after discovering the Hall effect, Hall conducted similar experiments on ferromagnetic materials. He observed that the Hall resistance vs. applied field displayed an unusually large slope at low fields. It was recognized that this was a result of the presence of a finite magnetization in the sample and the phenomenon became known as the anomalous Hall effect (AHE). It is important to emphasize here that the AHE is *not* simply due to the net effective field becoming larger because of the magnetization. Instead, it is generally believed that SO coupling is the origin of the AHE. The exact mechanism is nevertheless still subject to some debate. The AHE has been an enigmatic problem that has resisted theoretical and experimental assaults for almost a century. The main reason seems to be that, at its core, the AHE problem involves concepts based on topology and geometry that have been formulated only in recent times, such as the Berry phase.

One group ascribes the AHE to impurity-induced skew scattering and side jumps of carriers, which is referred to as the extrinsic mechanism. The other group believes that AHE results from properties of the electronic energy band structure of ferromagnetic materials, which is known as the intrinsic mechanism. In 1954, Karplus and Luttinger proposed a theory for the AHE that, in hindsight, provided a crucial step in unraveling the AHE problem. KL showed that when an external electric field is applied to a solid, electrons acquire an additional contribution to their group velocity. KL's anomalous velocity was perpendicular to the electric field and therefore could contribute to the Hall effects. In the case of ferromagnetic conductors, the sum of the anomalous velocity over all occupied band states can be nonzero, implying a contribution to the Hall conductivity ρ_{xy} . Because this contribution depends only on the band structure and is largely independent of scattering, it has recently been referred to as the intrinsic contribution to the AHE. The equation of motion for the position $\mathbf{r}$ of an electron wave-packet (Bloch wave) moving in a crystal:

$$\dot{\mathbf{r}} = \frac{\partial \varepsilon_n(\mathbf{k})}{\hbar \partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}_n(\mathbf{k}), \quad (24.2)$$

where ε_n is energy band n and $\boldsymbol{\Omega}_n$ is the Berry curvature which is non-zero if time-reversal symmetry or inversion symmetry is broken. Note that $\dot{\mathbf{k}} \propto \mathbf{E}$, so that an applied electric field (current) induces an anomalous perpendicular velocity if the Berry curvature is finite.

Since a ferromagnetic material maintains a spontaneous magnetization even when the external magnetic field is removed, the AHE can also be measured in zero magnetic field. The empirical relation between the Hall resistivity, the applied field H_z , and the magnetization M_z which applies to many materials over a broad range of external magnetic fields reads:

$$\rho_{xy} = R_0 H_z + R_s M_z. \quad (24.3)$$

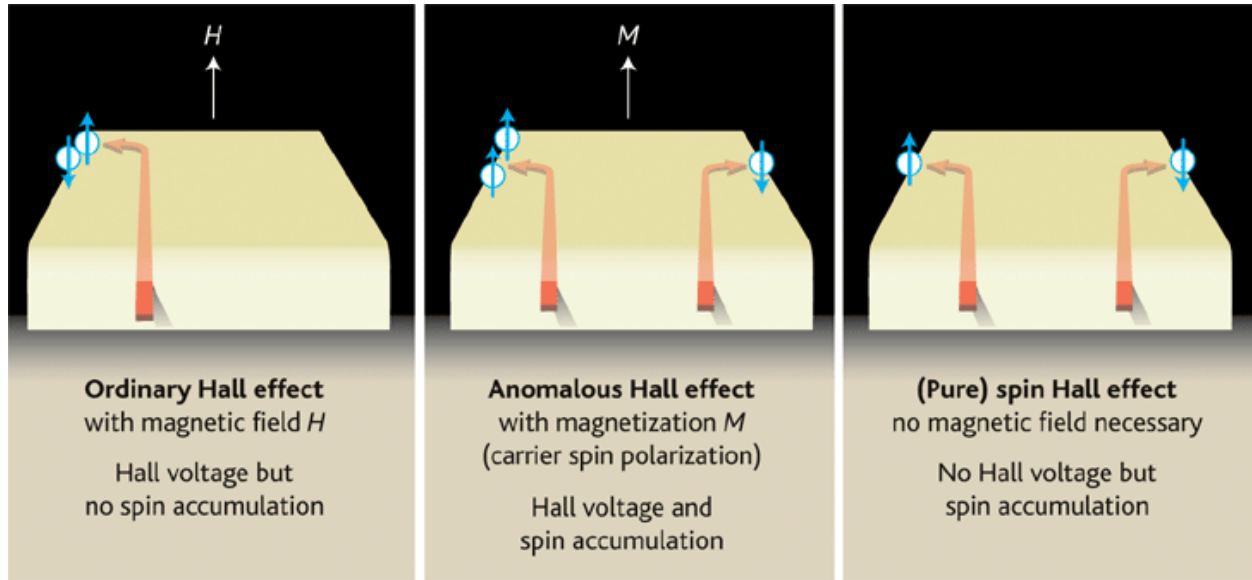


Figure 24.1: Three Hall effects [11]. (Left) The ordinary Hall effect is caused by deflection of carriers moving along an applied electric field (electrons or holes) by an applied magnetic field. Charge accumulation results in a Hall voltage, but there is no net spin accumulation because there are the same number of spin up carriers as spin down ones. (Middle) The anomalous Hall effect is the result of spin-dependent deflection of carrier motion, which produces a Hall voltage and spin accumulation at the edges. (Right) The pure spin Hall effect is caused by spin-dependent deflection of carriers and produces no Hall voltage when the numbers of deflected spin up and spin down electrons are the same but gives rise to spin accumulation. For simplicity, only the motion of a few carriers is shown in the figure panels.

The second term represents the Hall-effect contribution due to the spontaneous magnetization. R_0 depends mainly on the density of carriers. In contrast, R_s is found to depend on a variety of material specific parameters, including the longitudinal resistivity ρ_{xx} . Because of the different constants R_s and R_0 , it is clear that the anomalous Hall effect is not simply due to the renormalization $H_z \rightarrow H_z + M_z$.

Spin Hall effect

The last of the Hall trio is the spin Hall Effect (SHE). This is a transport phenomenon predicted by Russian physicists M.I. Dyakonov and V.I. Perel in 1971, which results in the appearance of spin accumulation on the lateral surfaces of an electric current-carrying sample. A net transverse spin current flow appears because of SO interactions which scatter opposite spins in opposite directions. Thus, the spin polarization of the induced spin accumulation is opposite on the opposing boundaries. Note that the transverse spin accumulation should not continue to build up indefinitely. The transverse spin current that arises due to the spin Hall effect reaches the edges of the sample and leads to a steady state of accumulated spins along the edges when a balance has been created between the spin current, spin diffusion, and spin relaxation. Such spin accumulation can be measured by Kerr rotation: a laser beam with linear polarization shining on the edge will be reflected, and its polarization will change with angle depending on the out-of-plane spin polarization.

It should be noted that in contrast to a charge current, a spin current can flow in devices which do

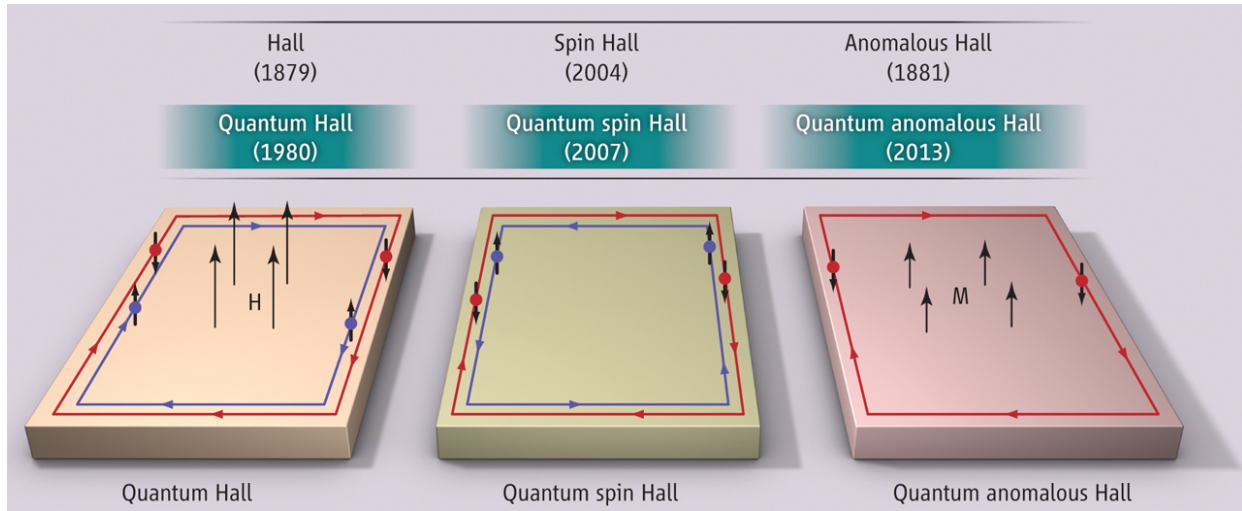


Figure 24.2: Quantum Hall trio [12]. Numbers in parentheses indicate the years of each discovery. H is the external magnetic field, and M is the magnetization. For all three quantum Hall effects, electrons flow through the lossless edge channels, with the rest of the system insulating. When there is a net forward flow of electrons for Hall resistance measurement, (left) those extra electrons occupy only the left edge channels in the quantum Hall system regardless of their spins, (center) opposite-spin electrons occupy opposite sides in the quantum spin Hall system, and (right) only spin-down electrons flow through the left edge in the quantum anomalous Hall system. The locking schemes between spin and flow direction, and the number of edge channels depend on the material details, and only the simplest cases are illustrated here.

not form closed circuits due to the non-conservation of spin in the presence of *e.g.* spin relaxation from magnetic impurities. For this reason, the transverse spin current can be sustained in the spin Hall effect, unlike the transverse charge current which is not sustained in the Hall effect.

No magnetic field is needed for the SHE which is a purely spin-based phenomenon. The SHE belongs to the same family as the anomalous Hall effect, known for a long time in ferromagnets, which also originates from spin-orbit interaction. The term "spin Hall effect" was introduced by Hirsch in 1999. Unaware of the work of Dyakonov and Perel, Hirsch used subtle physical reasoning based on the anomalous Hall effect to predict both the SHE and the inverse SHE. Experimentally, SHE was observed in semiconductors more than 30 years after the original prediction. The spin Hall effect can originate both from impurity spin-orbit scattering (extrinsic mechanism) or from *e.g.* Rashba-type spin-orbit coupling arising from the crystal structure (intrinsic mechanism).

The inverse spin Hall effect can also be measured in metals via spin pumping. The non-magnetic metal in which one desires to measure the SHE is attached to a ferromagnet. By causing the magnetization to precess, a spin current is pumped into the non-magnetic metal. This injected spin current then produces a charge current in the non-magnetic metal due to the inverse SHE. A transverse voltage drop can then be measured and acts as confirmation of the inverse SHE, which has been observed even at room temperature.

24.3 Quantum Hall effects

24.4 Basic considerations regarding the optical conductivity tensor and rotations

The conductivity tensor relates electric current and electric field:

$$\mathbf{J} = \sigma \mathbf{E} \quad (24.4)$$

and is in general a tensor. A transverse response is thus described by the off-diagonal components of σ . Now, the Hall response (whether it is induced by an external field or anomalous Hall due to time-reversal symmetry breaking in a system) is defined as the antisymmetric transverse part:

$$\sigma_H = (\sigma_{xy} - \sigma_{yx})/2 \quad (24.5)$$

rather than just σ_{xy} . But why not simply σ_{xy} which clearly describes a current arising transversely to the applied voltage stimulus?

The reason is that this definition extracts a transverse response which has a qualitatively different response than if we were to use σ_{xy} . To understand this, let us first examine the longitudinal response of the current described by the diagonal components of σ . In general, a material will have an easy direction(s) with large conductivity and a hard direction(s) with lower conductivity due to anisotropies in the crystal lattice. Aligning our x and y axis with these directions, the conductivity tensor can be written

$$\sigma = \begin{pmatrix} \sigma_0 + \Delta & 0 \\ 0 & \sigma_0 - \Delta \end{pmatrix}. \quad (24.6)$$

With this coordinate system, the system has no transverse response. However, let us now rotate the coordinate system an angle θ via a rotation matrix

$$R = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad (24.7)$$

one verifies that the σ_0 part of σ is invariant whereas the Δ part becomes

$$\Delta \begin{pmatrix} \cos 2\theta & -\sin 2\theta \\ -\sin 2\theta & -\cos 2\theta \end{pmatrix}. \quad (24.8)$$

In addition to having an anisotropic longitudinal conductivity, we now also have a transverse response in the new coordinate system. But this is not an intrinsic transverse response of the system in the sense that it depends on applying the current in a specific direction. It is simply a consequence of the system transporting current in different directions with different magnitudes for a given electric field.

Hall effects are different. They comprise an intrinsically transverse response which occurs regardless of which direction one applies the electric field: Hall effects generate a current in the perpendicular direction. In other words, this contribution should be invariant under a rotation of coordinate system. This manifests itself precisely as an antisymmetric contribution to the conductivity. Namely, if the conductivity tensor in a given coordinate system has a Hall response:

$$\sigma_H \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (24.9)$$

then one verifies that acting with the rotation matrix R on this matrix leaves it invariant.

In other words, just σ_{xy} does not describe solely a Hall response: it also includes any contribution that stems from anisotropies of longitudinal conductivities in the system. The antisymmetric part of σ , however, describes an intrinsic Hall effect and only appears in the absence of time-reversal symmetry in the charge sector. The spin Hall effect can occur without time-reversal symmetry breaking, on the other hand.

Chapter 25

Relativistic quantum mechanics and field theory

25.1 Can the Klein-Gordon wavefunction describe a relativistic quantum mechanical particle?

The Klein-Gordon equation may be motivated in a similar manner as one can motivate the Schrödinger equation: converting the expression for the energy into an operator eigenvalue equation. The expressions for the operators are motivated by de Broglie's hypothesis that particles have wave characteristics. Now, the wavefunction solutions to the SE can be interpreted as probability amplitudes. The solutions to the KGE cannot. Instead one interprets it as a field following that diff. equation and imposes yet another quantization procedure (by comparing it to the harm. oscillator and introducing creation/annihilation operators). This is the first step of a quantum field theory. But why is this necessary in the first place? Why does the solution to the KGE not describe a relativistic quantum mechanical wavefunction?

The problem with treating the solution ϕ of the Klein-Gordon equation (before second-quantization) as a wavefunction is that there is no positive probability density ρ associated with this field that satisfies a continuity equation of the type

$$\partial_t \rho + \nabla \cdot \mathbf{j} = 0. \quad (25.1)$$

This contrasts with the solution ψ of the Schrodinger equation, which has a positive definite probability density $\rho = |\psi|^2$ satisfying precisely the equation above.

Instead, one may derive from the KG equation a continuity equation of the above-mentioned type where the density ρ is something like

$$\rho \propto i(\phi^* \partial_t \phi - \partial_t \phi^* \phi). \quad (25.2)$$

The problem is then that this ρ is not necessarily always positive and cannot be interpreted as a probability density for a wavefunction. Hence, we cannot use the KG equation to describe a single-particle relativistic quantum wavefunction.

The step which seems a bit random - quantizing the KGE a second time - is motivated partly by the fact that doing so allows us to describe creation and annihilation of particles. This is not possible with e.g. the Schrodinger equation (first quantization), where the wavefunction cannot vanish due to probability conservation. Instead, when we promote ϕ to an operator (quantize a second time), we can describe physics which does not require particle number conservation. This is one motivation for quantizing a second time.

Chapter 26

Dirac, Majorana, and Weyl fermions

26.1 Dirac equation

The Dirac equation describes relativistic electrons and has the form

$$i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0. \quad (26.1)$$

As is well-known, the quantities γ^μ are matrices that must satisfy the Clifford algebra $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$ and thus ψ is a spinor with multiple components. There are infinitely many possible choices of γ^μ matrices that satisfy this algebra, but the smallest matrices that accomplishes this are 4×4 matrices. One common choice, used *e.g.* in the standard textbook by Griffiths, is:

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}. \quad (26.2)$$

A quantum field ψ that satisfies the Dirac equation is known as a *Dirac fermion*.

26.1.1 Non-relativistic limit of Dirac equation: Pauli equation and spin-orbit coupling

26.1.2 Majorana fermions

The components of ψ will in general be complex numbers. However, it was shown by Majorana that it is possible to choose the γ^μ matrices in a way so that they are purely imaginary, while still satisfying the Clifford algebra. By inspecting Eq. (26.1), we see that if γ^μ are all purely imaginary then the equation is real and can be solved by a real $\psi = \psi^*$. Such solutions are known as *Majorana fermions*.

26.1.3 Weyl fermions

To describe Weyl fermions, we have to consider the limit of zero mass, $m = 0$. In this case, one can again choose a particular set of γ^μ -matrices known as the chiral representation. The chiral representation is the same as Eq. (26.2) except that

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (26.3)$$

This allows one to split the Dirac equation into two decoupled equations each known as the *Weyl equation*:

$$\begin{aligned} i\hbar\partial_0\psi_R &= c(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})\psi_R, \\ i\hbar\partial_0\psi_L &= -c(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})\psi_L, \end{aligned} \quad (26.4)$$

where we have defined

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}. \quad (26.5)$$

In other words, a Dirac fermion ψ is a 4×1 spinor whereas a Weyl fermion is a 2×1 spinor. The subscripts R and L indicate that there are two kinds of particles: right- and left-handed corresponding to the $\pm$ signs. This property is known as chirality. For a chiral particle, its spin is determined from its momentum direction. For a positive energy state, a right-handed particle has its spin oriented along the momentum direction and conversely for a left-handed particle. Only massless particles are chiral at any energy. At high energies $E \gg mc^2$, a particle can be treated as chiral to a good approximation since the coupling between ψ_R and ψ_L via the mass term is negligible. Thus, the Weyl Hamiltonian

$$H = c(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) \quad (26.6)$$

describes a spin-1/2 massless fermion known as a Weyl fermion and the associated two-component spinor ψ_R is known as a Weyl spinor. Similarly for ψ_L . Both of these fermions has a well-defined chirality and a linear energy dispersion $E = \pm cp$ with two energy branches touching at a single point $p = 0$ known as the Weyl point.

Note that there is a distinction between a massless Dirac fermion and a Weyl fermion. A massless Dirac fermion is still a 4×1 spinor and indeed can be regarded as a direct sum of a left-handed *and* a right-handed Weyl fermion.

Now, it is clear from the above discussion that a Weyl point has a two-fold degeneracy in terms of particle occupancy since the linear bands $E = cp$ and $E = -cp$ touch at $p = 0$. A Dirac point, however, is four-fold degenerate since it can be regarded as consisting of two Weyl points of opposite chirality sitting on top of each other.

How can neutral Majorana fermions be detected via STM?

Firstly, we note that any charged fermion can be written as a linear combination of real (self-adjoint) Majorana operators:

$$c = \gamma_1 + i\gamma_2. \quad (26.7)$$

Thus, such a fermion is not its own antifermion as $c^\dagger = \gamma_1 - i\gamma_2 \neq c$. However, the Majorana fermions are their own antiparticles, satisfying $\gamma_i = \gamma_i^\dagger$, as can be seen by expressing them with c and $c^\dagger$:

$$\begin{aligned} \gamma_1 &= \frac{1}{2}(c + c^\dagger), \\ \gamma_2 &= \frac{i}{2}(c - c^\dagger). \end{aligned} \quad (26.8)$$

Two Majorana fermions thus form an ordinary Dirac fermion. Thus, in condensed matter systems they typically come in pairs. The charge degree of freedom in the fermion is encoded in the relative phase between γ_1 and γ_2 . Thus, the charge information can be encoded in a non-local way if one can spatially separate the Majorana fermions. In mathematical terms, we can use the Majoranas γ_1 and γ_2 to create a qubit: either a fermion state is present ($c^\dagger c = 1$) or it is absent ($c^\dagger c = 0$). Dephasing of the qubit is avoided in much the same way that one would hide the phase of a complex number by separately storing the real and imaginary parts. The complex Dirac fermion operator c of the qubit is split into two real Majorana fermion operators γ_1 and γ_2 . The quasiparticle parity $c^\dagger c = \frac{1}{2}(1 + i\gamma_1\gamma_2)$, which gives the two possible states of the qubit, is only accessible by a joint measurement on the two Majoranas.

To create Majorana fermions in condensed matter system, we can use superconductors where the quasiparticles are naturally superpositions of electrons and holes. At $E = 0$, the quasiparticle operators satisfy $\gamma = \gamma^\dagger$. If spin-degeneracy is lifted, such a state is then a Majorana fermion. Note that zero-energy states at interfaces of unconventional superconductors also satisfy $\gamma^\dagger = \gamma$, but this is a spin-degenerate situation and thus these zero-energy states bound to the interface are not Majorana fermions.

If Majorana particles are their own antiparticles, their charge must be zero and the Lagrangian describing such Majorana fermions must break $U(1)$ gauge symmetry so that no coupling to the vector potential is allowed. But several experiments claim to have found signatures of Majorana fermions via measurements of electric current using STM. How can this be?

To understand how Majorana fermions at one interface can give rise to a signature in STM-measurements despite being electrically neutral, let us first review what happens when zero-energy states form at the vacuum boundary of an unconventional superconductor.

Close to the vacuum edge, the pair potential is suppressed because of quasiparticle reflection at the interface. Therefore, there exists a thin region of length L close to the vacuum edge where electrons and holes may exist without a pair potential. Consider then an electron moving inwards toward the superconductor. This electron penetrates a distance ξ into the superconductor before it is Andreev-reflected as a hole. The hole is then scattered back from the vacuum edge, and inversely Andreev-reflected back as an electron. And so the process begins again. In other words, there is a formation of a bound-state right at the interface. In unconventional superconductors, this process happens with unit probability at zero energy in the tunneling limit $Z \rightarrow \infty$. In conventional superconductors, this process has zero probability in the same limit: there are no zero-energy bound states at the interface. Actually, a mathematical analysis shows that even in the limit $L \rightarrow 0$, zero-energy states exist in an unconventional superconductor. One shows this from the Bohr-Sommerfeld quantization condition for the total phase accumulated during one cycle of the electron-hole scattering.

Thus, we have established that there exists bound-states at the interface of an unconventional superconductor. If spin degeneracy is lifted, then we have precisely the situation required for Majorana fermions: the bound-state represents a Majorana fermion since it is a superposition of electron and hole states right at the interface [recall $\gamma_1 = \frac{1}{2}(c + c^\dagger)$]. The indices on the c -operators are now the same since spin-degeneracy is lifted, in contrast to *e.g.* d -wave high- T_c cuprates. The charge of the bound-state as a whole is zero, but as we will now discuss it can still mediate transfer of an electric current.

This happens due to the Andreev-reflection process. As shown by Asano *et al.* PRB 2003, the Andreev-reflection probability can be written as

$$|r_A|^2 = |t_N|^4 \left| \sum_{n=0}^{\infty} |r_N|^{2n} [-e^{i(\phi_- - \phi_+)}]^n \right|^2 \quad (26.9)$$

Here, t_N and r_N are the normal-state transmission and reflection coefficients which satisfy $|t_N|^2 + |r_N|^2 = 1$. The phases $\phi_{\pm}$ are the phases of the superconducting order parameter felt by a particle moving in the (k_x, k_y) direction and the $(-k_x, k_y)$ direction, respectively (i.e. reversing the component of the momentum perpendicular to the interface). In an s -wave superconductor, the gap is isotropic and $e^{i(\phi_- - \phi_+)} = 1$. In a d_{xy} -wave superconductor, the gap is anisotropic and satisfies $e^{i(\phi_- - \phi_+)} = -1$. By using that the geometries series satisfies

$$\sum_{n=0}^{\infty} r^n = \frac{1}{1-r} \text{ if } |r| < 1, \quad (26.10)$$

we therefore get

$$\begin{aligned} s\text{-wave: } |r_A|^2 &= \frac{2|t_N|^4}{(2 - |t_N|^2)^2}, \\ d\text{-wave: } |r_A|^2 &= 1, \end{aligned} \quad (26.11)$$

So the Andreev-reflection probability becomes unity in the d -wave case *even* if $t_N \rightarrow 0$ in the vacuum edge case. Thus, the bound-state at the edge of a chiral p -wave superconductor is a Majorana fermion which is a composite object of electrons and holes. It has total charge zero, but if we now attach a normal metal to the chiral p -wave edge, Andreev-reflection can occur and transmit a Cooper pair into the superconductor. This transport is mediated by the Majorana fermion which consists of counter-propagating electrons and holes, despite the fermion being neutral as a whole.

Thus, the point is that the zero-energy state at the end of a chiral p -wave superconductor is a Majorana fermion, and it is equivalent to a bound-state of electrons and holes at $E = 0$. Such a bound-state mediates charge transport despite being electrically neutral overall. Simply put, an electron moving to the right and a hole moving the left is electrically neutral as a whole. Yet an electric current of $-2e$ is flowing to the right. The zero-bias peak seen in STM is a result of the high density of zero-energy states at the interface which in turn mediate perfect Andreev reflection and thus charge transport. The situation is somewhat analogous to the quantum spin Hall state occurring in time-reversal invariant topological insulators at the edge. TRS is not broken, so there is no magnetism. Yet, a spin current can flow if $\uparrow$ are moving to the right and $\downarrow$ are moving to the left.

26.1.4 Relation to graphene

How is this related to *e.g.* graphene? One often speaks about the Dirac point in graphene. However, strictly speaking, the band crossings at K and K' in the Brillouin zones are in fact Weyl points. The Hamiltonian at the K ($\eta = +1$) and K' ($\eta = -1$) points are given by

$$H = v_F(\sigma_x p_x + \eta \sigma_y p_y) \quad (26.12)$$

It is thus slightly different from the Weyl Hamiltonian $H = -v_F(\boldsymbol{\sigma} \cdot \mathbf{p})$ for the valley $\eta = -1$, but it is immediately clear that for the valley $\eta = +1$ the electrons in graphene are Weyl fermions. Note that σ_i above refers to sublattice space Pauli matrices. There is an additional true spin-degree of freedom, but this does not affect the sublattice-chirality one can define from the above Hamiltonian.

Now, even though the Hamiltonian for graphene valleys is $H = v_F(\sigma_x p_x \pm \sigma_y p_y)$ rather than $H = \pm v_F(\sigma_x p_x + \sigma_y p_y)$, the fermions described by this Hamiltonian are still chiral in both valleys $\pm$ in the sense that for a given momentum direction $\mathbf{p}$, the direction of polarization corresponding to the σ -matrices is fixed. Therefore, the two Fermi points K and K' in graphene indeed each represent a 2D Weyl point such that the low-energy quasiparticle excitations are 2D chiral fermions.

The chirality in this case then refers to the sublattice projection with respect to the momentum direction instead of spin. The chirality operator is not the same in both valleys, i.e. it is $\boldsymbol{\sigma} \cdot \mathbf{p}/p$ in the $+$ valley and $\bar{\boldsymbol{\sigma}} \cdot \mathbf{p}/p$ in the $-$ valley with $\bar{\boldsymbol{\sigma}} = (\sigma_x, -\sigma_y)$, but in both cases the sublattice pseudospin is linked to the momentum direction.

26.1.5 Terminology

We again underline that the established terminology in the literature is slightly confusing regarding the usage of "Dirac points" and "Weyl points", especially in graphene. The band dispersions near the K and K' points in graphene are referred to as Dirac points, but they are in fact two overlapping Weyl points with the same chirality. Each band crossing at K or K' is described by a Weyl Hamiltonian with a definite chirality, and hence is a Weyl point. Accounting for spin doubles the degeneracy of the bands at both K and K' , but it does not affect the chirality since spin does not couple to $\mathbf{p}$ in the graphene Hamiltonian.

A closer correspondence with a Dirac point arises only if one *combines* the quasiparticles at the K and K' points into a single model such as

$$H = \begin{pmatrix} H_K & 0 \\ 0 & H_{K'} \end{pmatrix}. \quad (26.13)$$

Such a Hamiltonian indeed describes a pair of Weyl points of different chirality, but, importantly, they are located at different points in $\mathbf{k}$ -space.

26.1.6 Robustness of 2D and 3D Weyl points

It is worth commenting on the difference between 2D and 3D Weyl points in terms of robustness against perturbations. In both cases, one can write the Hamiltonian as $H = v\mathbf{p} \cdot \boldsymbol{\sigma}$, but in the presence of a magnetic field m_z the Hamiltonian gains an extra term $m_z \sigma_z$. This term acts very differently depending on whether we are considering 2D or 3D. In 2D, it opens a gap in the spectrum and is called a mass term since the dispersion relation is no longer linear:

$$E = \pm v_F \sqrt{p_x^2 + p_y^2 + m_z^2}. \quad (26.14)$$

The bands no longer touch at $p = 0$ and are instead separated by a gap $2v_F m_z$. In contrast, adding such a magnetic field term in 3D produces the dispersion relation

$$E = \pm v_F \sqrt{p_x^2 + p_y^2 + (p_z + m_z)^2}. \quad (26.15)$$

Therefore, the $\pm$ bands still touch each other at a different point than $p = 0$: specifically, they touch at $\mathbf{p} = (0, 0, -m_z)$. Therefore, the 3D Weyl point is a protected band crossing which survives the presence of a Zeeman term and is thus more robust than its 2D counterpart, the latter requiring additional symmetries to be stable. For instance, in the case of graphene sublattice symmetry, meaning that the A and B sublattices in graphene are equivalent, must be preserved in order for the Weyl points to be gapless. Mathematically, the sublattice symmetry requires that $\{H(\mathbf{k}), \sigma_z\} = 0$.

The realization of Weyl points in 3D materials requires that either time reversal symmetry $\mathcal{T}$ or inversion symmetry $\mathcal{P}$ is broken, because only then are exactly *two* states degenerate at a finite number of points in the Brillouin zone. This can be seen as follows. Consider the Hamiltonian at a given node to be $H = v\mathbf{p} \cdot \boldsymbol{\sigma}$ where now $\boldsymbol{\sigma}$ is true spin. Under inversion symmetry, $\mathbf{p} \rightarrow (-\mathbf{p})$ while $\boldsymbol{\sigma} \rightarrow \boldsymbol{\sigma}$. Therefore, a Weyl node at $\mathbf{p}$ is always accompanied by a Weyl node at $-\mathbf{p}$ with opposite chirality. On the other hand, if time reversal is preserved then there is also a node at $-\mathbf{p}$ with the same chirality since both $\mathbf{p}$ and $\boldsymbol{\sigma}$ change sign under $\mathcal{T}$. As a result, if both symmetries are preserved, every Weyl node that exists must be a doublet of nodes with opposite chiralities. Such doublets are precisely the four-component Dirac fermions we have discussed previously.

Therefore, for a possible Weyl point, the combined operation $\mathcal{PT}$ leads to a second Weyl point with opposite chirality at the same $\mathbf{k}$ -point, turning it into a Dirac point (a sum of Weyl points with opposite chirality) rather than a Weyl point.

26.2 Majorana bound state in chiral p -wave superconductors

Chapter 27

Lattice Hamiltonians and diagonalization

27.1 Ground-state of Fermi sea and eigenstates of $\hat{H}$

Assuming a translationally invariant system, we know that the second-quantized Hamiltonian has the form

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \quad (27.1)$$

where $\epsilon_{\mathbf{k}}$ is the band dispersion relation. The ground-state is the states with lowest energy, and this is obtained by successively filling up the lowest available energy states. Therefore, the ground-state can be written

$$|\text{GS}\rangle = \prod_{\epsilon_{\mathbf{k}} \leq E_F} c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\downarrow}^{\dagger} |0\rangle \quad (27.2)$$

Here, $|0\rangle$ is the vacuum state (no particles) and the product goes over $\mathbf{k}$ -wavevectors which are such that $\epsilon_{\mathbf{k}} \leq E_F$ and E_F is the Fermi energy. In the special case of a free-particle dispersion $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$, the product goes over all states $|\mathbf{k}| \leq k_F$. For a more complicated band-structure $\epsilon_{\mathbf{k}}$, multiple Fermi surfaces could appear in the first Brillouin zone if $\epsilon_{\mathbf{k}}$ does not increase monotonically as a function of $|\mathbf{k}|$.

The eigenstates of the above $\hat{H}$ are states where the occupation number $n_{\mathbf{k}\sigma}$ is specified for all single-particle states $(\mathbf{k}, \sigma)$. For instance, $|0, 0, 1, 0, 1, \dots\rangle$ is a possible eigenstates with belonging eigenvalue $E = \sum_{\text{occupied } \mathbf{k}, \sigma} \epsilon_{\mathbf{k}}$ where the sum runs over the states which have $n_{\mathbf{k}\sigma} = 1$.

27.2 Role of chemical potential

In a system which has a fixed number of electrons N_e and N lattice sites, we must have $N_e \leq 2N$ due to the Pauli principle. The occupation numbers of an eigenstate with N_e electrons then satisfies

$$\sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} = N_e. \quad (27.3)$$

As explained above, the ground state is obtained by filling the N_e states with lowest energy.

However, the constraint Eq. (27.3) is impractical to work with: if we fix N_e , there can be several possible eigenstates satisfying the constraint. If one for instance has three electrons, placing a spin-up or a spin-down particle in the second-lowest $\mathbf{k}$ -state both satisfy the constraint. Therefore, it is more convenient to use a formulation in which the particle number can vary and only the average number of particles is fixed. To do so, we let

$$\hat{H} \rightarrow \hat{H} - \mu \hat{N} \quad (27.4)$$

where $\hat{N}$ is the total particle number operator and μ is the so-called chemical potential. The point is then to choose μ in such a way that the average number of electrons $\langle \hat{N} \rangle$ equals N_e . The expectation value of $\hat{N}$ can be computed in the usual way by taking the trace of the density matrix times the operator $\hat{N}$ itself. Computing $\langle \hat{N} \rangle$, one finds that it depends on both μ and temperature T . Conversely, the resulting equation dictates what μ has to be for a fixed value of $\hat{N}$ and at a given temperature T and can generally be solved numerically.

The chemical potential μ is then used as a knob which we can change to tune the filling of the electron bands in the system (the average number of electrons). For a free-electron gas at zero temperature, the smallest eigenvalue is obtained by occupying all states below μ and keeping all states above μ available. It is clear that μ is in this case equal to the Fermi energy of the system. It is unproblematic from a physical point of view to add the μ -term to the Hamiltonian since it simply redefines the reference level for energies in the system.

27.3 Group theory applied to lattices

Here, we will discuss in more detail group theory and related concepts in crystal structures: space group, point group, Bravais lattice, irreducible representations, basis functions.

Space group: the symmetry group of an object in space, such as a crystal lattice, with elements (the symmetry operations) that leave the object unchanged. This includes translation of the lattice. There are 230 space groups in 3D.

Point group: the symmetry group of a crystal lattice with elements (the symmetry operations) that leave *at least* one point of the lattice fixed. In other words, point group symmetries do not include translation of the lattice, whereas space group symmetries do.

Bravais lattice: a collection of lattice sites where the system looks identical in any given direction regardless of which lattice site you look from. An equivalent definition is that any lattice point can be reached from any other site by the vector $\mathbf{r} = n\mathbf{a}_1 + m\mathbf{a}_2 + k\mathbf{a}_3$ where $\{n, m, k\}$ are integers and $\{\mathbf{a}_i\}$ are primitive lattice vectors. The choice of primitive lattice vectors are not unique. There are 14 Bravais lattices in 3D, and each belongs to one of the 7 lattice systems. There are 5 Bravais Lattices in 2D, and 1 in 1D.

Lattice system: a given crystal lattice is classified as part of a lattice system depending on what its Bravais lattice looks like. There are 7 lattice systems: triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, cubic.

There is a close relation between all the concepts above. For instance, the 230 space groups in three dimensions are made from combinations of the 32 crystallographic point groups with the 14

types of Bravais lattices. The Bravais lattices, in turn, each belong to one of 7 fundamental lattice systems. One can say that a given crystal consists of a lattice (how the atoms are repeated) and a basis (what is repeated). The Bravais lattice gives us information about *how* the lattice is repeated (translational symmetry) whereas the basis gives us information about *what* is repeated (point group symmetry). In this way, the combination of the translational symmetry described by the Bravais lattice and all other symmetries related to rotation, reflection, et.c. described by the point group symmetry that depends on what the basis looks like.

The physical properties of a material must reflect its underlying lattice structure. In effect, the symmetries of the point group of the material should manifest themselves in *e.g.* interactions between different types of particles (electrons, phonons) on the lattice. This is mathematically expressed using the concepts of irreducible representations and basis functions. We first go through all the theoretical concepts. Then, to see how this works in practice, we consider a specific example: a 2D square lattice.

27.3.1 Group properties

First, a brief reminder of the three defining properties of a group. A group is a set of elements $\mathcal{G}$ together with a multiplication rule for combining two elements in the group, such that the combination of any two elements g_1 and g_2 forms an element of $\mathcal{G}$, denoted $g_1 \cdot g_2$, in a manner so that the following three requirements are satisfied:

- Associativity
- Identity element exists
- Inverse element exists

An element g_1 is defined as *conjugate* to g_2 when

$$g_1 \equiv X g_2 X^{-1} \quad (27.5)$$

where X is an arbitrary element of the group. The elements of an Abelian group (where the elements commute) are clearly self-conjugate.

Moreover, a *class* $\mathcal{C}$ is the totality of all elements obtained from a given group element by conjugation. For instance, consider the permutation group $\mathcal{G} = P(3)$. It has the following elements:

$$\begin{aligned} E &= (1, 2, 3) \text{ [identity]}, \quad A = (2, 1, 3), \quad B = (1, 3, 2), \\ C &= (3, 2, 1), \quad D = (3, 1, 2), \quad F = (2, 3, 1). \end{aligned} \quad (27.6)$$

The three classes (or conjugate classes) of this group are $\mathcal{C}_1 = \{E\}$, $\mathcal{C}_2 = \{A, B, C\}$, $\mathcal{C}_3 = \{D, F\}$. For instance, we see that $ABA^{-1} = AF = C$, as consistent with the class designation. The identity element is always in a class by itself.

27.3.2 Irreducible representations and character tables

Moreover, a *representation* Γ of a group is a set of $n \times n$ matrices which have the same multiplication table (with respect to the multiplication rule in the group) as the group elements. This means that for each group element g , there exists an invertible matrix $D(g)$ so that

$$D(g_1)D(g_2) = D(g_1 g_2) \quad (27.7)$$

and $\Gamma = \{D(g)\}$, i.e. the set of $D(g)$ matrices. The dimension of the representation is equal to n . Any group has a trivial 1D representation $D(g) = 1$. Representations can be classified as reducible or irreducible. If there exists a fixed transformation matrix U for all elements g so that the transformation

$$D'(g) = UD(g)U^{-1} \quad (27.8)$$

brings the representation $D'(g)$ into a block-diagonal form

$$D'(g) = \begin{pmatrix} D'_1(g) & 0 \\ 0 & D'_2(g) \end{pmatrix} \quad (27.9)$$

then the representation $D'(g)$ is said to be reducible and it is decomposed into the sum of the representations D'_1 and D'_2 . Otherwise, it is called irreducible. An irreducible representation cannot be expressed in terms of representations of lower dimensionality. Any representation of a finite (compact) group can be brought to unitary form, so this is usually assumed a priori. Also, we note that the matrices in an irreducible representation of a group are not unique: any similarity transformation UDU^{-1} with a unitary matrix provides an equally good representation. However, the trace of the matrix remains invariant under such a similarity transformation, and therefore traces, known as *characters*, can be used to uniquely classify irreps, as we now discuss.

The character $\chi_D(g)$ of the matrix representation $D(g)$ of a group element is simply the trace of the matrix D :

$$\chi_D(g) = \text{Tr}\{D(g)\}. \quad (27.10)$$

Let us extend the notation slightly and write

$$\chi_D^{(j)}(g) = \text{Tr}\{D^{(j)}(g)\}. \quad (27.11)$$

where j is an index labelling the different representations $\Gamma^{(j)} = \{D^{(j)}(g)\}$. The representation $\Gamma^{(j)}$ will have the same number of characters as the number of classes, since all elements in a conjugate class have the same character (since a unitary transformation does not change the trace of a matrix). Informally, this property means that elements of the same class correspond to similar symmetry operations (*e.g.* a class corresponding to two-fold rotations or mirror operations).

Several extremely useful theorems can be used to identify the irreducible representations of a group (see <http://web.mit.edu/course/6/6.734j/www/group-full102.pdf> for proof):

- The number of irreducible representations is equal to the number of classes in a group.
- The dimensionalities l_j of these irreducible representations are found from $\sum_j l_j^2 = h$ where h is the number of elements in the group.
- The rest of the entries of a character table can be computed using various orthogonality relations between the characters for different classes and irreps.

For instance, for the permutation group $P(3)$ we have $h = 6$ and $l_1 = 1$. Thus, we get $1^2 + x^2 + y^2 + \dots = 6^2$. This equation only has one solution $x = 1, y = 2$. So $P(3)$ has two 1D representations and one 2D representation. The character table for $P(3)$ thus has the form

Irreps/Classes	$C_1 = E$	$C_2 = A, B, C$	$C_3 = D, F$
Γ_1	1	1	1
Γ_2	1	-1	1
Γ_3	2	0	-1

The way to obtain this in practice is to start by filling in 1 for the entire upper row (trivial irrep) and then the dimension of the irrep in the first column (identity element always has character equal to the dimension of the irrep). Then, the remaining characters are completed by using orthogonality relations for the characters.

27.3.3 Representation theory: what it means and why it is useful

See <https://sites.ualberta.ca/~vbouchar/MAPH464/chapter-representation.html> for a very pedagogical description.

27.3.4 Mulliken symbols

Various symbols, such as $A, B, E, T, \dots$ are used to classify different irreps. These are known as Mulliken symbols.

- A : 1D irrep which is symmetric with respect to rotation about a principal axis. In other words, it is an irrep which has $\chi(C_n) > 0$.
- B : 1D irrep which is antisymmetric with respect to rotation about a principal axis. In other words, it is an irrep which has $\chi(C_n) < 0$.
- E : 2D irrep.
- T : 3D irrep.

and so forth. The subscripts g and u stand for the German words *gerade* and *ungerade*, and refer to whether the character of the conjugate class containing inversion is positive or negative.

27.3.5 Basis functions

The different irreps can be associated with certain functions of coordinates which transform in the same way as the characters of the classes of the groups. For instance, consider the group C_{2v} which *e.g.* the H_2O molecule belongs to. It has four elements: $E, C_2, \sigma_v, \sigma'_v$. Thus, it has four 1D irreps:

Irreps/Classes	$C_1 = E$	$C_2 = C_2$	$C_3 = \sigma_v$	$C_4 = \sigma'_v$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

Now consider the coordinate z . It is invariant under any symmetry operation of the group. Thus, we can state that z transforms as A_1 in the group C_{2v} because the characters of the A_1 representation express the transformation properties of the coordinate z under the operations of C_{2v} . This is true since A_1 is a 1D representation and the matrices representing the symmetry operations are equal to their characters (since they are scalars). On the other hand, x transforms as B_1 and y transforms as B_2 . You can apply the same reasoning for other functions like $x^2 + y^2$, z^2 , or xz .

The above functions are examples of *basis functions*. The formal definition of a basis function (also known as partner functions) is as follows. A set $\{\phi_\alpha^{(j)}\}$ of functions that transform according to the representation $D^{(j)}$ with $\alpha = 1, \dots, d_j$. That is, if $\hat{g}$ is the operator that transforms ϕ according to $g \in \mathcal{G}$, then

$$\hat{g}\phi_\alpha^{(j)} = \sum_\beta \phi_\beta^{(j)} D_{\beta\alpha}^{(j)}(g) \quad (27.12)$$

for all $g \in \mathcal{G}$. Here, (j) labels the representation. Clearly, for 1D representations, the matrices D can be replaced by their characters. In this case, we see precisely what was alluded to above: the functions x , xz , et.c. are examples of basis functions. Note that different basis functions are orthogonal in the following sense: if $\phi_\alpha^{(j)}$ and $\phi_\beta^{(j')}$ are basis functions, then $\langle \phi_\alpha^{(j)} | \phi_\beta^{(j')} \rangle = \delta_{\alpha\beta} \delta_{jj'}$.

In general, there can be many basis functions for an 1D irrep. For instance, the A_1 representation of the group C_{2v} has basis functions $1, z, x^2 + y^2$. These are not all orthogonal since they all belong to the same 1D irrep. However, the A_2 irrep has basis function xy and this is orthogonal to all basis functions of A_1 .

For 2D irreps, there are doublets of basis functions. We will see an example of this for the square lattice.

27.3.6 Example: square lattice

Now consider a 2D square lattice where we will make use of all the concepts introduced above. The point group consists of all symmetry operations that leaves the lattice invariant except any form of translation. The point group is denoted D_4 or C_{4v} (they mean exactly the same thing, just the notation is different). There are 8 elements in this symmetry group:

$$E, C, C^2, C^3, \sigma_x, \sigma_y, \sigma_+, \sigma_-. \quad (27.13)$$

C denotes rotation by $\pi/2$ whereas σ is a rotation around the x, y axes or the two diagonals ($\pm$). One can then set up a multiplication table for these operations. By computing all conjugate elements (no easy way around this in general, just an exhaustive calculation), we obtain five conjugate classes $\mathcal{C}$:

$$\mathcal{C}_1 = \{E\}, \mathcal{C}_2 = \{C, C^3\}, \mathcal{C}_3 = \{C^2\}, \mathcal{C}_4 = \{\sigma_x, \sigma_y\}, \mathcal{C}_5 = \{\sigma_+, \sigma_-\}. \quad (27.14)$$

The character table for the square lattice point group can now be constructed.

Irreps/Classes	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

We will soon augment this character table to also show the basis functions of the irreps. In fact, we can already note that $x^2 + y^2$, z^2 transform as A_1 in C_{4v} , while $x^2 - y^2$ transforms as B_1 and xy transforms as B_2 . In the 2D irrep E , we have a doublet of basis functions written $[x, y]$: they

correspond to the α, β index in the definition of basis functions. In other words, an 1D irrep can have several possible basis functions that can be used individually, whereas the notation $[x, y]$ means that x and y *together* form a basis for a 2D irrep. Moreover, when basis functions are listed in a character table, only a selection of basis functions (usually the simplest which are linear or quadratic) are included. There can exist infinitely many basis functions for *e.g.* the A_1 irrep (any power of z^n for the group C_{4v} and so on).

Note how the zeros in the character table mean that when a symmetry operation corresponding to an element in the conjugate class acts on the basis function, it transform to something else than just $\pm$ of the original function.

Including the basis functions of the irreps of C_{4v} then aguments the table as follows.

Irreps/Classes	C_1	C_2	C_3	C_4	C_5	Basis functions
A_1	1	1	1	1	1	1
A_2	1	1	1	-1	-1	$xy(x^2 - y^2)$
B_1	1	1	-1	1	-1	$x^2 - y^2$
B_2	1	1	-1	-1	1	xy
E	2	-2	0	0	0	$[x, y]$

Sometimes basis functions are given in momentum space and in terms of cosines and sines. This is appropriate for lattices when working with lattice momentum $\mathbf{k}$, since functions are supposed to be periodic with $2n\pi$ in the components of $\mathbf{k}$. For instance, both $k_x k_y$ and $\sin k_x \sin k_y$ are basis functions of the B_2 irrep of C_{4v} , but only the latter satisfies the aforementioned periodicity requirement.

27.3.7 Expanding superconducting order parameter in basis functions of irreps

Neumann's principle tells us that physical properties of a lattice must have at least the same symmetries as the lattice itself. This means that the pairing interaction $V(\mathbf{r}, \mathbf{r}')$ must be invariant under the symmetry operations of the point group of the lattice. Because of this, one may show that the pairing potential can be expanded in terms of the basis functions of irreducible representations (Landau and Lifshitz, 1979). In turn, this results in the order parameter Δ itself transforming according to one of the irreps of the point group of the lattice. The actual physically realized order parameter will be the one that has the highest T_c of all possible forms of the order parameter. Assume then that it is the basis functions $\phi_\alpha^{(j)}$ of the irrep $\Gamma^{(j)}$ which give the highest T_c of the order parameter. In that case, one may write

$$\Delta(\mathbf{k}) = \sum_{\alpha=1}^{d_j} \eta_\alpha \phi_\alpha^{(j)} \quad (27.15)$$

where d_j is the dimensionality of the irrep $\Gamma^{(j)}$ and η_α is a complex number (invariant under all symmetry operations of the point group). For a 1D irrep, only one basis function is necessary, so the gap function can be described by a single complex order parameter. For a 2D irrep, two expansion coefficients η_α are required since the basis functions are doublets.

A special mention is useful for noncentrosymmetric lattices lacking inversion center. Consider for instance a tetragonal unit cell with an extra atom that breaks inversion symmetry along the z -axis [001]. The point group of the lattice then reduces to the square lattice, i.e. $D_4 = C_{4v}$. Here, we have basis functions with a definitive parity (even, odd), so the basis functions that the superconducting order parameter is expanded in have a well-defined parity even when the crystal

lacks inversion center. To be more precise, this pertains to the superconducting order parameter in the pseudospin-basis corresponding to pairing between time-reversed states. If the pairing is *not* between time-reversed states, the corresponding order parameter does not transform according to the irreducible representations of the point group. This can be shown using the transformation properties of the diagonalized fermion operators under a point group operation (see Curnoe *et al.* PRB 2004) and the fact that the full Hamiltonian must be invariant under space group operations and time reversal. A key point is that the order parameter acquires an additional phase factor upon applying a point group symmetry operation. On the other hand, when we consider pairing between time-reversed states, the corresponding order parameter does transform according to the irreps of the point group, and we can thus expand it in basis functions.

In the original fermion basis, the order parameter in contrast does not have a definite parity, but becomes a mix of singlet and triplet pairing.

27.4 Bravais lattices and periodic boundary conditions

The choice of primitive lattice vectors in a Bravais lattice is not unique. Two possible choices for the square lattice is shown in Fig. 27.1(a). The total system can be constructed by connecting unit cells to each other. There is no unique choice of unit cell: two possible choices for the square lattice are shown. But there is one particular unit cell that is special: the Wigner-Seitz cell, which is obtained by drawing a line from a given lattice point to all of its nearest-neighbors and then drawing a line intersecting each of those lines perpendicularly at their middle point. The resulting area is the W-S cell [Fig. 27.1(b)]. The unique thing about the W-S cell is that it is the unit cell with the highest symmetry of all unit cells, i.e. it has the same symmetry as the lattice itself.

Non-Bravais lattice, such as the graphene lattice (see below), can be thought of as Bravais lattices where each lattice site has a multi-atom basis. The recipe for constructing the Wigner-Seitz cell in that case is the same as above, only that one considers solely atoms on one fixed sublattice. This will be enough, since the other sublattice atoms have fixed positions relative a given sublattice.

27.4.1 Periodic boundary conditions

Periodic boundary conditions can be used to model translationally symmetric structures instead of having a finite size system with vacuum interfaces. PBC allow us to write fermion operators c_i in terms of a Fourier-series where only special values for the momentum indices are allowed. To see this, consider an operator c_i which is periodic in the sense that $c_i = c_{i+N}$. This means we can write

$$c_i = 1/\sqrt{N} \sum_k c_k e^{ikr_i}. \quad (27.16)$$

The property $c_i = c_{i+N}$ is guaranteed by only allowing k to take values such that $kNa = 2\pi n$ where n is an integer. The prefactor $1/\sqrt{N}$ is there to ensure that the number of degrees of freedom is conserved:

$$\sum_i c_i^\dagger c_i = \sum_k c_k^\dagger c_k. \quad (27.17)$$

This is due to the property

$$\sum_k e^{ik(r_i - r_{i'})} = N\delta_{ii'}. \quad (27.18)$$

We will see a proof of this relation soon (see also notes by J. O. Fjaerestad).

In the square lattice case, one often considers PBC in the x and y -directions. The allowed k -values are then $k_x, k_y = [0, 2\pi - 2\pi/Na]$. Since the values k and $k + 2\pi/a$ are identical, it is customary to shift the interval to $k_x, k_y = [-\pi/a, \pi/a - 2\pi/Na]$. In this way, the summation over k -values goes over the first BZ (the equivalent of the Wigner-Seitz cell in reciprocal space).

Similarly to the real space-treatment, once the reciprocal lattice geometry has been identified one constructs the Wigner-Seitz cell in reciprocal space (in effect, the 1st BZ) by considering only one nearest-neighbor reciprocal lattice vectors within the same reciprocal sublattice.

Note that we could also have considered PBC in different directions, for instance along the alternative set of primitive unit vectors shown in Fig.27.1(a). Then, we would have obtained different k -values to sum over, because the system geometry under consideration would have been different. We still would have performed a summation over k_x in the interval $[-\pi/a, \pi/a]$, but in contrast we would have to sum over $k_y \in [-\pi/a - k_x, \pi/a - k_x]$. This is no longer the 1st BZ of the square lattice.

Let us also see how the periodic boundary conditions are used for a non-square lattice, such as the hexagonal (triangular) lattice. Consider a lattice distance a between each site. We choose $\mathbf{a}_1 = a/\sqrt{2}(1, 1)$ and $\mathbf{a}_2 = a/\sqrt{2}(1, -1)$ as the primitive lattice vectors and then periodic boundary conditions along these directions with a period of N atoms [Fig. 27.1(b)]. Any lattice point on the triangular lattice may be written $\mathbf{r}_j = m_j\mathbf{a}_1 + n_j\mathbf{a}_2$ where n_j, m_j are integers. The PBC along $\mathbf{a}_1$ and $\mathbf{a}_2$ then give the conditions

$$\begin{aligned}\mathbf{k} \cdot N\mathbf{a}_1 &= 2\pi n_1, \\ \mathbf{k} \cdot N\mathbf{a}_2 &= 2\pi n_2\end{aligned}\tag{27.19}$$

where n_1, n_2 are integers. This gives us

$$\begin{aligned}k_x Na/\sqrt{2} + k_y Na/\sqrt{2} &= 2\pi n_1, \\ k_x Na/\sqrt{2} - k_y Na/\sqrt{2} &= 2\pi n_2,\end{aligned}\tag{27.20}$$

which can be rewritten to

$$\begin{aligned}k_x N\sqrt{2}a &= 2\pi(n_1 + n_2) \rightarrow k_x = \sqrt{2}\pi Na(n_1 + n_2), \\ k_y N\sqrt{2}a &= 2\pi(n_1 - n_2) \rightarrow k_y = \sqrt{2}\pi Na(n_1 - n_2).\end{aligned}\tag{27.21}$$

These are the allowed k -values. They probably together spawn the 1st BZ of the triangular lattice (haven't checked explicitly). Now, we want to show that the relation

$$\sum_{\mathbf{r}_j} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} = N^2 \delta_{\mathbf{k}\mathbf{k}'}\tag{27.22}$$

holds. Clearly, if $\mathbf{k} = \mathbf{k}'$, we get the result N^2 which is the number of lattice points. If $\mathbf{k} \neq \mathbf{k}'$, we have:

$$\begin{aligned}\sum_{\mathbf{r}_j} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} &= \sum_{\mathbf{r}_j} e^{im_j a/\sqrt{2}(k_x - k'_x + k_y - k'_y)} + e^{in_j a/\sqrt{2}(k_x - k'_x - k_y + k'_y)} \\ &= \sum_{m_j, n_j} x^{m_j} y^{n_j}\end{aligned}\tag{27.23}$$

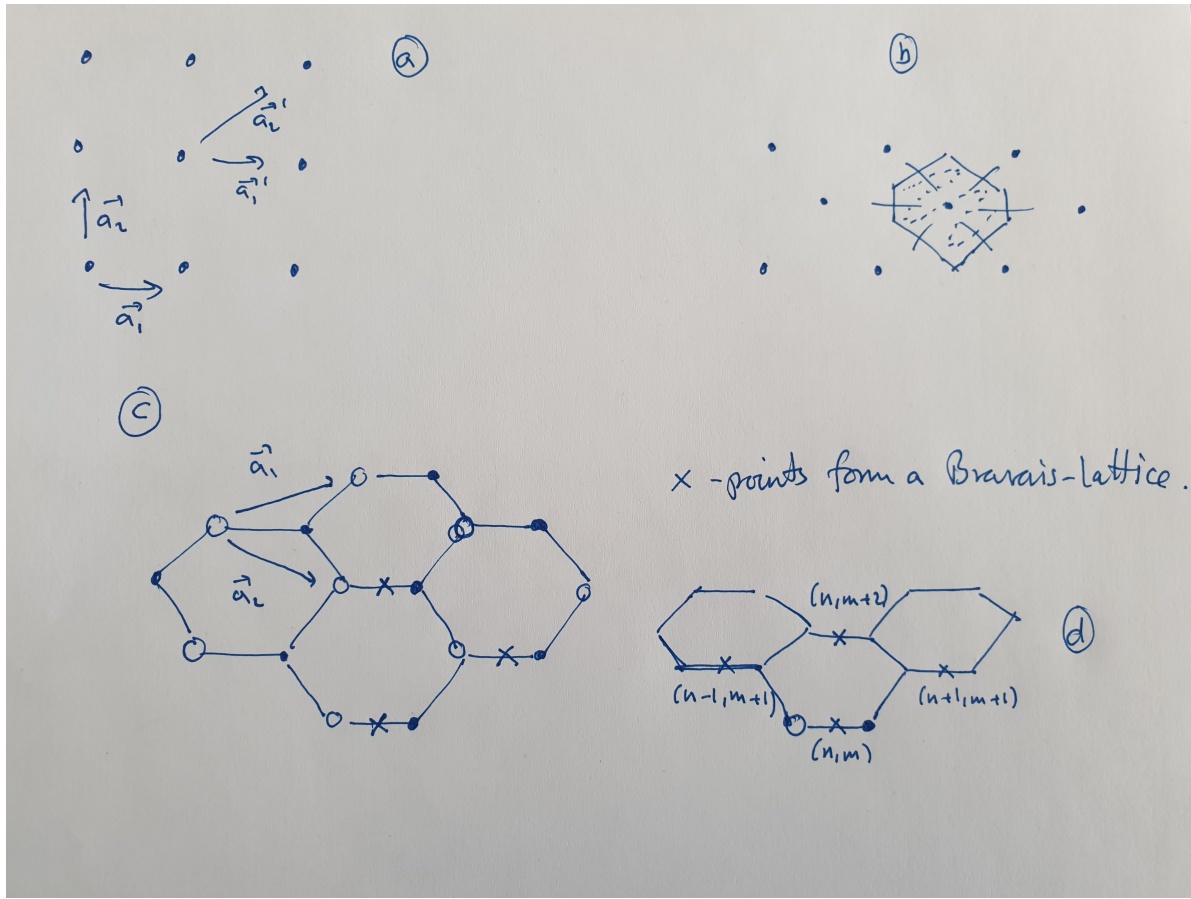


Figure 27.1: Various lattices and primitive unit vectors.

where we defined

$$x \equiv e^{2\pi i(n_1 - n'_1)/N}, \quad y \equiv e^{2\pi i(n_2 - n'_2)/N}. \quad (27.24)$$

Since

$$\sum_{m_j=0}^{N-1} x^{m_j} = \frac{1 - x^N}{1 - x} \quad (27.25)$$

and we know that $x \neq 1$ since $\mathbf{k} \neq \mathbf{k}'$ and $|n_1 - n'_1| < N$. Moreover, we have

$$x^N = e^{2\pi i(n_1 - n'_1)} = 1. \quad (27.26)$$

Therefore, the sum vanishes and the proof is complete.

Note that the summation over $\mathbf{k}$ does not necessarily have to be over the 1st BZ: it all depends on in which direction you apply the periodic boundary conditions for the lattice.

27.4.2 Non-Bravais lattice: graphene

All symmetric lattices are not necessarily Bravais lattices. Consider graphene. We can see straight away that this cannot be a Bravais lattice, since looking in a given direction the system does not

look identical if you stand on an A or B site. On all A sites, it looks the same. Therefore, the graphene lattice is a superposition of two hexagonal (Bravais) lattices. More formally, it can also be seen by considering that there does not exist two primitive lattice vectors $\mathbf{a}_1, \mathbf{a}_2$ which connects to all lattice points via $\mathbf{r} = n\mathbf{a}_1 + m\mathbf{a}_2$ where n and m are integers.

In the graphene, it is useful to consider instead the primitive vectors that connect the middle points of the "dumbbells" with an A and B atom on each side [Fig. 27.1(c)]. Each such middle point forms a triangular Bravais lattice. We can then label each such middle point by an index (n, m) for its x -position and y -position (see note from Annica on tight binding-BdG on graphene). One may then construct a basis so that

$$H = \sum_{ij} \begin{pmatrix} X_{i\uparrow}^\dagger & X_{j\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} H_0(i, j) & 0 \\ 6 = -H_0(i, j) & \end{pmatrix} \begin{pmatrix} X_{j\uparrow} \\ X_{j\downarrow} \end{pmatrix} \quad (27.27)$$

with

$$X_{i\sigma} = \begin{pmatrix} a_{i\sigma} \\ b_{i\sigma} \end{pmatrix} \quad (27.28)$$

Here, (i, j) are coordinates for each middle point of the "dumbbells", as shown in Fig. 27.1(d). Periodic boundary conditions can now be set up for each sublattice operator, for instance using armchair or zigzag interfaces. The allowed k -values will be different in those cases.

Regardless of if one uses an indexing of atom positions based on the middle points of the "dumbbells" or if one only operates with the direct atomic positions, it is useful to distinguish the operators on each sublattice since they each form a Bravais lattice, ensuring that summations of the type $\sum_i e^{i(k-k')i} = N\delta_{kk'}$ still hold. Moreover, the formulation of the PBC is easier when one uses two types of operators. Strictly speaking, one does not necessarily have to use two distinct operators for each sublattice, but then one has to be very careful with the allowed k -values coming from the PBC (which will be more challenging to set up in the first place) as well as summations over momenta (which do not become Kronecker δ -functions).

27.4.3 Non-Bravais lattice: Kagome lattice

Another interesting non-Bravais lattice (or, equivalently, Bravais lattice with basis) is the Kagome lattice. It is shown in Fig. 27.2: a triangular lattice with a 3-atom basis (labelled A,B,C). The W-S cell is constructed by drawing a line from, for instance, each A-atom to all neighboring A-atoms and then intersecting their middle with a perpendicular line. In the picture, this has been done along with an overall downwards translation of the W-S cell (which has no consequence).

The Kagome lattice can also be decorated with spins, as in arXiv:2309.01607. In this case, the W-S cell becomes larger since the distance between neighboring lattice sites with the same spin becomes larger. The 1st BZ therefore becomes smaller.

27.5 Charge continuity equation and definition of current

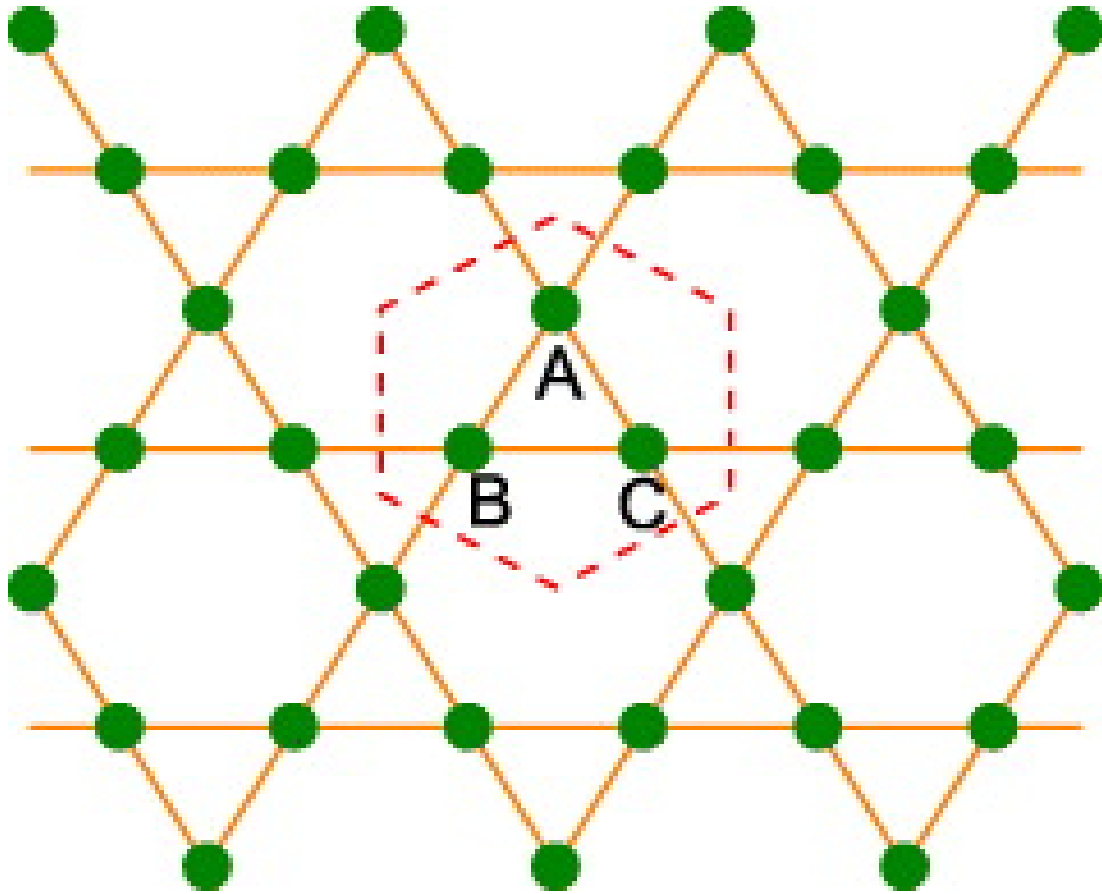


Figure 27.2: Kagome lattice and the Wigner-Seitz cell shown with dashed lines.

Chapter 28

Quasiclassical theory

28.1 The essence of the quasiclassical approximation

The key aspect of quasiclassical theory is to assume that the Fermi wavelength λ_F is the shortest length scale in the system. Therefore, the Fermi energy μ is the largest energy scale in the system. This means that λ_F must be smaller than the system length, the impurity scattering length, the superconducting coherence length, and so on. It turns out that the Gor'kov (exact) Green function of such a system consists of a part which is rapidly oscillating on a length scale of λ_F and an envelope function that varies on the other characteristic length scales of the system (such as the superconducting coherence length ξ). The rapidly oscillating part is technically problematic because it makes the derivatives of the Green function non-zero everywhere, whereas the envelope part contains information about how all self-energies and potentials in the system influence physical observables. Therefore, it is desirable to get rid off the rapid oscillations and only deal with the envelope function. This is what *quasiclassical theory* accomplishes.

The assumption that λ_F is the smallest length scale in the system is manifested in at least two places in the theory. The first place is the gradient expansion that is performed for the equation of motion for the Green function of the system, where an infinite series of derivations is truncated at first order of the derivative operator $\nabla_{\mathbf{R}}$ where $\mathbf{R}$ is the center of mass position coordinate. This is shown to be valid precisely when λ_F is the smallest length scale. We will prove this explicitly in one of the following subsections.

The second place it shows up is in how μ being the largest energy scale determines the momentum-dependence of the Gor'kov Green function $\check{G}(\mathbf{p}, E)$ which in turn justifies the definition of the quasiclassical Green function $g(\mathbf{p}_F)$:

$$\check{g}(\mathbf{p}_F, E) = \frac{i}{\pi} \int_{-\omega_c}^{\omega_c} d\xi_p \check{G}(\mathbf{p}, E) \quad (28.1)$$

where $\check{G}(\mathbf{p}, E)$ is the non-quasiclassical 8×8 Gor'kov Green function matrix in Keldysh space. The idea behind defining the quasiclassical Green function in this way is that the Gor'kov Green function can be shown to be strongly peaked near the Fermi momentum $\mathbf{p}_F$ when all energy scales in the system are much smaller than μ . Therefore, upon integrating over the magnitude $p = |\mathbf{p}|$ of the momentum, we keep only the contribution from $\check{G}$ close to p_F . Heuristically, a strongly peaked function near the Fermi-level can be approximated by

$$G(\mathbf{p}, E) \propto \delta(\xi_{\mathbf{p}}) g(\mathbf{p}) \quad (28.2)$$

since $\xi_{\mathbf{p}} = \mathbf{p}^2/2m - \mu = (p^2 - p_F^2)/2m$. Plugging the above form of $G(\mathbf{p}, E)$ into Eq. (28.1) gives the correct result. Note that since we do not integrate over angles, the quasiclassical Green function keeps the directional dependence $\Omega_{\mathbf{p}}$. Therefore, $\tilde{g}$ ends up depending on $\mathbf{p}_F$ in general.

Let us give a simplified mathematical justification for this. Consider a Gor'kov Green function for a homogeneous system, so that G only depends on the relative coordinate $\mathbf{r}$. We may then write

$$G(\mathbf{r}) = e^{i\mathbf{p}_F \cdot \mathbf{r}} f(\mathbf{r}). \quad (28.3)$$

Here, f is the envelope function which varies slowly compared to the rapidly oscillating exponential factor, which varies on the scale of λ_F . The Green function $\tilde{G}$ in momentum space is obtained via a Fourier-transformation

$$\tilde{G}(\mathbf{p}) = \int d\mathbf{r} e^{-i\mathbf{p} \cdot \mathbf{r}} G(\mathbf{r}) = \tilde{f}(\mathbf{p}_F - \mathbf{p}). \quad (28.4)$$

Here, we used that $\int e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} = \delta(\mathbf{q})$ and $\tilde{f}$ is the Fourier-transform of f . We see that we are left with only the envelope part of the Green function and that $\mathbf{p}_F$ enters its argument. If we now additionally integrate over all momenta $\mathbf{p}$, we get

$$\int d\mathbf{p} \tilde{f}(\mathbf{p}_F - \mathbf{p}) = g(\mathbf{p}_F) \quad (28.5)$$

The quantity g is the equivalent of the quasiclassical Green function: it contains information about the envelope part $\tilde{f}$ at the Fermi level $\mathbf{p}_F$. This can be seen by noting that if $f(\mathbf{r})$ is slowly varying, then its Fourier-transform $\tilde{f}(\mathbf{q})$ has to be sharply peaked. For instance, a constant function c has a Dirac-delta Fourier transform $c\delta(\mathbf{q})$. Therefore, $\tilde{f}(\mathbf{p}_F - \mathbf{p})$ should be sharply peaked at momenta $\mathbf{p} \simeq \mathbf{p}_F$ where its argument is zero. As the integral defining $g(\mathbf{p}_F)$ is performed, it is clear that the integrand mainly contributes close to the Fermi level, as stated initially. We note in passing that $g(\mathbf{p}_F)$ is also equal to $f(0)$, meaning that if we set the relative coordinate $\mathbf{r} \rightarrow 0$ right away in the Green function $G(\mathbf{r})$, we get rid off the rapidly oscillating part. However, the role of $\mathbf{p}_F$ is not clear in that case, whereas it is clear with the above derivation.

Based on the above discussion, it is possible to understand why it is occasionally stated in the literature that the quasiclassical approximation of the Green function can be thought of as simply writing

$$G(\mathbf{p}, E) \simeq \frac{\pi}{i} \delta(\xi_{\mathbf{p}}) g(\mathbf{p}) \quad (28.6)$$

where g is the quasiclassical Green function so that G is strongly peaked at $\mathbf{p} = \mathbf{p}_F$ (like a Dirac δ -function). But it is not immediately clear that Eq. (28.6) is a valid approximation as one considers free-electrons, because although $G(\mathbf{p}, E)$ is peaked at the Fermi level in this case, it is not peaked as a Dirac δ -function. Therefore, it is more appropriate to state that the definition of the quasiclassical Green function in Eq. (28.1) expresses that the main contribution to the integration over $\xi_{\mathbf{p}}$ comes from a very small interval near the Fermi level. We will prove analytically that in the simplest case of a free electron gas it turns out that the net contribution from G in Eq. (28.1) indeed has the form of a δ -function. We will prove this in the next section.

In the definition of the quasiclassical Green function, ω_c is a cutoff energy which we will show must satisfy the inequality:

$$\alpha \ll \omega_c \ll \mu. \quad (28.7)$$

Here, α is the largest energy scale of the system except for the Fermi energy. The requirement that $\alpha \ll \omega_c$ is necessary in order for $\tilde{G}(\mathbf{p}, E)$ to be strongly peaked near the Fermi level, which is true for $E \ll \mu$. Namely, in order for the quasiclassical Green function to capture all low-energy poles of the Gor'kov Green function, which are shifted away from $\xi_{\mathbf{p}}$ exactly equal zero when quasiparticle energy E , self-energies Σ , or potentials V are present, the integral must be taken over a region where $\alpha = \{E, \Sigma, V\} \ll \omega_c$. The second inequality $\omega_c \ll \mu$ will become clear later in the aforementioned *gradient approximation*.

We underline that the cutoff ω_c has no physical meaning in itself and should it appear in any expression for a physical quantity, it has to be replaced by a physical quantity that depends on it. This is similar to how the Debye frequency cutoff in the superconducting gap equation can be replaced by the superconducting critical temperature. We also close by mentioning that it is often stated in the literature that the high-energy part of the integral, when defining the quasiclassical Green function as $\int_{-\infty}^{\infty} d\xi_{\mathbf{p}} \tilde{G}$, does diverge, but that that part it is the same for all Green functions since that part is independent on the details near the Fermi level. Thus, one can discard it. This is not a good argument mathematically, and unclear physically. Using a cutoff to get rid of the high-energy part when defining the quasiclassical Green function solves this problem for the Green function itself, but the high-energy contribution to other quantities must still be discussed, which we now proceed to do.

What about the high-energy part of the integral?

If we integrate $\xi_{\mathbf{p}}$ only over the interval $[-\omega_c, \omega_c]$, we get the quasiclassical Green function. This is the definition of the quasiclassical Green function g , and we underline again that in order for g to be peaked close to the Fermi level, it implicitly assumes that E and all self-energies Σ are much smaller than ω_c . However, there are places in the derivation of quasiclassical theory (such as when computing physical observables) where one encounters integrals of the type $\int dE \int d\mathbf{p}$ which are proportional to

$$\int dE \int d\xi_{\mathbf{p}} p m \int d\Omega_{\mathbf{p}}. \quad (28.8)$$

The key point to note here is that the integral over $d\xi_{\mathbf{p}}$ is not confined to the interval $[-\omega_c, \omega_c]$, but instead to all possible values that $d\xi_{\mathbf{p}}$ can take. Similarly for the energy integral. In a free electron model, the limits are then $-\mu$ and ∞ . In a more realistic band-model in a material, the bandwidth W would define the size of the interval.

The retarded Green function itself takes the form of a free electron Green function outside $[-\omega_c, \omega_c]$, and so is proportional to the identity matrix and goes like $1/(E - \xi_{\mathbf{p}})$. Therefore, the integral diverges logarithmically, but if a finite bandwidth is included, there is no divergence. Nevertheless, the size of the integral outside the quasiclassical regime depends on how large the bandwidth is and is not necessarily negligible. An important point is that the Keldysh Green function instead goes like $1/(E - \xi_{\mathbf{p}})^2$, which means that any integral out to infinity in either E or $\xi_{\mathbf{p}}$ (not both) will give a convergent result.

Defining the quasiclassical Green function via a cutoff does not automatically eliminate the high-energy contribution to different quantities in the theory. The reason is, as explained above, that although we can choose to integrate the left-right subtracted Gor'kov equation (after the gradient approximation) over the interval defined by the cutoff (to get the Eilenberger equation), there are

other parts of the quasiclassical theory where the high-energy part of the integral is not as easily removed.

Two such parts are for self-energies (such as impurity scattering) and in the boundary conditions. The reason the high-energy part appears in these places is due to the Wigner-transformation where one changes from relative coordinates in time and space to energy and momentum. This transformation involves momentum-integrals which extend from $-\infty$ to ∞ , and thus not only the cutoff part that is used to define the quasiclassical Green function when integrating over $\xi_{\mathbf{p}}$. The type of integral shown above shows up at least two places: when computing the elastic impurity scattering in the Born approximation and when computing boundary conditions using Langreth's theorem and the Keldysh Green function (see later sections). *One question is then:* is it safe to disregard the contribution to the integral over $\xi_{\mathbf{p}}$ from the region outside $[-\omega_c, \omega_c]$, which is what is done in practice in both of the two places mentioned above? And what about the high-energy part of the integration over E in observables?

Self-energies and boundary conditions

For energy-dependent self-energies, this is not a problem since they appear in the commutator of the Usadel equation. To see why this is so, consider the expression for the self-energy before performing the quasiclassical approximation:

$$\check{\Sigma}_{\text{imp}}(\mathbf{R}, T, \mathbf{p}, E) = n_i \int \frac{d\mathbf{q}}{(2\pi)^3} |v(\mathbf{p} - \mathbf{q})|^2 \check{G}(\mathbf{R}, T, \mathbf{q}, E). \quad (28.9)$$

If we simply use $\int d\mathbf{q} \check{G} \propto \check{g}$, then we get the standard expression for the impurity self-energy. However, the definition of the quasiclassical Green function includes cutoffs in the momentum-integral, whereas the above expression for $\check{\Sigma}$ goes over all momenta. Therefore, it is correct to instead write

$$\check{\Sigma} \propto \check{g} + \check{\Sigma}_{\text{high}} \quad (28.10)$$

where $\check{\Sigma}_{\text{high}}$ is obtained by the integration outside of the cutoff range used to define the quasiclassical Green function. Nevertheless, one can ignore $\check{\Sigma}_{\text{high}}$ in the Usadel equation because it enters in a commutator and (ii) it is proportional to the identity matrix. The reason for the latter is that $\check{G} \propto \check{1}$ at large momenta, so long as we consider energies E close to the Fermi level. Therefore, $\check{\Sigma}_{\text{high}}$ drops out of the Usadel equation, even if it may be finite and large, simply because it commutes with anything. For energy-independent self-energies, like the superconducting gap Δ which is given by an additional integral $\int dE$, a different argument must be used. In the case of Δ , the high-energy part in E vanishes due to the introduction of a Debye cutoff, motivated by BCS theory.

The same reasoning as for the impurity scattering applies to the integrals used to derive boundary conditions for the quasiclassical Green function. Usually, commutators enter the right hand side of the generalized Kupriyanov-Lukichev boundary conditions, and the part of the Green function that comes from the high-energy part is proportional to identity and does not contribute. However, anticommutators can also enter in some cases (like the G_{MR} term in Cottet's boundary conditions), in which case one has to be more careful and see if the high-energy part can in fact give rise to additional terms in the boundary conditions. For example, in the case of the G_{MR} term mentioned above, the high-energy contribution renormalizes the G_{ϕ} term in the boundary condition.

Observables

For many observables, we are faced not only with an integration over momentum, or equivalently

over $\xi_{\mathbf{p}}$ after a variable change, but also an integral over all energies E (an exception to this is energy-resolved physical quantities, like the density of states).

One way to deal with this is to say that we want to compute the low-energy contribution in E to all observables. This is a valid approximation if we are considering physical quantities that have their main contribution from low energies E . But which physical quantities satisfy this? In normal metals (non-superconductors), this typically holds for non-equilibrium situations, i.e. for physical quantities that are zero in equilibrium: electric and spin currents, spin accumulation in non-magnetic metals, and so on, all have in common that it is electrons close to the Fermi level which determine these. They also have in common that the system must be driven out of equilibrium in order for the physical observables to be finite.

The equilibrium magnetization of a ferromagnet, in contrast, is an example of a physical quantity which is not correctly computed by only considering low energies E and the quasiclassical Green function. This is because all filled states contribute to the equilibrium magnetization of the system. The magnetization computed when only considering low energies E must therefore be interpreted as the *deviation* of the magnetization from its equilibrium value (isolated ferromagnet). For instance, the magnetization computed in a ferromagnet in a superconductor/ferromagnet bilayer is then the *deviation* from the equilibrium, bulk value of the isolated ferromagnet. To compute the entire magnetization, one has to integrate over all energies E .

In the superconducting state, physical quantities of interest, like the supercurrent, appears even in equilibrium. Is it then justified to neglect the high-energy contribution to the observable? Yes, because the supercurrent is only carried by states close to the Fermi level. In general, superconductivity affects only strongly single-particle states near the Fermi level, and thus the high-energy part of the integral in physical observables can be neglected even in equilibrium. In the case of current, the integral providing the current is over the odd part of the Keldysh Gor'kov Green function. In the high-energy regime $E \gg \Delta$, this is identically zero since the Gor'kov Green function is isotropic in $\mathbf{p}$ there (given by its normal-state value).

To make this argument more mathematical, consider then a time-independent situation, where the gradient approximation thus will give no derivatives with respect to energy since $\partial_T = 0$ where T is center of mass time. Generally, the expression for some observable $O(\mathbf{r})$ then looks like

$$O(\mathbf{r}) = \int dE \int d\Omega_{\mathbf{p}} \int d\xi_{\mathbf{p}} f[G(\mathbf{r}, E, \xi_{\mathbf{p}}), \mathbf{p}, E] \quad (28.11)$$

where f is a function of the non-quasiclassical Green function G and possibly momentum and energy as well. Typically, the Keldysh part of some product of such matrices is taken in f to compute the observable. The integral now has four parts in the integrations over E and $\xi_{\mathbf{p}}$

$$\int_{\text{low}} dE \int_{\text{low}} d\xi_{\mathbf{p}} + \int_{\text{low}} dE \int_{\text{high}} d\xi_{\mathbf{p}} + \int_{\text{high}} dE \int_{\text{low}} d\xi_{\mathbf{p}} + \int_{\text{high}} dE \int_{\text{high}} d\xi_{\mathbf{p}}. \quad (28.12)$$

Here, we defined

$$\begin{aligned} \int_{\text{low}} dE &= \int_{-\omega'}^{\omega'} dE, \\ \int_{\text{low}} d\xi_{\mathbf{p}} &= \int_{-\omega_c}^{\omega_c} d\xi_{\mathbf{p}} \end{aligned} \quad (28.13)$$

where ω' must be much smaller than ω_c (the cutoff in $\xi_{\mathbf{p}}$ used to define the quasiclassical Green function). This is necessary in order to be able to use the quasiclassical Green function, where E is assumed small compared to ω_c , in the integral $\int_{\text{low}} dE \int_{\text{low}} d\xi_{\mathbf{p}}$. So the $\int_{\text{low}} dE \int_{\text{low}} d\xi_{\mathbf{p}}$ gives the quasiclassical contribution to the observable. The integrations where either E or $\xi_{\mathbf{p}}$ is in a high-energy region are negligible since the Keldysh Green function goes like $1/(E - \xi_{\mathbf{p}})^2$. That means that we are left with the contribution from $\int_{\text{high}} dE \int_{\text{high}} d\xi_{\mathbf{p}}$ in addition to the quasiclassical one.

We may then write

$$\begin{aligned} O(\mathbf{r}) = & \int_{-\omega'}^{\omega'} dE \int d\Omega_{\mathbf{p}} f'[g(\mathbf{r}, E, \mathbf{p}_F), \mathbf{p}_F, E] \\ & + \int_{\text{high-energy}} dE \int_{\text{high-energy}} d\xi_{\mathbf{p}} f[G(\mathbf{r}, E, \xi_{\mathbf{p}}), \mathbf{p}, E]. \end{aligned} \quad (28.14)$$

In the first integral, we have used $\int d\xi_{\mathbf{p}}$ to convert $f(G, \mathbf{p}, E)$ into a different function $f'(g, \mathbf{p}_F, E)$ which depends on the quasiclassical Green function and where momentum is fixed at the Fermi level. This is the standard quasiclassical expression. Now what about the high-energy part? We can no longer use the argument that G^K goes like $1/(E - \xi_{\mathbf{p}})^2$ for large energies, because now *both* E and $\xi_{\mathbf{p}}$ are large and can cancel each other, giving a whole line of poles in the Green function where $E = \xi_{\mathbf{p}}$.

For some observables, the high-energy part in E and $\xi_{\mathbf{p}}$ can still be neglected for other reasons like angular averaging in the case of current. But yet other observables, like equilibrium magnetization, get an important contribution precisely from the high-energy part which cannot be neglected. Let us illustrate this with the equilibrium magnetization of a ferromagnet, following a note from E. Fyhn (2021). According to our reasoning, we should only get a contribution from the quasiclassical part and the high-energy integrals in both E and $\xi_{\mathbf{p}}$. First, the Keldysh Green function for a spatially and temporally uniform ferromagnet is

$$G^K = (G^R - G^A) \tanh(\beta E/2) \quad (28.15)$$

with

$$G^R = \frac{1}{\hat{\rho}_3(E + i\delta) + h\sigma_z - \xi_{\mathbf{k}}} \quad (28.16)$$

so that

$$G^K = \frac{-2i\delta\hat{\rho}_3}{(\xi_{\mathbf{k}} - \sigma_z h - \hat{\rho}_3 E)^2 + \delta^2} \tanh(\beta E/2), \quad (28.17)$$

which is to be understood as

$$G^K = -2i\delta \tanh(\beta E/2) \begin{pmatrix} \frac{1}{(\xi_{\mathbf{k}} - h - E)^2 + \delta^2} & 0 & 0 & 0 \\ 0 & \frac{1}{(\xi_{\mathbf{k}} + h - E)^2 + \delta^2} & 0 & 0 \\ 0 & 0 & \frac{1}{(\xi_{\mathbf{k}} - h + E)^2 + \delta^2} & 0 \\ 0 & 0 & 0 & \frac{1}{(\xi_{\mathbf{k}} + h + E)^2 + \delta^2} \end{pmatrix} \quad (28.18)$$

For small δ , G^K is close to being proportional to a Dirac delta-function distribution. Therefore, the integral over $\xi_{\mathbf{k}}$ will give 1 if $\xi_{\mathbf{k}} - \sigma_z h - \hat{\rho}_3 E = 0$ is within the integration regime. We obtain:

$$\int_{\text{high}} G^K d\xi_{\mathbf{k}} = -2i\delta \tanh(\beta E/2) \hat{\rho}_3 \begin{pmatrix} 1_{|E+h|>E_c} & 0 & 0 & 0 \\ 0 & 1_{|E-h|>E_c} & 0 & 0 \\ 0 & 0 & 1_{|E-h|>E_c} & 0 \\ 0 & 0 & 0 & 1_{|E+h|>E_c} \end{pmatrix} \quad (28.19)$$

since $\int_{\text{high}} d\xi_{\mathbf{p}} = \int_{\omega_c}^{\infty} d\xi_{\mathbf{p}} + \int_{-\infty}^{-\omega_c} d\xi_{\mathbf{p}}$. Then, the magnetization is

$$M = -\frac{ig\mu_B N_0}{32\pi} \int_{\text{high}} dE (-2i\pi) \tanh(\beta E/2) \text{Tr}\{\sigma_z \hat{\rho}_3 \begin{pmatrix} 1_{|E+h|>E_c} & 0 & 0 & 0 \\ 0 & 1_{|E-h|>E_c} & 0 & 0 \\ 0 & 0 & 1_{|E-h|>E_c} & 0 \\ 0 & 0 & 0 & 1_{|E+h|>E_c} \end{pmatrix}\} \\ + \text{quasiclassical contribution.} \quad (28.20)$$

This expression was obtained by starting out with the fundamental expression for magnetism in terms of expectation values of the field operators, for instance $M_Z \propto g\mu_B (\langle \psi_{\uparrow}^{\dagger} \psi_{\uparrow} - \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \rangle)$ and then converting this to be expressed in terms of the Green function matrix. The quasiclassical Keldysh Green function for a weak ferromagnet is $2\hat{\rho}_3 \tanh(\beta E/2)$, hence the quasiclassical contribution gives zero contribution after taking the trace. That the quasiclassical GF is equal to $2\hat{\rho}_3 \tanh(\beta E/2)$ can be verified directly from the bulk Usadel equation, or by explicitly computing $\int_{-\omega_c}^{\omega_c} -\omega_c G^K d\xi_{\mathbf{p}}$ for $E, h \ll \omega_c$ using the above expression for G^K . But the high-energy part gives the correct result for the total magnetization since:

$$M = -\frac{ig\mu_B N_0}{32\pi} \int_{\text{high}} dE (-4i\pi) \tanh(\beta E/2) [1_{|E+h|>\omega_c} - 1_{|E-h|>\omega_c}] \\ = -\frac{g\mu_B N_0}{8} \left[\int_{\omega_c-h}^{\omega_c+h} dE \tanh(\beta E/2) - \int_{\omega_c+h}^{\omega_c-h} dE \tanh(\beta E/2) \right] \\ = -\frac{g\mu_B N_0}{4} \int_{\omega_c-h}^{\omega_c+h} dE \tanh(\beta E/2) \\ \simeq -\frac{g\mu_B N_0 h}{2} \quad (28.21)$$

where we used that $\omega_c \gg h$, as assumed, and that $\tanh(x) \simeq 1$ for $x \gg 1$.

In summary, if we are dealing with observables where the contribution from $\int_{\text{high}} dE \int_{\text{high}} d\xi_{\mathbf{p}}$ integral vanishes, this justifies using only the quasiclassical expression

$$O(\mathbf{r}) = \int_{-\omega_c}^{\omega_c} dE \int d\Omega_{\mathbf{p}} f'[g(\mathbf{r}, E, \mathbf{p}_F), \nabla g(\mathbf{r}, E, \mathbf{p}_F)] \quad (28.22)$$

for instance for non-equilibrium resistive currents and equilibrium supercurrents. However, if we are dealing with observables that get a contribution from the entire Fermi sea, the high-energy part cannot be neglected and the quasiclassical contribution alone does not give the correct value for the observable.

28.1.1 Free electron

How is the quasiclassical approximation related to λ_F being the smallest length-scale? To see this, consider first a free electron-gas where the retarded Green function

$$G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) = -i\theta(t_1 - t_2) \langle \{\psi(\mathbf{r}_1, t_1), \psi^{\dagger}(\mathbf{r}_2, t_2)\} \rangle \quad (28.23)$$

obeys the following equation of motion

$$i\hbar \partial_{t_1} G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) = \hbar \delta(t_1 - t_2) \delta(\mathbf{r}_1 - \mathbf{r}_2) - i\theta(t_1 - t_2) \langle \{i\hbar \partial_{t_1} \psi(\mathbf{r}_1, t_1), \psi^{\dagger}(\mathbf{r}_2, t_2)\} \rangle \\ = \hbar \delta(t_1 - t_2) \delta(\mathbf{r}_1 - \mathbf{r}_2) + \hat{H}(\mathbf{r}_1) G^R(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2). \quad (28.24)$$

This can be seen from the time evolution of the field operators

$$i\hbar\partial_t\psi(\mathbf{r},t)=[\psi(\mathbf{r},t),\hat{H}(\mathbf{r})]. \quad (28.25)$$

For a stationary problem, we can Fourier-transform the relative coordinate $t_1 - t_2$ and one obtains

$$[E + i\delta - \hat{H}(\mathbf{r}_1)]G^R(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (28.26)$$

The reason for the appearance of the infinitesimal quantity $\delta \rightarrow 0$ is to ensure the proper boundary condition for the retarded Green function at very large relative times t , as has been explained in chapter 10.

For a free-electron gas, we have $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \mu$ and due to translational invariance we can also Fourier-transform in the relative coordinate $\mathbf{r}_1 - \mathbf{r}_2$. This results in

$$G^R(\mathbf{p}, E) = \frac{1}{E - \xi_{\mathbf{p}} + i\delta} \quad (28.27)$$

and $\xi_{\mathbf{p}} = \mathbf{p}^2/2m - \mu$ where μ is the Fermi level and $\delta \rightarrow 0^+$ is the inverse lifetime of the quasiparticles. For small quasiparticle energies $E \ll \mu$, it is clear that G is strongly peaked at $\mathbf{p} = \mathbf{p}_F$ since $\xi_{\mathbf{p}} \rightarrow 0$ there. Then, the quasiclassical approximation can be performed for the free-electron gas case. In this case, we had to assume that $\mu \gg E$, corresponding to μ being the largest energy scale in the problem as previously announced.

In performing the Fourier-transformation over $\mathbf{r}$, we had to discard a surface term of the type

$$i\mathbf{p}e^{i\mathbf{p}\cdot\mathbf{r}}G(\mathbf{r})\Big|_{\mathbf{r}\rightarrow-\infty}^{\mathbf{r}\rightarrow\infty} \quad (28.28)$$

This is justified if G vanishes in these limits which has to be verified in the end for the final result. We reveal already now that this is the case for both 2D and 3D free electrons (have not checked 1D yet).

We also briefly comment on the real-space form of the Gor'kov Green function in this free electron gas scenario, which takes the form

$$\begin{aligned} G^R(\mathbf{r}, E) &= \int G^R(\mathbf{p}, E)e^{i\mathbf{p}\cdot\mathbf{r}}d\mathbf{p} \\ &= \int d\mathbf{p} \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{E + \mu + i\delta - \mathbf{p}^2/2m}. \end{aligned} \quad (28.29)$$

Let (p, θ, ϕ) be spherical coordinates for $\mathbf{p}$ and choose the coordinate system so that $\mathbf{z}$ is parallel to $\mathbf{r}$. In this case, we obtain after performing the angular integration part (using *e.g.* that $\mathbf{p}\cdot\mathbf{r} = pr \cos \theta$):

$$G(\mathbf{r}, E) = \frac{\pi}{i|\mathbf{r}|} \int_0^\infty \frac{p(e^{ipr} - e^{-ipr})}{E + \mu + i\delta - p^2/2m} \quad (28.30)$$

where $p \equiv |\mathbf{p}|$ and $r \equiv |\mathbf{r}|$. Since the integrand is symmetric under $p \rightarrow (-p)$, we can extend the limit of integration to $-\infty$. Moreover, we define

$$k^2 = 2m(E + \mu) + i\delta. \quad (28.31)$$

We can rewrite this integral as

$$\begin{aligned} G(\mathbf{r}, E) &= \frac{m\pi}{ir} \int_{-\infty}^{\infty} \left(-\frac{1}{2p}\right) p (e^{ipr} - e^{-ipr}) \left(\frac{1}{p-k} + \frac{1}{p+k}\right) dp \\ &= \frac{m\pi i}{r} (I_1 - I_2). \end{aligned} \quad (28.32)$$

Here, we defined the quantities:

$$\begin{aligned} I_1 &= \int_{-\infty}^{\infty} e^{ipr} \left(\frac{1}{p-k} + \frac{1}{p+k}\right) dp, \\ I_2 &= \int_{-\infty}^{\infty} e^{-ipr} \left(\frac{1}{p-k} + \frac{1}{p+k}\right) dp. \end{aligned} \quad (28.33)$$

These integrals can be solved via Cauchy's integral formula:

$$f(z_0) = \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{f(z)}{z - z_0} dz \quad (28.34)$$

where f is an analytic function and $\mathcal{C}$ is a simple closed contour in the complex plane enclosing the point z_0 with positive orientation (it is traversed counterclockwise).

Let us choose $k = +\sqrt{2m(E + \mu) + i\delta}$ to begin with and later comment on the $k = -\dots$ choice. For I_1 , we choose the contour shown in Fig. ??(a) whereas for I_2 we choose the contour shown in Fig. ??(b) (note the orientation of the contour). The result is straightforwardly obtained:

$$I_1 = 2\pi i e^{ikr}, \quad I_2 = -2\pi i e^{ikr}. \quad (28.35)$$

The final result for the Green function in real space is then:

$$G(\mathbf{r}, E) = -\frac{4m\pi}{|\mathbf{r}_1 - \mathbf{r}_2|} e^{+ik|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (28.36)$$

We then also immediately know that

$$G(\mathbf{r}, E) = -\frac{4m\pi}{|\mathbf{r}_1 - \mathbf{r}_2|} e^{-ik|\mathbf{r}_1 - \mathbf{r}_2|} \quad (28.37)$$

is a solution to the Green function equation, since it satisfies the same equation as $+k$ as only k^2 enters the equation. There are thus two independent solutions for the Green function.

It is clear that it is rapidly oscillating as a function of the relative coordinate $|\mathbf{r}|$. Moreover, we see that the $i\delta$ -term gives rise to a localizing factor $e^{-\delta|\mathbf{r}|/v_F}$ in $G^R(\mathbf{r}, E)$. In other words, the Green function goes to zero for relative coordinates $|\mathbf{r}|$ which are much larger than $1/\delta$. Since $\delta \rightarrow 0$, the "mean free path" in this case is infinite. However, this observation will be useful later when we consider impurity scattering. When random impurity scattering is included in the equation for the Green function and treated as a self-energy, it is known that the retarded Green function takes the form

$$G^R(\mathbf{p}, E) \propto \frac{1}{E - \tilde{\xi}_{\mathbf{p}} + i/2\tau} \quad (28.38)$$

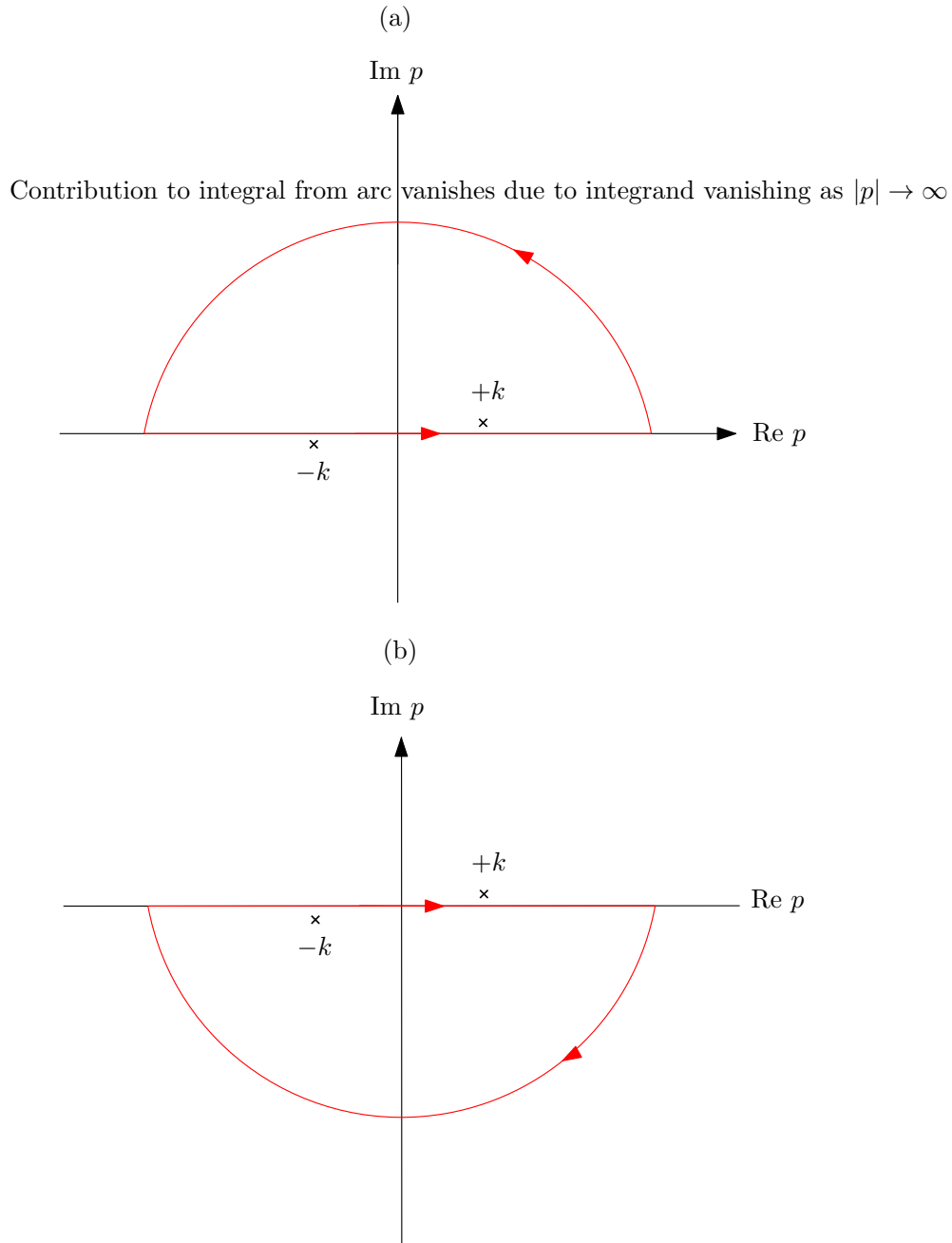


Figure 28.1: Contours to solve the integrals I_1 and I_2 .

where τ is the impurity scattering time so that $l_{\text{mfp}} = v_F \tau$. Now, we see that the localizing factor is $e^{-|\mathbf{r}|/l_{\text{mfp}}}$ and the Green function is zero unless the relative coordinate is $|\mathbf{r}| \ll l_{\text{mfp}}$. Physically, this is reasonable since the correlation between electrons should vanish when their relative distance exceeds the mean free path for the impurities, since scattering will then take place.

Finally, we can even directly compute the quasiclassical Green function. Let us absorb $E \ll \mu$ into

μ so that we are faced with the integral:

$$g^R(\mathbf{p}_F, \mathbf{R}) = \frac{i}{\pi} \int_{-\omega_c}^{\omega_c} d\xi_{\mathbf{p}} G^R(\mathbf{p}, \mathbf{R}). \quad (28.39)$$

Note that by absorbing E into μ , we are effectively assuming that the quasiparticle energy is very small. The quasiclassical Green function is thus only useful for small energies E . Nevertheless, physical observables are often computed by integrating over all possible energies. We will comment on how to reconcile this with the definition of the quasiclassical Green function later.

It is important that we take the limit $\delta \rightarrow 0$ after we perform the integration. Let us first rewrite the above equation as:

$$g^R(\mathbf{p}_F, \mathbf{R}) = \lim_{\delta \rightarrow 0} \frac{i}{\pi} \int_{-\omega_c}^{\omega_c} d\xi_{\mathbf{p}} \left[-\frac{\xi_{\mathbf{p}}}{\xi_{\mathbf{p}}^2 + \delta^2} - \frac{i\delta}{\xi_{\mathbf{p}}^2 + \delta^2} \right]. \quad (28.40)$$

The first term is antisymmetric in $\xi_{\mathbf{p}}$ and gives zero as result. The second term is a Lorentzian function and when taking the limit $\delta \rightarrow 0$ it becomes proportional to a Dirac delta-function $\delta(\xi_{\mathbf{p}})$. We are thus only left with the contribution from the second term and we obtain:

$$g^R(\mathbf{p}_F, \mathbf{R}) = \frac{i}{\pi} (-i\pi) = 1. \quad (28.41)$$

This is what we meant above when we wrote that the quasiclassical Green function can be obtained by replacing G^R with a $\delta(\xi_{\mathbf{p}})$ -function: strictly speaking, there is also another part which is antisymmetric in $\xi_{\mathbf{p}}$, but it gives no contribution to the quasiclassical Green function for a free electron.

We also note that if we instead had considered the advanced Green function, we should let $\delta \rightarrow (-\delta)$ which results in $g^A = -1$, as is consistent with the well-known result in quasiclassical theory. In the case where we don't have free electrons, g^R will take a different value than unity. We remind the reader that the cutoff must satisfy $\alpha \ll \omega_c$ in order for the quasiclassical Green function to contain the contribution to the integral defining it from poles of $G^R(\mathbf{p}, \mathbf{R})$.

28.1.2 Free electron + slowly varying potential V

Let us now consider a more general situation, namely where we additionally have a slowly varying potential $V(\mathbf{r})$ present in the Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - \mu + V(\mathbf{r}). \quad (28.42)$$

Following the same steps as before, we derive the following equation of motion for the retarded Green function

$$[E + \frac{\hbar^2}{2m} \nabla_{\mathbf{r}_1}^2 + \mu - V(\mathbf{r}_1)] G^R(\mathbf{r}_1, \mathbf{r}_2, E) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (28.43)$$

Note that we can no longer immediately Fourier-transform in the relative-coordinate due to the presence of the potential V . By proceeding in the usual manner and subtracting the left- and right-handed Gor'kov equation to get rid off the δ -function, switching to the mixed representation, and then Fourier-transforming, the term $V(\mathbf{r}_1) G^R(\mathbf{r}_1, \mathbf{r}_2)$ turns into (see chapter 4 in JP Morten thesis for details regarding how the star product appears)

$$\begin{aligned} V(\mathbf{r}_1) G^R(\mathbf{r}_1, \mathbf{r}_2) &\rightarrow V(\mathbf{R}) \otimes G^R(\mathbf{R}, \mathbf{p}) = e^{i\nabla_{\mathbf{R}}^V \nabla_{\mathbf{p}}^G / 2} V(\mathbf{R}) G^R(\mathbf{R}, \mathbf{p}) \\ &\simeq V(\mathbf{R}) G^R(\mathbf{R}, \mathbf{p}) + (i/2) \nabla_{\mathbf{R}} V(\mathbf{R}) \nabla_{\mathbf{p}} G^R(\mathbf{p}, \mathbf{R}). \end{aligned} \quad (28.44)$$

The last equality is known as the first order gradient approximation. We now wish to clarify which conditions the potential V has to satisfy in order for this to be valid. When we apply the quasiclassical approximation to the above term, the first term is trivial and turns into $V(\mathbf{R})g^R(\mathbf{R}, \mathbf{p}_F)$. For the second term, we need to find the quasiclassical approximation of $\nabla_{\mathbf{p}}G^R(\mathbf{R}, \mathbf{p})$. Here, we do this by integrating directly over $\int d\xi_{\mathbf{p}}$. Note that when higher order terms in the gradient approximation are included, it can actually be more practical to integrate over $\int d^3p$ to directly get an angular averaging and go to the Usadel equation rather than to first the Eilenberger equation. In spherical coordinates, we obtain

$$\nabla_{\mathbf{p}}G^R(\mathbf{p}, \mathbf{R}) = \partial_p G^R(\mathbf{p}, \mathbf{R})\hat{p} + \frac{1}{p}\nabla_{\Omega}G^R(\mathbf{p}, \mathbf{R}), \quad (28.45)$$

where $p = |\mathbf{p}|$ and $\nabla_{\Omega} \equiv \partial_{\theta}\hat{\theta} + \frac{1}{\sin\theta}\partial_{\phi}\hat{\phi}$ indicates the change in direction of $\mathbf{p}$. Upon defining the quasiclassical Green function, this is to be integrated over the quantity $\xi_{\mathbf{p}}$. Generally, we have

$$\partial_p = \frac{p}{m}\partial_{\xi}, \quad (28.46)$$

and so integration over the first term in Eq. (28.45) gives:

$$\int_{-\omega_c}^{\omega_c} d\xi_{\mathbf{p}} \sqrt{\frac{2(\mu + \xi_{\mathbf{p}})}{m}} \partial_{\xi_{\mathbf{p}}} G^R = \sqrt{\frac{2(\mu + \xi_{\mathbf{p}})}{m}} G^R \Big|_{-\omega_c}^{\omega_c} - \int_{-\omega_c}^{\omega_c} \frac{1}{\sqrt{2m(\mu + \xi_{\mathbf{p}})}} G^R d\xi_{\mathbf{p}} \quad (28.47)$$

by using a partial integration. Now, the surface term can be safely neglected, which can be seen more clearly by assuming that $\omega_c \ll \mu$, giving $\sqrt{2(\mu + \xi_{\mathbf{p}})} \simeq \sqrt{2\mu}$ so that:

$$\sqrt{\frac{2(\mu + \xi_{\mathbf{p}})}{m}} G^R \Big|_{-\omega_c}^{\omega_c} \simeq \frac{p_F}{m} [G^R(\xi_{\mathbf{p}} = \omega_c) - G^R(\xi_{\mathbf{p}} = -\omega_c)]. \quad (28.48)$$

First of all, the factor p_F/m is very small since $\mu/m \sim 10^{-5}$. Moreover, G^R itself should be close to its free-electron form when $\xi_{\mathbf{p}} = \pm\omega_c$, so G should also be negligible since $\alpha \ll \omega_c$.

Thus, only the second term on the right hand side of Eq. (28.47) remains. Under the assumption that the main contribution to the integral comes from energies $\xi_{\mathbf{p}} \simeq 0$ close to the Fermi level, like in the free-electron case, which we are allowed to assume since all self-energies and potentials are supposed to be of order $\alpha \ll \omega_c$, we may substitute

$$\sqrt{2m(\mu + \xi_{\mathbf{p}})} \simeq \sqrt{2m\mu} = p_F \quad (28.49)$$

and thus obtain finally

$$\int d\xi_{\mathbf{p}} \partial_p G^R(\mathbf{p}, \mathbf{R}) = -\frac{1}{p_F} \int_{-\omega_c}^{\omega_c} G^R d\xi_{\mathbf{p}} = -\frac{\pi}{ip_F} g^R. \quad (28.50)$$

Here, we thus assumed that $\omega_c \ll \mu$ in order to be able to neglect $\xi_{\mathbf{p}}$ compared to μ . This was the second and missing inequality we needed to obtain Eq. (28.7).

As for the second term in Eq. (28.45), we may for the same reason make the replacement $\frac{1}{p} \rightarrow \frac{1}{p_F}$ if the integral over $G^R(\mathbf{R}, \mathbf{p})$ has its main contribution from energies near the Fermi level. This should be a safe assumption so long as the inequality Eq. (28.7) is satisfied.

The quasiclassical version of the gradient term in total ends up as

$$\nabla_p G^R(\mathbf{p}, \mathbf{R}) \rightarrow \frac{1}{p_F} [-g^R(\mathbf{p}_F, \mathbf{R})\hat{p} + \nabla_\Omega g^R(\mathbf{p}_F, \mathbf{R})]. \quad (28.51)$$

We have thus obtained after the integration over ξ_p :

$$V(\mathbf{r}) \otimes G^R(\mathbf{p}, \mathbf{R}) \rightarrow V(\mathbf{R})g^R(\mathbf{p}_F, \mathbf{R}) + \frac{i}{2p_F} \nabla_{\mathbf{R}} V(\mathbf{R}) \cdot [-g^R(\mathbf{p}_F, \mathbf{R})\hat{p} + \nabla_\Omega g^R(\mathbf{p}_F, \mathbf{R})]. \quad (28.52)$$

It is then clear that we could have replaced $V(\mathbf{r}_1) \rightarrow V(\mathbf{R})$ at the very start Eq. (28.43) if $V(\mathbf{R})$ varies so slowly that the second term in Eq. (28.52) can be neglected compared to the first. If we can argue that $\nabla_\Omega g^R(\mathbf{p}_F, \mathbf{R})$ is at most of the same order of magnitude as $g^R(\mathbf{p}_F, \mathbf{R})$, we obtain the criterion

$$\frac{i}{p_F} \nabla_{\mathbf{R}} V(\mathbf{R}) \ll V(\mathbf{R}) \quad (28.53)$$

for when we can make the substitution $V(\mathbf{r}_1) \rightarrow V(\mathbf{R})$. In effect, the potential has to vary slowly on the Fermi wavelength, which is consistent with the quasiclassical approximation.

If we are in the diffusive limit, where the Green function g^R is almost completely isotropic, it is clear that $\nabla_\Omega g^R$ will be negligible and the above condition is fulfilled. If we are not in the diffusive limit, we still know that the Green function for $V = 0$ is isotropic in momentum space. The same is true for $V = \text{constant}$ since this can be absorbed into the chemical potential. Therefore, any angular anisotropy in g^R must be induced by a spatially varying potential V . The slower V varies, the smaller $\nabla_\Omega g^R$ must be. Therefore, it is qualitatively consistent to neglect the second term when V varies very slowly even without impurity scattering.

28.1.3 Free electron + self-energies

Finally, if a self-energy $\Sigma(\mathbf{p}, E)$ is present, the Green function can be determined from the Dyson equation. The real part of the self-energy renormalizes the single particle excitation spectrum, whereas the imaginary part leads to a finite lifetime for the particles. We will show via a detailed derivation below that so long as $\Sigma(\mathbf{p}, E)$ does not have any strong momentum dependence and satisfies $\Sigma(\mathbf{p}, E) \ll \mu$, we can still perform the quasiclassical approximation by integrating over ξ_p to obtain the quasiclassical Green function $g(\mathbf{p}_F, \mathbf{R})$.

But first, we discuss the Dyson equation and how it may be used to define a self-energy in the case of randomly distributed impurities which in turn enters the equation of motion for the Green function.

28.2 Dyson equation and impurity self-averaging

Let us begin by briefly reminding ourselves of from where the Dyson equation comes. First, one defines Green functions which expresses propagators and correlations in a system. The motivation for introducing these is that physical observables, such as susceptibility and current, can be expressed through them. The Green functions are in general time-dependent and the difficult task is to find their time-dependence when interactions are present. The basic idea is to express the exact Green

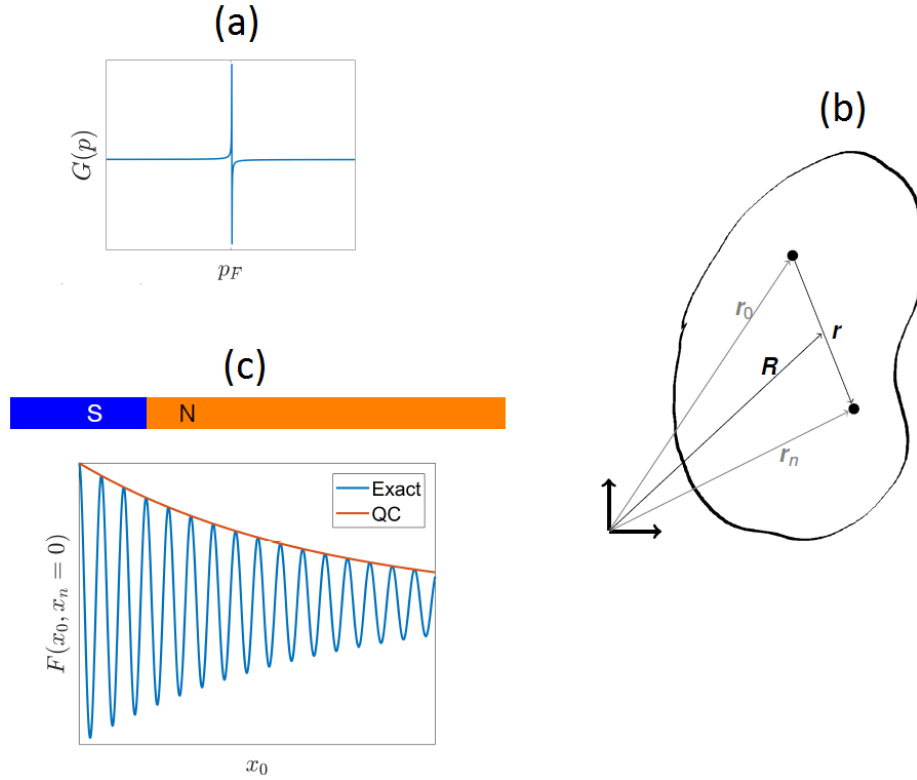


Figure 28.2: (a) The Gor'kov Green function for a free electron is strongly peaked near the Fermi momentum p_F , corresponding to $\xi_p = p^2/2m - \mu = 0$ since $\mu = p_F^2/2m$. (b) Definition of the relative and center-of-mass coordinates via the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ (denoted $\mathbf{r}_0$ and $\mathbf{r}_n$ in this particular figure). (c) Solution of the anomalous Gor'kov Green function an SN bilayer and the quasiclassical anomalous Green function. At $x = 0$, the two Green functions coincide if one uses continuous boundary conditions. Figures adapted from presentation given by M. Amundsen (2018).

function G as a perturbation expansion of the Green function G_0 that is evaluated *without* interactions in the system. The latter can be solved for exactly. To find such a perturbation expansion, one uses the Heisenberg equations of motion for the field operators that define the Green function G to obtain an expression for G via the interaction $V(t)$ through the so-called S -matrix.

If one now expands this equation for G in higher and higher order terms of the interaction $V(t)$, a pattern emerges which makes it natural to define the concept of a self-energy. The self-energy is defined in terms of integrals over the unperturbed Green function multiplied with the relevant interaction $V(t)$ and has higher and higher order terms.

The retarded Green function $G(1, 2)$ satisfies the equation of motion

$$[i\partial_{t_1}\hat{\rho}_3 - H(\mathbf{r}_1)]G(1, 2) = \delta(1 - 2). \quad (28.54)$$

as can be shown from Heisenberg's equation of motion for the field operators $\{\psi, \psi^\dagger\}$. To keep the notation light, we here omit any spin indices and $H(\mathbf{r}_1)$ is the first-quantized Hamiltonian of the system. Let us first consider the case without any scalar potential acting on the electrons, i.e. no

impurities, in which case the Hamilton-operator is H_0 and G_0 satisfies:

$$[i\partial_{t_1}\hat{\rho}_3 - H_0(\mathbf{r}_1)]G_0(1, 2) = \delta(1 - 2). \quad (28.55)$$

The ultimate goal is to find an equation of motion for the Green function including randomly distributed impurities, which should correspond to a realistic scenario in metals.

We start off, however, by considering a simpler scenario where a scalar potential $V(1)$ is included in the Hamiltonian, so that $H = H_0 + V$. This could be for instance the potential from a single impurity configuration. In this case, we can write

$$[i\partial_{t_1}\hat{\rho}_3 - H_0(\mathbf{r}_1)]G(1, 2) - V(1)G(1, 2) = \delta(1 - 2). \quad (28.56)$$

By defining the quantity $F(1, 2)$ such that it satisfies

$$\int d3 G_0(1, 3)F(3, 2) = \delta(1 - 2), \quad (28.57)$$

and writing

$$G(1, 2) = \int d3 \int d4 G_0(1, 4)F(4, 3)G(3, 2) \quad (28.58)$$

we can after a few steps bring the above equation for $G(1, 2)$ to the form:

$$G(1, 2) = G_0(1, 2) + \int d3 G_0(1, 3)V(3)G(3, 2). \quad (28.59)$$

By iterating this equation (inserting rhs into lhs), we obtain

$$G(1, 2) = G_0(1, 2) + \int d3 G_0(1, 3)V(3)G_0(3, 2) + \int d3 \int d4 G_0(1, 3)V(3)G_0(3, 4)V(4)G(4, 2) + \dots \quad (28.60)$$

This corresponds to a perturbation expansion in V to find the exact Green function $G(1, 2)$ since $G_0(1, 2)$ is assumed known. This expansion can be written diagrammatically via Feynman diagrams by defining the following rules:

Picture with diagrams coming

In the more general case of for instance two-body interactions or electron-phonon interactions, it is useful to generalize Eq. (28.59) to

$$G(1, 2) = G_0(1, 2) + \int d3 \int d4 G_0(1, 3)\Sigma(3, 4)G(4, 2). \quad (28.61)$$

This is the definition of the irreducible self-energy Σ . For the case of a scalar potential, we see that $\Sigma(3, 4) = V(3)\delta(3 - 4)$. This is the standard form of the Dyson equation in real-space coordinates. The advantage of this formulation is that it again permits an elegant diagrammatic representation by iterating the equation and defining corresponding Feynman rules.

Physical motivation for impurity averaging describing a single sample

We will come back and find a use for Eq. (28.61), but let us first consider the problem of impurity averaging. If the total scalar potential $V(\mathbf{r})$ above originates from N impurities located at positions $\mathbf{R}_j$, we obtain (writing now only the space-coordinate for simplicity):

$$V(\mathbf{r}_1) = \sum_{j=1}^N U(\mathbf{r}_1 - \mathbf{R}_j) \quad (28.62)$$

where U is the potential from one single impurity. This means that

$$G(\mathbf{r}_1, \mathbf{r}_2) = G_0(\mathbf{r}_1, \mathbf{r}_2) + \sum_{j=1}^N \int d\mathbf{r}' G_0(\mathbf{r}_1, \mathbf{r}') U(\mathbf{r}' - \mathbf{R}_j) G(\mathbf{r}', \mathbf{r}_2). \quad (28.63)$$

However, we are not interested in a theory which is only valid for one specific sample, i.e. one specific impurity configuration. Therefore, we expect that a more generic description for metals should be obtained by averaging the Green function over all possible impurity configurations. This becomes a necessity if we wish to develop a quasiclassical theory where the total potential $V(\mathbf{r})$ does not vary on a short length-scale, unlike the individual potentials $U(\mathbf{r} - \mathbf{R}_j)$ which do vary on short length-scales thanks to Coulomb potential screening in a metal.

It is possible to justify this point of view better physically, following the text in section 11.4 of the Bruus and Flensberg textbook.

"If the electron wavefunctions are completely coherent throughout the entire disordered metal each true electronic eigenfunction exhibit an extremely complex diffraction pattern spawned by the randomly positioned scatterers. If one imagine changing some external parameter, *e.g.* the average electron density or an external magnetic field, each individual diffraction pattern will of course change drastically due to the sensitivity of the scattering phases of the wavefunctions. Significant quantum fluctuations must therefore occur in any observable at sufficiently low temperatures.

Using modern nano-technology to fabricate small (but still macroscopic) samples, and standard cryogenic equipment to cool down these samples to ultra-low temperatures, one can in fact obtain an experimental situation where the electrons can traverse the sample without losing their quantum-mechanical phase coherence. In Fig. (a) below is shown the conductance trace of a GaAs nano-device, such as the one shown at 0.31 K as a function of the electron density. This density can be controlled by applying a gate voltage V_g on an external electrode. The conductance G is seen to fluctuate strongly for minute changes of V_g . These fluctuations turn out to be perfectly reproducible as V_g is swept up and down several times.

As the temperature of a given sample is raised, the amount of electron-electron and electron-phonon scattering increases because of an increased phase space for scattering and an increased number of phonons. The quantum mechanical phase of each individual electron is changed by a small random amount at each inelastic scattering event, and as a result the coherence length l_ϕ for the electrons diminishes. At sufficiently high temperature (*e.g.* 4.1 K) l_ϕ is much smaller than the size of the device, and we can think of the device as being composed as a number of phase-independent small phase coherent sub-systems. Therefore, when one measures an observable the result is in fact an incoherent average of all these sub-systems. Note that this average is imposed by the physical properties of the system itself, and this effective averaging is consequently denoted self-averaging. This

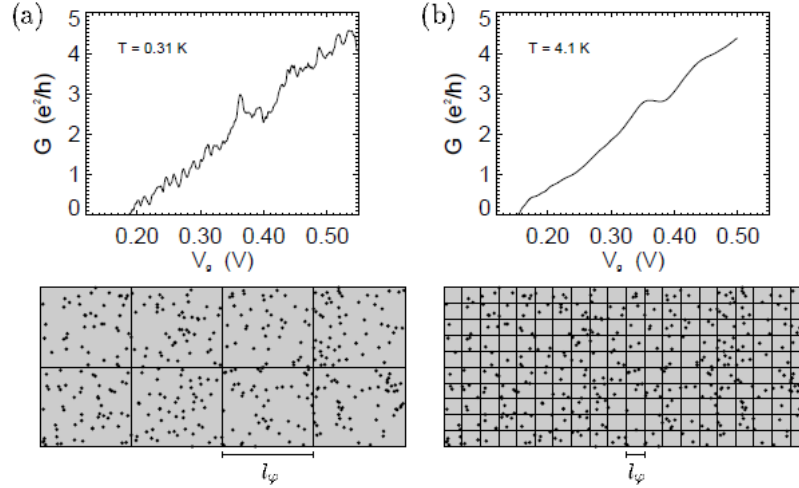


Figure 28.3: (a) The measured conductance of a disordered GaAs sample at $T = 0.31$ K displaying random but reproducible quantum fluctuations as a function of a gate voltage V_g controlling the electron density. The fluctuations are due to phase coherent scattering against randomly positioned impurities. Below is indicated that the phase coherence length l_ϕ is large compared to the size of the sample. (b) The same system at $T = 4.1$ K. The fluctuations are almost gone due to the smallness of l_ϕ at this temperature. The sample now contains a large number of independent but phase-coherent sub-systems of size l_ϕ . As a result a substantial self-averaging occurs, which suppresses the quantum fluctuations. Figure and caption taken from Fig. 11.2 in Bruus and Flensberg.

effect is illustrated in Fig. (b) where the conductance trace at 4.1 K is seen to be much smoother than the one at 0.31 K, and where the many small phase coherent sub-systems of the sample are indicated below the experimental graph.

For very large (mm sized) macroscopic samples l_ϕ is much smaller than the sample size at all experimental realizable temperatures ($T > 10$ mK for electron gases in metals and semiconductors), and we are in the impurity self-averaging case. Mathematically, the impurity average is performed by summing over all the phase-independent coherent sub-systems and dividing by their number N_{sys} . But due to the random distribution of the impurities, this average is the same as an average over the impurity position within a single subsystem - as can be seen from the figure. However, even on the rather small length scale l_ϕ the system is already homogeneous, and one can as well perform the position average over the entire volume of the sample.”

Technical details of impurity averaging

The impurity averaging of a quantity X is accounted for by the operation $\frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots X \equiv \langle X \rangle_{\text{av}}$, where $\mathcal{V}$ is the system volume, and performing this operation on the above equation gives

$$\begin{aligned}
 \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots G(\mathbf{r}_1, \mathbf{r}_2) &\equiv G_{\text{av}}(\mathbf{r}_1, \mathbf{r}_2) \\
 &= G_0(\mathbf{r}_1, \mathbf{r}_2) + \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots \sum_{j=1}^N G_0(\mathbf{r}_1, \mathbf{r}') U(\mathbf{r}' - \mathbf{R}_j) G(\mathbf{r}', \mathbf{r}_2).
 \end{aligned}
 \tag{28.64}$$

since G_0 is independent on $\{R_j\}$. We now insert Eq. (28.63) into Eq. (28.64) to obtain

$$\begin{aligned}
 G_{\text{av}}(\mathbf{r}_1, \mathbf{r}_2) &= G_0(\mathbf{r}_1, \mathbf{r}_2) + \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots \sum_{j=1}^N \int d\mathbf{r}' G_0(\mathbf{r}, \mathbf{r}') U(\mathbf{r}' - \mathbf{R}_j) G_0(\mathbf{r}', \mathbf{r}_2) \\
 &+ \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots \sum_{j=1}^N \sum_{j'=1}^N \int d\mathbf{r}' \int d\mathbf{r}'' G_0(\mathbf{r}_1, \mathbf{r}') U(\mathbf{r}' - \mathbf{R}_j) \\
 &\times G_0(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'' - \mathbf{R}_{j'}) G(\mathbf{r}'', \mathbf{r}_2). \tag{28.65}
 \end{aligned}$$

Note that the equation is still exact. By the way, note that if we had considered the case of spin-orbit impurities, $U(\mathbf{r}) \rightarrow U_{\text{soc}}(\mathbf{r})$ would have been a matrix and an operator, due to the gradient-operator appearing in $U_{\text{soc}}(\mathbf{r})$. Then, the second U on the last line of Eq. (28.65) acts on $G(\mathbf{r}'', \mathbf{r}_2)$. This causes the final self-energy to be on the (qualitative) form $\langle U_{\text{soc}} G_0 U_{\text{soc}} \rangle$ where the second U_{soc} in this expression would be an operator acting on whatever comes after. However, we can avoid this by doing a partial integration on the last line of Eq. (28.65), so that $U_{\text{soc}}(\mathbf{r}'' - \mathbf{R}_{j'})$ acts to the *left* on $G_0(\mathbf{r}', \mathbf{r}'')$ instead and also acquires a minus-sign due to the partial integration. Doing so still gives us a self-energy on the form $\langle U_{\text{soc}} G_0 U_{\text{soc}} \rangle$, but now the second U_{soc} has an extra minus sign compared to the first and also acts to the left on G_0 .

To make further progress we make some assumptions. First of all, for randomly distributed impurities we expect that the average potential should be a constant. Whatever its value, it can simply be absorbed into the definition of chemical potential. This can readily be seen by looking at the original Gor'kov Green function and thus we ignore the term:

$$\langle V(\mathbf{r}) \rangle_{\text{av}} \equiv \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots \sum_{j=1}^N U(\mathbf{r} - \mathbf{R}_j). \tag{28.66}$$

This means that we effectively assume $\langle V \rangle = 0$, which is equivalent to $\langle U \rangle = 0$. In doing so, the first term in Eq. (28.65) vanishes. Its actual value is equal to $Nv(0)$ where $v(0)$ is the zero-momentum contribution in the Fourier-transform of the potential:

$$U(\mathbf{r}) = \sum_i U(\mathbf{r} - \mathbf{r}_i) = \sum_i \sum_{\mathbf{q}} v(\mathbf{q}) e^{i\mathbf{q}(\mathbf{r} - \mathbf{r}_i)}, \tag{28.67}$$

but as explained we ignore this relative the Fermi energy μ . Since each $U(\mathbf{r} - \mathbf{r}_i)$ is sharply localized near each impurity, it is clear that $v(\mathbf{q})$ should depend very weakly on the magnitude of the momentum. The fact that we're setting $\langle V \rangle = 0$ is consistent with the treatment in section 4.5.2 of JP Morten's thesis, where the $\mathbf{q} = \mathbf{q}' = 0$ term in the lower line of Eq. (4.42) is ignored even if it is non-zero (this is because it is much smaller than the sum of remaining terms in the upper line of the same equation). The actual value $v(0) \propto \langle V \rangle$ appears in the final expression for the self-energy, so we are just ignoring $v(0)$ whenever there are other terms present in a given expression featuring it which are much larger.

As for the second term in Eq. (28.65), we see that we have to evaluate $\langle U(\mathbf{r}' - \mathbf{R}_j) G_0(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'' - \mathbf{R}_{j'}) G(\mathbf{r}'', \mathbf{r}_2) \rangle_{\text{av}}$. Looking at the expression for G in Eq. (28.63), we see that to lowest order in the impurity potential U [$\mathcal{O}(U^0)$ to be precise] we have $G = G_0$, so that:

$$\langle U(\mathbf{r}' - \mathbf{R}_j) G_0(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'' - \mathbf{R}_{j'}) G(\mathbf{r}'', \mathbf{r}_2) \rangle_{\text{av}} = \langle U(\mathbf{r}' - \mathbf{R}_j) G_0(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'' - \mathbf{R}_{j'}) \rangle_{\text{av}} G_0(\mathbf{r}'', \mathbf{r}_2). \tag{28.68}$$

by inserting $G = G_0$ on the left-hand side. In a more compact symbolical notation, we have thus used $\langle UG_0UG \rangle \simeq \langle UG_0U \rangle G_0$ to lowest in the impurity potential. This is an approximation, but we will later verify its validity by comparing with the exact expression obtained from the Dyson equation. Note that G_0 and U are in general matrices, so that we must keep the G_0 between the two U 's. Using this in Eq. (28.65), we get:

$$G_{\text{av}}(\mathbf{r}_1, \mathbf{r}_2) = G_0(\mathbf{r}_1, \mathbf{r}_2) + \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots \sum_{j=1}^N \sum_{j'=1}^N \int d\mathbf{r}' \int d\mathbf{r}'' G_0(\mathbf{r}_1, \mathbf{r}') \times U(\mathbf{r}' - \mathbf{R}_j) G_0(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'' - \mathbf{R}_{j'}) G_0(\mathbf{r}'', \mathbf{r}_2) \quad (28.69)$$

which we can write as

$$G_{\text{av}}(1, 2) = G_0(\mathbf{r}_1, \mathbf{r}_2) + \int d\mathbf{r}_3 \int d\mathbf{r}_4 G_0(\mathbf{r}_1, \mathbf{r}_3) \Sigma(\mathbf{r}_3, \mathbf{r}_4) G_0(4, 2). \quad (28.70)$$

Here, $G_{\text{av}}(1, 2)$ is the impurity-averaged Green function and

$$\begin{aligned} \Sigma(\mathbf{r}, \mathbf{r}') &= \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots \sum_j \sum_{j'} U(\mathbf{r}' - \mathbf{R}_j) G_0(\mathbf{r}', \mathbf{r}'') U(\mathbf{r}'' - \mathbf{R}_{j'}) \\ &= \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \int d\mathbf{R}_2 \dots V(\mathbf{r}') G_0(\mathbf{r}', \mathbf{r}'') V(\mathbf{r}'') \\ &= \langle V(\mathbf{r}') G_0(\mathbf{r}, \mathbf{r}') V(\mathbf{r}'') \rangle_{\text{av}}. \end{aligned} \quad (28.71)$$

At this point, we make an approximation: we replace $G_0(\mathbf{r}, \mathbf{r}')$ in Σ and $G_0(4, 2)$ in Eq. (28.70) with G_{av} . Before justifying this mathematically, it makes sense physically that it is a better approximation to use the full Green function propagator inside the expression for the self-energy for the following reason. Using the non-interacting Green function G_0 in $\Sigma(\mathbf{r}, \mathbf{r}')$ means that the background (virtual) particles contributing to the self-energy are treated as non-interacting. In reality, of course, these particles also move in an average potential coming from the presence of all the other particles and should be renormalized as well. Thus instead of using G_0 in Σ , we expect it to be a better approximation to use the exact Green function G_{av} . This is known as the *self-consistent* Born approximation. In the special case of a translationally invariant system, this can be shown rigorously in the momentum representation (see chapter 11 the textbook "*Many-Body Quantum Theory in Condensed Matter Physics: An Introduction*" by Bruus and Flensberg). The same argument also applies to using $G_{\text{av}}(4, 2)$ instead of $G_0(4, 2)$ in Eq. (28.70): this should give a more accurate result than truncating the expansion of G_{av} at second order by using $G_0(4, 2)$.

Let us now formally show why the selfconsistent Born approximation should be better than using G_0 (i.e. truncating completely at second order in V). First, we note that the exact equation for G before impurity averaging is

$$G = G_0 + G_0 V G. \quad (28.72)$$

Products are here bullet products involving convolution integrals in spatial coordinates as above, but we write it simply like this for brevity of notation. Therefore, the impurity averaged Green function is:

$$\begin{aligned} \langle G \rangle &= G_0 + G_0 \langle V G \rangle \\ &= G_0 + G_0 \langle V G_0 V \rangle G_0 + G_0 \langle V G_0 V G_0 V \rangle G_0 + \dots \end{aligned} \quad (28.73)$$

since $\langle G_0 \rangle = G_0$ and we assumed, as before, that $\langle V \rangle = 0$. Now, in the Born approximation we have:

$$\langle G \rangle = G_0 + G_0 \langle V G_0 V \rangle G_0 \quad (28.74)$$

As seen, this just contains the first three terms in the exact expression Eq. (28.73). Now, can the selfconsistent Born approximation do better than that? Let us check. We defined the selfconsistent Born approximation as:

$$\langle G \rangle = G_0 + G_0 \langle V \langle G \rangle V \rangle \langle G \rangle. \quad (28.75)$$

Now, iterating this equation by reinserting $\langle G \rangle$ on the right hand side then gives:

$$\begin{aligned} \langle G \rangle = & \overbrace{G_0}^{\text{0th order terms}} \\ & + \overbrace{G_0 \langle V G_0 V \rangle G_0}^{\text{2nd order terms}} \\ & + \overbrace{G_0 \langle V G_0 V \rangle G_0 \langle V G_0 V \rangle G_0 + G_0 \langle V G_0 \langle V G_0 V \rangle G_0 V \rangle G_0}^{\text{4th order terms}} + \dots \end{aligned} \quad (28.76)$$

Notice how the selfconsistent Born approximation gives no contribution to third order in the potential V since we assumed $\langle V \rangle = 0$. Look now at the fourth order terms for $\langle G \rangle$ in the exact expression and in the selfconsistent Born approximation. All the diagrams contained in the fourth order terms in the selfconsistent Born approximation

$$G_0 \langle V G_0 V \rangle G_0 \langle V G_0 V \rangle G_0 + G_0 \langle V G_0 \langle V G_0 V \rangle G_0 V \rangle G_0 \quad (28.77)$$

are also contained in the fourth order term in the exact expression for $\langle G \rangle$:

$$G_0 \langle V G_0 V G_0 V G_0 V \rangle G_0. \quad (28.78)$$

We illustrate this in the figure below. We note in passing that had we not assumed $\langle V \rangle = 0$, the selfconsistent Born approximation would have additional fourth order terms which are not included here. In the diagrams, the straight lines are free propagators G_0 , the dashed lines represent impurity potentials, and the crosses represent impurity averaging. Specifically, the Feynman rules which have been used to set up the diagrams are as follows:

- For each straight line from $\mathbf{r}_1$ to $\mathbf{r}_2$, multiply a factor $G_0(\mathbf{r}_1, \mathbf{r}_2)$.
- For each dashed line from a point at $\mathbf{r}$ to a cross labelled i , multiply a factor $U(\mathbf{r} - \mathbf{R}_i)$.
- For each cross labelled i , perform an integration and summation according to $\frac{1}{\mathcal{V}} \int \sum_i d\mathbf{R}_i$.

Note that even if some terms using the selfconsistent Born approximation have two impurity averages for instance in the fourth order terms, this gives rise to more terms than the single impurity average occurring in the exact expression. But there are also twice as many $1/\mathcal{V}$ factors in the selfconsistent expression due to the impurity averaging, so it does not mean that the expression in the selfconsistent case is larger. Moreover, it does not give rise to more Feynman diagrams than in the exact expression: the diagrams are almost the same, except for *e.g.* the crossing line diagram. We simply average over impurity positions more times in the selfconsistent case, but also reduce the magnitude by accompanying $1/\mathcal{V}$ factors.

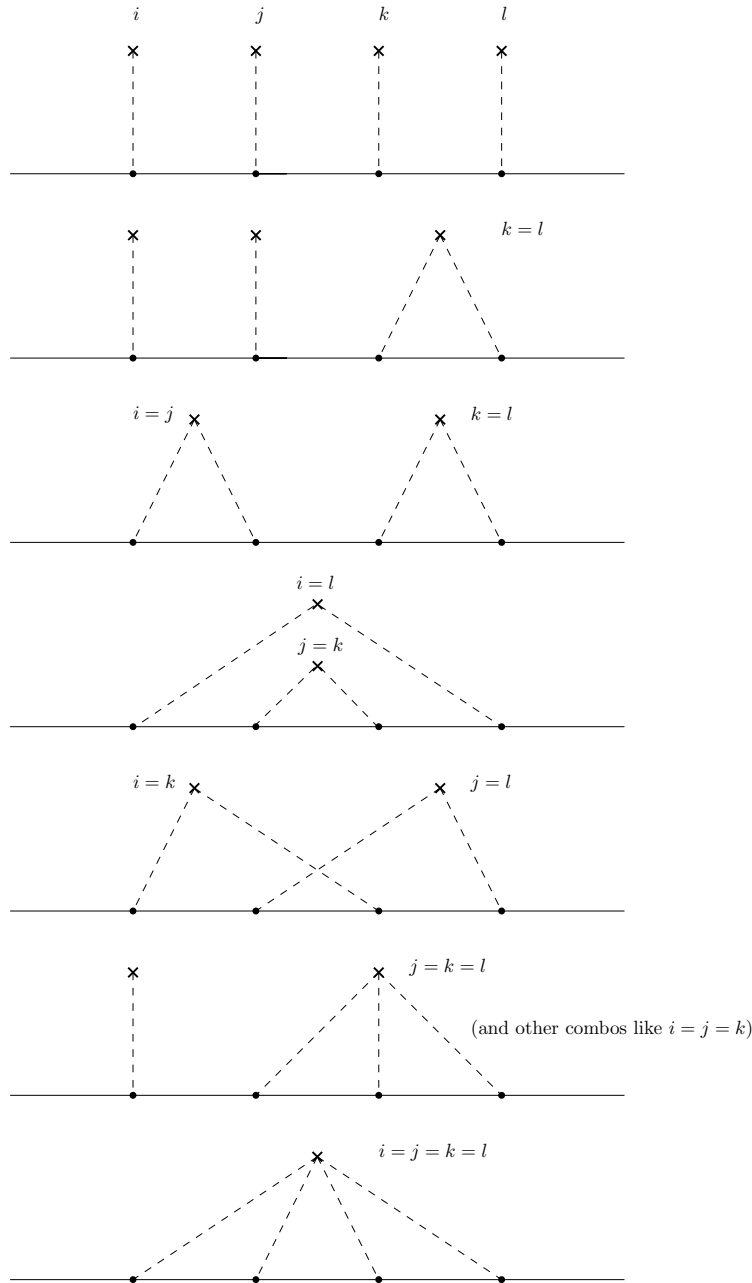


Figure 28.4: Some of the diagrams produced by fourth order term in V_0 in the expression for $\langle G \rangle$ in the exact expression and the selfconsistent Born approximation. The diagram at the bottom and the one with crossed lines do not appear in the selfconsistent Born approximation. Moreover, the diagrams having crosses with a single dashed line all vanish when $\langle V \rangle = 0$ is assumed, as we have done above.

To see precisely why the exact expression for $\langle G \rangle$ captures more diagrams than the selfconsistent Born approximation expression, consider the *first* of the two fourth order terms in the selfconsistent

Born approximation case:

$$\begin{aligned}
 G_0 \langle V G_0 V \rangle G_0 \langle V G_0 V \rangle G_0 &= G_0 \left(\frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \dots \int d\mathbf{R}_N \sum_{i=1, j=1}^N U_i G_0 U_j \right. \\
 &\quad \left. \times G_0 \frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \dots \int d\mathbf{R}_N \sum_{k=1, l=1}^N U_k G_0 U_l \right) \times G_0
 \end{aligned} \tag{28.79}$$

Note that there is an integration over the internal coordinates of the G_0 propagators as well: the notation for this has just been suppressed. The contribution from $i = j$ and $k = l$ gives

$$G_0 \left(\frac{1}{\mathcal{V}} \int \sum_i d\mathbf{R}_i U_i G_0 U_i \right) G_0 \left(\frac{1}{\mathcal{V}} \int \sum_k d\mathbf{R}_k U_k G_0 U_k \right). \tag{28.80}$$

We see that $N - 2$ of the volume factors cancel against the impurity position integrals. This corresponds to one of the diagrams in the figure. However, we see that there is no way we can get an expression of the form

$$G_0 \left(\frac{1}{\mathcal{V}_N} \sum_i \int d\mathbf{R}_i U_i G_0 U_i G_0 U_i G_0 U_i \right) \tag{28.81}$$

which corresponds to the $i = j = k = l$ diagram in the figure. Also, neither of the fourth order terms in the selfconsistent Born approximation can give an $i = k$ and $j = l$ diagram.

In contrast, the exact expression for $\langle G \rangle$ to fourth order:

$$G_0 \left(\frac{1}{\mathcal{V}^N} \int d\mathbf{R}_1 \dots d\mathbf{R}_N \sum_{ijkl} U_i G_0 U_j G_0 U_k G_0 U_l \right) G_0 \tag{28.82}$$

We see that we can get the same expression as Eq. (28.80) by considering the contribution to the above summation from $i = j$ and $k = l$, which gives precisely

$$G_0 \left(\frac{1}{\mathcal{V}^2} \sum_{ik} \int d\mathbf{R}_i d\mathbf{R}_k U_i G_0 U_i G_0 U_k G_0 U_k \right) G_0 = G_0 \left(\frac{1}{\mathcal{V}^2} \int \sum_i d\mathbf{R}_i U_i G_0 U_i G_0 \int \sum_k d\mathbf{R}_k U_k G_0 U_k \right) G_0. \tag{28.83}$$

Note that it is implicit in this expression that $i \neq k$. This should therefore be indicated in the Feynman diagram when labelling the cross so that *e.g.* the summation over k excludes $k = i$. This is because the diagram for $i = j, k = l$ while simultaneously $i = l$ in the exact expression corresponds to scattering on a *single* impurity, which qualitatively changes the diagram (to the $i = j = k = l$ diagram in the figure).

However, we also get a contribution from the exact expression which cannot be obtained in the selfconsistent Born approximation, namely the contribution from $i = j = k = l$ in Eq. (28.81). So the exact expression contains the same terms as in selfconsistent Born, but also additional terms which give rise to different Feynman diagrams.

Finally, we note that the diagram with $i = l$ and $j = k$ in the figure comes from the first of the two 4th order terms in the selfconsistent Born approximation. Moreover, it is clear that the $i = k$ and

$j = l$ diagram in the figure above (crossing lines) cannot be obtained with *any* of the two 4th order terms in the Born approximation, since none of these term include an averaging over the first and third potential V in the expression.

We also note that in the actual evaluation of Σ , which is done at a later stage during the derivation of the quasiclassical Usadel equation, it is a common approximation to take the random impurity potential to have a Gaussian distribution meaning that $\langle V(\mathbf{r})V(\mathbf{r}') \rangle_{\text{av}} = \delta(\mathbf{r} - \mathbf{r}')$ which in turn can be understood physically as the impurity density being so low that the potential at different points are not correlated.

The above procedure then demonstrates the so-called selfconsistent Born approximation and matches the expression for the self-energy in JP Morten's thesis:

$$\Sigma(\mathbf{r}, \mathbf{r}') = \langle V(\mathbf{r})G_{\text{av}}(\mathbf{r}, \mathbf{r}')V(\mathbf{r}') \rangle_{\text{av}}. \quad (28.84)$$

Relation to self-energy in Usadel equation

The self-energy in the derivation of the Usadel equation originally enters the Gor'kov equation as

$$[i\partial_{t_1}\rho_3 - H(1)]\langle G(1, 2) \rangle - \int d3 \Sigma(1, 3)\langle G(3, 2) \rangle = \delta(1 - 2). \quad (28.85)$$

This equation is equivalent to the Dyson equation

$$\langle G \rangle = G_0 + G_0 \Sigma \langle G \rangle. \quad (28.86)$$

where G_0 is the solution of the Gor'kov equation for $\Sigma = 0$. Now, we would like to find an approximate expression for Σ . In order to see how well our approximate expression for Σ is, we can compare it to the exact expression for $\langle G \rangle$ up to a certain order in the impurity potential.

First, start with the Dyson equation for the Green function G which solves the Gor'kov equation for a specific impurity configuration V :

$$G = G_0 + G_0 V G. \quad (28.87)$$

As before, products are really bullet products (convolution integrals). Now iterate this expression and take impurity average:

$$\langle G \rangle = G_0 + G_0 \langle V G_0 V G \rangle \quad (28.88)$$

due to $\langle V \rangle = 0$. So far, this is still exact. Now we make an approximation on the above equation by saying

$$\begin{aligned} \langle G \rangle &\simeq G_0 + G_0 \langle V \langle G \rangle V \rangle \langle G \rangle \\ &= G_0 + G_0 \Sigma \langle G \rangle \end{aligned} \quad (28.89)$$

where $\Sigma = \langle V \langle G \rangle V \rangle$. While we are free to make such an approximation, the question is now if this is a *good* approximation. We can check this by comparing with the exact expression for $\langle G \rangle$ to third order in V :

$$\begin{aligned} \langle G \rangle &= G_0 + G_0 \langle V G \rangle \\ &= G_0 + G_0 \langle V G_0 V \rangle G_0 + \mathcal{O}(V^4). \end{aligned} \quad (28.90)$$

As shown in the previous section, we get exactly the same result to $\mathcal{O}(V^2)$ if we iterate Eq. (28.89), but not to $\mathcal{O}(V^3)$ since the selfconsistent Born approximation in fact gives *no* terms to third order in the potential.

To capture third order terms in the potential, we have to go beyond the selfconsistent Born approximation. By using a selfenergy

$$\Sigma = \langle V \langle G \rangle V \rangle + \langle V \langle G \rangle V \langle G \rangle V \rangle \quad (28.91)$$

in Eq. (28.89) instead and then iterating Eq. (28.89), we indeed get an identical expression as the exact result for $\langle G \rangle$ up to and including $\mathcal{O}(V^3)$. This is consistent with Espedal PRB 2017.

In principle, one can also include additional terms in the self-energy Σ if one allows $\langle V \rangle \neq 0$. In that case, using

$$\Sigma = \langle V \rangle + \langle V \langle G \rangle V \rangle - \langle V \rangle \langle G \rangle \langle V \rangle \quad (28.92)$$

gives identical result to the exact expression up to, and including, $\mathcal{O}(V^2)$. The linear term simply renormalizes the chemical potential. Note that the lone $\langle V \rangle$ term should be understood to include a $\delta(1-2)$ since $\Sigma = \Sigma(1-2)$.

Momentum-space version of Dyson equation for translationally invariant system. We mention in passing that due to the impurity averaging, we expect that if no other translational-invariance breaking processes are present (such as a spatially varying superconducting order parameter), the impurity-averaged Green function $G_{\text{av}}(1,2)$ should also be translationally invariant just like $G_0(1,2) = G_0(1-2)$. Let us then assume that $G_{\text{av}}(1,2) = G_{\text{av}}(1-2)$ and $\Sigma(1,2) = \Sigma(1-2)$ (this is not assumed in the above real-space derivation). Starting with the exact Dyson equation

$$G_{\text{av}}(1-2) = G_0(1-2) + \int d3 \int d4 G_0(1-3) \Sigma(3-4) G_{\text{av}}(1-2), \quad (28.93)$$

and performing $\int d\mathbf{k} e^{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)}$ as well as inserting the inverse Fourier-transformations

$$G_0(1-3) = \int d\mathbf{q} e^{-i\mathbf{q}(\mathbf{r}_1-\mathbf{r}_3)} \quad (28.94)$$

and correspondingly for Σ and G , straight-forward resolution of the integrals provides

$$G_{\text{av}}(\mathbf{k}) = G_0(\mathbf{k}) + G_0(\mathbf{k}) \Sigma(\mathbf{k}) G_{\text{av}}(\mathbf{k}) \quad (28.95)$$

with the solution

$$G_{\text{av}} = \frac{1}{G_0^{-1}(\mathbf{k}) - \Sigma(\mathbf{k})}. \quad (28.96)$$

28.2.1 Random phase approximation

See section 13.1 in Bruus & Flensberg textbook for a detailed and intuitive description. The RPA essentially consists of keeping self-energy diagrams which are expected to be larger than other self-energy diagrams (more divergent). This is estimated on the basis of looking at how many internal interaction lines in the diagram (which diverge like $1/q^2$ per line for $q \rightarrow 0$ for the Coulomb interaction) that have the same internal momentum. The diagram with the most lines is estimated to be the most important. In contrast, diagrams with the same amount of internal lines but with different momenta (like $1/q^2 \times 1/(q-p)^2$) are neglected which amounts to saying that these terms can be viewed as interference-like terms with random phases that cancel out.

28.2.2 More details on self-energies and the Dyson equation

Impurity scattering in the Usadel equation is typically treated in the Born approximation, which means that the strength of the impurity potential (the phase-shift imposed on the electron wavefunction when it scatters on the impurity) is sufficiently weak, although the impurity concentration may still be high. This is in contrast to the opposite regime of the unitary limit where the scattering potential is strong, imposing a large phase-shift. In effect, the Born treatment assumes that the strength of the impurity potential is so weak that it imposes a phase-shift δ on the electron wavefunction upon scattering satisfying $\delta \ll 1$.

Dyson equation

We now sketch how impurity scattering may be accounted for in the Usadel equation technically. If one starts out with an impurity potential $V_{\text{imp}}(\mathbf{r})$ in the Hamiltonian according to:

$$H_{\text{imp}} = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}, t) V_{\text{imp}}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}), \quad (28.97)$$

the Eilenberger equation takes the form

$$[\varepsilon \hat{\rho}_3 + i v_F \nabla - V_{\text{imp}} \hat{1} - \hat{\Delta} \otimes \hat{g}] = 0 \quad (28.98)$$

where V_{imp} in the commutator is now evaluated at $\mathbf{R}$ (the center of mass coordinate), just like $\hat{g}$. See *e.g.* appendix D2 in [20]. The product $\otimes$ will in a time-independent situation and in the quasiclassical approximation (see pages 35-37 in [20]) be reduced to simple matrix multiplication.

However, instead of specifying the impurity potential (which may be quite complicated if it *e.g.* arises from several randomly distributed impurities) one can incorporate impurity scattering via a self-energy through a diagrammatic expansion. The idea is that the exact Green function G in the system can be written as the Green function G_0 *without* impurity scattering plus all types of interactions with impurities which start and end with G_0 . This idea can then also be generalized to include electron-electron interactions via for instance phonons or photons, and is schematically shown in Fig. 28.5 where the double line represents G , the single line G_0 , and the wavy line represents some interaction (for instance a phonon or photon).

Let us introduce the concept of a self-energy Σ which represents the interaction of G_0 with the surrounding many-particle system. The self-energy leads to a renormalization of the Green function into G , and G is determined by the so-called Dyson equation. Let us now explain this in more detail. Formally, we introduce Σ as shown in Fig. 28.6.

and the corresponding analytical expression is given by

$$G(\mathbf{r}, t; \mathbf{r}', t') = G_0(\mathbf{r}, t; \mathbf{r}', t') + \int d1 \int d2 G_0(\mathbf{r}, t; 1) \Sigma(1, 2) G_0(2; \mathbf{r}', t'). \quad (28.99)$$

We used the abbreviation $1 \equiv (\mathbf{r}_1, t_1)$ and $\int d1 \equiv d\mathbf{r}_1 \int dt_1$, so that one integrates over all possible positions and times at which the interactions can take place. This is similar as in particle physics Feynman diagrams where one integrates over all possible momenta of the virtual particles mediating interactions.

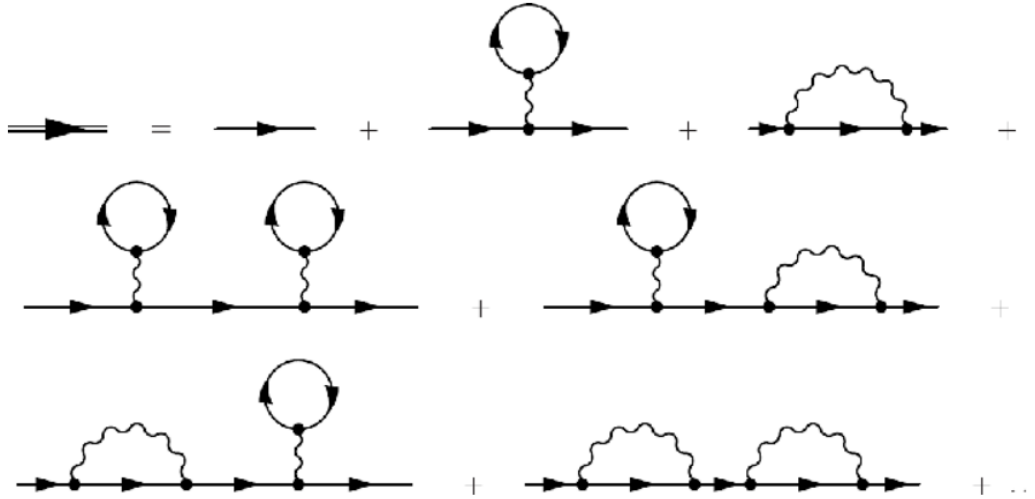
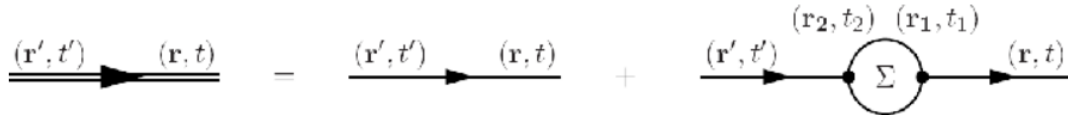


Figure 28.5: The Green's function expanded in terms of connected diagrams.

Figure 28.6: The Feynman diagrams showing how the renormalized Green function G is expressed via the bare Green function G_0 and the self-energy Σ .

Another important concept is the *proper self-energy* which is a piece of the self-energy diagrams that cannot be separated into two pieces by cutting a single-particle line. By definition, the total proper self-energy is the sum of all irreducible (also called proper) self-energy contributions and will be denoted Σ^* . First-order irreducible self energies are shown in Fig. 28.7 - note how they cannot be reduced to two pieces by cutting a single-particle line. They are referred to as the Hartree-Fock self-energies¹.

It follows from the above definitions that all self-energy diagrams can be put together by using irreducible self-energy diagrams and connecting these with G_0 . Therefore, the total self-energy including all contributions, reducible and irreducible, is given by:

$$\Sigma(\mathbf{r}, t; \mathbf{r}', t') = \Sigma^*(\mathbf{r}, t; \mathbf{r}', t') + \int d1 \int d2 \Sigma^*(\mathbf{r}, t; 1) G_0(1, 2) \Sigma^*(2, \mathbf{r}', t') + \dots \quad (28.100)$$

Inserting this expression for Σ into Eq. (28.99), the total renormalized Green function can be

¹The Hartree-Fock method is originally an approximate, iterative computational method for solving the time-independent Schrodinger equation of many-body electronic systems. A proper description of atomic systems is only possible by applying quantum mechanics rules and solving the Schrodinger equation, which explains the motion of atomic and subatomic particles. The Hartree Fock approximation breaks down a multi-electron wave function into a set of one-electron wave functions, called molecular orbitals, which then are obtained by an iterative method. We also call the Hartree Fock method the self-consistent field method because of its particular iterative way of solving the Schrodinger equation solution. The Hartree Fock method itself cannot account for strong electron-electron correlations since the core of its approximation is that it treats the Coulomb interaction between electrons in a mean-field way, so that each electron feels the average Coulomb field of all other electrons as an external field. Thus, the Hartree-Fock method is a self-consistent method. Performing a mean-field approximation on the Hubbard Hamiltonian interaction term in the particle channel (i.e. setting $\langle c_{\sigma}^{\dagger} c_{\sigma} \rangle = n_{\sigma}$) is therefore referred to as a mean-field decoupling in the Hartree or Hartree-Fock channel.

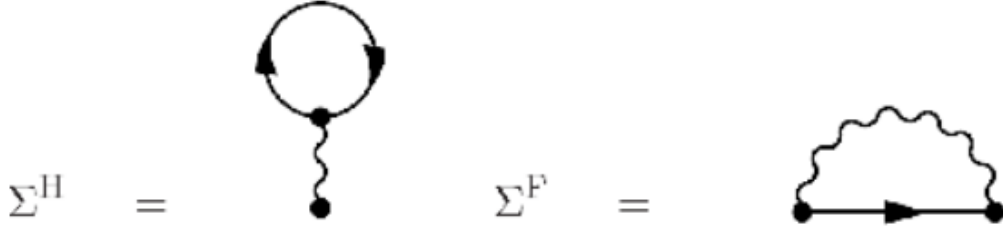


Figure 28.7: The Feynman diagrams of the first-order irreducible self-energies.

written as:

$$G(\mathbf{r}, t; \mathbf{r}', t') = G_0(\mathbf{r}, t; \mathbf{r}', t') + \int d1 \int d2 G_0(\mathbf{r}, t; 1) \Sigma^*(1, 2) G_0(2; \mathbf{r}', t') + \dots \quad (28.101)$$

By inspecting the higher order terms appearing in Eq. (28.101), one can verify that this equation in fact reads:

$$G(\mathbf{r}, t; \mathbf{r}', t') = G_0(\mathbf{r}, t; \mathbf{r}', t') + \int d1 \int d2 G_0(\mathbf{r}, t; 1) \Sigma^*(1, 2) G(2; \mathbf{r}', t'). \quad (28.102)$$

The diagrammatic representation of this equation is shown in Fig. 28.8.

The validity of Eq. (28.102) can be directly verified by iterating the right-hand side, which then

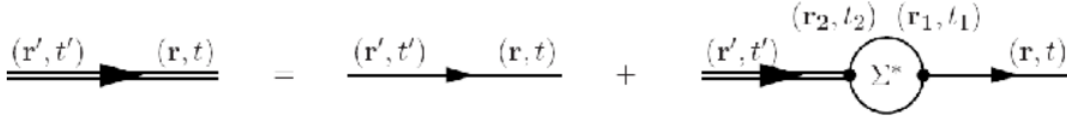


Figure 28.8: The Feynman diagrams representing Dyson's equation.

reproduces Eq. (28.101) term by term after renaming some auxiliary integration variables. In a similar manner, one can show that the Dyson equation can alternatively be written as:

$$G(\mathbf{r}, t; \mathbf{r}', t') = G_0(\mathbf{r}, t; \mathbf{r}', t') + \int d1 \int d2 G(\mathbf{r}, t; 1) \Sigma^*(1, 2) G_0(2; \mathbf{r}', t'). \quad (28.103)$$

Quasiclassical approximation for self-energy term

Let us now use the Dyson equation for the Green function in matrix form (Keldysh space, ...) reads. To do this, we make use of Eq. (28.102) as well as the equation for the bare Green function:

$$[i\partial_{t_1} \hat{\rho}_3 - \hat{\xi}(\mathbf{r}_1)] \check{G}_0(1; 2) = \delta(1 - 2) \hat{1}. \quad (28.104)$$

This equation is derived *e.g.* in JP Morten thesis. Let us define the operator:

$$\check{\check{G}}_0^{-1}(1) \equiv i\partial_{t_1} \hat{\rho}_3 - \hat{\xi}(\mathbf{r}_1) \quad (28.105)$$

We defined $\hat{\xi}_1 = (-\nabla_1/2m)\hat{1}$. We now operate on Eq. (28.102) with $\check{\check{G}}_0^{-1}$ from the left and move the integral over to the left side. After renaming some variables and noting that $\check{\check{G}}_0^{-1}$ only acts on the bare Green function G_0 inside the integral on the right hand side of Eq. (28.102), we obtain:

$$\check{\check{G}}_0^{-1}(1) \check{G}(1, 2) - \int dx_3 \check{\Sigma}(1, 3) \check{G}(3, 2) = \delta(1 - 2) \hat{1} \quad (28.106)$$

and $\check{\Sigma}(1, 2)$ contains the irreducible self-energies in the problem. The same result is found in *e.g.* Rammer & Smith RMP 1986 or Mahan eq. (3.331). Keep in mind that $x = (\mathbf{r}, t)$. This includes impurity scattering which can then be treated in the Born approximation, so that $\check{\Sigma}_{\text{imp}}(1, 2) = \langle V_{\text{imp}}(1) \check{G}(1, 2) V_{\text{imp}}(2) \rangle$ and the averaging is over the positions of the impurities. The fact that the self-energy takes this form can be seen by inspecting the diagram that gives rise to it, namely the interaction (vertex) between the impurity scattering potential and the Green function at point 1, propagation of the Green function up to point 2, and a new interaction between impurity potential and Green function and point 2 (see *e.g.* Fig. 21.3 in [47]).

The last step is to get the convolution integral $\int dx_3 \check{\Sigma}(1, 3) \check{G}(3, 2)$ onto the Fourier-transformed form which enters the Eilenberger and Usadel equations with the Fourier-transformed quantities $\check{\Sigma}(\mathbf{R}, \mathbf{p}, E)$ and $\check{G}(\mathbf{R}, \mathbf{p}, E)$ (assuming no explicit time-dependence). Using xxx, it follows by acting with $[\check{G}_0^{-1}(2)]$ from the right side that:

$$\check{G}(1, 2) [\check{G}_0^{-1}(2)] - \int dx_3 \check{G}(1, 3) \check{\Sigma}(3, 2) = \delta(1 - 2) \check{1}. \quad (28.107)$$

Subtracting Eq. (28.107) from (28.106), we see that the contribution from the self-energy is:

$$- \int dx_3 \check{\Sigma}(1, 3) \check{G}(3, 2) + \int dx_3 \check{G}(1, 3) \check{\Sigma}(3, 2). \quad (28.108)$$

We now want to Fourier-transform this, in which case we find

$$- \int dx_3 \int d(x_1 - x_2) e^{-ip(x_1 - x_2)} [\check{\Sigma}(1, 3) \check{G}(3, 2) - \check{G}(1, 3) \check{\Sigma}(3, 2)]. \quad (28.109)$$

One can prove (see *e.g.* equation D.1 in JP thesis) that this is equal to:

$$\begin{aligned} -(\check{\Sigma} \otimes \check{G})(X, p) + (\check{G} \otimes \check{\Sigma})(X, p) &= -e^{i(\partial_{X_\Sigma} \partial_{p_G} - \partial_{p_\Sigma} \partial_{X_G})/2} \check{\Sigma}(X, p) \check{G}(X, p) \\ &\quad + -e^{i(\partial_{X_G} \partial_{p_\Sigma} - \partial_{p_G} \partial_{X_\Sigma})/2} \check{G}(X, p) \check{\Sigma}(X, p). \end{aligned} \quad (28.110)$$

If there is no explicit time-dependence and we do a gradient approximation (meaning we only keep derivatives in space and momentum up to first order), this simplifies to:

$$\begin{aligned} -(\check{\Sigma} \otimes \check{G})(X, p) + (\check{G} \otimes \check{\Sigma})(X, p) &= -[\check{\Sigma}, \check{G}] - \frac{i}{2} (\nabla_{\mathbf{R}} \check{\Sigma} \nabla_{\mathbf{p}} \check{G} - \nabla_{\mathbf{p}} \check{\Sigma} \nabla_{\mathbf{R}} \check{G}) \\ &\quad + \frac{i}{2} (\nabla_{\mathbf{R}} \check{G} \nabla_{\mathbf{p}} \check{\Sigma} - \nabla_{\mathbf{p}} \check{G} \nabla_{\mathbf{R}} \check{\Sigma}). \end{aligned} \quad (28.111)$$

To lowest order, we keep only the first term $[\check{\Sigma}, \check{G}]$ which leaves us with only the commutator between the Fourier-transformed quantities $\check{\Sigma}(\mathbf{R}, \mathbf{p}, E)$ and $\check{G}(\mathbf{R}, \mathbf{p}, E)$ as originally announced.

28.2.3 Impurity scattering selfenergy

It is shown by a detailed calculation in JP Morten thesis that the self-energy for an ensemble-average of randomly located impurities in the self-consistent Born approximation takes the form

$$\check{\Sigma}_{\text{imp}}(\mathbf{R}, T, \mathbf{p}, E) = n_i \int \frac{d\mathbf{q}}{(2\pi)^3} |v(\mathbf{p} - \mathbf{q})|^2 \check{G}(\mathbf{R}, T, \mathbf{q}, E), \quad (28.112)$$

where n_i is the impurity density at position $\mathbf{r}_i$. Moreover, $v(\mathbf{q})$ is the Fourier-transformation of the real-space impurity potential $\mathcal{V}(\mathbf{r} - \mathbf{r}_i)$ where the total potential from N impurities at positions $\mathbf{r}_i$ can be written:

$$V(\mathbf{r}) = \sum_i \mathcal{V}(\mathbf{r} - \mathbf{r}_i) = \sum_i \sum_{\mathbf{q}} v(\mathbf{q}) e^{i\mathbf{q}(\mathbf{r} - \mathbf{r}_i)}. \quad (28.113)$$

In order for the above self-energy $\check{\Sigma}_{\text{imp}}(\mathbf{R}, T, \mathbf{p}, E)$ to have a weak momentum dependence, i.e. vary slowly and smoothly in momentum space, it is clear that $v(\mathbf{p} - \mathbf{q})$ should not depend strongly on the magnitude of the momentum. Physically, this is a reasonable situation in a metal where the potential from impurity charges are screened effectively so that the corresponding real-space potential is localized in space. A localized real-space potential corresponds to a slowly varying momentum-space potential, as described above. This can be seen from the very definition of the Fourier-transformation. We emphasize that in the derivation of the above self-energy, an averaging over many impurity configurations has been performed. If the impurity density is high, the total potential $\langle V(\mathbf{r}) \rangle$ can still be slowly varying in real space, in accordance with quasiclassical theory, even if the potential $\mathcal{V}(\mathbf{r} - \mathbf{r}_i)$ around each individual impurity is localized.

Since the potential $v(\mathbf{p} - \mathbf{q})$ depends weakly on the magnitude of the momentum, we can carry out the $\int d\mathbf{q}$ integration to obtain the quasiclassical Green function:

$$\check{\Sigma}_{\text{imp}}(\mathbf{R}, T, \mathbf{p}, E) \simeq \frac{\pi}{i} N_0 n_i \int \frac{d\Omega_{\mathbf{q}}}{(2\pi)^3} |v(\mathbf{p} - \mathbf{q}_F)|^2 \check{g}(\mathbf{R}, T, \mathbf{q}_F, E) \equiv \check{\sigma}(\mathbf{R}, T, \mathbf{p}, E). \quad (28.114)$$

We swapped notation from $\Sigma \rightarrow \sigma$ to indicate that the selfenergy is now a functional of the quasiclassical Green function g rather than the full Green function G . We also mention here how the selfenergy ends up looking in the Eilenberger equation. Recall first that the the gradient approximation produces a term of the type

$$[\check{\Sigma}(\mathbf{p}), \check{G}(\mathbf{p})]_- \quad (28.115)$$

in the equation of motion for the Green function $\check{G}(\mathbf{p})$. To obtain the quasiclassical Eilenberger equation from this, one integrates the equation over the kinetic energy $\int d\xi_{\mathbf{p}}$. Now, we just saw that due to the weak-momentum dependence of $v(\mathbf{p} - \mathbf{q})$, we have $\check{\Sigma}(\mathbf{p}) \simeq \check{\sigma}(\mathbf{p})$. Therefore, integrating the equation of motion via $\int d\xi_{\mathbf{p}}$ and using that:

$$\int d\xi_{\mathbf{p}} \check{\sigma}(\mathbf{p}) \check{G}(\mathbf{p}) = \int d\xi_{\mathbf{p}} \check{\sigma}(\mathbf{p}) \check{g}(\mathbf{p}_F) \delta(\xi_{\mathbf{p}}) = \check{\sigma}(\mathbf{p}_F) \check{g}(\mathbf{p}_F), \quad (28.116)$$

we see that we end up with the standard form of the Eilenberger equation, except that above Σ is used instead of σ . We can also write $\check{\sigma}$ in the customary manner:

$$\check{\sigma}(\mathbf{p}_F) = -i\pi n_i N_0 \int d\Omega_{\mathbf{q}} |v(\mathbf{p}_F - \mathbf{q}_F)|^2 \check{g}(\mathbf{R}, T, \mathbf{q}_F, E) \simeq -\frac{i}{2\tau} \check{g}_s \quad (28.117)$$

with $\check{g}_s$ being the isotropic (in momentum space) part of $\check{g}(\mathbf{q}_F)$. In effect, we set $\check{g}(\mathbf{R}, T, \mathbf{q}_F, E) = \check{g}_s$ above. This comes about since we assume that the impurity scattering is so frequent that the Green function is dominantly isotropic. Moreover, the impurity scattering time τ is defined via:

$$\frac{1}{\tau} \equiv 2\pi n_i N_0 \int d\Omega_{\mathbf{q}} |v(\mathbf{p}_F - \mathbf{q}_F)|^2. \quad (28.118)$$

In practice, since we have assumed that v is slowly varying in momentum space, the angular integration should essentially give a factor 4π whereas $|v(\mathbf{p}_F - \mathbf{q}_F)|^2 \simeq |v(0)|^2$ can be pulled outside.

If we include the next-order terms in the gradient approximation, we would have obtained terms like

$$\Sigma(\mathbf{p}, \mathbf{R}) + \frac{i}{2} \nabla_{\mathbf{R}} \Sigma(\mathbf{p}, \mathbf{R}) \nabla_{\mathbf{p}} G^R(\mathbf{p}, \mathbf{R}) - \frac{i}{2} \nabla_{\mathbf{p}} \Sigma(\mathbf{p}, \mathbf{R}) \nabla_{\mathbf{R}} G(\mathbf{p}, \mathbf{R}). \quad (28.119)$$

The two last type of terms should then be discardable compared to the first as long as the self-energy is slowly varying in $\mathbf{p}$ (corresponding to localized impurities, as discussed above) and so long as $G(\mathbf{R})$ has a slow spatial variation (which has to come from a varying potential V). Under these assumptions, the smallness of $\nabla_{\mathbf{R}} \Sigma$ and $\nabla_{\mathbf{R}} G^R$ justify keeping only the first order term. Note that if $\nabla_{\mathbf{R}} G^R$ is small, then $\nabla_{\mathbf{R}} \Sigma$ must also be small since its spatial dependence comes from precisely G^R . However, these terms need to be kept if one wants to compute spin Hall phenomena.

28.2.4 Relation to impurity scattering in lattice model

In a lattice model, impurities are added as on-site potentials and then one averages any quantity of interest (such as Green function, order parameter or current) over several impurity configurations. How is this related to the treatment of impurities shown above? To lowest order in the self-energy (first order Born approximation), the self-energy due to impurity scattering takes the form

$$\Sigma_{\mathbf{k}}(i\omega_n) = -i \operatorname{sgn}(\omega_n) \frac{1}{2\tau_{\mathbf{k}}} \quad (28.120)$$

where ω_n is a fermionic Matsubara frequency (see treatment in Bruus & Flensberg textbook), and the Matsubara Green function is obtained as

$$G_{\mathbf{k}}(i\omega_n) = \frac{1}{i\omega_n - \xi_{\mathbf{k}} + i \frac{\operatorname{sgn}(\omega_n)}{2\tau_{\mathbf{k}}}} \quad (28.121)$$

where the retarded/advanced Green function is obtained by $i\omega_n \rightarrow \omega$ and $\operatorname{sgn}(\omega_n) = \pm 1$. Due to the imaginary self-energy, this causes a broadening of the spectral weight.

At first glance, this looks somewhat different than the on-site potentials in the lattice model. Can one expect this to give rise to a broadening of a spectral weight? The answer is that the two methods (lattice and analytical) are based on the same fundamental assumptions, so the answer is yes. In both cases, the impurities are added as a spatially varying potential: in the analytical case, the starting point is

$$\sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) V(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \quad (28.122)$$

and then writes this as a self-energy and averages the Green function over several configurations $V(\mathbf{r})$ after truncating the Dyson equation at some order, assuming a weak impurity potential, and assuming that the impurity averaging restores translational invariance. But this is the same treatment as in the lattice model, except that we compute the exact Green function for each impurity configuration $V(\mathbf{r})$. Therefore, the fundamental treatment of the impurity potential is the same in the lattice and analytical case apart from some simplifying assumptions in the analytical case.

28.2.5 Spin-orbit impurity scattering selfenergy

The impurity potential also gives rise to extrinsic spin-orbit coupling for the itinerant electrons passing by. The corresponding potential takes the form

$$\begin{aligned} V_{\text{so}}(\mathbf{r}) &= \sum_i \mathcal{V}_{\text{so}}(\mathbf{r} - \mathbf{r}_i) \\ &= \gamma \sum_i \boldsymbol{\sigma} \times \nabla V(\mathbf{r} - \mathbf{r}_i) \cdot \hat{\mathbf{p}}. \end{aligned} \quad (28.123)$$

Here, $\hat{\mathbf{p}} = \hbar \nabla / i$ is the momentum operator and $\gamma > 0$ is the strength of the spin-orbit scattering. Note how it is the same potential $V(\mathbf{r} - \mathbf{r}_i)$ that enters the spin-orbit impurity scattering potential as the impurity scattering potential. The above potential can be generalized to spin-Nambu space (4×4) in the following manner:

$$V_{\text{so}}(\mathbf{r}) = \gamma \sum_i [\rho_3 \boldsymbol{\alpha} \times \nabla V(\mathbf{r} - \mathbf{r}_i)] \cdot \hat{\mathbf{p}} \quad (28.124)$$

where $\boldsymbol{\alpha} = \text{diag}(\boldsymbol{\sigma}, \boldsymbol{\sigma}^*)$.

The spin-orbit impurity selfenergy, $\check{\Sigma}_{\text{so}}(1, 2) = \langle V_{\text{so}}(1) \check{G}(1, 2) V_{\text{so}}(2) \rangle$ entering the Usadel equation is computed in the same way as for impurity scattering, $\check{\Sigma}_{\text{imp}}(1, 2) = \langle V_{\text{imp}}(1) \check{G}(1, 2) V_{\text{imp}}(2) \rangle$. In both cases, one averages over impurity positions. Note that the momentum operator $\hat{\mathbf{p}}$ in Eq. (28.123) acts on the Green function $\check{G}(1, 2)$ and so produces a factor $\mathbf{p}$ after expressing $\check{G}(1, 2)$ in the Wigner-representation (as an integral over $\check{G}(\mathbf{p}, E, \mathbf{R}, T)$). In the end, one should end up with an expression along the lines of

$$\check{\sigma}_{\text{so}} = -\frac{i\gamma^2}{2} \left\langle \frac{1}{\tau(\mathbf{p} - \mathbf{q})} \rho_3 \boldsymbol{\alpha} \cdot (\mathbf{p} \times \mathbf{q}) \check{g}(\mathbf{R}, \mathbf{q}, E, T) \rho_3 \boldsymbol{\alpha} \cdot (\mathbf{p} \times \mathbf{q}) \right\rangle_F \quad (28.125)$$

where $\langle \dots \rangle_F$ denotes an angular average with respect to $\mathbf{q}$ at the Fermi surface. The same result obtained in a slightly different manner can be found in Espedal *et al.*, PRB 2016.

Finally, it is instructive to consider the momentum-space representation of the impurity potential and the spin-orbit impurity potential. Since the first-quantized potential in the Hamiltonian has the form

$$V_{\text{tot}}(\mathbf{r}) = V_{\text{imp}}(\mathbf{r}) + \gamma \boldsymbol{\sigma} \cdot (\nabla V_{\text{imp}}(\mathbf{r}) \times \hat{\mathbf{p}}) \quad (28.126)$$

the second-quantized Hamiltonian in momentum-space reads

$$H = \frac{1}{V} \sum_{s, s', \mathbf{k}, \mathbf{k}'} \psi_{\mathbf{k}, s}^\dagger U_{\mathbf{k}, \mathbf{k}', s, s'} \psi_{\mathbf{k}', s'} \quad (28.127)$$

where according to the general prescription we have that

$$U_{\mathbf{k}, \mathbf{k}'} = \langle \mathbf{k} | V_{\text{tot}}(\mathbf{r}) | \mathbf{k}' \rangle. \quad (28.128)$$

Note that $U_{\mathbf{k}, \mathbf{k}'}$ as written above is a matrix in spin space. To evaluate $U_{\mathbf{k}, \mathbf{k}'}$, we make use of position eigenfunctions $|\mathbf{r}\rangle$ and their completeness relation $\int d\mathbf{r} |\mathbf{r}\rangle \langle \mathbf{r}| = 1$. This allows us to write

$$U_{\mathbf{k}, \mathbf{k}'} = \int d\mathbf{r} \phi_{\mathbf{k}}(\mathbf{r})^* V_{\text{tot}}(\mathbf{r}) \phi_{\mathbf{k}'}(\mathbf{r}) \quad (28.129)$$

where $\phi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k} \rangle = e^{i\mathbf{k} \cdot \mathbf{r}}$ is a plane-wave basis. Alternatively, one could also multiply the plane-wave with function $u(\mathbf{r})$ which has the same periodicity as the crystal lattice, turning $\phi_{\mathbf{k}}(\mathbf{r})$ into a Bloch function. Sticking with the pure plane-wave basis, we see now that the potential matrix in momentum space is

$$\begin{aligned}
 U_{\mathbf{k},\mathbf{k}'} &= \int d\mathbf{r} e^{-i\mathbf{k}\mathbf{r}} \left(V_{\text{imp}} + \gamma \boldsymbol{\sigma} \cdot \nabla V_{\text{imp}} \times \frac{\nabla}{i} \right) e^{i\mathbf{k}'\mathbf{r}} \\
 &= \int d\mathbf{r} e^{-i\mathbf{k}\mathbf{r}} \left[\sum_{j\mathbf{q}} v(\mathbf{q}) e^{i(\mathbf{r}-\mathbf{r}_j)} - \gamma \sum_{j\mathbf{q}} v(\mathbf{q}) e^{i(\mathbf{r}-\mathbf{r}_j)\mathbf{q}} \boldsymbol{\sigma} \cdot \mathbf{q} \times \mathbf{k}' \right] e^{i\mathbf{k}'\mathbf{r}} \\
 &= \sum_{j\mathbf{q}} \int d\mathbf{r} e^{i\mathbf{r}(\mathbf{q}-\mathbf{k}+\mathbf{k}')} v(\mathbf{q}) e^{-i\mathbf{r}_j\mathbf{q}} - \sum_{j\mathbf{q}} \int d\mathbf{r} e^{i\mathbf{r}(\mathbf{q}-\mathbf{k}+\mathbf{k}')} \gamma v(\mathbf{q}) e^{-i\mathbf{r}_j\mathbf{q}} \boldsymbol{\sigma} \cdot \mathbf{q} \times \mathbf{k}' \\
 &= \sum_j v(\mathbf{k} - \mathbf{k}') e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}_j} - \sum_j \gamma v(\mathbf{k} - \mathbf{k}') e^{-i\mathbf{r}_j(\mathbf{k}-\mathbf{k}')} \boldsymbol{\sigma} \cdot (\mathbf{k} - \mathbf{k}') \times \mathbf{k}' \\
 &= V_{\mathbf{k},\mathbf{k}',\text{imp}} - \gamma V_{\mathbf{k},\mathbf{k}',\text{imp}} \boldsymbol{\sigma} \cdot (\mathbf{k} \times \mathbf{k}').
 \end{aligned} \tag{28.130}$$

Here, we used that $\int d\mathbf{r} e^{i\mathbf{r}(\mathbf{k}_2-\mathbf{k}_1)} = \delta(\mathbf{k}_2 - \mathbf{k}_1)$ and defined

$$V_{\mathbf{k},\mathbf{k}',\text{imp}} \equiv \sum_j v(\mathbf{k} - \mathbf{k}') e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}_j}. \tag{28.131}$$

28.2.6 Impurity scattering in antiferromagnets

To see why non-magnetic impurities in antiferromagnets enter the Usadel equation with an additional spin-flip term which looks like magnetic impurities, consider first a normal metal with magnetic impurities that point in the z -direction. The potential in the Hamilton-operator then has the form $V_0 + \sigma V_m$ to begin with. The total (magnetic + non-magnetic) impurity scattering selfenergy obtained using the selfconsistent Born approximation then acquires the form (consider only the electron-sector for simplicity instead of the full Nambu space):

$$\begin{pmatrix} V_0 + V_m & 0 \\ 0 & V_0 - V_m \end{pmatrix} g \begin{pmatrix} V_0 + V_m & 0 \\ 0 & V_0 - V_m \end{pmatrix} \tag{28.132}$$

The terms $\propto V_0^2$ give the usual non-magnetic impurity scattering self-energy, whereas the V_m^2 terms give the spin-flip self-energy $V_m^2 \sigma_z g \sigma_z$. The cross-terms $\propto V_0 V_m$ vanish upon averaging over impurity positions, since the magnetic and non-magnetic impurities are independent of each other.

Consider now the AFM case. We start with an impurity potential from the A and B sublattices. Consider again only the electron-sector, which now will be a 4×4 matrix since we have spin and sublattice degrees of freedom. In the selfconsistent Born approximation, we obtain

$$\begin{pmatrix} V_{A,\uparrow} & 0 & 0 & 0 \\ 0 & V_{A,\downarrow} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} g \begin{pmatrix} V_{A,\uparrow} & 0 & 0 & 0 \\ 0 & V_{A,\downarrow} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ V_{B,\uparrow} & 0 & 0 & 0 \\ 0 & V_{B,\downarrow} & 0 & 0 \end{pmatrix} g \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ V_{B,\uparrow} & 0 & 0 & 0 \\ 0 & V_{B,\downarrow} & 0 & 0 \end{pmatrix} \tag{28.133}$$

where $V_{A,B,\uparrow,\downarrow}$ is the impurity potential acting on spin $\uparrow, \downarrow$ on sublattice A, B . These all have the same value V since we have non-magnetic impurities. Now, we want to find a theory for the conduction band. This means that we have to project the Green function in spin and sublattice

space onto the conduction band by a unitary transformation S (which diagonalizes the Hamiltonian in spin-sublattice space). In essence, this means that we transform $\Sigma \rightarrow S\Sigma S^\dagger$, which leads to prefactors in front of the potentials $V_{A,B,\uparrow,\downarrow} = V$ correspond to their weight in the conduction band for each spin. The self-energy for the conduction band Green function (which is now 2×2 since we only have spin degrees of freedom):

$$\begin{pmatrix} V_{\uparrow}^{\text{big}} & 0 \\ 0 & V_{\downarrow}^{\text{small}} \end{pmatrix} g_c \begin{pmatrix} V_{\uparrow}^{\text{big}} & 0 \\ 0 & V_{\downarrow}^{\text{small}} \end{pmatrix} + \begin{pmatrix} V_{\uparrow}^{\text{small}} & 0 \\ 0 & V_{\downarrow}^{\text{big}} \end{pmatrix} g_c \begin{pmatrix} V_{\uparrow}^{\text{small}} & 0 \\ 0 & V_{\downarrow}^{\text{big}} \end{pmatrix} \quad (28.134)$$

The first term is the contribution from the A sublattice, which has a large weight in the spin- $\uparrow$ conduction band and small weight in the spin- $\downarrow$ conduction band. Opposite for the second term, which is the contribution from the B sublattice. To see the physics more easily, it is useful to parametrize the small and big potentials as

$$V_{\uparrow,\downarrow}^{\text{big}} = V_0 + V_m, \quad V_{\uparrow,\downarrow}^{\text{small}} = V_0 - V_m. \quad (28.135)$$

The V_m term becomes bigger the larger J is. For $J = 0$, $V_m = 0$. With this parametrization, we get

$$\begin{pmatrix} V_0 + V_m & 0 \\ 0 & V_0 - V_m \end{pmatrix} g_c \begin{pmatrix} V_0 + V_m & 0 \\ 0 & V_0 - V_m \end{pmatrix} + \begin{pmatrix} V_0 - V_m & 0 \\ 0 & V_0 + V_m \end{pmatrix} g_c \begin{pmatrix} V_0 - V_m & 0 \\ 0 & V_0 + V_m \end{pmatrix} \quad (28.136)$$

The first term looks exactly like the normal-metal term with a magnetic impurity potential. So does the second term, except that $V_m \rightarrow -V_m$. Therefore, the crossterms $V_0 V_m$ cancel each other (due to the opposite signs, and not due to the impurities being independent). The V_0^2 term gives the usual impurity term whereas the V_m^2 term gives an effective magnetic impurity term $V_m^2 \sigma_z g_c \sigma_z$.

28.3 Gradient approximation and derivation of Eilenberger equation

As shown in the thesis by JP Morten, one obtains an equation of motion (setting $\mathbf{A} = 0$ for simplicity) after performing the Wigner-transformation:

$$[E\hat{\rho}_3 + i\frac{\nabla \mathbf{R}}{m}\hat{1} - e\phi\hat{1} - \hat{\Delta} + \check{\Sigma}_{\text{imp}}(\mathbf{p}, E) \overset{\otimes}{\check{G}}]_- = 0 \quad (28.137)$$

where $\Sigma_{\text{imp}}(\mathbf{p}, E)$ is the impurity selfenergy that is discussed in more detail below. Now, the starproduct above is defined as an expansion in powers of derivatives. In the *gradient approximation* one neglects short-range oscillations in space by assuming that all quantities vary slowly (in comparison to the Fermi wavelength). In this way, we can write

$$A \otimes B \simeq A \circ B + \frac{i}{2}(\nabla_{\mathbf{R}} A \nabla_{\mathbf{p}} B - \nabla_{\mathbf{p}} A \nabla_{\mathbf{R}} B) \quad (28.138)$$

by keeping only derivatives up to first order in space. However, we have kept all orders of derivatives with respect to time in the $\circ$ product. If the system is translationally invariant in time, the $\circ$ product reduces to ordinary matrix multiplication.

We can now proceed in two ways. First, we could use Eq. (28.138) and keep first order terms, which would give us anticommutators of the form $\{\nabla_{\mathbf{R}}\check{\Sigma}, \nabla_{\mathbf{p}}\check{G}\}$ and $\{\nabla_{\mathbf{p}}\check{\Sigma}, \nabla_{\mathbf{R}}\check{G}\}$ in the equation of motion. Here, we defined the notation

$$\check{\Sigma}(\mathbf{p}, E) \equiv E\hat{\rho}_3 + i\mathbf{p} \cdot \frac{\nabla_{\mathbf{R}}}{m}\hat{1} - e\phi\hat{1} - \hat{\Delta} + \check{\Sigma}_{\text{imp}}(\mathbf{p}, E). \quad (28.139)$$

If this is done, it is not clear how one should obtain the Eilenberger equation by integrating over the magnitude of the momentum. This is also mentioned in the appendix of Ref. [48]. The solution to this problem is to integrate the equation of motion (after performing the gradient approximation and keeping up to first order terms) over $\mathbf{p}$, in effect both magnitude and direction, and in this way go straight to the Usadel equation without going via the Eilenberger equation. This is possible since $\int d\mathbf{p}$ includes both integration over magnitude of momentum, necessary to obtain the quasiclassical Green function, and the directional dependence of $\mathbf{p}$, giving the angular averaging necessary to get the Usadel equation. This is the strategy used in Ref. [48].

It is also worth noting that *if* there is no impurity scattering in the problem, performing the gradient approximation to first order only gives an extra term $\{E\nabla_{\mathbf{R}}\hat{\Delta}, \nabla_{\mathbf{p}}\check{G}\}$ since there is no part of the total selfenergy that is dependent on momentum. If we now integrate over $\mathbf{p}$ and perform a partial integration, a boundary term of the type

$$(\nabla_{\mathbf{R}}\hat{\Delta})\check{G}\Big|_{|\mathbf{p}| \rightarrow p_c} \quad (28.140)$$

appears, but this is negligible since $\check{G}$ should vanish at $|\mathbf{p}| \rightarrow p_c$ (it falls off as $1/\xi_{\mathbf{p}}$ where p_c is the cutoff in momentum corresponding to the cutoff $\xi_{\mathbf{p}} = \omega_c$). Therefore, the extra term in the equation of motion coming from the first order terms in the gradient approximation does not give any contribution. However, in that case we cannot argue that the Green function should be essentially isotropic either since there is no impurity averaging, so this does not help us much.

Instead, the second approach is to simply keep the lowest order term in the gradient approximation and set $A \otimes B \simeq A \circ B = A \cdot B$. In this case, no gradients $\nabla_{\mathbf{p}}$ appear in the equation of motion and we can integrate over $\xi_{\mathbf{p}}$ to obtain the Eilenberger equation without any problem.

To account for spin-charge coupling, giving rise to spin Hall effects in the presence of extrinsic spin-orbit impurity scattering, one thus has to skip the Eilenberger equation and go straight to the Usadel equation by performing $\int d\mathbf{p}$ (and also the same equation multiplied by $\mathbf{p}$ before performing $\int d\mathbf{p}$). This is necessary for the reason described above, namely that terms of the type $\{\nabla_{\mathbf{R}}\check{\Sigma}, \nabla_{\mathbf{p}}\check{G}\}$ and $\{\nabla_{\mathbf{p}}\check{\Sigma}, \nabla_{\mathbf{R}}\check{G}\}$ in the equation of motion does not allow one to obtain any Eilenberger-type of equation.

It is also worth to note that one may rewrite

$$\{\nabla_{\mathbf{R}}\check{\Sigma}, \nabla_{\mathbf{p}}\check{G}\} + \{\nabla_{\mathbf{p}}\check{\Sigma}, \nabla_{\mathbf{R}}\check{G}\} \quad (28.141)$$

after integrating over $\int d^3p$ and doing a partial integration (discarding a surface term, which may be justified in the same way as for Eq. 28.47) to

$$\int d^3p \nabla_{\mathbf{R}} \{\nabla_{\mathbf{p}}\check{\Sigma}, \check{G}\}. \quad (28.142)$$

28.4 Derivation of electric current and electromagnetic response of superconducting proximity systems

Before starting, there is actually a very elegant way of deriving the expression for the current in the diffusive limit of transport. Instead of starting with the QM expression for current, start with the QM expression for charge density ρ (see Espedal PRB 2017 appendix) which involves the time-derivative of the Keldysh Green function. By virtue of the continuity equation for charge, the time derivative of ρ has to equal the divergence of the current. By computing the time-derivative of G , and expressing in Wigner-coordinates (energy rather than time), one identifies that $d\rho/dt \propto \int dE \text{Tr}\{\epsilon\rho_3, g\}^K$ for a time-independent system (can still be non-equilibrium). This equation is identically zero, but that does mean the current is zero: it means that $\nabla \cdot \mathbf{j} = 0$. Thus, since the term $[\epsilon\rho_3, g]$ enters the Usadel equation, we can substitute that term by minus the rest of the terms in Usadel. Then, we can pull out a gradient ∇ and in this way identify the expression for $\mathbf{j}$. This method is particularly convenient when the Usadel equation contains higher order terms in the gradient expansion coming from *e.g.* spin-orbit impurity scattering.

Let us start with the general quantum mechanical expression for electric current, including a vector potential $\mathbf{A}$. Here, $(1) = (\mathbf{r}_1, t_1)$ as usual.

$$\begin{aligned} \mathbf{j}(1) &= \frac{-\hbar|e|}{2mi} \left\langle \sum_{\sigma} \left[\psi_{\sigma}^{\dagger}(1)(\nabla_1 + i|e|\mathbf{A}(1))\psi_{\sigma}(1) - [(\nabla_1 - i|e|\mathbf{A}(1))\psi_{\sigma}^{\dagger}(1)]\psi_{\sigma}(1) \right] \right\rangle \\ &= \frac{-\hbar|e|}{2mi} \sum_{\sigma} \lim_{1 \rightarrow 2} \left[(\nabla_1 + i|e|\mathbf{A}(1)) - (\nabla_2 - i|e|\mathbf{A}(2)) \right] \langle \psi_{\sigma}^{\dagger}(2)\psi_{\sigma}(1) \rangle. \end{aligned} \quad (28.143)$$

The origin of Eq. (28.143) is that one considers the Heisenberg equations of motion for the field operators $\psi(\mathbf{r}, t)$ and $\psi^{\dagger}(\mathbf{r}, t)$ (see *e.g.* equations 3.27 and 3.32 in JP thesis) and then uses these to derive a continuity equation for the density operator $n = \psi^{\dagger}\psi$. One then finds the above expression. Note that equation 3.56 in JP thesis is not strictly correct.

We know that $G_{\sigma\sigma'}^K(1, 2) = -i\langle \psi_{\sigma}(1)\psi_{\sigma'}^{\dagger}(2) - \psi_{\sigma'}^{\dagger}(2)\psi_{\sigma}(1) \rangle$. Using the anticommutation rule for fermion field operators in this definition, we obtain that:

$$\langle \psi_{\sigma}^{\dagger}(2)\psi_{\sigma}(1) \rangle = \frac{G_{\sigma\sigma'}^K(1, 2)}{2i} + \frac{\langle \delta(1-2) \rangle}{2}. \quad (28.144)$$

Now, insert this into the above equation for $\mathbf{j}$ and obtain:

$$\mathbf{j} = -\frac{\hbar|e|}{2mi} \sum_{\sigma} \lim_{1 \rightarrow 2} [(\nabla_1 + i|e|\mathbf{A}(1)) - (\nabla_2 - i|e|\mathbf{A}(2))] \left(\frac{G_{\sigma\sigma'}^K(1, 2)}{2i} + \frac{\langle \delta(1-2) \rangle}{2} \right). \quad (28.145)$$

This can be rewritten as:

$$\begin{aligned} \mathbf{j} &= \frac{\hbar|e|}{4m} \text{Tr} \left\{ \lim_{1 \rightarrow 2} [(\nabla_1 + i|e|\mathbf{A}(1)) - (\nabla_2 - i|e|\mathbf{A}(2))] \underline{G}^K(1, 2) \right\} \\ &+ \frac{i\hbar|e|}{4m} \sum_{\sigma} \left\{ \lim_{1 \rightarrow 2} [(\nabla_1 + i|e|\mathbf{A}(1)) - (\nabla_2 - i|e|\mathbf{A}(2))] \langle \delta(1-2) \rangle \right\}. \end{aligned} \quad (28.146)$$

Here, $\underline{G}^K$ is the 2×2 Keldysh Green function matrix. The first term in the above equation is exactly the one in Morten's thesis, eq. 3.59 (note that his $e = -|e|$). Now, what about the second

term. Why does it vanish? Consider first the terms with the derivative operators. We know that $\delta(1-2) = \delta(2-1)$ is a fundamental property of the Dirac delta function. Thus, one may write $\nabla_2\delta(1-2) = \nabla_2\delta(2-1)$. If I now rename 2 to 1, we see that the derivative terms in the second term cancel each other. We are thus left with the following part of the 2nd term:

$$\frac{-\hbar|e|^2}{4m} \sum_{\sigma} \lim_{1 \rightarrow 2} (\mathbf{A}_1 + \mathbf{A}_2) \langle \delta(1-2) \rangle. \quad (28.147)$$

In the absence of any gauge potential (external field), this term is zero since $\mathbf{A} = 0$. Then, our derivation is already complete. If $\mathbf{A} \neq 0$, how can we see that it vanishes? It is, contrary to what it looks like at first glance, gauge-independent. If you transform $\mathbf{A} \rightarrow \mathbf{A}'$ and $\psi \rightarrow \psi'$ in the original expression, the δ -function also gets transformed because it comes from the anticommutation of two fermion fields. So there has to be another reason for why it vanishes.

The reason is in fact quite subtle: it comes down to the fact that we cannot let $1 \rightarrow 2$ in such a way that they become exactly equal. If we go back to Eq. (28.143), we see that what allows us to extract the operators outside of the expectation value is that we are assigning the arguments of the ψ 's to be different, namely 1 and 2. If we let 1 become exactly equal to 2 in the second line of that expression, it vanishes. Thus, we must take the limit $1 \rightarrow 2$ (with the times being equal, $t_1 = t_2$, in order to use the anticommutation relation of the field operators) but without letting 1 becoming identically equal to 2. Now, if 1 is never identically equal to 2, it is clear that the δ -function contribution vanishes, and hence we have solved the problem with the last term.

Some additional comments are that we must let the times in 1 and 2 be equal in order to be able to use the anticommutation relation, i.e. above we have $1 = (\mathbf{r}_1, t_1)$ and $2 = (\mathbf{r}_2, t_1)$. Moreover, the last term Eq. (28.147) does not show up for any of the spin current components. For instance, for the z -component of the spin current one would have to replace $\sum_{\sigma} \dots \rightarrow \sum_{\sigma} \sigma \times \dots$, which would cancel Eq. (28.147) since it is independent on σ . For the x and y components of the spin current, the δ -function never shows up in the first place, because the anticommutation between field operators $\psi_{\uparrow}$ and $\psi_{\downarrow}$ gives zero.

Generalization to Nambu space, matrix-current, and $\mathbf{A}$ -contribution

Above, we have strictly speaking only derived the electronic current (that is, the contribution from electrons). Since we can also have hole excitations, which must included in the description of a superconducting systems due to the mixed nature of quasiparticles there and the necessity to work in $\text{spin} \otimes \text{Nambu}$ space, it is of relevance to compute the *total electric current* including the contribution from holes.

In order to accomplish this, we start from a generalized charge operator

$$\hat{Q} = -|e| \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (28.148)$$

so that the charge density ρ becomes:

$$\rho = \langle \Psi^{\dagger} \hat{Q} \Psi \rangle = -|e| \sum_{\sigma} [\langle \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) - \psi_{\sigma}(\mathbf{r}) \psi_{\sigma}^{\dagger}(\mathbf{r}) \rangle]. \quad (28.149)$$

We want to derive a continuity equation of the type

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (28.150)$$

and in this manner identify an expression for the total electric current $\mathbf{j}$. This gives

$$\frac{\partial \rho}{\partial t} = -|e| \sum_{\sigma} \langle \partial_t \psi_{\sigma}^{\dagger} \psi_{\sigma} + \psi_{\sigma}^{\dagger} \partial_t \psi_{\sigma} - \partial_t \psi_{\sigma} \psi_{\sigma}^{\dagger} - \psi_{\sigma} \partial_t \psi_{\sigma}^{\dagger} \rangle \quad (28.151)$$

which when inserting the Heisenberg equations

$$\begin{aligned} i\partial_t \psi_{\sigma} &= -\frac{1}{2m} (\nabla + i|e|\mathbf{A})^2 \psi_{\sigma}, \\ i\partial_t \psi_{\sigma}^{\dagger} &= \frac{1}{2m} (\nabla - i|e|\mathbf{A})^2 \psi_{\sigma}^{\dagger}, \end{aligned} \quad (28.152)$$

yields the expression

$$\partial_t \rho = \frac{ie}{2m} \nabla \cdot \sum_{\sigma} \langle (\nabla - i|e|\mathbf{A}) \psi_{\sigma}^{\dagger} \psi_{\sigma} - \psi_{\sigma}^{\dagger} (\nabla + i|e|\mathbf{A}) \psi_{\sigma} + \{i \rightarrow (-i) \text{ \& } \psi_{\sigma} \leftrightarrow \psi_{\sigma}^{\dagger}\} \rangle \quad (28.153)$$

since the $\mathbf{A}^2$ terms cancel each other. Therefore, we may identify the total current

$$\mathbf{j} = \frac{-i|e|}{2m} \sum_{\sigma} \langle (\nabla - i|e|\mathbf{A}) \psi_{\sigma}^{\dagger} \psi_{\sigma} - \psi_{\sigma}^{\dagger} (\nabla + i|e|\mathbf{A}) \psi_{\sigma} + (\nabla + i|e|\mathbf{A}) \psi_{\sigma} \psi_{\sigma}^{\dagger} - \psi_{\sigma} (\nabla + i|e|\mathbf{A}) \psi_{\sigma}^{\dagger} \rangle. \quad (28.154)$$

Proceeding now in exactly the same manner as in the original treatment of the electronic current above (introducing the limit $\lim_{1 \rightarrow 2}$), we obtain

$$\begin{aligned} \mathbf{j} &= \lim_{1 \rightarrow 2} \frac{i|e|}{2m} \sum_{\sigma} \left[\left(\nabla_1 - \nabla_2 + i|e|[\mathbf{A}(1) + \mathbf{A}(2)] \right) \left[-\frac{i}{2} G_{\sigma\sigma}^K(1, 2) \right] \right. \\ &\quad \left. + \left(\nabla_1 - \nabla_2 - i|e|[\mathbf{A}(1) + \mathbf{A}(2)] \right) \left[\frac{i}{2} G_{\sigma\sigma}^K(1, 2) \right]^* \right] \end{aligned} \quad (28.155)$$

which can be rewritten by noting that

$$\hat{G}^K(1, 2) = \begin{pmatrix} \underline{G}^K(1, 2) & 0 \\ 0 & -[\underline{G}^K(1, 2)]^* \end{pmatrix}. \quad (28.156)$$

We then obtain:

$$\mathbf{j}(\mathbf{R}) = \lim_{1 \rightarrow 2} \frac{|e|}{4m} \text{Tr} \{ (\nabla_1 - \nabla_2) \hat{\rho}_3 \hat{G}^K(1, 2) + i|e|[\mathbf{A}(1) + \mathbf{A}(2)] \hat{G}^K \}. \quad (28.157)$$

For the first term, we see that the electron and hole sector of the Keldysh Green function contribute to the current with opposite sign due to the ρ_3 , as is reasonable since they carry opposite charge. However, the electrons and holes contribute with equal sign in the $\mathbf{A}$ -term. This is due to the fact that the vector potential in the Hamilton-operator also changes sign in the hole sector since the charge is opposite, giving a cancelling minus sign in the current. Thus, there should be no ρ_3 in the $\mathbf{A}$ -term. This is correctly treated in E. Fyhn's master thesis, but incorrect in M. Amundsen's

master thesis.

The total quasiclassical electric current then reads in the diffusive limit of transport:

$$\mathbf{j} = \frac{-N_0|e|D}{4\hbar} \int dE \text{Tr}\{\hat{\rho}_3(\tilde{g}\tilde{\nabla}\tilde{g})^K\} + \frac{-N_0|e|}{4m\hbar} \int dE \text{Tr}\{\mathbf{A}\hat{g}^K\}, \quad (28.158)$$

where $\tilde{\nabla}$ is the covariant derivative. Examining the second term in equilibrium so that $\hat{g}^K = (\hat{g}^R - \hat{g}^A) \tanh(\beta E/2)$, one obtains by using that $g^A = -\rho_3(g^R)^\dagger \rho_3$ and that the diagonal part of $\hat{g}^R$ is $\text{diag}[g_\uparrow(E), g_\downarrow(E), -g_\uparrow^*(-E), -g_\downarrow^*(-E)]$:

$$\begin{aligned} \mathbf{A} \int dE \text{Tr}\{\hat{g}^K\} &= \mathbf{A} \int dE \text{Tr}\{\hat{g}^R - \hat{g}^A\} \tanh(\beta E/2) \\ &= \mathbf{A} \int dE \sum_\sigma \text{Tr}\{g_\sigma(E) - g_\sigma^*(-E) + g_\sigma^*(E) - g_\sigma(-E)\} \tanh(\beta E/2) \\ &= 4 \int dE \tanh(\beta E/2) \sum_\sigma \text{Re}(g_\sigma(E)) \\ &= 2 \int dE \tanh(\beta E/2) N(E) \\ &= 0. \end{aligned} \quad (28.159)$$

since the density of states $N(E) = \text{Tr}\{g^R(E)\}$ is symmetric around $E = 0$. Above, we assumed a gauge $\phi = 0$ since charge neutrality in general requires that the integral over the trace of $\hat{g}^K$ equals ϕ (see section at the end of this chapter). Note that the so-called diamagnetic term $\propto \mathbf{A}$ in the expression for $\mathbf{j}$ also has a high-energy contribution in ξ_p before doing the quasiclassical approximation, which is not zero. However, as discussed in previous literature states, the total diamagnetic contribution to the current is cancelled by the high-energy part of the first term in $\mathbf{j}$ that is neglected when doing the quasiclassical approximation (over ξ_p).

This means that the linear Meissner response to a supercurrent, whether we're considering a BCS superconductor or the proximity-induced Meissner response of a non-superconducting material, should be described by the $\mathbf{A}$ -dependent part of the expression $\mathbf{j} = \frac{-N_0|e|D}{4\hbar} \int dE \text{Tr}\{\hat{\rho}_3(\tilde{g}\tilde{\nabla}\tilde{g})^K\}$. Writing out the $\mathbf{A}$ -dependent part explicitly, one arrives at

$$\mathbf{j} \propto |e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \text{Im}\{\text{Tr}\{\underline{g}^2 + \underline{f}\tilde{f}\}\}. \quad (28.160)$$

Since the normalization of the Green function dictates that $\underline{g}^2 - \underline{f}\tilde{f} = \underline{1}$, we see that

$$\text{Im}\{\text{Tr}\{\underline{g}^2 + \underline{f}\tilde{f}\}\} = 2\text{Im}\{\text{Tr}\{\underline{f}\tilde{f}\}\}, \quad (28.161)$$

and thus

$$\mathbf{j} \propto |e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \text{Im}\{\text{Tr}\{\underline{f}\tilde{f}\}\}. \quad (28.162)$$

However, here we have to be careful. There is another contribution to the current which is linear in $\mathbf{A}$ and which comes from the $\tilde{g}\tilde{\nabla}\tilde{g}$ -term. Such a term can in general arise since the Usadel equation itself depends on $\mathbf{A}$, and thus the solution $\tilde{g}$ can also do that. But a lot of literature seems to only include the explicitly $\mathbf{A}$ -dependent part in the supercurrent to linear response. We now discuss this issue in detail.

28.4.1 Linear-response expression for supercurrent

We begin by some general considerations. The proportionality between $\mathbf{J}$ and $\mathbf{A}$ may be written as $\mathbf{J} = -K\mathbf{A}$. This relation is valid only in a specific gauge, namely the London gauge $\nabla \cdot \mathbf{A} = 0$ where the vector potential additionally must satisfy the same boundary conditions as the current itself. Thus, the normal component of the supercurrent at any surface should be equal to $A_\perp$. If the surface borders vacuum, we need $A_\perp = \mathbf{n} \cdot \mathbf{A} = 0$ where $\mathbf{n}$ is the surface normal.

Specifying $\nabla \cdot \mathbf{A} = 0$ is not sufficient to uniquely identify a gauge and, as explained above, not sufficient to guarantee the validity of $\mathbf{J} = -K\mathbf{A}$. For instance, for a magnetic field $\mathbf{B} \parallel \mathbf{z}$, we have two choices that satisfy $\nabla \cdot \mathbf{A} = 0$, namely $\mathbf{A} = B(0, -x, 0)$ and $\mathbf{A} = B(y, 0, 0)$. The first gauge is ok to use near an edge $x = 0$, since the current should then flow only in the y -direction. Instead, we cannot use the second gauge near an edge $x = 0$, since it would give a current flowing in the x -direction, i.e. out into vacuum.

So although $\mathbf{J} = -K\mathbf{A}$ is clearly not gauge-invariant, it is physically correct so long as we choose a specific gauge. Mathematically, the following equations uniquely determine the vector potential for which $\mathbf{J} = -K\mathbf{A}$ is valid:

- 1) $\nabla \cdot \mathbf{A} = 0$ (London gauge),
 - 2) $\mathbf{n} \cdot \mathbf{A} = 0$ (expresses current conservation at edges),
 - 3) Real order parameter Δ .
- (28.163)

To derive $\mathbf{J} = -K\mathbf{A}$, we now discuss the linear response expression both in the Eilenberger and the Usadel formalism.

Eilenberger

It is useful to start by considering the Eilenberger equation without impurity scattering (see J. Ouassou *et al.*, PRL 2019). If one includes a vector potential, one can analytically derive the relation $\mathbf{J} = -K\mathbf{A}$ quasiclassically if one assumes (1) a London gauge, (2) that the Green function for $\mathbf{A} = 0$ is such that no current flows, (3) a spatially slowly varying vector potential $\mathbf{A}$, (4) disregard any boundaries in the system, and (5) that Δ is fixed to be real when $\mathbf{A}$ is present. The latter means that there is no gradient in the superconducting order parameter. Does this make sense physically if we let $\mathbf{A}$ vary so slowly that it is in fact a constant? A constant $\mathbf{A}$ gives zero magnetic field $\mathbf{B} = 0$, so why should there be a supercurrent?

The answer lies in the fact that we have not solved for Δ selfconsistently, but instead fixed it to be real. This means that although we consider a state with $\mathbf{B} = 0$, we do consider a state where a supercurrent is present. This corresponds to an excited state of the system. Had we instead solved Eilenberger with constant $\mathbf{A}$ selfconsistently, we would have found a Δ which was such that the total supercurrent was zero: in effect, the ground-state.

Belzig *et al.* generalized the Eilenberger equation to include an impurity self-energy and a vector potential, showing that as one takes the dirty limit, one obtains Zaikin's expression. One could thus take the viewpoint that by fixing Δ as real, we are choosing the gauge so that the supercurrent is determined exclusively from the explicitly $\mathbf{A}$ -dependent part of the supercurrent expression in the Usadel equation. We now proceed to discuss how this is justified mathematically.

Usadel

When $\mathbf{A}$ is present in the Usadel equation, it can induce a variation in $\hat{g}$ along its direction. This variation will in general contain a term which is linear in $\mathbf{A}$. Thus, to lowest order, we have $\nabla g \sim \mathbf{A}$. If this term is non-zero, one has to keep it in order to make the current gauge-invariant.

At first glance, this gives reason to question papers which have used the approach of only keeping the $f^2 \mathbf{A}$ term to linear order in the current, where f is the anomalous Green function. unless there is something special about the particular gauge chosen (see Zaikin, 1982 for screening in S/N structures) which actually justifies dropping the $\tilde{g} \nabla \tilde{g}$ term that gives $\tilde{f} \nabla f$ in the supercurrent. So, is there some gauge choice which allows us to only keep the $f^2 \mathbf{A}$ term and get physically correct results?

We wish to discuss the linear-response expression in the Usadel framework for the supercurrent in several different systems to prove mathematically under which circumstances keeping only the $\mathbf{A} f^2$ term gives physically correct results.

We first note some useful mathematical relations which will help us in the discussion below. Gauge-invariance is obtained under the following transformation:

$$\begin{aligned}\mathbf{A} &\rightarrow \mathbf{A} + \nabla \chi, \\ \Delta &\rightarrow \Delta e^{2i\chi}, \\ \psi(\mathbf{r}) &\rightarrow \psi(\mathbf{r}) e^{i\chi/2}.\end{aligned}\tag{28.164}$$

The transformation on the field operators ψ leads to a corresponding transformation on the Green function matrix in the system. We won't need the explicit expression for this transformation in what follows. Moreover, the solution for the Green function in a superconductor with a uniform current reads

$$g = \frac{1}{\sqrt{\epsilon^2 - \Theta^2}} \begin{pmatrix} \epsilon & \Theta e^{i\phi} i\sigma_y \\ \Theta e^{-i\phi} i\sigma_y & -\epsilon \end{pmatrix}.\tag{28.165}$$

Here, ϕ is the SC phase which winds in the presence of a current as $\phi(x) = ux/\xi$ where x is position and u is the constant winding rate. The function Θ is determined by:

$$\Theta = \frac{|\Delta|}{1 + u^2/2\sqrt{\Theta^2 - \epsilon^2}},\tag{28.166}$$

and the gap equation reads

$$|\Delta| = \frac{1}{\text{acosh}(\omega_c)} \int_0^{\omega_c} d\epsilon \text{Re} \left(\frac{\Theta}{\sqrt{\epsilon^2 - \Theta^2}} \right) \tanh(\pi\epsilon/2e^\gamma T)\tag{28.167}$$

where γ is the Euler-Mascheroni constant. It is clear that to first order in the winding rate u , we get $\Theta = |\Delta|$ and the Green function is the BCS one, but with a linearly varying phase.

Now, we consider the specific systems.

28.4.2 Bulk homogeneous superconductor

We consider a homogeneous superconductor and apply a magnetic field described by a vector potential $\mathbf{A}$. A supercurrent is generated. We wish to compute this supercurrent to linear-response in the vector potential $\vec{A}$. The Usadel equation reads

$$D\nabla(g\nabla g) + i[E\rho_3 + \Delta, g] = 0,\tag{28.168}$$

the gap equation reads

$$\Delta \propto \int dE \text{Tr}\{\rho_{\Delta} g\} \quad (28.169)$$

and finally the supercurrent expression is

$$\mathbf{J} \propto \int dE (\tilde{f} \nabla f - f \nabla \tilde{f} - 4\mathbf{A} f \tilde{f}). \quad (28.170)$$

Here, we have dropped matrix notation for the Green function, omitted constants of proportionality, and ρ_{Δ} is an appropriate matrix which projects out the anomalous Green function content of g .

Without a field, the system is assumed to be a bulk homogeneous BCS superconductor. To compute the effect of the field $\mathbf{A}$, let us do a perturbation expansion by assuming a small $\mathbf{A}$. We write

$$\begin{aligned} g &= g^{(0)} + g^{(1)} + \dots \\ \Delta &= \Delta^{(0)} + \Delta^{(1)} + \dots \end{aligned} \quad (28.171)$$

so that for instance $g^{(1)}$ is the correction to the Green function to first order in $\mathbf{A}$. To $\mathcal{O}(\mathbf{A}^0)$, the Usadel and gap equation take their standard form and are solved by the BCS solution.

To $\mathcal{O}(\mathbf{A}^1)$, we find that the Usadel equation reads

$$g^{(0)} \left(\nabla^2 g^{(1)} - i[\rho_3(\nabla \cdot \mathbf{A}), g^{(0)}] \right) = i[\Delta^{(1)}, g^{(0)}]. \quad (28.172)$$

We have used that $\nabla g^{(0)} = 0$.

Based on the above, we may conclude that $\Delta^{(1)}$ and $g^{(1)}$ are both zero for the following reasons:

1. $g^{(1)}$ can only depend on $\nabla \cdot \mathbf{A}$ and $\Delta^{(1)}$ for a homogeneous superconductor, as seen from the Usadel equation Eq. (28.172) and the gap equation. We return below to the issue of how $\mathbf{A}$ can enter through boundary conditions in a finite system (non-homogeneous).
2. If $\nabla \cdot \mathbf{A} = 0$, $g^{(1)}$ and thus $\Delta^{(1)}$ have no dependence on $\mathbf{A}$ through the Usadel or gap equation.
3. Since $g^{(1)}$ and $\Delta^{(1)}$ are first order in $\mathbf{A}$, they therefore have to be zero unless $\mathbf{A}$ enters through boundary conditions.
4. What about boundary conditions then? As long as $\mathbf{n} \cdot \mathbf{A} = 0$ at boundaries, $\mathbf{A}$ will not enter the quasiclassical boundary conditions for the derivative of the Green functions, and thus there can be no additional $\mathbf{A}$ -dependence.

Thus, the conclusion is that there is no correction to the Green function in the superconductor to first order in $\mathbf{A}$. Considering the supercurrent expression, we can safely conclude that in the London gauge $\nabla \cdot \mathbf{A}$, the linear-response is of the form

$$\mathbf{j} = -K\mathbf{A}. \quad (28.173)$$

Note that if an edge is present, our London gauge-choice must also satisfy $\mathbf{n} \cdot \mathbf{A} = 0$ in order for this expression to be valid. This is because the vector potential must satisfy the same boundary

condition as the supercurrent when they are proportional.

In other words, since $g^{(1)}$ is supposed to be linear in $\mathbf{A}$, we may conclude that it has to be zero since there is nothing in the system of equations determining it that depends on $\mathbf{A}$.

Relation to gauge-transformation (reconciling with Ali's note)

At the same time, we know that gauge-transformation from zero $\mathbf{A}$ to constant $\mathbf{A}$ would give *e.g.* $\Delta = \Delta_0 e^{-2ie\mathbf{A}\cdot\mathbf{r}}$. This shows that $g^{(1)}$ and $\Delta^{(1)}$ would not be zero for a constant gauge $\mathbf{A}$. but in this case, $\mathbf{n} \cdot \mathbf{A} = 0$ is not satisfied at all boundaries, and thus we cannot use the reasoning described above.

28.4.3 S/N bilayers

Case I: Zero magnetic field and zero supercurrent

Zero magnetic field can be described using a constant gauge-field $\mathbf{A} = (0, A_0, 0)$ everywhere. We will neglect the inverse proximity effect in the superconductor. To ensure zero supercurrent there when the gauge-field is constant, we need to use an order parameter $\Delta = \Delta_0 e^{i\theta} = \Delta_0 e^{2ieA_0 y/\hbar}$ so that the gauge-invariant phase $\nabla\theta - 2e\mathbf{A}/\hbar$ is zero.

The question is now: what is the linear-response current in the normal metal? There is no field and no supercurrent in S, thus there should be no supercurrent in N either. Clearly, we cannot have a contribution only from the $\mathbf{A}f\tilde{f}$ term in the supercurrent in N, because that would give a finite supercurrent. Instead, the gradient term $f\nabla\tilde{f}$ will now also contribute as to cancel the total current.

To see why this happens, let us gauge away the vector potential in the system by performing a gauge-transformation. This gives us $\mathbf{A} = 0$ and $\Delta = \Delta_0$ in the superconductor. In the normal metal, we see that the solution for the Green function $\check{g}(\mathbf{A} = 0)$ without the vector potential is obtained from the solution with the vector potential $\check{g}[\mathbf{A} = (0, A_0, 0)]$ according to a transformation on the field operators $\psi(\mathbf{r})$ as shown in Eq. (28.164). This has the consequence that the anomalous Green function is

$$f(\mathbf{A} = 0) = e^{-2ieA_0 y} f(\mathbf{A} \neq 0). \quad (28.174)$$

Now, we know that the solution for the Green function in the normal metal in the gauge where $\mathbf{A} = 0$ does not carry any supercurrent since it is in contact with a BCS superconductor with $\mathbf{A} = 0$ in that gauge. Therefore, the supercurrent in the gauge where $\mathbf{A} \neq 0$ gets a contribution both from the $\mathbf{A}f\tilde{f}$ term and the $f\nabla\tilde{f}$ term which are equal and opposite. This gives zero supercurrent in both gauges, as it should be.

Case II: Zero magnetic field and finite supercurrent in S

Zero magnetic field can be described using a constant gauge-field $\mathbf{A} = (0, A_0, 0)$ everywhere, as before. But now we allow for a finite supercurrent flowing in the superconducting region. In the present gauge $\mathbf{A}$, we do this simply by letting the order parameter be real. Let us now do the same trick as above, namely we gauge away the vector potential everywhere. This means that the order parameter is transformed to $\Delta_0 e^{-2ieA_0 y}$ and that $\mathbf{A} = 0$ in the covariant derivative in both S and N. The solution for the Green function in N in such a scenario is that the y -dependence is given by $f \propto e^{-2ieA_0 y}$. This can be directly verified by considering *e.g.* the linearized Usadel equation in the

normal metal with KL boundary conditions to a superconductor with a y -dependent phase as shown above. In fact, the solution for the Green function in N will have the form $f = p(x, \mathbf{A})e^{-2ieA_0y}$ where p solves $\partial^2 p / \partial x^2 + (2iE - 4e^2 \mathbf{A}^2)p = 0$. Thus, the lowest order correction in $\mathbf{A}$ to p is second order. Computing the supercurrent in the normal metal now gives a contribution only from the $f \nabla \tilde{f}$ term to $\mathcal{O}(\mathbf{A}^1)$.

But we know that the solution for the Green function in the gauge with $\mathbf{A} \neq 0$ is related to the one in the gauge $\mathbf{A} = 0$ according to Eq. (28.174). It follows that f is independent on $\mathbf{A}$ to $\mathcal{O}(\mathbf{A}^1)$ in the original gauge. Therefore, only the $\mathbf{A} f \tilde{f}$ term will contribute the supercurrent to first order and result in a finite supercurrent. The result is the same in both gauges, as it should be.

Case III: Finite magnetic field in N

We now consider the scenario where a finite magnetic field exists in the N region. The superconductor is assumed to screen the field completely so that no gauge field or supercurrent exists in S. This is the standard setup considered in the literature that computes the Meissner response of S/N bilayers. Thus we have a vector potential $\mathbf{A} = (0, A(x), 0)$ in the N region and a real Δ and BCS bulk solution in the S part with $\mathbf{A} = 0$ there.

The question is now what the correct expression for the supercurrent linear-response is in the N part of this system. The one that is used in the standard literature is that only a contribution comes from the $\mathbf{A} f \tilde{f}$ term. Note that since $B \neq 0$ in the N region, we cannot gauge away the vector potential there now. If the $\mathbf{A} f \tilde{f}$ term is supposed to be the only contribution, we need to show that the $\mathcal{O}(\mathbf{A})$ contribution to the Green function in N is zero. Considering the wide-junction limit and without any edges along the y -direction (infinite system along y), we need to show (to $\mathcal{O}(\mathbf{A}^1)$) that the solution for the Green function matrix g is translationally invariant along the y -axis in the chosen gauge and thus $\partial_y g = 0$. To be more precise, we need $\partial_y f = 0$ where f is the anomalous Green function.

Choosing a gauge $\mathbf{n} \cdot \mathbf{A} = 0$ at the S/N interface and a real Δ in S gives an Usadel equation and boundary conditions in the x -direction for the $\mathcal{O}(\mathbf{A})$ correction $g^{(1)}$ that are independent on $\mathbf{A}$. This is true since we also have $\nabla \cdot \mathbf{A} = 0$. If the S/N bilayer is now infinite in the y -direction, it follows that there can be no y -dependence in this direction if S has a real order parameter and no $\mathbf{A}$ -field. Therefore, the Green function in N cannot depend on $\mathbf{A} \cdot \mathbf{r}$ since that would also break translational invariance (homogeneity in the y -direction). Note that this solution explicitly assumes no edges in y -direction, since it clearly does not hold close to y -edges.

Also note that this argument does not contradict the gauge-transformation result for constant $\mathbf{A}$ and no edges, where we found that there is an y -dependence and the Green function g does depend on $\mathbf{A} \cdot \mathbf{r}$ through the factor $e^{-2i\mathbf{A} \cdot \mathbf{r}}$. The reason for why it does not contradict is that in that case Δ had an y -dependence which also causes g to have a y -dependence. One way to see this is to consider a superconductor with $\mathbf{A} = 0$, but with a gradient in the order parameter. This will give rise to a gradient in f and a finite supercurrent. If we now gauge away the gradient in order parameter to get a real Δ , we also acquire a finite $\mathbf{A}$. The solution for f will now be y -independent and also have zero $\mathcal{O}(\mathbf{A}^1)$ contribution, but the $\mathbf{A} f^2$ term gives a supercurrent. There is thus a finite supercurrent in both gauges. Therefore, it is in fact consistent to assume g independent on y to $\mathcal{O}(\mathbf{A}^1)$ when we have real OP and $\mathbf{A} \parallel \mathbf{y}$.

Finally, we mention that if one does not determine Delta self-consistently, an infinite system *must*

be assumed along the y -direction if one considers $\mathbf{A}||\mathbf{y}$ in the N part with real Δ in S. Otherwise, this gauge choice violates boundary conditions that would exist at y -edges.

28.4.4 Meissner response for a BCS superconductor

For a BCS bulk superconductor without any phase gradient, we have $\underline{f} = s i \sigma_2$ where we have chosen a real SC order parameter. In this case, we have $s = -\tilde{s}$ and

$$s^2 = \frac{\Delta^2}{E^2 - \Delta^2}. \quad (28.175)$$

In the BCS case, we thus obtain:

$$\mathbf{j} \propto |e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \text{Im}\{s^2\}. \quad (28.176)$$

At first glance, this seems problematic: we just saw that s^2 is purely real, suggesting that there should be no Meissner response! At the same time, it is known [31] that in the Matsubara formalism (meaning that we have converted from a real energy representation to Matsubara frequencies), one obtains

$$\mathbf{j} \propto T \sum_n \frac{\Delta^2}{\Delta^2 + \omega_n^2} \neq 0 \quad (28.177)$$

with $\omega_n = (2n+1)\pi k_B T$. The resolution to this problem lies in a small detail that usually can be overlooked, but which is crucial in this particular case. Since we are dealing with the retarded Green function, the energy argument E strictly speaking has an infinitesimally small imaginary quantity η , so that one has

$$s^2 = \lim_{\eta \rightarrow 0} \frac{\Delta^2}{(E + i\eta)^2 - \Delta^2}. \quad (28.178)$$

To see why it is important to take into account this, note first that the definition of the $\delta(x)$ function reads

$$\delta(x) = \frac{1}{\pi} \lim_{\gamma \rightarrow 0} \frac{\gamma}{x^2 + \gamma^2}, \quad x \in \mathbb{R}. \quad (28.179)$$

Now, in our system we have that $E \in \mathbb{R}$. We can rewrite our expression for s^2 as:

$$s^2 = \lim_{\eta \rightarrow 0} \frac{\Delta^2(E^2 - \Delta^2 - \eta^2 - 2iE\eta)}{(E^2 - \Delta^2 - \eta^2)^2 + 4E^2\eta^2} \quad (28.180)$$

which means that the imaginary contribution that enters the integral for $\mathbf{j}$ gives:

$$\mathbf{j} \propto \lim_{\eta \rightarrow 0} -2|e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \frac{\Delta^2 E \eta}{(E^2 - \Delta^2 - \eta^2)^2 + 4E^2\eta^2}. \quad (28.181)$$

If we now define $x \equiv \sqrt{(E^2 - \Delta^2)^2 + \eta^4}$ and use the definition of the $\delta(x)$ -function given above, the integral provides

$$\mathbf{j} \propto \lim_{\eta \rightarrow 0} -2|e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \frac{\Delta^2 E \eta}{(E^2 - \Delta^2 - \eta^2)^2 + 4E^2\eta^2}. \quad (28.182)$$

Collecting the $\mathcal{O}(\eta)$ part, we get:

$$\begin{aligned} \mathbf{j} &\propto \lim_{\eta \rightarrow 0} -|e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \frac{\Delta^2 E}{E^2 + \Delta^2} \frac{\eta}{(x^2/(2E^2 + 2\Delta^2) + \eta^2)} \\ &\propto \lim_{\gamma \rightarrow 0} -|e|^2 \mathbf{A} N_0 v_F \int dE \tanh(\beta E/2) \frac{\Delta E}{E^2 + \Delta^2} \frac{\gamma}{\frac{x^2}{2\Delta^2(E^2 + \Delta^2)} + \gamma^2} \end{aligned} \quad (28.183)$$

where we defined the dimensionless number $\gamma \equiv \eta/\Delta$. The last factor in the integrand is precisely the definition we previously gave for the $\delta(x)$ -function, and gives a contribution to the integral for $E = \pm\Delta$. We thus finally obtain the answer for the supercurrent response, *which we emphasize is independent on η (or γ)*:

$$\mathbf{j} \propto -2|e|^2 \mathbf{A} N_0 v_F \tanh(\beta\Delta/2). \quad (28.184)$$

This expression is physically reasonable: it vanishes in the absence of SC ($\Delta \rightarrow 0$) and it decreases with increasing temperature [both via the temperature dependence of $\Delta(T)$ and via the $\beta = 1/(k_B T)$ dependence].

The contribution from the infinitesimal part η is only important in the BCS case: if we compute the Meissner response due to the proximity effect, $\underline{f}\underline{f}$ is complex even when ignoring η and keeping η gives only a negligible contribution. If the reader finds it difficult to accept that η must be kept up until a certain point in the calculation before one can take the limit $\eta \rightarrow 0$ in order to get the correct result, one could argue that inelastic scattering enters in exactly the same manner as η (an imaginary contribution to the energy) and since this always is present to some degree in real materials, $\mathbf{j}$ remains non-zero. However, we emphasize that the above treatment shows that inelastic scattering is not strictly speaking required to obtain a Meissner response, in accordance with established theory.

28.4.5 More general discussion regarding paramagnetic and diamagnetic response to a magnetic field

In general, a material can feature both a paramagnetic and diamagnetic contribution to the current-response in the presence of a vector potential $\mathbf{A}$. For a time-independent potential $\mathbf{A}$, there is no electric field associated with such a potential and hence no voltage can be present to drive a normal, dissipative current. In non-superconducting materials, the paramagnetic and diamagnetic contributions thus cancel each other (there can be an additional paramagnetic effect from the spin of the electrons providing a net paramagnetic response of the material).

Superconductors are exceptions. Qualitatively, one can state that a superconductor is robust against small perturbations since there is a gap Δ prohibiting excitations as $T \rightarrow 0$ as long as the perturbation energy is smaller than the gap. In this case, there is only a diamagnetic response to the current. Let us do the math to back up this statements. In the London limit (where the magnitude of the superconducting order parameter is constant whereas the phase can vary) and in the absence of impurity scattering (for simplicity), one obtains [32] a supercurrent that is locally related to the vector potential via a tensor equation:

$$\mathbf{j}_i = - \sum_j R_{ij} \mathbf{A}_j \quad (28.185)$$

where the symmetric response tensor is:

$$R_{ij} = \frac{e^2}{4\pi^3\hbar c} \oint_{\text{FS}} dS \left[\frac{v_F^i v_F^j}{|\mathbf{v}_F|} \left(1 + 2 \int_{\Delta(\mathbf{k})}^{\infty} \frac{\partial f(E)}{\partial E} \frac{N(E)}{N(0)} dE \right) \right]. \quad (28.186)$$

Here, $f(E)$ is the Fermi function (a step function at $T = 0$) and E is the quasiparticle energy. The density of states reads $N(E)/N(0) = E/\sqrt{E^2 - [\Delta(\mathbf{k})]^2}$ and v_F^i are the components of the Fermi velocity. The $\oint$ is the angular integral taken over the Fermi surface, which only has consequences for the second part of the integrand since that one depends (potentially) on momentum via $\Delta(\mathbf{k})$. For an s -wave superconductor $\Delta(\mathbf{k}) = \Delta$, the averaging has no effect.

The first part of the integrand is the diamagnetic part, which is always present. The second part of the integrand is the paramagnetic contribution, which is seen to depend crucially on the nature of $N(E)$. For instance, for a superconductor at $T = 0$, the derivative of $f(E)$ gives a δ -function so that there is only a contribution from $E = 0$. But the integral itself starts at Δ (since the DOS is zero for $E < \Delta$ in a superconductor), and hence the second term makes no contribution at all. In contrast, if $\Delta = 0$, the second term completely cancels the first one since $N(E)/N_0 = 1$ and the integral yields a factor $-1/2$.

It is clear from Eq. (28.186) that as soon as one moves away from $T = 0$, the derivative of the distribution function will allow a small, but finite contribution from the paramagnetic term in R_{ij} , thus reducing the diamagnetic response. The paramagnetic response increases continuously until $T = T_c$ where it completely cancels the diamagnetic response. However, it is interesting to note that in the case of a d -wave superconductor which features zero-energy Andreev bound states at certain crystallographic orientations of its surface to vacuum, the paramagnetic term leads to a non-monotonic behavior of the Meissner response vs. temperature since $N(E = 0)$ is strongly enhanced. This non-linear Meissner effect has been experimentally verified.

Interestingly, this observation also offers a possible explanation for why odd-frequency superconductivity can also give rise to a paramagnetic effect. As is known from the literature, odd-frequency pairing has a renormalizing effect on the quasiparticle mass rather than gapping the spectrum, which as an effect gives rise to a similar zero-bias peak in the density of states as in the d -wave case. Therefore, it is reasonable to expect that the available quasiparticles at subgap energies also give rise to a paramagnetic contribution to the Meissner effect, similarly to the case described above.

We end by confirming our treatment above using the Ginzburg-Landau formalism. The free energy reads

$$F_S = F_N + \int dV \left[\alpha(T)|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*} \left| \left(\hbar \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right|^2 + \frac{B^2}{8\pi} \right] \quad (28.187)$$

where ψ is the superconducting order parameter, so that $m^* = 2m_e$ is the Cooper pair mass and $e^* = -2|e|$ is the Cooper pair charge. The current density is obtained from the Ginzburg-Landau equations, providing

$$\mathbf{j} = -\frac{ie\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{2e^2}{mc} |\psi|^2 \mathbf{A}. \quad (28.188)$$

The last term is the diamagnetic contribution that we have discussed above, and is thus proportional to the number of superconducting electrons $|\psi|^2 = n_s$. The paramagnetic contribution is the first

term which in the London limit depends on the gradient of the superconducting phase. Due to the phase rigidity of Cooper pairs, twisting the phase costs energy, and the paramagnetic contribution is zero at $T = 0$ whereas it becomes finite at $T \neq 0$.

28.4.6 Conservation for total electric current

The total charge current $\mathbf{I}$ through a system is composed of contributions from both resistive terms (proportional to gradients in distribution functions) and supercurrents (proportional to distribution functions and instead involving gradients in spectral quantities). It has to be conserved both in and out of equilibrium. Let us see how this follows from the Usadel equation and its belonging kinetic equations.

The Usadel equation in a superconductor may be written

$$D\nabla(\check{g}\nabla\check{g}) + i[E\check{\rho}_3 + \check{\Delta}, \check{g}] = 0. \quad (28.189)$$

Here, $\check{\Delta} = \text{diag}(\hat{\Delta}, \hat{\Delta})$ and $\Delta = \text{offdiag}(\Delta, -\Delta, \Delta^*, -\Delta^*)$. We also know that the electric current is

$$\mathbf{I} = \int dE \text{Tr}\{\hat{\rho}_3(\check{g}\nabla\check{g})^K\} \quad (28.190)$$

and it has to be conserved both in and out of equilibrium: $\nabla \cdot \mathbf{I} = 0$. This is completely general. Assume now that we have only singlet correlations, but allow for a non-equilibrium situation. Then, the self-consistency equation for the gap is

$$\Delta = \int dE f_{\uparrow\downarrow}^K. \quad (28.191)$$

For both Δ and $\mathbf{I}$, we have for simplicity omitted constant prefactors which are not important for the present discussion. We then see that the Usadel equation can in fact be written as the divergence of the electric current by taking the Keldysh part, multiplying with $\hat{\rho}_3$ from the left, taking the trace, and integrating over all energies:

$$D\nabla \cdot \mathbf{I} + \int dE \text{Tr}\{\hat{\rho}_3(i[E\hat{\rho}_3 + \hat{\Delta}, \hat{g}^K])\} = 0. \quad (28.192)$$

Thus, current conservation demands that

$$\int dE \text{Tr}\{\hat{\rho}_3(i[E\hat{\rho}_3 + \hat{\Delta}, \hat{g}^K])\} = 0. \quad (28.193)$$

The energy-part of the integrand vanishes even before integrating due to the commutation. What remains is

$$\int dE \text{Tr}\{\hat{\rho}_3([\hat{\Delta}, \hat{g}^K])\} = 0. \quad (28.194)$$

Now use that $f_{\uparrow\downarrow}^K = -f_{\downarrow\uparrow}^K$ if we only have singlet superconductivity in the system (that's where this assumption comes in). We then get

$$\int dE \text{Tr}\{\hat{\rho}_3([\hat{\Delta}, \hat{g}^K])\} \propto \int dE (-\Delta \tilde{f}_{\uparrow\downarrow}^K + \Delta^* f_{\uparrow\downarrow}^K). \quad (28.195)$$

Further, we use

$$\Delta^* = \int dE \tilde{f}_{\uparrow\downarrow}^K \quad (28.196)$$

as can be seen by shifting variables $E \rightarrow -E$. We then obtain

$$\int dE \text{Tr}\{\hat{\rho}_3([\hat{\Delta}, \hat{g}^K])\} \propto \int dE dE' [-f^K(E) \tilde{f}^K(E') + \tilde{f}^K(E) f^K(E')] = 0. \quad (28.197)$$

This shows that the electric current is conserved when we treated the gap self-consistently - otherwise, it is not.

It is important to note that the phase of the superconducting order parameter and the phase of f^R when using the θ -parametrization of the retarded Green function are in general not the same. To see this, write $f_{\uparrow\downarrow}^R = \chi e^{i\theta}$ and χ, θ are in general both position and energy-dependent quantities. Generally, the gap equation for a singlet superconductor takes the form

$$\Delta = \int dE [h_L \text{Re}(\chi) - i h_T \text{Im}(\chi)] e^{i\theta}. \quad (28.198)$$

This is derived by inserting what $f_{\uparrow\downarrow}^K$ is when using $\hat{g}^K = \hat{g}^R \hat{h} - \hat{h} \hat{g}^A$ where $\hat{h} = h_L \hat{1} + h_T \hat{\rho}_3$ is only assumed to have a charge and energy mode for simplicity whereas $\hat{g}^A = -(\hat{\rho}_3 \hat{g}^R \hat{\rho}_3)^\dagger$. In equilibrium, where $h_T = 0$, we see that the phase of the superconducting order parameter and θ can be the same quantity, if we assume that θ is energy-independent. This is true even if we have a pure supercurrent in the system, so that θ is not a constant, since h_T can still be zero then.

However, if $h_T \neq 0$, the phase θ_Δ of the order parameter $\Delta = |\Delta| e^{i\theta_\Delta}$ cannot be the same as θ , since Δ now acquires an extra phase from the complex square bracket in Eq. (28.198). This has to be taken into account in the kinetic equations in order to get a correct form which implies current conservation when using the self-consistent form of the gap. For instance, this is not taken into account in the papers by JP Morten who writes the source term in the kinetic equation for the charge current as $\alpha_T T h_T$ with $\alpha_T T = \text{Im}(\chi) |\Delta|$. This does not give current conservation, since both $\text{Im}(\chi)$ and h_T are symmetric in E and do not vanish under integration. The resolution is that the expression he gives is only valid for $h_T = 0$, since he has assumed that θ_Δ and θ are identical. In fact, by assuming this we arrive at precisely $\alpha_T T h_T$ from the above expression $(-\Delta \tilde{f}_{\uparrow\downarrow}^K + \Delta^* f_{\uparrow\downarrow}^K)$.

28.4.7 Correct normalization (prefactor) for the quasiclassical current and current conservation

The correction prefactor is $N_0 e D A / 8$ for the total current (without A , it is current density). Note that in some of Ali's paper we have an extra factor L in the prefactor, but this is not correct. However, we will see why the extra L is there and it does not affect the results obtained in those papers in practice.

The KL boundary conditions are

$$2L_i \zeta_i g_i \partial_x g_i = [g_1, g_2], \quad i = 1, 2. \quad (28.199)$$

Here, we have defined the ratio of barrier resistance to normal-state resistance for material i :

$$\zeta_i = \frac{R_B}{R_i}, \quad R_i = \frac{L_i}{\sigma_i A}, \quad \sigma_i = N_{0,i} e^2 D_i. \quad (28.200)$$

The latter is the Drude conductivity and $N_{0,i}$ is the density of states per unit volume in material i . By using that $N_0 = k_F m / 2\pi^2$ and that the electron density is $n \propto k_F^3$ while $D_i \propto v_{F,i}^2 \tau_i$ (excluding numerical prefactors), one proves that $\sigma_i = n_i e^2 \tau_i / m_i$, as usual. Note that this means that the general boundary condition can be rewritten as

$$2R_B \sigma_i A g_i \partial_x g_i = [g_1, g_2], \quad i = 1, 2. \quad (28.201)$$

The point is now that we usually take the interface parameter ζ_i to be the same on both sides of a material. In effect, we write something like

$$2L_i g_i \partial_x g_i = \frac{G_T}{G_0} [g_1, g_2], \quad i = 1, 2. \quad (28.202)$$

However, in doing so, we are thus forcing the quantity σ_i / L_i to be a constant, as can be seen by computing $1/\zeta_i = G_T / G_0$.

With this in mind, let us return to the definition of the current. We have

$$I = \frac{N_0 e D A}{8} \int dE \text{Tr} \{ \rho_3 (g \partial_x g)^K \}. \quad (28.203)$$

We can rewrite this as

$$I = \frac{R_B \sigma_i A}{4} \int dE \text{Tr} \{ \rho_3 (g \partial_x g)^K \}. \quad (28.204)$$

Then, it is clear from Eq. (28.201) that this quantity is conserved regardless of which side of the interface we evaluate it on.

Now, we consider our specific choice of boundary condition parameters where σ_i / L_i is a constant. Denote this constant C . So multiply Eq. (28.205) with L_i / L_i to obtain

$$I = \frac{R_B C A}{4} \int dE \text{Tr} \{ \rho_3 (L_i g \partial_x g)^K \}. \quad (28.205)$$

We then see that when we choose G_T / G_0 to be the same value on both sides of the interface, then it follows from Eq. (28.202) that the integrand in Eq. (28.205) is indeed constant. The prefactor is material-independent, so total current is conserved, as it should.

28.5 Boundary conditions: derivation of Kupriyanov-Lukichev form

There exists many extensions of boundary conditions for the quasiclassical Green functions, depending on which type of interface one deals with: tunneling, high-transparency, magnetic, and so forth. The derivation of these boundary conditions is a technically challenging task if done mathematically rather strictly.

Below, we demonstrate how the t -matrix formalism can be used to derive the Kupriyanov-Lukichev boundary condition which are the most commonly used boundary conditions in the literature.

28.5.1 Non-magnetic interface derivation using t -matrix

The t -matrix

We start by defining our Fourier transformation conventions. Note that we are using the symbol G for all functions, even if strictly speaking the functions are different when changing argument. For instance, if we have $G(\mathbf{r}_1, \mathbf{r}_2)$, we can express the function in terms of $\mathbf{R}$ and $\mathbf{r}$ instead. This would give $G(\mathbf{r}_1, \mathbf{r}_2) = G'(\mathbf{R}, \mathbf{r})$, where G' is a different function than G . As mentioned, we suppress the notational difference between the functions.

We define

$$\begin{aligned} G(\mathbf{k}_1, \mathbf{k}_2) &= \int \int d\mathbf{r}_1 d\mathbf{r}_2 G(\mathbf{r}_1, \mathbf{r}_2) e^{-i\mathbf{k}_1 \mathbf{r}_1 + i\mathbf{k}_2 \mathbf{r}_2}, \\ G(\mathbf{r}_1, \mathbf{r}_2) &= \int \int \frac{d\mathbf{k}_1}{(2\pi)^3} \frac{d\mathbf{k}_2}{(2\pi)^3} G(\mathbf{k}_1, \mathbf{k}_2) e^{i\mathbf{k}_1 \mathbf{r}_1 - i\mathbf{k}_2 \mathbf{r}_2}. \end{aligned} \quad (28.206)$$

The relative and center-of-mass coordinates in position and momentum are

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{k} = \frac{\mathbf{k}_1 + \mathbf{k}_2}{2}, \quad \Delta\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2. \quad (28.207)$$

In the mixed representation, we have

$$\begin{aligned} G(\mathbf{k}, \mathbf{R}) &= \int d\mathbf{r} G(\mathbf{r} + \frac{1}{2}\mathbf{R}, \frac{1}{2}\mathbf{R} - \mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} \\ &= \int d\mathbf{r} G(\mathbf{r}, \mathbf{R}) e^{-i\mathbf{k}\mathbf{r}}. \end{aligned} \quad (28.208)$$

or alternatively

$$G(\mathbf{k}, \mathbf{R}) = \int \frac{d\Delta\mathbf{k}}{(2\pi)^3} G(\mathbf{k} + \frac{1}{2}\Delta\mathbf{k}, \mathbf{k} - \frac{1}{2}\Delta\mathbf{k}) e^{i\Delta\mathbf{k}\mathbf{R}}. \quad (28.209)$$

Note that the different signs in the exponent for the arguments in Eq. (28.206) are required in order to be consistent with the Fourier transformation in the mixed representation Eq. (28.208). We also have

$$\delta(\mathbf{r}) = \int \frac{d\mathbf{y}}{(2\pi)^3} e^{i\mathbf{y}\mathbf{r}}. \quad (28.210)$$

Finally, we assume that the system is large enough that we may use

$$\frac{1}{V} \sum_{\mathbf{k}} \simeq \int \frac{d\mathbf{k}}{(2\pi)^3}. \quad (28.211)$$

Consider now the presence of an impurity potential $V(\mathbf{r}_0)$ that is strongly localized in real space. Here, $\mathbf{r}_0$ is the position vector. This impurity is assumed distinct from all other impurities that we perform an impurity average over in the selfconsistent Born approximation. Assume that the potential is a scalar (possibly with a matrix structure) and not an operator. The latter would be the case for a spin-orbit impurity potential in real space.

Our definition of the T -matrix requires, as we will show below, that a quantity G_0 satisfies:

$$G(1, 2) = G_0(1, 2) + \int G_0(1, 3)V(3)G(3, 2)d3. \quad (28.212)$$

Here, 123 are spatial coordinates. In the PRB we say that G_0 is the solution to the Gor'kov equation without V , but with Σ_{imp} . The question is now which Green function that Σ_{imp} is a functional of: is it G or G_0 ? It turns out that it must be G , as proven below. Therefore, the isotropization zone treatment given later in this derivation will end up showing that the quasiclassical Green function g_0 satisfying impenetrable boundary conditions (meaning no coupling between the two sides of the interface) will equal the diffusive Green function g satisfying *penetrable* boundary conditions at the beginning of the isotropization zone. This will allow us to produce the standard Kupriyanov-Lukichev boundary conditions with g on both lhs and rhs. The proof goes as follows (let $\Sigma \equiv \Sigma_{\text{imp}}$ for brevity).

We know that $G(1, 2)$ satisfies:

$$[H_0(1) - V(1)]G(1, 2) - \int \Sigma[G(1, 3)]G(3, 2)d3 = \delta(1 - 2). \quad (28.213)$$

The claim is now that if $G_0(1, 2)$ satisfies

$$H_0(1)G_0(1, 2) - \int \Sigma[G(1, 3)]G_0(3, 2)d3 = \delta(1 - 2), \quad (28.214)$$

then Eq. (28.212) is fulfilled. In contrast, Eq. (28.212) would *not* have been fulfilled if we used $\Sigma[G_0(1, 3)]$ in Eq. (28.214). Let us verify this. Start with the expression:

$$H_0(1)G(1, 2) - \int \Sigma[G(1, 4)]G(4, 2)d4 \quad (28.215)$$

and now insert Eq. (28.212). We get:

$$\begin{aligned} H_0(1)G_0(1, 2) + \int H_0(1)G_0(1, 3)V(3)G(3, 2)d3 - \int \Sigma[G(1, 4)]G_0(4, 2)d4 \\ - \int \int \Sigma[G(1, 4)]G_0(4, 3)V(3)G(3, 2)d3d4. \end{aligned} \quad (28.216)$$

The first and third term combined equal $\delta(1 - 2)$ according to Eq. (28.214). Thus, we are left with

$$\begin{aligned} \delta(1 - 2) + \int \left(H_0(1)G_0(1, 3) - \int \Sigma[G(1, 4)]G_0(4, 3)d4 \right) V(3)G(3, 2)d3 \\ = \delta(1 - 2) + \int \delta(1 - 3)V(3)G(3, 2)d3 \\ = \delta(1 - 2) + V(1)G(1, 2). \end{aligned} \quad (28.217)$$

Thus, we have proven that

$$H_0(1)G(1, 2) - \int \Sigma[G(1, 4)]G(4, 2)d4 = \delta(1 - 2) + V(1)G(1, 2), \quad (28.218)$$

and this is identical with Eq. (28.213). This completes the proof.

To define the t -matrix, we therefore start with the Gor'kov equation in real space:

$$[\epsilon\check{\rho}_3 - \frac{1}{2m}\nabla^2 + \mu - V(\mathbf{r}_0)]\check{G}(\mathbf{r}_0, \mathbf{r}_n) - \int \check{\Sigma}[G(\mathbf{r}_0, \mathbf{r}')] \check{G}(\mathbf{r}', \mathbf{r}_n) d\mathbf{r}' = \delta(\mathbf{r}_0 - \mathbf{r}_n). \quad (28.219)$$

Here, $\check{\cdot}$ denotes a matrix in Keldysh space (8×8) and $\check{\Sigma}$ contains the effect of all other impurities that we average over configurations for. The ∇ -operator acts on the $\mathbf{r}_0$ coordinate. The absence of $\check{\cdot}$ on some terms means that they are proportional to the unit matrix in Keldysh space. As shown above, we may reformulate the equation above as:

$$\check{G}(\mathbf{r}_0, \mathbf{r}_n) = \check{G}_0(\mathbf{r}_0, \mathbf{r}_n) + \int d\mathbf{r}_1 \check{G}_0(\mathbf{r}_0, \mathbf{r}_1) V(\mathbf{r}_1) \check{G}(\mathbf{r}_1, \mathbf{r}_n), \quad (28.220)$$

where $\check{G}_0$ solves the Gor'kov equation in the absence of the distinguished impurity $V(\mathbf{r}_0)$, but with a self-energy that is a functional of the full Green function $\check{G}$. In other words, $\check{G}_0$ is the impurity-averaged Green function where the self-energy is obtained using $\check{G}$. Therefore, $\check{G}_0$ does not correspond to the solution for an actual physical system, but is an auxiliary useful mathematical object that will be eliminated from the expressions in the end. From now on, drop $\check{\cdot}$ for brevity of notation.

We can recast the above equation into momentum-space by multiplying the whole equation with $e^{-i\mathbf{k}_0\mathbf{r}_0+i\mathbf{k}_n\mathbf{r}_n}$ and integrating over $\mathbf{r}_0$ and $\mathbf{r}_n$:

$$\begin{aligned} G(\mathbf{k}_0, \mathbf{k}_n) &= G_0(\mathbf{k}_0, \mathbf{k}_n) + \int \int \int d\mathbf{r}_1 d\mathbf{r}_0 d\mathbf{r}_n e^{-i\mathbf{k}_0\mathbf{r}_0+i\mathbf{k}_n\mathbf{r}_n} G_0(\mathbf{r}_0, \mathbf{r}_1) V(\mathbf{r}_1) G(\mathbf{r}_1, \mathbf{r}_n) \\ &= G_0(\mathbf{k}_0, \mathbf{k}_n) + \int d\mathbf{r}_1 d\mathbf{r}_0 d\mathbf{r}_n \frac{d\mathbf{p}_1 d\mathbf{p}_2}{(2\pi)^6} \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} G_0(\mathbf{p}_1, \mathbf{p}_2) e^{i\mathbf{p}_1\mathbf{r}_0-i\mathbf{p}_2\mathbf{r}_1} V(\mathbf{r}_1) G(\mathbf{q}_1, \mathbf{q}_2) \\ &\quad \times e^{i\mathbf{q}_1\mathbf{r}_1-\mathbf{q}_2\mathbf{r}_n} e^{-i\mathbf{k}_0\mathbf{r}_0+i\mathbf{k}_n\mathbf{r}_n}. \end{aligned} \quad (28.221)$$

Defining the Fourier-transform of the potential

$$V(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{r}\mathbf{q}} V(\mathbf{r}), \quad (28.222)$$

we obtain, after using the definition of the Dirac delta-function, that

$$G(\mathbf{k}_0, \mathbf{k}_n) = G_0(\mathbf{k}_0, \mathbf{k}_n) + \int \int \frac{d\mathbf{k}_1 d\mathbf{k}_2}{(2\pi)^6} G_0(\mathbf{k}_0, \mathbf{k}_1) V(\mathbf{k}_1 - \mathbf{k}_2) G(\mathbf{k}_2, \mathbf{k}_n). \quad (28.223)$$

Repeated iteration of this equation provides us with the t -matrix:

$$G(\mathbf{k}_0, \mathbf{k}_n) = G_0(\mathbf{k}_0, \mathbf{k}_n) + \int \int \frac{d\mathbf{k}_1 d\mathbf{k}_2}{(2\pi)^6} G_0(\mathbf{k}_0, \mathbf{k}_1) T(\mathbf{k}_1, \mathbf{k}_2) G_0(\mathbf{k}_2, \mathbf{k}_n), \quad (28.224)$$

where

$$T(\mathbf{k}_0, \mathbf{k}_n) = V(\mathbf{k}_0 - \mathbf{k}_n) + \int \int \frac{d\mathbf{k}_1 d\mathbf{k}_2}{(2\pi)^6} V(\mathbf{k}_0 - \mathbf{k}_1) G_0(\mathbf{k}_1, \mathbf{k}_2) T(\mathbf{k}_2, \mathbf{k}_n). \quad (28.225)$$

Note how the t -matrix only couples to G_0 , and not G , which will turn out to be an advantage.

Now, we assumed that the impurity potential was localized, say at $\mathbf{r}_0 = \mathbf{R}_0$. For instance, if the potential was delta-function localized, it means that the Fourier transformation of the potential is

$$\begin{aligned} V(\mathbf{q}) &= \int d\mathbf{r} e^{-i\mathbf{r}\mathbf{q}} V(\mathbf{r}) \\ &= \int d\mathbf{r} e^{-i\mathbf{r}\mathbf{q}} V_0 \delta(\mathbf{r} - \mathbf{R}_0) \\ &= V_0 e^{-i\mathbf{q}\mathbf{R}_0}. \end{aligned} \quad (28.226)$$

Therefore, we can write

$$V(\mathbf{q}) = V_0(\mathbf{q}) e^{-i\mathbf{q}\mathbf{R}_0} \quad (28.227)$$

to a good approximation where V_0 varies very slowly with $\mathbf{q}$. Recall again that $V(\mathbf{q})$ is a perturbation to a system where all other self-energies are present.

With the above particular form of $V(\mathbf{q})$, the t -matrix satisfies

$$T(\mathbf{k}_0, \mathbf{k}_n) = T_0(\mathbf{k}_0, \mathbf{k}_n) e^{-i(\mathbf{k}_0 - \mathbf{k}_n)\mathbf{R}_0} \quad (28.228)$$

where we defined

$$T_0(\mathbf{k}_0, \mathbf{k}_n) = V_0(\mathbf{k}_0 - \mathbf{k}_n) + \int \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} V_0(\mathbf{k}_0 - \mathbf{q}_1) G_0(\mathbf{q}_1, \mathbf{q}_2) T_0(\mathbf{q}_2, \mathbf{k}_n) e^{i(\mathbf{q}_1 - \mathbf{q}_2)\mathbf{R}_0}. \quad (28.229)$$

So far, our treatment of the t -matrix is exact. Now we make some approximations. In the end, we will only be interested in a low-energy theory relative the Fermi level. For such low energies, particles must have momenta close to $\mathbf{q}_F$. Thus, both $\mathbf{q}_1$ and $\mathbf{q}_2$ are close to $\mathbf{q}_F$ so that the momentum transfer $\mathbf{q} = \mathbf{q}_1 - \mathbf{q}_2$ is small relative $\mathbf{q}_F$. For all other momenta differences, we assume that the Green function is negligible. Moreover, we know that G is strongly peaked near $\mathbf{k} = \mathbf{k}_F$. For instance, in the normal state we have

$$G(\mathbf{k}, E) \propto \frac{1}{E - \xi_{\mathbf{k}} + i\delta}. \quad (28.230)$$

where $\mathbf{k} = (\mathbf{k}_1 + \mathbf{k}_2)/2$. Based on this, the main contribution to the integral giving T_0 has to come from a region in $\mathbf{q}$ -space where $\mathbf{q} = \mathbf{q}_1 - \mathbf{q}_2$ is small. We may then set:

$$\begin{aligned} T_0(\mathbf{k}_0, \mathbf{k}_n) &= V_0(\mathbf{k}_0 - \mathbf{k}_n) + \int \int \frac{d\mathbf{Q}}{(2\pi)^3} \frac{d\mathbf{q}}{(2\pi)^3} V_0(\mathbf{k}_0 - \mathbf{Q} - \mathbf{q}/2) \\ &\quad \times G_0(\mathbf{Q}, \mathbf{q}) T_0(\mathbf{Q} - \mathbf{q}/2, \mathbf{k}_n) e^{i\mathbf{q}\mathbf{R}_0} \\ &= V_0(\mathbf{k}_0 - \mathbf{k}_n) + \int \frac{d\mathbf{Q}}{(2\pi)^3} V_0(\mathbf{k}_0 - \mathbf{Q}) \\ &\quad \times \int \frac{d\mathbf{q}}{(2\pi)^3} G_0(\mathbf{Q}, \mathbf{q}) e^{i\mathbf{q}\mathbf{R}_0} T_0(\mathbf{Q}, \mathbf{k}_n) \end{aligned} \quad (28.231)$$

since the Jacobian of the coordinate change $(\mathbf{q}_1, \mathbf{q}_2) \rightarrow (\mathbf{Q}, \mathbf{q})$ is 1 and since V_0 , and thus T_0 , have to be slowly varying functions of their momenta. For T_0 , this can be seen by looking at the $\mathbf{k}_0$ and $\mathbf{k}_n$ dependence in the above equation upon iteration. Thus, we obtain

$$T_0(\mathbf{k}_0, \mathbf{k}_n) = V_0(\mathbf{k}_0 - \mathbf{k}_n) + \int \frac{d\mathbf{Q}}{(2\pi)^3} V_0(\mathbf{k}_0 - \mathbf{Q}) G_0(\mathbf{Q}, \mathbf{R}_0) T_0(\mathbf{Q}, \mathbf{k}_n). \quad (28.232)$$

Now, from the equation of motion

$$G(\mathbf{k}_0, \mathbf{k}_n) = G_0(\mathbf{k}_0, \mathbf{k}_n) + \int \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} G_0(\mathbf{k}_0, \mathbf{q}_1) T(\mathbf{q}_1, \mathbf{q}_2) G_0(\mathbf{q}_2, \mathbf{k}_n), \quad (28.233)$$

we know that $\mathbf{k}_0 \simeq \mathbf{k}_n$ to give a non-zero G or G_0 for low-energy scattering. This means that $\mathbf{q}_1$ has to be close to $\mathbf{q}_2$ inside the integral in order for G_0 to give a contribution. Therefore, we may approximate

$$T(\mathbf{q}_1, \mathbf{q}_2) \simeq T(\mathbf{q}, \mathbf{q}) \quad (28.234)$$

where $\mathbf{q} = (\mathbf{q}_1 + \mathbf{q}_2)/2$ is the center-of-mass coordinate. It follows that $T_0(\mathbf{k}_0, \mathbf{k}_n) \simeq T_0(\mathbf{k}, \mathbf{k})$. In the mixed representation, we then have

$$\begin{aligned} T(\mathbf{k}, \mathbf{R}) &= \int \frac{d\Delta\mathbf{k}}{(2\pi)^3} T(\mathbf{k}, \Delta\mathbf{k}) e^{i\Delta\mathbf{k}\mathbf{R}} \\ &\simeq \int \frac{d\Delta\mathbf{k}}{(2\pi)^3} T(\mathbf{k}, \mathbf{k}) e^{i\Delta\mathbf{k}\mathbf{R}} \\ &= \int \frac{d\Delta\mathbf{k}}{(2\pi)^3} T_0(\mathbf{k}, \mathbf{k}) e^{i\Delta\mathbf{k}\mathbf{R} - i\Delta\mathbf{k}\mathbf{R}_0} \\ &= T_0(\mathbf{k}, \mathbf{k}) \delta(\mathbf{R} - \mathbf{R}_0). \end{aligned} \quad (28.235)$$

$$(28.236)$$

Above, we used that $T(\mathbf{k}, \Delta\mathbf{k}) = T'(\mathbf{k}_1, \mathbf{k}_2) \simeq T'(\mathbf{k}, \mathbf{k})$ where T' is a different function than T (as remarked initially in this section) and then dropped the ' notation on the T .

We now want to write down the equation of motion in the mixed representation in differential form. We make use of our previous results for the normal impurity self-energy, namely that an integral equation of the type

$$G(\mathbf{k}_0, \mathbf{k}_n) = G_0(\mathbf{k}_0, \mathbf{k}_n) + \int \int \frac{d\mathbf{k}_1 d\mathbf{k}_2}{(2\pi)^6} G_0(\mathbf{k}_0, \mathbf{k}_1) \Sigma(\mathbf{k}_1, \mathbf{k}_2) G(\mathbf{k}_2, \mathbf{k}_n) \quad (28.237)$$

[which follows by rewriting the real-space version $G(1, 2) = G_0(1, 2) + \int d3d4 \dots$ into momentum-space] takes the following form in the mixed representation (see Amundsen thesis section 2.4):

$$[\epsilon\check{\rho}_3 + \frac{1}{2m}(\mathbf{i}\mathbf{k} + \nabla_{\mathbf{R}}/2)^2 + \mu - \check{\Sigma}(\mathbf{k}, \mathbf{R})] \otimes \check{G}(\mathbf{k}, \mathbf{R}) = 1. \quad (28.238)$$

As a side note, after subtracting the "right-handed version" of this equation, one obtains the standard starting point for doing the quasiclassical approximation. Above, $\otimes$ is the Moyal product:

$$G_A(\mathbf{k}, \mathbf{R}) \otimes G_B(\mathbf{k}, \mathbf{R}) = \exp \left[\frac{i}{2} (\nabla_{\mathbf{R}}^A \nabla_{\mathbf{k}}^B - \nabla_{\mathbf{k}}^A \nabla_{\mathbf{R}}^B) G_A(\mathbf{k}, \mathbf{R}) G_B(\mathbf{k}, \mathbf{R}) \right] \quad (28.239)$$

which to the lowest order approximation is a normal product. In particular, if Σ and G are both slowly varying in $\mathbf{R}$ relative the Fermi wavelength, we have $\check{\Sigma} \otimes \check{G} \simeq \check{\Sigma}\check{G}$.

Based on the above equivalence between equations of motion, it follows that since our integral equation for the Green function matrix is

$$G(\mathbf{k}_0, \mathbf{k}_n) = G_0(\mathbf{k}_0, \mathbf{k}_n) + \int \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} G_0(\mathbf{k}_0, \mathbf{q}_1) T(\mathbf{q}_1, \mathbf{q}_2) G_0(\mathbf{q}_2, \mathbf{k}_n), \quad (28.240)$$

the corresponding mixed representation differential equation has to be

$$[\epsilon\check{\rho}_3 + \frac{1}{2m}(\mathbf{i}\mathbf{k} + \nabla_{\mathbf{R}}/2)^2 + \mu - \check{\Sigma}(\mathbf{k}, \mathbf{R})] \otimes \check{G}(\mathbf{k}, \mathbf{R}) - T(\mathbf{k}, \mathbf{R}) \otimes G_0(\mathbf{k}, \mathbf{R}) = 1. \quad (28.241)$$

The expression for $T(\mathbf{k}, \mathbf{R})$ can be written in terms of the quasiclassical Green function

$$g(\mathbf{p}_F, \mathbf{R}) = \frac{\mathbf{i}}{\pi} \int d\xi_{\mathbf{p}} G(\mathbf{p}, \mathbf{R}). \quad (28.242)$$

By using that

$$\int \frac{d\mathbf{Q}}{(2\pi)^3} = \frac{N_0}{V} \int d\xi_{\mathbf{Q}} \int \frac{d\Omega_{\mathbf{Q}}}{4\pi}, \quad (28.243)$$

we obtain

$$\begin{aligned} T(\mathbf{k}, \mathbf{R}) &= \delta(\mathbf{R} - \mathbf{R}_0) T_0(\mathbf{k}, \mathbf{k}) \\ &= \delta(\mathbf{R} - \mathbf{R}_0) [V_0(0) + \int \frac{d\mathbf{Q}}{(2\pi)^3} V_0(\mathbf{k} - \mathbf{Q}) G_0(\mathbf{Q}, \mathbf{R}_0) T_0(\mathbf{Q}, \mathbf{k})] \\ &\simeq \delta(\mathbf{R} - \mathbf{R}_0) [V_0(0) + \frac{N_0}{V} \frac{\pi}{\mathbf{i}} \int \frac{d\Omega_{\mathbf{Q}}}{4\pi} V_0(\mathbf{k} - \mathbf{Q}_F) g_0(\mathbf{Q}_F, \mathbf{R}_0) T_0(\mathbf{Q}_F, \mathbf{k})]. \end{aligned} \quad (28.244)$$

Here, we used that V_0 and T_0 vary slowly with momentum. For the same reason, we may fix $\mathbf{k}$ at $\mathbf{k}_F$. To indicate the approximations we have made, we replace the notation $T \rightarrow t$ and thus obtain

$$t(\mathbf{k}_F, \mathbf{R}) = \delta(\mathbf{R} - \mathbf{R}_0) t_0(\mathbf{k}_F, \mathbf{k}_F) \quad (28.245)$$

where

$$t_0(\mathbf{k}_F, \mathbf{k}_F) = V_0(0) + \frac{N_0}{V} \frac{\pi}{\mathbf{i}} \int \frac{d\Omega_{\mathbf{Q}}}{4\pi} V_0(\mathbf{k}_F - \mathbf{Q}_F) g_0(\mathbf{Q}_F, \mathbf{R}_0) t_0(\mathbf{Q}_F, \mathbf{k}_F). \quad (28.246)$$

Iterating this equation and truncating at second order in V_0 , we obtain

$$t_0 = V_0(0) - \mathbf{i}[\tilde{V}_0(0)]^2 g_0(\mathbf{q}_F, \mathbf{R}_0) \quad (28.247)$$

where we absorbed some coefficients into $\tilde{V}_0(0)$. Since V_0 is weakly dependent on momentum, we approximated $V_0(\mathbf{k}_F - \mathbf{Q}_F) \simeq V_0(0)$. The usual derivation of the Eilenberger equation applied on the extra term $t(\mathbf{k}_F, \mathbf{R}) G(\mathbf{k}, \mathbf{R})$ then gives after applying the left-right trick:

$$\mathbf{i}\hbar \mathbf{v}_F \cdot \nabla_{\mathbf{R}} g + [\epsilon\rho_3 - \Sigma, g] - [t_0, g_0] \delta(\mathbf{R} - \mathbf{R}_0) = 0 \quad (28.248)$$

where $t_0 = -\mathbf{i}\tilde{V}_0^2 g_s(\mathbf{R}_0)$ and g_s is the diffusive quasiclassical Green function (angularly averaged over all momenta directions). The lone $V_0(0)$ in t_0 falls out since it commutes with g_s .

Note that the above result, derived for a single point-impurity. For a line of such impurities requires a modified treatment since the form of $V(\mathbf{q})$ in the case of *e.g.* two impurities located at $\mathbf{R}_a$ and $\mathbf{R}_b$ will be

$$V(\mathbf{q}) = V_a(\mathbf{q}) e^{-\mathbf{i}\mathbf{q}\mathbf{R}_a} + V_b(\mathbf{q}) e^{-\mathbf{i}\mathbf{q}\mathbf{R}_b}. \quad (28.249)$$

In turn, this changes the expression for $T(\mathbf{k}_0, \mathbf{k}_n)$ used above. In Amundsen PRB, one models the interface as an entire plane instead which modifies the treatment further. Thus, the derivation given here is for the simplest case of a single point-impurity acting as the interface. Physically, one would expect that this gives qualitatively similar results as a line of point-impurities if the distance between the impurities is large enough that one may disregard any interference effects because by pairs of them.

Coupling the two materials

With the t -matrix in hand, we now want to couple two materials via an interface. We can do this by expanding Hilbert space into two domains which represent the two sides of the interface. The Green function in this space can then be written as

$$\check{g} = \begin{pmatrix} \check{g}_{11} & \check{g}_{12} \\ \check{g}_{21} & \check{g}_{22} \end{pmatrix} \quad (28.250)$$

where the subscripts 1 and 2 indicate the two materials (could be denoted L and R, alternatively). The matrices $\check{g}_{12(21)}$ are built up from creation and annihilation operators on both sides of the interface. Therefore, they are to be considered as drone amplitudes with no physical meaning. We will ultimately eliminate them from the theory and they need not be specified further. Note that we have both a position coordinate $\mathbf{R}$ and an index $\{1, 2\}$ which now distinguishes the two sides of the interface. Formally, we let all $\check{g}_{ij}$ be defined for all $\mathbf{R}$, but in the end we will be interested in how $\check{g}_{11}$ for $\mathbf{R} \leq \mathbf{R}_0$ couples to $\check{g}_{22}$ for $\mathbf{R} \geq \mathbf{R}_0$ at the interface $\mathbf{R} = \mathbf{R}_0$.

Now, the interface itself is here described as an infinite line of point impurities which mediates tunneling between its two sides (this is different from Amundsen PRB. By the way, note that there is a ρ_3 missing in the definition of $\check{V}$ in the SOC paper with Amundsen). Thus, the point impurities scatter fermions from one side to the other. For simplicity, consider the case of a single point impurity describing the interface below. Such a potential may be described as

$$\check{V} = \begin{pmatrix} 0 & \check{V}_0 \\ \check{V}_0 & 0 \end{pmatrix} \quad (28.251)$$

and this interface potential may be treated as a perturbation in order to use the t -matrix formalism we derived above.

Note that if $\check{V}_0$ is zero, there is no coupling between the two sides 1 and 2. Thus, the unperturbed Green function denoted $\check{g}_0$ takes the form:

$$\check{g}_0 = \begin{pmatrix} \check{g}_{0,1} & 0 \\ 0 & \check{g}_{0,2} \end{pmatrix}. \quad (28.252)$$

It is clear that $\check{g}_0$ satisfies the following equation of motion

$$i\mathbf{k}_F \cdot \nabla \check{g}_0 + [\check{\Sigma}, \check{g}_0] = 0, \quad (28.253)$$

where

$$\check{\Sigma} = \begin{pmatrix} E\check{\rho}_3 + \check{\Sigma}_1 - \check{\Sigma}_{\text{imp}} & 0 \\ 0 & E\check{\rho}_3 + \check{\Sigma}_2 - \check{\Sigma}_{\text{imp}} \end{pmatrix}. \quad (28.254)$$

For the coupled Green function $\check{g}$, we can write the equation of motion in a similar way:

$$i\mathbf{k}_F \cdot \nabla \check{g} + [\check{\Sigma}, \check{g}] = [\check{t}, \check{g}_0]\delta(\mathbf{R} - \mathbf{R}_0), \quad (28.255)$$

which is clearly satisfied by both $\check{g}_{11}$ and $\check{g}_{22}$, as seen from the treatment in the previous subsection. At this point, a mathematically strict derivation requires that we introduce the S -matrix which relates incoming and outgoing trajectories relative the interface as follows:

$$\check{g}_0^{\text{out}} = \check{S} \check{g}_0^{\text{in}} \check{S}^\dagger \quad (28.256)$$

where incoming or outgoing is determined by the sign of $\mathbf{k}_F \cdot \mathbf{n}_{\text{int}}$ where $\mathbf{n}_{\text{int}}$ is the interface normal, to be defined below. The above relation between the Green functions and S can be derived by using boundary conditions for the wavefunctions that are used to construct $\check{g}$, see appendix Amundsen PRB 2019. A few extra details are given here. The relation between G^{in} and G^{out} via the S -matrix is valid at the interface, i.e. $r_{\perp} = 0$. Therefore, we have

$$G^{\text{out}}(\mathbf{r}_{\parallel}, \mathbf{r}'_{\parallel}, r_{\perp} = 0, r'_{\perp} = 0) = S(\mathbf{k})G^{\text{in}}(\mathbf{r}_{\parallel}, \mathbf{r}'_{\parallel}, r_{\perp} = 0, r'_{\perp} = 0)S^{\dagger}(\mathbf{k}). \quad (28.257)$$

We now express the GFs in center of mass and relative coordinate and then Fourier-transform the $\parallel$ component of the relative coordinate to get:

$$G^{\text{out}}(\mathbf{k}_{\parallel}, \mathbf{R}_{\parallel}, R_{\perp} = 0, r_{\perp} = 0) = S G^{\text{in}}(\mathbf{k}_{\parallel}, \mathbf{R}_{\parallel}, R_{\perp} = 0, r_{\perp} = 0)S^{\dagger}. \quad (28.258)$$

The center of mass coordinate $\mathbf{R} = (R_{\perp}\hat{n} = 0, \mathbf{R}_{\parallel})$ corresponds to a point on the interface. Let us drop these coordinates and thus implicitly work with the Green functions at the interface. Since

$$G(r_{\perp} = 0) \propto \int dk_{\perp} G(k_{\perp}) \quad (28.259)$$

in general, we may write

$$\int dk_{\perp} G^{\text{out}}(\mathbf{k}) = S \int dk_{\perp} G^{\text{in}} S^{\dagger}. \quad (28.260)$$

But precisely such an integral over $k_{\perp}$ is dealt with when deriving the quasiclassical t -matrix for the interface potential earlier in the paper. Using the general Green function gives essentially $g^{+} + g^{-}$ where g is the quasiclassical Green function and $\pm$ indicates momentum toward or away from interface. Therefore, the $^{\text{out}}$ and $^{\text{in}}$ GFs give rise to either g^{+} or g^{-} in the above case. This completes the derivation.

Consider now the upper left block of Eq. (28.255) and integrate it from $\mathbf{R}_0^{-}$ to $\mathbf{R}_0^{+}$. Recall that we are interested in $\check{g}_{11}$ for $\mathbf{R} \leq \mathbf{R}_0$ and $\check{g}_{22}$ for $\mathbf{R} \geq \mathbf{R}_0$, even though both objects are defined formally for all $\mathbf{R}$. That is, $\check{g}_{11}$ is described by $E\check{\rho}_3 + \check{\Sigma}_1 - \check{\Sigma}_{\text{imp}}$ in its equation of motion even for $\mathbf{R} \geq \mathbf{R}_0$. Now, since we are integrating from $\mathbf{R}_0^{-}$ to $\mathbf{R}_0^{+}$ and $\mathbf{n}_{\text{int}}$ from now on is defined to point from 1 to 2 (R_0^{-} to R_0^{+}), we obtain

$$\check{g}_{11}(\mathbf{k}_F, R_0^{+}) - \check{g}_{11}(\mathbf{k}_F, R_0^{-}) = \frac{1}{i\mathbf{k}_F \cdot \mathbf{n}_{\text{int}}} [\check{t}_{11}, \check{g}_{0,11}(R_0)] \quad (28.261)$$

where

$$\check{t}_{11} = -i\tilde{V}_0 g_{0,22,s} \tilde{V}_0. \quad (28.262)$$

The s subscript means it is the isotropic (diffusive) component of the Green function. Above, we have only written out the dependence on $R_0^{\pm}$ which we define as the x -component of the vector $\mathbf{R}_0^{\pm}$. Here, one could if desirable define "in" and "out" notation depending on whether the Green function is evaluated for a trajectory pointing away from or toward the interface. For instance, one could define

$$\begin{aligned} \check{g}_{11}^{\text{in}}(R_0^{-}) &\equiv \check{g}_{11}[\text{sign}(\mathbf{k}_F \cdot \mathbf{n}_{\text{int}}) > 0, R_0^{-}], \\ \check{g}_{11}^{\text{out}}(R_0^{-}) &\equiv \check{g}_{11}[\text{sign}(\mathbf{k}_F \cdot \mathbf{n}_{\text{int}}) < 0, R_0^{-}], \\ \check{g}_{11}^{\text{in}}(R_0^{+}) &\equiv \check{g}_{11}[\text{sign}(\mathbf{k}_F \cdot \mathbf{n}_{\text{int}}) < 0, R_0^{+}], \\ \check{g}_{11}^{\text{out}}(R_0^{+}) &\equiv \check{g}_{11}[\text{sign}(\mathbf{k}_F \cdot \mathbf{n}_{\text{int}}) > 0, R_0^{+}]. \end{aligned} \quad (28.263)$$

since $\mathbf{n}_{\text{int}}$ was defined to point from left to right (1 to 2).

To formulate boundary conditions on one side of the interface, for instance for $\check{g}_{11}$ at R_0^- , we need to eliminate $\check{g}_{11}(\mathbf{k}_F, R_0^+)$ from Eq. (28.261). This can be done by making use of a generalized normalization condition due to Shelankov. Details of how to derive this normalization condition is given in Appendix A in the paper by Amundsen. In what follows, we outline this procedure for the objects $\check{g}$ and $\check{g}_0$. However, note that due to the matrix structure of these objects given earlier in this text, the normalization condition also holds for $\check{g}_{11}$ and $\check{g}_{22}$.

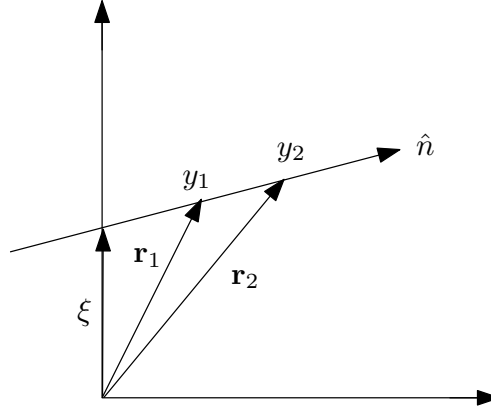


Figure 28.9: (Color online) The coordinates that are used to define the trajectory Green function $\check{g}_{\mathbf{n}}$.

The procedure makes use of the trajectory Green function $g_{\mathbf{n}}(y_1, y_2)$ which can be used to express the quasiclassical Green function via (see Shelankov)

$$\check{g}(\mathbf{k}_F, \mathbf{R}) = \check{g}_+(\mathbf{k}_F, \mathbf{r}_p, y, y) + \check{g}_-(\mathbf{k}_F, \mathbf{r}_p, y, y), \quad (28.264)$$

where

$$\check{g}_{\pm}(\mathbf{n}, \mathbf{r}_p, y, y) = \lim_{\epsilon \rightarrow 0} \check{g}_{\mathbf{n}}(\mathbf{r}_p, y \pm \epsilon, y). \quad (28.265)$$

The parameters y_1 and y_2 are two points connected by a straight line that is collinear with $\mathbf{k}_F$ and $\mathbf{r}_p$ is the location of the interface potential in a plane perpendicular to this straight line. Thus, $\mathbf{R} = y\hat{\mathbf{k}}_F + \mathbf{r}_p$. Thus, y_1 and y_2 are here coordinates along a straight line trajectory which is not the actual y -axis in general. We can also define the trajectory Green function more generally as follows

$$\check{g}_{\mathbf{n}}(y_1, y_2) = \begin{cases} \check{g}_+(\xi + y_1\mathbf{n}, \xi + y_2\mathbf{n}) & \text{if } y_1 > y_2, \\ \check{g}_-(\xi + y_1\mathbf{n}, \xi + y_2\mathbf{n}) & \text{if } y_1 < y_2. \end{cases} \quad (28.266)$$

The objects $g_{\pm}$ satisfy equations of motions (see Shelankov and Amundsen thesis):

$$\pm i\hbar v_F \hat{\mathbf{r}} \cdot \nabla_1 \check{g}_{\pm} + [\epsilon \check{\rho}_3 - \check{V}] \check{g}_{\pm} = 0. \quad (28.267)$$

Here, $\nabla_1 = \nabla_{\mathbf{r}_1}$ and $\hat{\mathbf{r}}$ is a unit vector in the $(\mathbf{r}_1 - \mathbf{r}_2)$ direction. Because of this, the trajectory Green function can be shown to satisfy the equation of motion

$$i\hbar v_F \frac{\partial}{\partial y_1} \check{g}_{\mathbf{n}} + [\epsilon \check{\rho}_3 - \check{V}(y_1)] \check{g}_{\mathbf{n}} = i\hbar v_F \delta(y_1 - y_2). \quad (28.268)$$

Its validity for $y_1 - y_2 = 0$ becomes clear after introducing Eq. (28.270) below, but its validity for $y_1 \neq y_2$ can be seen as follows. First, consider the case $y_1 > y_2$. In that case, the derivative term above is $i\hbar v_F \frac{\partial}{\partial y_1} g_+(y_1, y_2)$. This is consistent with Eq. (28.267) by noting that $\nabla_1 = \nabla_{\mathbf{r}_1} = \frac{\partial}{\partial y_1} \hat{n}$ since $\mathbf{r}_1 = \xi + y_1 \mathbf{n}$ where ξ is a constant. Moreover, for $y_1 > y_2$ we have $\hat{r} = +\hat{n}$ as seen by subtracting $\mathbf{r}_1$ and $\mathbf{r}_2$. Therefore, we get $+i\hbar v_F \hat{r} \cdot \nabla_1 g_+ = i\hbar v_F \frac{\partial}{\partial y_1} g_+$.

If we instead had $y_1 < y_2$, then Eq. (28.268) has a derivative term $i\hbar v_F \frac{\partial}{\partial y_1} g_-(y_1, y_2)$. This is consistent with Eq. (28.267) by noting that $\nabla_1 = \nabla_{\mathbf{r}_1} = \frac{\partial}{\partial y_1} \hat{n}$ still holds since $\mathbf{r}_1 = \xi + y_1 \mathbf{n}$ where ξ is a constant. Moreover, for $y_1 < y_2$ we have $\hat{r} = -\hat{n}$ as seen by subtracting $\mathbf{r}_1$ and $\mathbf{r}_2$. Therefore, we get $+i\hbar v_F \hat{r} \cdot \nabla_1 g_- = -i\hbar v_F \frac{\partial}{\partial y_1} g_-$.

By considering the Gor'kov equation where the derivative is with respect to $\mathbf{r}_2$ rather than $\mathbf{r}_1$, one derives an analogous equation to Eq. (28.267) from which it follows that the trajectory Green function also satisfies:

$$-i\hbar v_F \frac{\partial}{\partial y_2} \check{g}_{\mathbf{n}} + \check{g}_{\mathbf{n}}[\epsilon \check{\rho}_3 - \check{V}(y_2)] = i\hbar v_F \delta(y_1 - y_2). \quad (28.269)$$

Here, $\check{V}$ is for instance an impurity potential experienced by the particle, but not the interface potential. The above equations may be generalized to include self-energies as well, but this is not included here to keep the notation lighter and does not change the following procedure.

The trajectory Green function satisfies two important relations (see Shelankov):

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} [\check{g}_{\mathbf{n}}(y + \epsilon, y) + \check{g}_{\mathbf{n}}(y - \epsilon, y)] &= \check{g}(\mathbf{n}, y), \\ \lim_{\epsilon \rightarrow 0} [\check{g}_{\mathbf{n}}(y + \epsilon, y) - \check{g}_{\mathbf{n}}(y - \epsilon, y)] &= \check{1}. \end{aligned} \quad (28.270)$$

In other words, we can obtain the quasiclassical Green function $\check{g}(\mathbf{k}_F, \mathbf{R})$ by computing the trajectory Green function for a trajectory $\mathbf{n} \parallel \mathbf{k}_F$. This is seen by noting that (see Amundsen thesis eqs. 2.58, 2.63, 2.71):

$$\check{g}(\mathbf{n}) = \frac{i}{\pi} \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} d\xi_k \cos[\xi_k \epsilon / \hbar v_F] \check{G}(\mathbf{R}, k\mathbf{n}), \quad (28.271)$$

whereas the standard definition of the quasiclassical Green function is

$$\check{g}(\mathbf{k}_F) = \frac{i}{\pi} \int_{-\omega_c}^{\omega_c} d\xi_k \check{G}(\mathbf{R}, \mathbf{k}). \quad (28.272)$$

with $\xi_k = \mathbf{k}^2/2m - \mu$. The only difference is that a hard cutoff is used in the latter equation. So $\mathbf{n}$ in $\check{g}$ is equivalent to $\mathbf{k}_F$ in the quasiclassical Green function.

Consider now the object

$$\check{A}(y) = \check{g}_{\mathbf{n}}(y_1, y) \check{g}_{\mathbf{n}}^0(y, y_2) \quad (28.273)$$

where $\check{g}_{\mathbf{n}}$ is the trajectory Green function. Consider the region $y < y_1 < y_2 < y^*$ where y^* is the position of the interface along the trajectory. Now choose a trajectory $\mathbf{n}$ directed toward the interface on side 1, as shown in Fig. 28.10(a). Moving deep into material 1 (i.e. in the direction of $\mathbf{s}$) along this trajectory corresponds to $y \rightarrow -\infty$ when $\mathbf{n} = -\mathbf{s}$, as seen from the definition of $\check{g}_{\mathbf{n}}$. For $y \rightarrow -\infty$, $\check{A} = 0$ since the relative coordinate of the Green function becomes infinite. One may

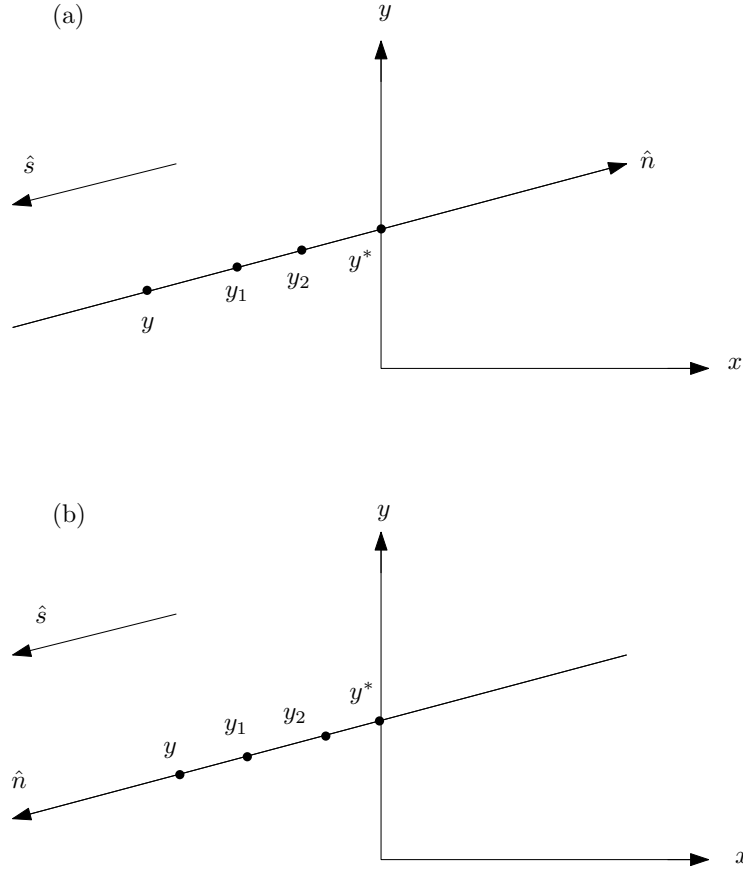


Figure 28.10: (Color online) The geometries considered to derive generalized normalization conditions, starting with the object $\check{A}(y)$ and various trajectories relative the interface. The situations depicted are relevant to derive generalized normalization conditions on the left side of the interface, R_0^- . Note that the y -coordinate along $\hat{n}$ is a different coordinate than the y -axis indicated.

show that $d\check{A}/dy = 0$ except at special points by using Eqs. (28.268) and (28.270) (see Amundsen thesis), and thus we conclude that $\check{A} = 0$ at all points y such that $y < y_1 < y_2 < y^*$. We then take the limit $y = y_2 - \epsilon$ with $\epsilon \rightarrow 0^+$. This gives

$$\check{g}_+(y, y)\check{g}_-^0(y, y) = 0. \quad (28.274)$$

Using that $\check{g} = \check{g}_+ + \check{g}_-$ and $\check{g}_+ - \check{g}_- = I$, it follows that

$$(\check{g}_{11} + I)(\check{g}_{0,11} - I) = 0 \quad (28.275)$$

We can derive a similar normalization condition

$$(\check{g}_{0,11} + I)(\check{g}_{11} - I) = 0 \quad (28.276)$$

again for $\text{sgn}(\mathbf{n} \cdot \mathbf{s}) = 1$ by doing the same analysis on the object $\check{A}(y) = \check{g}_\mathbf{n}^0(y_1, y)\check{g}_\mathbf{n}(y, y_2)$ instead.

Now, we still consider material 1, i.e. a point R_0^- , but a trajectory $\mathbf{n} \parallel \mathbf{s}$, i.e. a trajectory $\mathbf{n}$ pointing away from the interface. In this case, the bulk of material 1 is reached for $y \rightarrow \infty$.

Therefore, considering now $y > y_1 > y_2 > y^*$ and an outgoing trajectory $\text{sgn}(\mathbf{n} \cdot \mathbf{s}) = -1$, one obtains

$$\begin{aligned}(\check{g}_{11} - I)(\check{g}_{0,11} + I) &= 0, \\ \check{g}_{0,11} - I)(\check{g}_{11} + I) &= 0.\end{aligned}\tag{28.277}$$

We have now derived a generalized normalization condition for the Green function on side 1, i.e. R_0^- for both a trajectory toward and away from the interface. We can repeat the same analysis on side 2, i.e. the point R_0^+ . In that case, we see that for a trajectory $\mathbf{n}$ pointing into the bulk of material 2, it is $y \rightarrow \infty$ that corresponds to that bulk region where $\check{A} = 0$. Thus, for such a trajectory $\mathbf{n} \parallel \mathbf{n}_{\text{int}}$, we consider $y > y_1 > y_2 > y^*$ and get

$$\begin{aligned}(\check{g}_{11} + I)(\check{g}_{0,11} - I) &= 0, \\ \check{g}_{0,11} + I)(\check{g}_{11} - I) &= 0.\end{aligned}\tag{28.278}$$

For the opposite trajectory $\mathbf{n} \parallel -\mathbf{n}_{\text{int}}$, we have to consider $y < y_1 < y_2 < y^*$ since it is $y \rightarrow \infty$ that reaches the bulk of material 2. Thus, we get

$$\begin{aligned}(\check{g}_{11} - I)(\check{g}_{0,11} + I) &= 0, \\ \check{g}_{0,11} - I)(\check{g}_{11} + I) &= 0.\end{aligned}\tag{28.279}$$

Both of the above equations are thus valid for R_0^+ .

This means that the generalized normalization condition finally takes the following general form

$$\begin{aligned}[\check{g}_\sigma(R_0^\pm) \mp \sigma][\check{g}_{0,\sigma}(R_0^\pm) \pm \sigma] &= 0, \\ [\check{g}_{0,\sigma}(R_0^\pm) \mp \sigma][\check{g}_\sigma(R_0^\pm) \pm \sigma] &= 0\end{aligned}\tag{28.280}$$

where $\sigma = \text{sgn}(\mathbf{n} \cdot \mathbf{n}_{\text{int}})$ with $\mathbf{n}_{\text{int}}$ pointing from 1 to 2. In the above equation, $\check{g}$ may be replaced with $\check{g}_{jj}$, as we did above. Note that R_0^- is in material 1 and R_0^+ is in material 2.

From now on, consider only $\check{g}_{11}$ and omit the $\check{\cdot}$ and $_{11}$ notation for brevity. Then, we know from Eq. (28.261) that

$$g_\sigma(R_0^+) - g_\sigma(R_0^-) = \frac{\sigma}{i|v_n|}[t, g_0(R_0)].\tag{28.281}$$

To formulate the boundary condition for material 1, we wish to eliminate $g(R_0^+)$ from the above equation. To do so, insert the equation into Eqs. (28.280) evaluated for R_0^+ to eliminate $g(R_0^+)$:

$$\begin{aligned}[g_\sigma(R_0^-) + D_\sigma - \sigma][g_{0,\sigma}(R_0^+) + \sigma] &= 0, \\ [g_{0,\sigma}(R_0^+) - \sigma][g_\sigma(R_0^-) + D_\sigma + \sigma] &= 0.\end{aligned}\tag{28.282}$$

We defined

$$D_\sigma \equiv \frac{\sigma}{i|v_n|}[t, g_0(R_0)].\tag{28.283}$$

We see that we also need to eliminate $g_{0,\sigma}(R_0^+)$ in order to formulate boundary conditions involving exclusively Green functions depending on the R_0^- coordinate. Since $g_{0,\sigma}$ satisfies Eq. (28.281) with $t = 0$, we may set $g_{0,\sigma}(R_0^+) = g_{0,\sigma}(R_0^-)$. Although g_0 is referred to as the Green function

satisfying impenetrable boundary conditions, this means in practice that there is no coupling between g_{11} and g_{22} . It does not prevent g_{jj} from existing on both sides of R_0 , as previously remarked.

We are then left with

$$\begin{aligned} [(g_\sigma(R_0^-) + \sigma) + D_\sigma - 2\sigma][(g_{0,\sigma}(R_0^-) - \sigma) + 2\sigma] &= 0, \\ [(g_{0,\sigma}(R_0^-) + \sigma) - 2\sigma][(g_\sigma(R_0^-) - \sigma) + D_\sigma + 2\sigma] &= 0. \end{aligned} \quad (28.284)$$

We can now use Eqs. (28.280) for R_0^- to simplify the above to:

$$\begin{aligned} (g_\sigma(R_0^-) + \sigma)2\sigma + (D_\sigma - 2\sigma)(g_{0,\sigma}(R_0^-) - \sigma) + 2\sigma(D_\sigma - 2\sigma) &= 0, \\ (g_{0,\sigma}(R_0^-) + \sigma)(D_\sigma + 2\sigma) - 2\sigma(g_\sigma(R_0^-) - \sigma) - 2\sigma(D_\sigma + 2\sigma) &= 0. \end{aligned} \quad (28.285)$$

Subtract these equations to obtain

$$4\sigma g_\sigma(R_0^-) + 4\sigma D_\sigma + (D_\sigma - 2\sigma)(g_{0,\sigma}(R_0^-) - \sigma) - (g_{0,\sigma}(R_0^-) + \sigma)(D_\sigma + 2\sigma) = 0. \quad (28.286)$$

Dividing on 4σ and cancelling terms, we get

$$g_\sigma(R_0^-) = g_{0,\sigma}(R_0^-) - \frac{D_\sigma}{2} - \frac{1}{4\sigma}[D_\sigma, g_{0,\sigma}(R_0^-)]. \quad (28.287)$$

The commutator is

$$\begin{aligned} [D_\sigma, g_{0,\sigma}] &= \frac{\sigma}{i|v_n|} [[t, g_{0,\sigma}], g_{0,\sigma}] \\ &= \frac{\sigma}{i|v_n|} [[t, g_{0,\sigma} + \sigma], g_{0,\sigma} - \sigma]. \end{aligned} \quad (28.288)$$

Now we can use that

$$[g_{0,\sigma} \pm 1][g_{0,\sigma} \mp 1] = 0 \quad (28.289)$$

since $(g_{0,\sigma})^2 = 1$. The commutator then ends up as:

$$[D_\sigma, g_{0,\sigma}] = \frac{\sigma}{i|v_n|} (2t - 2g_{0,\sigma}tg_{0,\sigma}). \quad (28.290)$$

Above, all occurrences of $g_{0,\sigma}$ are $g_{0,\sigma}(R_0^-)$. By approximating $g_{0,\sigma}(R_0^-) \simeq g_{0,\sigma}(R_0)$ [which is reasonable since we know that $g_{0,\sigma}(R_0^-) = g_{0,\sigma}(R_0^+)$], we get

$$\check{g}_{\sigma,11}(R_0^-) = \check{g}_{0,\sigma,11}(R_0^-) - \frac{\sigma}{2i|v_n|} [\check{t}, \check{g}_{0,\sigma,11}(R_0^-)] - \frac{\check{t}}{2i|v_n|} + \frac{1}{2i|v_n|} \check{g}_{0,\sigma,11}(R_0^-) \check{t} \check{g}_{0,\sigma,11}(R_0^-). \quad (28.291)$$

This can be rewritten as

$$\check{g}_{\sigma,11}(R_0^-) = \check{g}_{0,\sigma,11}(R_0^-) + \frac{1}{2i|v_n|} [\check{g}_{0,\sigma,11}(R_0^-) - \sigma] \check{t} [\check{g}_{0,\sigma,11}(R_0^-) + \sigma]. \quad (28.292)$$

which is precisely the corresponding equations in Amundsen PRB 2019 and also agrees with Eschrig NJP 2015. Recall that $\sigma = \text{sgn}(\mathbf{k}_F \cdot \mathbf{n}_{\text{int}})$.

At this point, we make use of the fact that the matrix current flowing in the $\mathbf{n}_{\text{int}}$ -direction defined as

$$\begin{aligned}\check{I}_{jj} &= \int dE d\Omega_{\mathbf{p}_F} \mathbf{n}_{\text{int}} \cdot \mathbf{p}_F \check{g}_{jj} \\ &= \int dE d\Omega_{\mathbf{p}_F, \text{half}} \mathbf{n}_{\text{int}} \cdot \mathbf{p}_F (\check{g}_{jj}^{\text{in}} - \check{g}_{jj}^{\text{out}})\end{aligned}\quad (28.293)$$

is conserved across the isotropization zone, as shown in Cottet *et al.* PRB 2009. The integral on the second line is over a hemisphere relative the interface, since we distinguished between incoming and outgoing trajectories in the second line when doing the angular average. As a corollary, the electric current obtained by taking trace of $\check{\rho}_3 \check{I}$ is naturally also conserved, actually not just across the isotropization zone but also when going from material 1 to 2. The matrix current, however, is generally not conserved when going from material 1 to 2.

In the diffusive limit, the matrix current flowing in the $\mathbf{n}_{\text{int}}$ -direction takes the form (shown in JP Morten thesis):

$$\check{I}_{jj} \propto \int dE \check{g}_{jj,s} \partial_{n_{\text{int}}} \check{g}_{jj,s}. \quad (28.294)$$

Here, we will consider material 1, $jj = 11$. We now wish to consider the above expression right at the beginning of the isotropization zone and connect it to Eq. (28.293). Recall that $\check{g}_0$ is the Green function solving the Usadel equation without the t -matrix, but *with* the full Green function $\check{g}$ in the impurity self-energy. Thus, $\check{g}_0$ has to equal $\check{g}$ at the beginning of the isotropization zone, which is shown in Sec. 28.5.1. But first, a brief discussion about the angular integration in Eq. (28.293) in different dimensions.

Angular averaging of current

Eq. (15) in <https://ntnuopen.ntnu.no/ntnu-xmlui/bitstream/handle/11250/2635872/qcsoc.pdf?sequence=1&isAllowed=y> comes from the left-hand side of eq. (46) in https://ntnuopen.ntnu.no/ntnu-xmlui/bitstream/handle/11250/2462583/Eschrig_2015_New_J._Phys._17_083037.pdf?sequence=4.

In other words, eq. (15) expresses a summation over $g^i - g^o$ for all possible transverse modes. This is the lhs of the equation in Eschrig's paper. As an integral over angles, we have obtained the equation (28.293).

Consider first 1D. There are no transverse modes. Hence, there is only one term in the $\sum_n$ in Eschrig's paper and only the normal mode contributes.

Consider now 2D. There exists transverse modes. Assume the interface normal is x so that the transverse modes are k_y . The summation turns into an integral as follows:

$$\sum_n \propto \int dk_y \quad (28.295)$$

Now, we can parametrize $k_y = k_F \sin \phi$ where $\phi \in [-\pi/2, \pi/2]$ in order to cover all values from $k_y = -k_F$ to $k_y = k_F$. Assume $k_F = 1$ for simplicity. Then, we get

$$\int_{-1}^1 dk_y = \int_{-\pi/2}^{\pi/2} d\phi \cos \phi. \quad (28.296)$$

It is clear that normal-modes $\phi = 0$ are weighted the most strongly in the angular averaging over transverse modes due to the $\cos \phi$ factor.

Consider now 3D. In this case, just like in 1D and 2D, one might expect physically that the normal mode also contributes the strongest. However, this turns out to not be the case. Assume the interface normal is z , as in Amundsen PRB 2019. Thus, we need to perform a summation over all transverse modes k_x and k_y :

$$\sum_n \propto \int \int dk_x dk_y. \quad (28.297)$$

We need to perform this summation with the restriction that the length of $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$ is constant (equal to $k_F = 1$). Therefore, we need to perform the double integral over a circle in the $k_x - k_y$ -plane with radius 1. That will include all possible transverse modes. So we have

$$\sum_n I_{nn} \propto \int \int_{\text{unit circle in } k_x - k_y\text{-plane}} dk_x dk_y (g^i - g^o). \quad (28.298)$$

The unit circle can be written in terms of two new coordinates: r and ϕ where r is the radius in the $k_x - k_y$ -plane. In effect, we are switching to polar coordinates. We get:

$$\int \int_{\text{unit circle in } k_x - k_y\text{-plane}} dk_x dk_y (g^i - g^o) = \int_0^1 \int_0^{2\pi} r dr d\phi (g^i - g^o). \quad (28.299)$$

But the radius r in the $k_x - k_y$ -plane does not depend on ϕ : it depends only on the polar angle θ (in other words, the interface normal angle θ), namely $r = k_F \sin \theta = \sin \theta$ since $k_F = 1$. Then $dr = \cos \theta d\theta$ and we may rewrite:

$$\sum_n I_{nn} \propto \int_0^{\pi/2} \int_0^{2\pi} \cos \theta \sin \theta d\theta d\phi. \quad (28.300)$$

Despite the normal mode $\theta = 0$ having zero weight, this makes sense after all since in 3D there are much fewer modes available at $\theta = 0$ (no ϕ -dependence there) than at finite θ (where all ϕ can contribute).

Thus, we obtain the matrix current

$$\check{I} = \int_{\text{hemisphere}} \frac{d\Omega}{2\pi} \hat{n} \cdot \mathbf{v}_F (\check{g}_{jj}^i - \check{g}_{jj}^o) \propto \int_0^{\pi/2} \int_0^{2\pi} \sin \theta d\theta d\phi \hat{n} \cdot \mathbf{v}_F (\check{g}_{jj}^i - \check{g}_{jj}^o). \quad (28.301)$$

In the final boundary condition, we will end up with a $1/|v_n|$ factor which cancels the $\cos \theta$. The remaining integral over $\sin \theta$ is finite.

Isotropization zone

The discussion so far has been concerned with Green functions that solve the Gor'kov and, later, the Eilenberger equation. However, the ultimate aim is to derive boundary conditions for the diffusive Green function satisfying the Usadel equation. A key insights is that regardless of how dirty a material is, a particle having tunneled through the interface will travel at least a distance l_{mfp} before it encounters its first impurity. This means that, surrounding the interface, there will always be a thin boundary layer in which the particles are governed by ballistic Green functions. This is

known as the ballistic zone.

Far away from the interface, many scatterings have randomized the motion of the particle which is not diffusive. This is the diffusive zone. But what happens between the ballistic and diffusive zone? This is the so-called isotropization zone. In this region, it is assumed that the impurity potential dominates all other self-energies. The size of the isotropization zone should also be on the scale of the mean free path, so that it is much smaller than the length scale over which the diffusive Green function $\check{g}_s$ varies. In the isotropization zone, the Eilenberger equation reduces to:

$$\mathbf{v}_F \cdot \nabla \check{g}_{0,11} + \frac{1}{2\tau} [\check{g}_{s,11}, \check{g}_{0,11}] = 0. \quad (28.302)$$

Consider an incoming Green function along a trajectory directed along $\mathbf{n}_{\text{int}}$, meaning $\mathbf{k}_F \parallel \mathbf{n}_{\text{int}}$, and let r denote the coordinate along this trajectory. Moreover, let r_0 denote the intersection between this trajectory and the interface. The equation of motion then becomes

$$\frac{d}{dr} \check{g}_{0,11}^{\text{inc}} + \frac{1}{2\tau v_F} [\check{g}_{s,11}, \check{g}_{0,11}^{\text{inc}}] = 0. \quad (28.303)$$

The following ansatz is a reasonable solution describing the transition from a ballistic to a diffusive Green function as one moves away from the interface:

$$\check{g}_{0,11}^{\text{inc}}(r) = [\check{g}_{0,11}^{\text{inc}}(r_0) - \check{g}_{s,11}] e^{-|r-r_0|/\tau v_F} + \check{g}_{s,11}. \quad (28.304)$$

Here, r_0 is the point where the trajectory intersects the interface. Thus, the solution interpolates between the ballistic Green function $g_{0,11}$ at $r = r_0$ satisfying impenetrable boundary conditions and the diffusive Green function $g_{s,11}$ at the beginning of the isotropization zone where $r - r_0$ is of order a few mean free paths l_{mfp} . Inserting the ansatz into the Eilenberger equation, we see that in order for it to be a solution, the following has to be satisfied:

$$2[\check{g}_{0,11}^{\text{inc}}(r_0) - \check{g}_{s,11}] = -[\check{g}_{s,11}, \check{g}_{0,11}^{\text{inc}}(r_0)]. \quad (28.305)$$

Squaring both sides of this equation and using the normalization of both $\check{g}_0$ and $\check{g}$, we get

$$4[2 - \{g_{0,11}^{\text{inc}}, g_{s,11}\}] = \left(\{g_{0,11}^{\text{inc}}, g_{s,11}\} + 2\right) \left(\{g_{0,11}^{\text{inc}}, g_{s,11}\} - 2\right) \quad (28.306)$$

where we dropped the $\check{\cdot}$ notation for brevity. The above equation is clearly satisfied when

$$\{g_{0,11}^{\text{inc}}, g_{s,11}\} = 2. \quad (28.307)$$

Combining Eqs. (28.305) and (28.307), we find that the incoming Green function must satisfy the conditions

$$\begin{aligned} (g_{0,11}^{\text{inc}} + 1)(g_{s,11} - 1) &= 0, \\ (g_{s,11} + 1)(g_{0,11}^{\text{inc}} - 1) &= 0. \end{aligned} \quad (28.308)$$

A similar analysis for the outgoing Green function with $\mathbf{k}_F \parallel -\mathbf{n}_{\text{int}}$ yields

$$\begin{aligned} (g_{0,11}^{\text{out}} - 1)(g_{s,11} + 1) &= 0, \\ (g_{s,11} - 1)(g_{0,11}^{\text{out}} + 1) &= 0. \end{aligned} \quad (28.309)$$

This is derived by considering a trajectory $\mathbf{k}_F \parallel -\mathbf{n}_{\text{int}}$. Letting r still be a coordinate along the $\mathbf{k}_F \parallel +\mathbf{n}_{\text{int}}$ trajectory, so that r and r_0 have the same meaning as before, we get

$$-\frac{d}{dr}\check{g}_{0,11}^{\text{out}} + \frac{1}{2\tau v_F}[\check{g}_{s,11}, \check{g}_{0,11}^{\text{out}}] = 0. \quad (28.310)$$

Then, we can use the same ansatz as before.

These equations provide an important relationship between the diffusive Green function at the beginning of the isotropization zone and their ballistic counterparts right at the interface. For plain interfaces with $S = 1$, we see from an earlier equation that $g_{0,11}^{\text{inc}} = g_{0,11}^{\text{out}}$. Thus, the above equations can only be satisfied if $g_{0,11}^{\text{inc}} = g_{0,11}^{\text{out}} = g_{11,s}$. It is for this reason that we did not need to specify whether $g_{0,11}$ in the commutator obtained when integrating the Eilenberger equation was incoming or outgoing: the result is the same in both cases.

Therefore, since $\check{g}_{0,11}^{\text{inc}} = \check{g}_{0,11}^{\text{out}} = \check{g}_{11,s}$ for a plain interface, and similarly $\check{t}_{11} \rightarrow \check{t}_{11,s}$, we get from Eq. (28.292) that

$$\begin{aligned} \check{g}_{11}^{\text{inc}} &= \check{g}_{11,s} + \frac{1}{2i|v_n|}(\check{g}_{11,s} - I)\check{t}_{s,11}(\check{g}_{11,s} + I), \\ \check{g}_{11}^{\text{out}} &= \check{g}_{11,s} + \frac{1}{2i|v_n|}(\check{g}_{11,s} + I)\check{t}_{s,11}(\check{g}_{11,s} - I). \end{aligned} \quad (28.311)$$

Since we need the difference $\check{g}_{11}^{\text{out}} - \check{g}_{11}^{\text{inc}}$ for the boundary conditions [here, we are using the out and in notation defined earlier, which really refers to the direction of $\mathbf{k}_F$ relative the interface normal $\mathbf{n}_{\text{int}}$], we use Eq. (28.311) to subtract the equations and get:

$$\check{g}_{11}^{\text{out}} - \check{g}_{11}^{\text{inc}} = \frac{i}{|v_n|}[\check{t}_{11,s}, \check{g}_{11,s}]. \quad (28.312)$$

Inserting this into Eq. (28.293), we finally obtain

$$\check{g}_{11,s}\partial_{n_{\text{int}}}\check{g}_{11,s} \propto \tilde{V}_0^2[\check{g}_{11,s}, \check{g}_{22,s}]. \quad (28.313)$$

where we reinstated the $\check{\cdot}$ notation. This is the standard Kupriyanov-Lukichev boundary condition and completes the derivation. Note that if we wanted the boundary conditions for $\check{g}_{22,s}$, we would have used

$$\begin{aligned} \check{g}_{22}^{\text{in}} &= \check{g}_{22,s} + \frac{1}{2i|v_n|}(\check{g}_{22,s} + I)\check{t}_{s,22}(\check{g}_{22,s} - I), \\ \check{g}_{22}^{\text{out}} &= \check{g}_{22,s} + \frac{1}{2i|v_n|}(\check{g}_{22,s} - I)\check{t}_{s,22}(\check{g}_{22,s} + I) \end{aligned} \quad (28.314)$$

which we showed how to derive earlier. This gives an extra sign change so that

$$\check{g}_{22}^{\text{out}} - \check{g}_{22}^{\text{inc}} = -\frac{i}{|v_n|}[\check{t}_{22,s}, \check{g}_{22,s}]. \quad (28.315)$$

But in addition, g_{22}^{in} and g_{22}^{out} change place in the matrix current since "in" denotes opposite directions in material 1 and 2 (similarly for "out"). This compensates the above sign change. Therefore, we also get

$$\check{g}_{22,s}\partial_{n_{\text{int}}}\check{g}_{22,s} \propto \tilde{V}_0^2[\check{g}_{11,s}, \check{g}_{22,s}]. \quad (28.316)$$

A note in the context of antiferromagnetic quasiclassical theory and compensated vs. uncompensated interfaces. It is interesting to note that one can escape the requirement of an isotropization zone close to the interface, and still approximate the quasiclassical Green function as close to isotropic near the interface, if one assumes a rough interface. The rough interface will strongly suppress *e.g.* *d*-wave superconductivity even without impurities, whereas it has no effect on *s*-wave superconductivity. In this way, assuming a rough interface, one does not have to postulate an isotropization zone and the diffusive Green function can be applied right up to the interface (rather than a few mean free paths away from it).

This becomes a bit more complicated when considering antiferromagnetic interfaces which can be compensated or uncompensated. A compensated interface can still be considered rough, since the assumption of a rough interface is still consistent with equally many atoms from each sublattice (on average) next to the interface. An uncompensated interface is more tricky to reconcile with interface roughness, since an uncompensated interface is supposed to be atomically sharp in order to have all atoms belonging to the same sublattice at the interface.

However, there is a way out of this conundrum. If the antiferromagnet consists of a material where different atoms provide localized spins up and spin down, then one of the atoms can have a stronger coupling to the other material than the other type of atom. Then, even in the presence of a rough interface, the effective coupling across the interface acts as uncompensated. Depending on which AFM material one uses, one may thus more easily end up with an uncompensated (if the spin sublattices are comprised of different atoms, which does not appear to be the case in *e.g.* metallic antiferromagnet IrMn) rather than compensated interface which persists even in the presence of interface roughness.

28.6 Normalization condition for the Green function

Upon subtracting the conjugate Gor'kov equation from the original Gor'kov equation, we get rid off a δ -function which allows us to proceed with the derivation of the Eilenberger equation. However, upon doing so we lose a degree of freedom since the Eilenberger equation is homogeneous. This means that if $\check{g}$ is a solution, then so is $c\check{g}$ where c is a constant. Therefore, we need an extra condition to determine the Green function matrix uniquely.

It is possible to solve analytically for $\check{g}$ in a bulk normal metal or a bulk superconductor, and the solution satisfies $\check{g}^2 = \check{1}$. One can also derive an equation of motion for $\check{g}^2$ explicitly, as done in JP Morten thesis, and it is seen that $\check{g}^2$ also satisfies the Eilenberger equation in general (even for non-bulk systems) if $\check{g}$ satisfies the Eilenberger equation. Since $\check{g}^2 = \check{1}$ clearly is a solution of the Eilenberger equation, one usually simply takes this as the normalization condition everywhere in the system (not only in the bulk).

Below, we provide two more detailed discussions on how to justify the normalization condition mathematically.

28.6.1 Consistency with unique solution

Physically, we require that the solution to the Eilenberger equation + boundary conditions has to be unique so that a physical system described by an equation of motion and a set of boundary conditions has uniquely determined physical properties. Assume then that $g = f(x, E)$ is a solution (consider 1D for simplicity). We cannot prove that this is the *only* mathematical solution, since

there may exist a solution $g = h(x, E)$ that we do not know about.

However, given that $g = f(x, E)$ is a solution, we can say something about which properties this solution must have in order for the fact that $g = f(x, E)$ is a solution is *consistent* with that $g = f(x, E)$ is a unique solution.

We know that f^n is a solution if f is a solution, by iterating the Eilenberger equation. This is then inconsistent with f being a unique solution. but the following two conditions make $g = f(x, E)$ being a solution consistent with it being the only solution:

- $f^2 = 1$.
- The solution $g = f(x, E)$ give the same result as the quasiclassical approximation applied to the solution of the Gor'kov equation.

The first condition ensures that f^n is not a new solution when n is odd, since $f^n = f$ for such n . The second condition enables us to discard the solution $f^n = 1$ as a solution for even n , since this solution does not agree with the quasiclassical approximation of the Gor'kov solution. This can be seen for instance in the high-energy limit where Gor'kov gives the solution $g = \rho_3$ and not identity. In other words: if g solves the Eilenberger + boundary conditions and satisfies $g^2 = 1$, $g \neq 1$ (thus satisfying the two above bullet points), then this is consistent with that g can be a unique, physical solution.

We note that the above rationale does not preclude that there might exist other solutions $g = h(x, E)$ which satisfy the same requirements, but the above properties at least make it the set of equations comprised of Eilenberger + boundary conditions + normalization internally consistent with $g = f(x, E)$ being a unique solution.

28.6.2 Importance of normalization with respect to Usadel equation

The normalization condition is used for several purposes. Firstly, it makes the Green function unique, which it must be in order to compute physical observables from it. Secondly, it is used to derive the analytical expression for many observables, such as DOS and magnetization, in the weak proximity effect regime (see subsection below for more details). Thirdly, it is in fact used to derive the Usadel equation from the Eilenberger equation. This is because one first expands $g = g_s + \mathbf{e}_F \cdot \mathbf{g}_p$, and then use that $g^2 = 1$ gives $g_s^2 = 1$ and $\{g_s, \mathbf{g}_p\} = 0$. In order for the Usadel equation to be consistent with $g_s^2 = 1$, one must be able to write the entire Usadel equation (including the gradient terms) in the form

$$[A, g_s] = 0. \quad (28.317)$$

where A is some matrix that may depend on g_s . This can be seen as follows. If we can write Usadel as $[A, g_s] = 0$, then multiply with g_s from the right and add and subtract $g_s^2 A - g_s^2 A$, which gives the equation $[A, g_s^2] = 0$. This is consistent with $g_s^2 = 1$. Note that the usual Usadel equation $D\nabla(g\nabla g) + i[E + \Sigma, g] = 0$ (dropping subscript s) can indeed be written as $[A, g_s] = 0$ if $g_s^2 = 1$. This can be seen by noting that

$$[\nabla^2 g, g] = -2\nabla(g\nabla g) \quad (28.318)$$

when using that $\nabla(g^2) = g\nabla g + \nabla g g = 0$.

Add clarification normalization condition Huang PRB 2018 and Virtanen PRB 2021, and relation to inverse spin Hall arXiv: 23:

28.6.3 Shelankov's proof

This proof was originally done by Shelankov and is shown in more detail in M. Amundsen's Ph.D thesis section 2.5. A few comments regarding this derivation:

- The original motivation in section 2.5 of Morten's thesis for considering the limit $\mathbf{k} \cdot \mathbf{r} \gg 1$ is not strictly needed: it is sufficient to say that we consider this limit because it will lead us to the quasiclassical GF and its normalization condition.
- One goes from (2.64) to (2.65) by setting $x = \xi_k \epsilon / \hbar v_F$ and integrating.
- (2.66) contains both (2.60), as seen when setting $\eta_1 \neq \eta_2$, and (2.65), as seen by integrating η_1 over an infinitesimal interval $[\eta_2 - \delta, \eta_2 + \delta]$. This holds for all η_2 .

The derivation done by Amundsen is shown for the case of a potential $V(\mathbf{r})$ in the original Hamiltonian. It would be desirable to extend this proof to the case where a self-energy is included in the Gor'kov equation, since this is the case for the impurity-averaged Green function. This proof is sketched again by Shelankov, but not given in detail. We here give more details which makes the proof easier to understand.

First, we note that the Gor'kov equation for the Green function and its adjoint version, without self-energies, are given as (see E. Fyhn master thesis):

$$\begin{aligned} \left(i\partial_t \hat{\rho}_3 - \check{H} \right) \check{G}(\mathbf{r}, t\mathbf{r}', t') &= \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'), \\ \check{G}(\mathbf{r}, t, \mathbf{r}', t') \left(i\partial_{t'} \hat{\rho}_3 - \hat{\rho}_3 \check{H}(\mathbf{r}') \hat{\rho}_3 \right)^\dagger &= \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (28.319)$$

Above, the $\dagger$ means matrix transpose and complex conjugation. With self-energies, they take the form

$$\begin{aligned} \left(i\partial_t \hat{\rho}_3 - \check{H} \right) \check{G}(\mathbf{r}, t\mathbf{r}', t') - \int d3 \check{\Sigma}(1, 3) \check{G}(3, 2) &= \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'), \\ \check{G}(\mathbf{r}, t, \mathbf{r}', t') \left(i\partial_{t'} \hat{\rho}_3 - \hat{\rho}_3 \check{H}(\mathbf{r}') \hat{\rho}_3 \right)^\dagger - \int d3 \check{G}(1, 3) \check{\Sigma}(3, 2) &= \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \quad (28.320)$$

Ignore the time-dependence for the moment (it gives rise to a circle-product which is an internal integration over time variables in general, but it is not important for the normalization argument), so that $\int d3 = \int d\mathbf{r}_3$. By inserting the approximation for $\check{G}$ in terms of g_+ and g_- in Morten's thesis, we find that the g_+ equation becomes

$$e^{ik_F r_{12}} / r_{12} \left(\pm i\hbar v_F \hat{\mathbf{r}} \cdot \nabla_1 \check{g}_\pm + (E\check{\rho}_3 - \check{V}) \check{g}_\pm \right) - \int d\mathbf{r}_3 \Sigma(\mathbf{r}_1, \mathbf{r}_3) g_+(\mathbf{r}_3, \mathbf{r}_2) e^{ik_F r_{32}} / r_{32} = 0. \quad (28.321)$$

In the last term, we do the following:

$$\begin{aligned} \int d\mathbf{r}_3 \Sigma(\mathbf{r}_1, \mathbf{r}_3) g_+(\mathbf{r}_3, \mathbf{r}_2) e^{ik_F r_{32}} / r_{32} &= e^{ik_F r_{12}} \int d\mathbf{r}_3 \Sigma(\mathbf{r}_1, \mathbf{r}_3) g_+(\mathbf{r}_3, \mathbf{r}_2) e^{ik_F r_{31}} / r_{32} \\ &\simeq e^{ik_F r_{12}} / r_{12} \int d\rho \Sigma(\mathbf{r}_1 + \rho/2, \mathbf{r}_1 - \rho/2) g_+(\mathbf{r}_1, \mathbf{r}_2) e^{ik_F r_{31}}. \end{aligned} \quad (28.322)$$

To get the last line, we used that Σ is peaked at $\mathbf{r}_1 - \mathbf{r}_3 \simeq 0$, so that we could replace $\mathbf{r}_3 \simeq \mathbf{r}_1$ in the exponential and inverse radial position in the integrand. The fact that it is peaked at relative coordinate close to zero can be seen from the expression given earlier:

$$\Sigma_{\text{imp}}(\mathbf{R}, \mathbf{p}) = n_i \int \frac{d\mathbf{q}}{(2\pi)^3} |v(\mathbf{p} - \mathbf{q})|^2 G(\mathbf{R}, \mathbf{q}). \quad (28.323)$$

Since

$$\Sigma_{\text{imp}}(\mathbf{R}, \mathbf{r}) = \frac{1}{(2\pi)^3} \int \Sigma_{\text{imp}}(\mathbf{R}, \mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{r}}, \quad (28.324)$$

we see that $\Sigma_{\text{imp}}(\mathbf{R}, \mathbf{r})$ is almost like a $\delta(\mathbf{r})$ function when the individual impurity potential v is weakly dependent on momentum.

Moreover, we rewrote the self-energy as $\Sigma(\mathbf{r}_1, \mathbf{r}_3) = \Sigma(\mathbf{R} + \rho/2, \mathbf{R} - \rho/2)$ where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_3)/2$ and ρ is relative coordinate. Now, Σ is peaked when the relative coordinate $\rho \equiv \mathbf{r}_1 - \mathbf{r}_3$ is $\simeq 0$. Thus, by assuming that it varies slowly on the scale of k_F^{-1} , so that we can effectively replace the center of mass coordinate with $\mathbf{r}_1$ [just like we showed was the case for a slowly varying potential in section 25.1.2 [$V(\mathbf{r}_1) \rightarrow V(\mathbf{R})$], we get the transition to the last line above.

Having done this and now cancelling the common factor $e^{ik_F r_{12}}/r_{12}$, the equation for g_+ takes the form:

$$\pm i\hbar v_F \hat{\mathbf{r}} \cdot \nabla_1 \check{g}_{\pm} + (E\check{\rho}_3 - \check{V})\check{g}_{\pm} - \left(\int d\rho \Sigma(\mathbf{r}_1 + \rho/2, \mathbf{r}_1 - \rho/2) e^{ik_F \rho} \right) g_+(\mathbf{r}_1, \mathbf{r}_2) = 0. \quad (28.325)$$

This is essentially the same form that Shelankov has. Therefore, the equation for g_+ depends only on fields $(\check{V}, \check{\Sigma})$ which in turn depend on $\mathbf{r}_1$. Moreover, the equation describes motion along a straight line connecting $\mathbf{r}_1$ and $\mathbf{r}_2$, since you have to integrate along the $\hat{\mathbf{r}}$ -direction to solve it. This is because of the derivative term which is projected along the $\hat{\mathbf{r}}$ -direction. Shelankov has an additional $\mathbf{n} = \mathbf{r}_1 - \mathbf{r}_2$ dependence in the integrand for the self-energy, but that does not change the argument in Morten's thesis since it still describes motion along the straight line connecting $\mathbf{r}_1$ and $\mathbf{r}_2$.

Thus, we can write the equation for g_+ as

$$\pm i\hbar v_F \hat{\mathbf{r}} \cdot \nabla_1 \check{g}_{\pm}(\mathbf{r}_1, \mathbf{r}_2) + (E\check{\rho}_3 - \check{V})\check{g}_{\pm}(\mathbf{r}_1, \mathbf{r}_2) - \check{\Sigma}(\mathbf{r}_1)g_+(\mathbf{r}_1, \mathbf{r}_2) = 0. \quad (28.326)$$

by defining $\check{\Sigma}$ as the $(\dots)$ factor.

Now consider the adjoint equation, which after inserting $G \sim g_+ + g_-$ gives the extra term

$$- \int d\mathbf{r}_3 g_+(\mathbf{r}_1, \mathbf{r}_3) \Sigma(\mathbf{r}_3, \mathbf{r}_2) e^{ik_F r_{13}}/r_{13} = e^{ik_F r_{12}} \int d\mathbf{r}_3 g_+(\mathbf{r}_1, \mathbf{r}_3) \Sigma(\mathbf{r}_3, \mathbf{r}_2) e^{ik_F r_{23}}/r_{13}. \quad (28.327)$$

Rewriting $\Sigma(\mathbf{r}_2 + \rho/2, \mathbf{r}_2 - \rho/2)$ with $\rho \equiv \mathbf{r}_2 - \mathbf{r}_3$ this time, we get after letting $\mathbf{r}_3 \simeq \mathbf{r}_2$ in g_+ and the inverse radial variable (just like above):

$$e^{ik_F r_{12}}/r_{12} \int d\mathbf{r}_3 g_+(\mathbf{r}_1, \mathbf{r}_2) \Sigma(\mathbf{r}_2 + \rho/2, \mathbf{r}_2 - \rho/2) e^{ik_F \rho}. \quad (28.328)$$

Thus, the total adjoint equation after cancelling common factors becomes:

$$\mp i\hbar v_F \hat{\mathbf{r}} \cdot \nabla_2 \check{g}_{\pm}(\mathbf{r}_1, \mathbf{r}_2) + \check{g}_{\pm}(\mathbf{r}_1, \mathbf{r}_2) (E\check{\rho}_3 - \check{V}) - g_+(\mathbf{r}_1, \mathbf{r}_2) \check{\Sigma}(\mathbf{r}_2) = 0. \quad (28.329)$$

It is now straight forward to convert these to the 2.66 and 2.67 equations in Morten's thesis, but now including the self-energy term, and then differentiate 2.68 and insert 2.66 and 2.67 to show that $dA/d\eta = 0$ also with the self-energy. This completes the proof.

28.6.4 Zero-energy correction to DOS

From the normalization condition of the Green function, one can derive an expression for the DOS in the weak proximity effect which shows that the singlet will suppress the Fermi-level DOS whereas the odd-frequency triplets increases it.

We start by writing the 4×4 retarded Green function $\hat{g}$ as follows:

$$\hat{g} = \hat{g}_0 + \hat{f} + \hat{g}_2 \quad (28.330)$$

for a material in contact with a superconductor. Assuming a weak proximity effect, we have thus expanded the solution $\hat{g}$ in orders of the interface transparency: $\hat{g}_0$ is the solution to zero order (bulk non-superconducting material), $\hat{f}$ is a first order correction, $\hat{g}_2$ is a second order correction. It follows that $\hat{g}_0 = \hat{\rho}_3$. To find $\hat{f}$ and $\hat{g}_2$, we use the normalization condition for the Green function, $\hat{g}^2 = 1$. We get the following terms, discarding terms that are third order corrections or higher:

$$\begin{aligned} \text{Zeroth order (should equal 1): } & \hat{\rho}_3^2 \\ \text{First order (should equal 0): } & \hat{\rho}_3 \hat{f} + \hat{f} \hat{\rho}_3 \\ \text{Second order (should equal 0): } & \hat{\rho}_3 \hat{g}_2 + \hat{g}_2 \hat{\rho}_3 + \hat{f}^2. \end{aligned} \quad (28.331)$$

The zeroth order term is fulfilled. The first order term equation shows that $\hat{f}$ must be off-diagonal. According to the general structure of a retarded quasiclassical Green function, it must therefore have the form

$$\hat{f} = \begin{pmatrix} 0 & f \\ -\tilde{f} & 0 \end{pmatrix} \quad (28.332)$$

where f is a 2×2 matrix. The second order term equation shows that any off-diagonal elements in $\hat{g}_2$ will automatically fulfil the equation since they anticommute with $\hat{\rho}_3$. The diagonal terms of $\hat{g}_2$ are what give the correction to the DOS and magnetization, and these do not have to be non-zero due to the $\hat{f}^2$ term. Setting the off-diagonal terms of $\hat{g}_2$ to zero (since we do not need them anyway), we must have

$$\hat{g}_2 = \begin{pmatrix} g & 0 \\ 0 & -\tilde{g} \end{pmatrix} \quad (28.333)$$

where g is a 2×2 matrix. The second order term equation then gives us

$$2g = f\tilde{f}. \quad (28.334)$$

Thus, the correction to the normal part of the Green function (to second order) is:

$$1 + g = 1 + f\tilde{f}/2 \quad (28.335)$$

so that the DOS reads

$$N(E)/N_0 = \frac{1}{2} \text{Tr}\{1 + f\tilde{f}/2\}. \quad (28.336)$$

Inserting

$$f = \begin{pmatrix} f_{\uparrow} & f_t + f_s \\ f_t - f_s & f_{\downarrow} \end{pmatrix} \quad (28.337)$$

gives us

$$N(0)/N_0 = 1 - \frac{|f_s(0)|^2}{2} + \frac{|f_t(0)|^2}{2} + \frac{|f_{\uparrow}(0)|^2}{4} + \frac{|f_{\downarrow}(0)|^2}{4} \quad (28.338)$$

28.6.5 A few more details regarding quasiclassical approximation

In computing the quasiclassical Green function, we are performing an integral over the kinetic energy relative the Fermi energy, $\xi_p = p^2/2m - \mu$. The problem with this integral is that it has one part which falls off like $\sim 1/\xi_p$. Thus, the integral formally diverges when the integration limits are $\pm\infty$. This is usually handled by introducing a large cut-off and assuming that the limits are taken symmetrically, so that the $1/\xi_p$ part of the integral vanishes due to symmetry. However, it is worth to note that Shelankov (1985) also derived the quasiclassical equations without using the ξ_p integration, obtaining the same result as with the former method.

We here derive the result:

$$\int \frac{d^3p}{(2\pi)^3} \rightarrow N_0 \int d\xi_p \int \frac{d\Omega_p}{4\pi} \quad (28.339)$$

where N_0 is the normal-state density of states at the Fermi energy per spin and per unit volume which is valid for free electrons in 3D in the quasiclassical approximation. Recall the general definition of DOS per unit volume:

$$N(E) = \frac{1}{V} \sum_i \delta(E - E_i) \quad (28.340)$$

where E_i are the allowed energy states in the system. It is a textbook result that the normal-state DOS at energy E per spin per volume for 3D free electrons with a quadratic dispersion is:

$$N_0(E) = \frac{m}{2\pi^2} \sqrt{2mE} \quad (28.341)$$

so that at the Fermi level $\mu = p_F^2/(2m)$, one gets $N_0 = \frac{m}{2\pi^2} \sqrt{2m\mu}$. The unit of the DOS per volume is $\text{m}^{-3} \text{eV}$. Now, we can do the following:

$$\begin{aligned} \int \frac{d^3p}{(2\pi)^3} &= \frac{1}{(2\pi)^3} \int p^2 dp \int d\Omega_p = \frac{1}{2\pi^2} \int p^2 dp \int \frac{d\Omega_p}{4\pi} \\ &= \frac{1}{2\pi^2} \int p m d\xi_p \int \frac{d\Omega_p}{4\pi} \simeq \frac{mp_F}{2\pi^2} \int d\xi_p \int \frac{d\Omega_p}{4\pi}. \end{aligned} \quad (28.342)$$

In the last step, we used a quasiclassical approximation $p \rightarrow p_F$ and pulled it out of the integral. Since $p_F = \sqrt{2m\mu}$, we now see that we have recovered the desired result since the prefactor is N_0 , in effect the density of states per spin per volume.

We can use this to further justify the normalization condition $g^2 = 1$ for the quasiclassical Green function. The energy-resolved density of states per volume is given by the spectral weight A of the system as

$$DOS(\varepsilon) = \frac{1}{V} \sum_{\mathbf{k}} A(\mathbf{k}, \varepsilon) \quad (28.343)$$

where V is the volume of the system. The spectral weight, in turn, is given as

$$A(\mathbf{k}, \varepsilon) = -\frac{1}{\pi} \text{Im}\{G^R(\mathbf{k}, \varepsilon)\} \quad (28.344)$$

where G^R is the retarded Green function. In the continuum limit, we have

$$\frac{1}{V} \sum_{\mathbf{k}} = \int \frac{d^3k}{(2\pi)^3}. \quad (28.345)$$

Thus, we obtain

$$\begin{aligned} DOS(\varepsilon) &= \int \frac{d^3k}{(2\pi)^3} A(\mathbf{k}, \varepsilon) \\ &= -\frac{1}{\pi} \int \frac{d^3k}{(2\pi)^3} \text{Im}\{G^R(\mathbf{k}, \varepsilon)\}. \end{aligned} \quad (28.346)$$

Now make use of the result derived above:

$$\int \frac{d^3p}{(2\pi)^3} \rightarrow N_0 \int d\varepsilon_p \int \frac{d\Omega_p}{4\pi} \quad (28.347)$$

in order to obtain

$$\begin{aligned} DOS(\varepsilon) &= \int \frac{d^3k}{(2\pi)^3} A(\mathbf{k}, \varepsilon) \\ &= N_0 \int d\varepsilon_k \int \frac{d\Omega_k}{4\pi} \text{Re}\left\{\frac{i}{\pi} G^R(\mathbf{k}, \varepsilon)\right\}. \end{aligned} \quad (28.348)$$

Using the definition of the quasiclassical GF:

$$g^R = \frac{i}{\pi} \int d\varepsilon_k G^R \quad (28.349)$$

we get

$$\begin{aligned} DOS(\varepsilon) &= \int \frac{d^3k}{(2\pi)^3} A(\mathbf{k}, \varepsilon) \\ &= N_0 g_s^R(\varepsilon) \end{aligned} \quad (28.350)$$

where $_s$ indicates the isotropic part of the Green function (due to the angular averaging).

Now comes the connection to the normalization of the Green function. The solution of the Eilenberger equation, even in a spatially inhomogeneous state, will for sufficiently large energies ϵ be equal to $g_s^R = c\rho_3$ where c is a constant. More precisely, large energies ε compared to the other

energy scales in the problem, such as Δ , or the inverse length scale associated with the spatial inhomogeneity, but still within the quasiclassical regime. Now, the Eilenberger equation only determines the Green function up to the multiplicative constant c , but does not allow us to determine what c is in the accompanying normalization condition $(g_s^R)^2 = c^2$. However, the above expression for the DOS does. Namely, if we want the expression $DOS(\varepsilon) = N_0 g_s^R(\varepsilon)$ to be valid at sufficiently large energies above the Fermi level, we must have $c = 1$ so that $DOS(\varepsilon)$ then equals N_0 . Thus, the normalization condition $(g_s^R)^2 = 1$ enforces that the density of states given by the quasiclassical Green function is correct for $\varepsilon \gg \Sigma$ for any inhomogeneous state.

The applicability for quasiclassical theory is usually taken as the requirement that the Fermi wavelength λ_F is the smallest length scale in the system, compared to *e.g.* the superconducting coherence length ξ , the length of the system L , or the mean free path l_{mfp} . In the dirty limit where l_{mfp} is small, one additionally assumes that l_{mfp} is smaller than any of the other energy scales (except λ_F), in which case one may use the Usadel equation rather than the Eilenberger equation. Equivalent to the above formulation, one can state that the applicability for quasiclassical theory is that the Fermi energy E_F is the largest energy scale in the system. In the dirty limit where the Usadel equation is valid, one would then have:

$$E_F \gg \tau^{-1} \gg \Delta, h, \varepsilon_T. \quad (28.351)$$

where τ is the impurity scattering time, Δ is the superconducting gap, h is the exchange field, while ε_T is the Thouless energy.

However, some care is required when there are multiple length or energy scales in the system in order to state when the quasiclassical theory is valid. For instance, consider an S/F layer. If we keep terms of order h^2 , then the quasiclassical approach remains valid only if terms of order ΔE_F are much larger than h^2 . In effect, it means that although E_F is the largest energy scale of the problem, the quasiclassical theory is strictly speaking not valid ...

The full 8×8 matrix in Keldysh space is:

$$\check{g} = \begin{pmatrix} \hat{g}^R & \hat{g}^K \\ 0 & \hat{g}^A \end{pmatrix} \quad (28.352)$$

A 4×4 matrix acting on $\check{g}$ should be understood as two 4×4 matrices along the diagonal of an 8×8 matrix, so that for instance $\hat{\rho}_3 \check{g} = \text{diag}(\hat{\rho}_3, \hat{\rho}_3) \check{g}$.

The matrices read:

$$\hat{\Delta} = \begin{pmatrix} 0 & \Delta i \sigma_y \\ \Delta^* i \sigma_y & 0 \end{pmatrix}, \quad \hat{M} = \begin{pmatrix} \mathbf{h} \cdot \boldsymbol{\sigma} & 0 \\ 0 & (\mathbf{h} \cdot \boldsymbol{\sigma})^* \end{pmatrix}. \quad (28.353)$$

The $\sim$ operation denotes complex conjugation and $\varepsilon \rightarrow (-\varepsilon)$, so that $\check{g}(X, \varepsilon) = \underline{g}^*(X, -\varepsilon)$. From the definitions of the Green's functions, we have that:

$$\hat{g}^R = \begin{pmatrix} \underline{g}^R & \underline{f}^R \\ -\underline{\tilde{f}}^R & -\underline{\tilde{g}}^R \end{pmatrix}, \quad \hat{g}^A = \begin{pmatrix} \underline{g}^A & \underline{f}^A \\ -\underline{\tilde{f}}^A & -\underline{\tilde{g}}^A \end{pmatrix}. \quad (28.354)$$

Moreover, since $\hat{g}^A = -(\hat{\rho}_3 \hat{g}^R \hat{\rho}_3)^\dagger$, we also have:

$$\hat{g}^A = \begin{pmatrix} -(\underline{g}^R)^\dagger & -(\underline{\tilde{f}}^R)^\dagger \\ (\underline{\tilde{f}}^R)^\dagger & (\underline{\tilde{g}}^R)^\dagger \end{pmatrix} \quad (28.355)$$

. The Keldysh part has the symmetry structure:

$$\hat{g}^K = \begin{pmatrix} g^K & f^K \\ \bar{f}^K & \bar{g}^K \end{pmatrix} \quad (28.356)$$

28.6.6 Deriving quasiclassical boundary conditions using the Keldysh-contour and Langreth's theorem

Consider two regions R and L separated by a tunneling interface. We then have

$$H = H_R + H_L + H_T, \quad (28.357)$$

where

$$\begin{aligned} H_L &= \sum_{ps} \xi_p a_{ps}^\dagger a_{ps} + \sum_p (\Delta_L a_{p\uparrow}^\dagger a_{-p\downarrow}^\dagger + \text{h.c.}), \\ H_R &= \sum_{ps} \xi_p b_{ps}^\dagger b_{ps} + \sum_p (\Delta_R b_{p\uparrow}^\dagger b_{-p\downarrow}^\dagger + \text{h.c.}), \\ H_T &= \sum_{pp'ss'} (T_{pp'ss'} a_{ps}^\dagger b_{p's'} + \text{h.c.}). \end{aligned} \quad (28.358)$$

We have assumed that the L and R regions act as reservoirs where the Hamiltonian has no spatial dependence (on the center of mass coordinate). However, to justify that the boundary conditions we are about to derive are valid also for the case where the L and R regions are not spatially homogeneous, we can consider a region close enough to the interface where the above Hamiltonians are valid. The boundary conditions will then be valid using the value of the Green functions at the interface.

The equation of motion for the operators becomes:

$$i\partial_t a_{ps} = [a_{ps}, H], \quad (28.359)$$

and equivalently for b_{ps} . Let us for compactness define the annihilation column operator A_p in spin $\otimes$ Nambu space:

$$A_p = \begin{pmatrix} a_{p\uparrow} \\ a_{p\downarrow} \\ a_{-p\uparrow}^\dagger \\ a_{-p\downarrow}^\dagger \end{pmatrix} \quad (28.360)$$

and equivalently for B_p . These operators can then be shown, by evaluating the above commutator, to satisfy the following equation of motions:

$$\begin{aligned} i\hat{\rho}_3 \partial_t A_p &= \mathcal{H}_L A_p + \sum_{p'} \Gamma_{pp'} B_{p'}, \\ i\hat{\rho}_3 \partial_t B_p &= \mathcal{H}_R B_p + \sum_{p'} \tilde{\Gamma}_{pp'} A_{p'}. \end{aligned} \quad (28.361)$$

where we defined

$$\mathcal{H}_{L,R} \equiv \xi_p + \hat{\Delta}_{L,R} \quad (28.362)$$

while the quantities $\Gamma_{pp'}$, $\tilde{\Gamma}_{pp'}$ are matrices. Their elements for arbitrary tunneling matrix elements can be derived by using that

$$\begin{aligned} [a_{ps}, H_T] &= \sum_{q\gamma} T_{pq\gamma} b_{q\gamma}, \\ [a_{-ps}^\dagger, H_T] &= - \sum_{q\gamma} T_{-p,q\gamma}^* b_{q\gamma}^\dagger, \\ [b_{ps}, H_T] &= \sum_{q\gamma} T_{qp\gamma}^* a_{q\gamma}, \\ [b_{-ps}^\dagger, H_T] &= - \sum_{q\gamma} T_{q,-p,\gamma} a_{q\gamma}^\dagger. \end{aligned} \quad (28.363)$$

It then follows that

$$\begin{aligned} \Gamma_{pp'} &= \begin{pmatrix} T_{pp'\uparrow\uparrow} & T_{pp'\uparrow\downarrow} & 0 & 0 \\ T_{pp'\downarrow\uparrow} & T_{pp'\downarrow\downarrow} & 0 & 0 \\ 0 & 0 & T_{-p,-p'\uparrow\uparrow}^* & T_{-p,-p'\uparrow\downarrow}^* \\ 0 & 0 & T_{-p,-p'\downarrow\uparrow}^* & T_{-p,-p'\downarrow\downarrow}^* \end{pmatrix}, \\ \tilde{\Gamma}_{pp'} &= \begin{pmatrix} T_{p'p\uparrow\uparrow}^* & T_{p'p\downarrow\uparrow}^* & 0 & 0 \\ T_{p'p\uparrow\downarrow}^* & T_{p'p\downarrow\downarrow}^* & 0 & 0 \\ 0 & 0 & T_{-p',-p,\uparrow\uparrow} & T_{-p',-p,\downarrow\uparrow} \\ 0 & 0 & T_{-p',-p,\uparrow\downarrow} & T_{-p',-p,\downarrow\downarrow} \end{pmatrix}. \end{aligned} \quad (28.364)$$

A few special cases can be mentioned. If the tunneling is spin- and momentum-independent and real, we simply have $\Gamma_{pp'} = \tilde{\Gamma}_{pp'} = T\hat{1}$. If the tunneling elements are momentum-independent (as usually assumed when modelling magnetic boundary conditions), we have $\Gamma_{pp'} = \tilde{\Gamma}_{pp'}^\dagger$. In general, they are however different.

Note that the assumption $\xi_p = \xi_{-p}$ has been used and that we defined

$$\hat{\Delta}_i = \begin{pmatrix} 0 & 0 & 0 & \Delta_i \\ 0 & 0 & -\Delta_i & 0 \\ 0 & \Delta_i^* & 0 & 0 \\ -\Delta_i^* & 0 & 0 & 0 \end{pmatrix}. \quad (28.365)$$

Moreover, $\hat{\rho}_3 = \text{diag}(1, 1, -1, -1)$.

Now, the tunneling current in the system can be computed as

$$I = e \frac{d}{dt} \langle N \rangle, \quad (28.366)$$

where the number operator is

$$N = \sum_{ps} a_{ps}^\dagger(t) a_{ps}(t). \quad (28.367)$$

We wrote the time-dependence explicitly just to remind ourselves that the operators are in fact time-dependent. We can now express the number operator as follows:

$$N = \frac{1}{2} \sum_{pp's} (a_{ps}^\dagger a_{ps} + 1 - a_{-ps} a_{-ps}^\dagger) = \sum_p (1 + \frac{1}{2} A_p^\dagger \hat{\rho}_3 A_p). \quad (28.368)$$

To proceed from here, we first consider for simplicity now the case of spin-independent tunneling. Then, we consider the case of arbitrary tunneling.

Spin-independent tunneling

In this case, Γ and $\tilde{\Gamma}$ are both proportional to the identity matrix. Thus, we let Γ and $\tilde{\Gamma}$ from now on denote scalars. Differentiating with respect to time and using the Heisenberg equations of motion provides

$$\begin{aligned}\langle \dot{N} \rangle &= \frac{i}{2} \sum_{pp'} \langle A_p^\dagger(t) \mathcal{H}_L^\dagger A_p(t) \delta_{pp'} + B_{p'}^\dagger(t) \tilde{\Gamma}_{p'p} A_p(t) - A_p^\dagger(t) \mathcal{H}_L A_p(t) \delta_{pp'} - A_p^\dagger(t) \Gamma_{pp'} B_{p'}(t) \rangle \\ &= \frac{1}{2} \sum_{pp'} \text{Tr} \{ \tilde{\Gamma}_{p'p} C_L^<(p, t; p', t) - \Gamma_{p'p} C_R^<(p, t; p', t) \}.\end{aligned}\quad (28.369)$$

In the above equation, the $\mathcal{H}_L$ terms do not immediately cancel because the presence of superconductivity ensures that $\mathcal{H}_L^\dagger \neq \mathcal{H}_L$. However, we still discarded those term in the last line which can be justified as follows. We are looking for the current due to tunneling and this can alternatively be computed according to $\langle \dot{N} \rangle = \frac{1}{i} [N, H_T]$. In effect, using only H_T rather than the full Hamiltonian H gives us the contribution from tunneling. In that case, one ends up with just tunneling-dependent terms as in the last line. An alternative approach to the above is to compute $\dot{N}$ simply from $[N, H_T]$, in which case one ends up with a dependence only on one of the C -matrices. In that case, one also has to compute $\dot{N}$ on the right hand side ($b^\dagger b$) and subtract the currents to get the total current across the junction.

We have defined the composite Green functions

$$\begin{aligned}C_L^<(p, t; p', t') &= i \langle \left[\left(B_{p'}^\dagger(t') \right)^{\text{tr}} \left(A_p(t) \right)^{\text{tr}} \right]^{\text{tr}} \rangle, \\ C_R^<(p, t; p', t') &= i \langle \left[\left(A_{p'}^\dagger(t') \right)^{\text{tr}} \left(B_p(t) \right)^{\text{tr}} \right]^{\text{tr}} \rangle.\end{aligned}\quad (28.370)$$

In the above summation, we also used that

$$\sum_{pp'} T_{pp'} C_R^<(p', t; p, t) = \sum_{pp'} T_{p'p} C_R^<(p, t; p', t) \quad (28.371)$$

which follows simply from renaming indices. Moreover, defining the Green function:

$$C_L^>(p, t; p', t) = -i \langle A_p(t) B_{p'}^\dagger(t) \rangle, \quad (28.372)$$

we notice as a useful property for later that at equal times:

$$C_L^<(p, t; p', t) = C_L^>(p, t; p', t). \quad (28.373)$$

The superscripts denote lesser and greater Green functions, to be consistent with the usual definitions in the literature of these quantities. Let us moreover define the time-ordered ($\mathcal{T}$) and *contour-ordered* ($\mathcal{T}_c$) Green functions (where the contour is the Keldysh contour, allowing us to work out of equilibrium)

$$C^{\mathcal{T}} = -i\rho_3 \langle \mathcal{T} A_p(t) B_{p'}^\dagger(t') \rangle, \quad C^{\mathcal{T}_c} = -i\rho_3 \langle \mathcal{T}_c A_p(t) B_{p'}^\dagger(t') \rangle. \quad (28.374)$$

Again, these are the standard definitions for these types of Green functions (same sign for i and time-arguments): the only unusual thing is that we are using two different operators A and B ,

whereas usually one only works with one type of operator ψ . Note also that all the Green functions $C^<, C^>, C^T, C^{\mathcal{T}c}$ above are matrices, we have simply dropped the $\hat{\cdot}$ for brevity of notation. Finally, for later use we give the definition of the Keldysh Green function:

$$C^K(p, p', t, t') = -i\rho_3 \langle [A_p(t), B_{p'}^\dagger(t')] \rangle \quad (28.375)$$

where the commutator should be understood as:

$$[A_p(t), B_{p'}^\dagger(t')] \equiv A_p(t)B_{p'}^\dagger(t) - \left[\left(B_{p'}^\dagger(t') \right)^{\text{tr}} \left(A_p(t) \right)^{\text{tr}} \right]^{\text{tr}}. \quad (28.376)$$

Interlude: the Keldysh contour

Let us comment a bit further on the Keldysh contour mentioned above, following the notes of Jauho and Kamenev. The central quantity in constructing the perturbation theory for Green functions in equilibrium is the matrix $S(\infty, -\infty)$ which describes the evolution of the system from $t = -\infty$ to $t = +\infty$. At both of these endpoints, the system is assumed to be noninteracting and the interactions $V(t)$ are turned on and off adiabatically so that they exist only in between these times. Therefore, the state of the system at $t = \pm\infty$ must be identical except for an overall phase factor.

In nonequilibrium, however, there is no guarantee that the system returns to its initial state for asymptotically large times. In fact, often it does not. Consider, for example, an important problem in surface physics, where atoms or molecules impinging on a surface exchange charge with the surface, and hence the initial state at $t = -\infty$ is very different from the final state at $t = +\infty$. Thus, one should avoid any reference to the asymptotically large times in the nonequilibrium theory. The general formulation of the theory is slightly more complicated than in the equilibrium case. However, the abstract structure of the theory bears a close resemblance to the equilibrium theory and we shall make use of this below.

Let us now formalize the arguments made above to see how this necessitates the introduction of a *Keldysh contour* when dealing with nonequilibrium situations. We consider a quantum many-body system governed by a time-dependent Hamiltonian $\hat{H}(t)$. Initially, at $t = -\infty$, the system is in a state specified by a many-body density matrix operator $\hat{\rho}(-\infty)$. The density matrix operator evolves according to the equation of motion

$$\partial_t \hat{\rho}(t) = i[\hat{\rho}(t), \hat{H}(t)] \quad (28.377)$$

which can be derived from the time-dependent Schrodinger equation. Formally, the solution takes the form

$$\hat{\rho}(t) = \hat{U}(t, -\infty) \hat{\rho}(-\infty) \hat{U}^\dagger(-\infty, t) \quad (28.378)$$

where the evolution operator is defined by the time-ordered exponent

$$\hat{U}(t, t') = \mathcal{T} e^{-i \int_{t'}^t \hat{H}(\tau) d\tau} = \lim_{N \rightarrow \infty} e^{-i\hat{H}(t)\delta} e^{-i\hat{H}(t-\delta)\delta} \dots e^{-i\hat{H}(t'+\delta)\delta}, \quad (28.379)$$

with an infinitesimal time-step $\delta = (t - t')/N$.

What we are typically interested in is the expectation value for an observable $\hat{\mathcal{O}}$ (such as a current or density) at a time t , which is defined as:

$$\langle \hat{\mathcal{O}} \rangle(t) \equiv \text{Tr}\{\hat{\mathcal{O}} \hat{\rho}(t)\} = \text{Tr}\{\hat{U}(-\infty, t) \hat{\mathcal{O}} \hat{U}(t, -\infty) \hat{\rho}(-\infty)\} = \text{Tr}\{\hat{\mathcal{O}}_H \hat{\rho}_H\} \quad (28.380)$$

where $\hat{\rho}(-\infty)$ is the density matrix in the Heisenberg picture, where it is time-independent. The traces are performed over the many-body Hilbert space of the system. The expression in the last trace describes (reading from right to left) an evolution from $t = -\infty$, where the initial density matrix is specified, forward to t , where the observable is calculated, and then backward to $t = -\infty$. The time-dependence on the left hand side is written outside of the expectation value to underline that the expectation value is identical regardless of whether one evaluates it in the Schrodinger or Heisenberg picture. The $\hat{\mathcal{O}}$ is the operator in the Schrodinger picture, while $_H$ indicates an operator in the Heisenberg picture. Note that although we haven't written it explicitly above, the operator $\hat{\mathcal{O}}$ in the Schrodinger picture can have an explicit time-dependence.

This forward-backward evolution is avoided in equilibrium by a particular trick. To see this, recall that in zero temperature quantum field theory in equilibrium one deals with expectation values of the type $\langle \text{GS} | \hat{\mathcal{O}}(t) | \text{GS} \rangle = \langle 0 | \hat{U}(-\infty, t) \hat{\mathcal{O}}(t) \hat{U}(t, -\infty) | 0 \rangle$. Here, $|\text{GS}\rangle = \hat{U}(t, -\infty) | 0 \rangle$ is the ground-state of the full interacting system and so the evolution operator describes the evolution of the noninteracting ground state $|0\rangle$ toward $|\text{GS}\rangle$ upon adiabatically switching on the interactions.

Here comes the trick that can be used in equilibrium, but not out of equilibrium. We use that

$$\langle 0 | \hat{U}(+\infty, -\infty) = \langle 0 | e^{i\phi}. \quad (28.381)$$

What this means is that when the interactions are adiabatically turned on and off, the system must revert to its original ground-state except for the possibility of an overall phase-factor $e^{i\phi}$. Since the system adiabatically follows its instantaneous ground-state, the only result of evolving the noninteracting ground state along the entire time-axis is acquiring $e^{i\phi}$. Therefore, we may write

$$\begin{aligned} \langle \text{GS} | \hat{\mathcal{O}}(t) | \text{GS} \rangle &= \langle 0 | \hat{U}(+\infty, -\infty) \hat{U}(-\infty, t) \hat{\mathcal{O}}(t) \hat{U}(t, -\infty) | 0 \rangle / e^{i\phi} \\ &= \langle 0 | \hat{U}(+\infty, t) \hat{\mathcal{O}}(t) \hat{U}(t, -\infty) | 0 \rangle / e^{i\phi}. \end{aligned} \quad (28.382)$$

In effect, we only need to describe the evolution along the forward time axis, in effect from $-\infty$ to t and then further to ∞ , *without* the backward segment. The price to pay is that one has to deal with $e^{i\phi}$, which can be shown to be removed by subtracting so-called disconnected diagrams. For instance, for a time-ordered 2-point correlator one gets rid of the phase-factor by dividing the correlator on the norm of the vacuum $\langle \text{GS} | \text{GS} \rangle$.

This trick *does not work out of equilibrium*, as we have already alluded to above. Driving the system out of equilibrium means that the final state of its evolution does not have to coincide with the initial one. Instead, the final state can depend on the details of the switching procedure as well as on the history of the system. Therefore, we cannot get rid of the backward position of the evolution history that is present in Eq. (28.380).

Therefore, we have to accept that the evolution operators used in the expectation values of nonequilibrium quantum field theory do act on a different time contour than in equilibrium (straight line from $-\infty$ to ∞), namely a so-called *closed time contour*: along with the conventional forward path, one also has the backward one (back to $-\infty$). In this way, one avoids the need to know the state of the system at $t = +\infty$. Consequently, it is natural for the Green functions used in nonequilibrium quantum field theory to reside on this so-called Keldysh contour which is depicted in Fig. 28.11. We mention in passing that this contour is *topologically* equivalent to the forward time-axis (just imagine you bend it upwards): by defining a variable τ which follows the contour, we have exactly

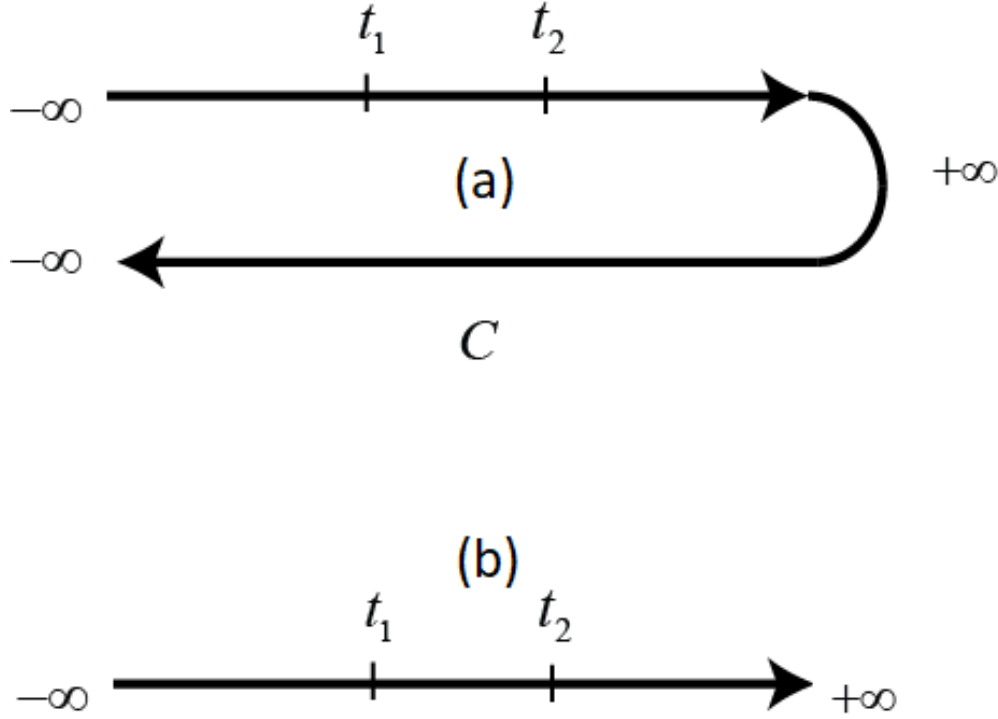


Figure 28.11: (Color online) (a) Keldysh contour. In practice, one can also extend the Keldysh contour so that the system evolves back to $-\infty$ after t_1 before it goes to t_2 . This operation is equal to the identity operation (see argument in Kamenev) and does not require any additional assumptions. The mathematical reason for this is that $\hat{U}(t_1, -\infty)\hat{U}(-\infty, t_1) = \hat{1}$. (b) Forward time-axis line.

the same scenario as real time t increasing along forward time-axis. We will make use of this topological equivalent in the boundary conditions below.

Return to the derivation of boundary conditions

We return now to the derivation of the KL boundary conditions, where the idea is to compute an expression for the current using the above framework and compare it with the general expression for the current in quasiclassical theory. To find an expression for I with the above framework, we see from Eq. (28.421) that we need to determine $C_{L,R}^<(p, t; p', t)$. To do this, we have to take a small detour and consider the time-ordered Green function C_L^T . Assume now for simplicity that $\Gamma_{pp'} = T$, i.e. proportional to identity matrix, and note that all momentum labels are really vectors, i.e. p is really $\mathbf{p}$. The equation of motion for this Green function, with the help again of the Heisenberg equations of motion, is:

$$\begin{aligned} i\hat{p}_3\partial_t C_L^T(p, t; p', t') &= -i\langle T i\hat{p}_3\partial_t A_p(t) B_{p'}^\dagger(t') \rangle \\ &= \mathcal{H}_L C_L^T(p, t; p', t') + \sum_q T G_R^T(q, t; p', t'). \end{aligned} \quad (28.383)$$

We here used the definition of the time-ordered Green function in the right reservoir:

$$G_R^T(p, t; p', t') = -i\rho_3\langle T B_p(t) B_{p'}^\dagger(t') \rangle. \quad (28.384)$$

To proceed, we note that we can rewrite Eq. (28.383) as:

$$(i\hat{\rho}_3\partial_t - \mathcal{H}_L)C_L^\mathcal{T}(p, t; p', t') = \sum_q TG_R^\mathcal{T}(q, t; p', t'). \quad (28.385)$$

The operator $i\hat{\rho}_3\partial_t - \mathcal{H}_L$ also appears in the equation of motion that determines the unperturbed (no tunneling) time-ordered reservoir Green function:

$$\left[i\hat{\rho}_3\partial_t - \mathcal{H}_L(p)\right]G_{L,0}^\mathcal{T}(p, t, p', t') = \delta(t - t')\delta_{pp'} \quad (28.386)$$

where we now also wrote the momentum-dependence of the Hamilton-operator to be precise. This equation can be derived by using the Heisenberg equations for the $A_p(t)$ -operators (spinors). The appearance of the δ -functions here, which did not appear above in the equation of motion for $C_L^\mathcal{T}$, can be seen to arise due to the definition of the time-ordering operator:

$$\mathcal{T}\langle B_p(t)B_{p'}^\dagger(t')\rangle = \theta(t - t')\langle B_p(t)B_{p'}^\dagger(t')\rangle - \theta(t' - t)\langle \left[B_{p'}^\dagger(t')\right]^\text{tr} \left[B_p(t)\right]^\text{tr} \rangle. \quad (28.387)$$

since $B_p(t)$ contains fermionic operators and $^\text{tr}$ means matrix transpose. When acting on the time-ordered Green function with ∂_t , we get $\delta(t - t')$ functions [since $\delta(x) = \delta(-x)$]. One of these survives when we anticommute the operator-spinors in the last term. Note that the ρ_3 in the definition of $G_{R(L)}^\mathcal{T}(p, t; p', t')$ [and correspondingly in $G_{R(L),0}^\mathcal{T}$] is necessary in order to give just δ -functions in Eq. (28.386) on the right-hand side without any additional ρ_3 .

We start by *defining* the quantity $F_{L,0}^\mathcal{T}$ such that it satisfies

$$\int d\tau \int dk G_{L,0}^\mathcal{T}(p, k, t, \tau) F_{L,0}^\mathcal{T}(k, p', \tau, t') = \delta(t - t')\delta_{pp'}. \quad (28.388)$$

In the literature, the quantity $F_{L,0}^\mathcal{T}$ is referred to as the inverse of the time-ordered Green function operator. Using this definition, it follows that we can rewrite:

$$C_L^\mathcal{T}(p, p', t, t') = \int \int \int \int dk_1 dk_2 dt_3 dt_4 G_{L,0}^\mathcal{T}(p, k_1, t, t_3) F_{L,0}^\mathcal{T}(k_1, k_2, t_3, t_4) C_L^\mathcal{T}(k_2, p', t_4, t'). \quad (28.389)$$

Let us now insert this expression for $C_L^\mathcal{T}$ into the left hand side of Eq. (28.385):

$$\begin{aligned} \int \int \int \int dk_1 dk_2 dt_3 dt_4 \overbrace{[i\hat{\rho}_3\partial_t - \mathcal{H}_L(p)]G_{L,0}^\mathcal{T}(p, k_1, t, t_3) F_{L,0}^\mathcal{T}(k_1, k_2, t_3, t_4) C_L^\mathcal{T}(k_2, p', t_4, t')}^{\delta(t-t_3)\delta_{pk_1}} \\ = \sum_q TG_R^\mathcal{T}(q, p', t, t') \end{aligned} \quad (28.390)$$

so that the equation reduces to

$$\int dt_4 \int dk_2 F_{L,0}^\mathcal{T}(p, k_2, t, t_4) C_L^\mathcal{T}(k_2, p', t_4, t') = \sum_q TG_R^\mathcal{T}(q, t, p', t'). \quad (28.391)$$

Now, multiply the entire equation with $G_{L,0}^\mathcal{T}(q_1, p, t_1, t)$ from the left and integrate $\int \int dp dt$:

$$\begin{aligned} \int \int \int \int dt dp dk_2 dt_4 G_{L,0}^\mathcal{T}(q_1, p, t_1, t) F_{L,0}^\mathcal{T}(p, k_2, t, t_4) C_L^\mathcal{T}(k_2, p', t_4, t') \\ = \int \int dt dp G_{L,0}^\mathcal{T}(q_1, p, t_1, t) \sum_q TG_R^\mathcal{T}(q, p', t, t'). \end{aligned} \quad (28.392)$$

Using Eq. (28.388) once more, we see that this equation turns into:

$$C_L^T(q_1, p', t_1, t') = \int \int dt dp G_{L,0}^T(q_1, p, t_1, t) \sum_q T G_R^T(q, p', t, t') \quad (28.393)$$

and after renaming variables we arrive at:

$$C_L^T(p, p', t, t') = \int \int d\tau dk G_{L,0}^T(p, k, t, \tau) \sum_q T G_R^T(q, p', \tau, t') \quad (28.394)$$

We have then managed to find an expression for the time-ordered Green function $C_L^T(p, p', t, t')$, but we were really looking for $C_L^<(p, p', t, t')$. This can be achieved as follows. Recall first our comment about the Keldysh contour and the forward time-axis contour being topologically equivalent. This means that if Eq. (28.394) holds for the time-ordered Green function on the forward time-axis, the following equation must hold for the *contour-ordered* Green function on the Keldysh contour:

$$C_L^{Tc}(p, p', t, t') = \int \int d\tau dk G_{L,0}^{Tc}(p, k, t, \tau) \sum_q T G_R^{Tc}(q, p', \tau, t') \quad (28.395)$$

where the integral $\int_c$ is now taken over the Keldysh contour. The next step is to use Langreth's theorem, which is explained in the notes by Jauho, allowing us to write:

$$\rho_3 C_L^<(p, p', t, t') = \sum_q \int \int d\tau dk T [G_{L,0}^R(p, k, t, \tau) \rho_3 G_R^<(q, p', \tau, t') + \rho_3 G_{L,0}^<(p, k, t, \tau) G_R^A(q, p', \tau, t')]. \quad (28.396)$$

This can be derived straightforwardly by dividing the Keldysh contour into two parts, as shown in the notes by Jauho. The advantage is that we now work on the real time-axis again. The ρ_3 matrices appear because we have used ρ_3 in the fundamental definitions above of the retarded, advanced, and time/contour-ordered Green functions, but we have not done so in the lesser/greater Green functions. More precisely, the ρ_3 is necessary in the definition of the matrices given above in order for them to satisfy the proper Dyson or Gor'kov equation, *e.g.* without any ρ_3 on the δ -function side. Then, for eq. 17 in Jauho's review to be consistent with the definitions given by the various Green functions, we have to add an extra multiplicative ρ_3 for the $G^>$ and $G^<$. This produces Eq. (28.396).

Similarly, one derives

$$\rho_3 C_L^>(p, p', t, t') = \sum_q \int \int d\tau dk T [G_{L,0}^R(p, k, t, \tau) \rho_3 G_R^>(q, p', \tau, t') + \rho_3 G_{L,0}^>(p, k, t, \tau) G_R^A(q, p', \tau, t')]. \quad (28.397)$$

It can be verified from the definitions we have given of the greater, lesser, and Keldysh Green function that

$$C^K(p, p', t, t') = \hat{\rho}_3 [C^>(p, p', t, t') + C^<(p, p', t, t')] \quad (28.398)$$

Moreover, we noted above the relation

$$C^<(p, p', t, t) = C^>(p, p', t, t). \quad (28.399)$$

Therefore, at equal times we have generally:

$$C^K(p, p', t, t') = 2\hat{\rho}_3 C^<(p, p', t, t'). \quad (28.400)$$

Adding Eqs. (28.396) and (28.397) gives the Keldysh component of the Langreth rule:

$$C_L^K(p, p', t, t') = \sum_q \int \int d\tau dk T [G_{L,0}^R(p, k, t, \tau) G_R^K(q, p', \tau, t') + G_{L,0}^K(p, k, t, \tau) G_R^A(q, p', \tau, t')]. \quad (28.401)$$

Setting $t = t'$ and multiplying with $\hat{\rho}_3/2$ gives us:

$$C_L^<(p, p', t, t) = \frac{\hat{\rho}_3}{2} \sum_q \int \int d\tau dk T [G_{L,0}^R(p, k, t, \tau) G_R^K(q, p', \tau, t) + G_{L,0}^K(p, k, t, \tau) G_R^A(q, p', \tau, t)]. \quad (28.402)$$

Assuming that the Green functions have no dependence on center-of-mass time, so that we have a stationary but non-equilibrium situation, we now use that for arbitrary functions f and g :

$$\begin{aligned} \int d\tau f(t - \tau) g(\tau - t') &= \int d\tau \int \int \frac{dE}{2\pi} \frac{dE'}{2\pi} f(E) g(E') e^{i\tau(E-E')} e^{-iEt + iE't'} \\ &= \int \frac{dE}{2\pi} f(E) g(E) e^{-iE(t-t')}. \end{aligned} \quad (28.403)$$

We then obtain

$$C_L^<(p, p', t, t) = \frac{\hat{\rho}_3}{2} \sum_q \int \int \frac{dE}{2\pi} dk T [G_{L,0}^R(p, k, E) G_R^K(q, p', E) + G_{L,0}^K(p, k, E) G_R^A(q, p', E)]. \quad (28.404)$$

Similarly $C_R^<$ is found by interchanging subscripts R and L. The latter substitution is verified by comparing the Heisenberg equations of motion for the operators A_p and B_p . Now, we can finally go back to Eq. (28.421) and evaluate the current. Convert the summations over momenta into integrals according to

$$\sum_q = \frac{V}{(2\pi)^3} \int dq \quad (28.405)$$

where V is the volume, so that

$$\begin{aligned} I &= \frac{e}{2(2\pi)^6} \frac{V^3}{2(2\pi)^3} \int \int \int \int \int \frac{dE}{2\pi} dp dp' dk dq \text{Tr} \left\{ \rho_3 T^2 [G_{L,0}^R(p, k, E) G_R^K(q, p', E) \right. \\ &\quad + G_{L,0}^K(p, k, E) G_R^A(q, p', E)] - \rho_3 T^2 [G_{R,0}^R(p, k, E) G_L^K(q, p', E) \\ &\quad \left. + G_{R,0}^K(p, k, E) G_L^A(q, p', E)] \right\}. \end{aligned} \quad (28.406)$$

Since the Jacobian of the transformation from (p, k) to center-of-mass and relative coordinate $(p + k)/2$ and $p - k$ is unity, we can, exactly, regard p and k in the above equation as center-of-mass and relative momentum and similarly for q and p' . The integrals over the relative momentum then gives

the Green functions evaluated at center-of-mass coordinate $R = 0$ whereas the integrals over center-of-mass momentum immediately gives us the diffusive (isotropic), quasiclassical Green function g since

$$\int d\mathbf{p} G(\mathbf{p}) = \frac{\pi}{i} g. \quad (28.407)$$

In the above equation, I have disregarded a possible constant prefactor involving electron mass m and also wrote $\mathbf{p}$ explicitly to indicate that it is a vector. Therefore, we end up with:

$$I = \frac{e}{2(2\pi)^6} \frac{V^3 T^2}{2(2\pi)^3} \int \frac{dE}{2\pi} \text{Tr} \left\{ \rho_3 [g_{L,0}^R(E) g_R^K(E) + g_{L,0}^K(E) g_R^A(E)] \right. \\ \left. - \rho_3 [g_{R,0}^R(E) g_L^K(E) + g_{R,0}^K(E) g_L^A(E)] \right\}. \quad (28.408)$$

Here, all quasiclassical, isotropic Green functions are evaluated at $R = 0$. Note that if we had kept the momentum-dependence in T_{kp} , we would have had contributions from the p -wave component of the quasiclassical Green function as well. In turn, this would give us gradient terms in the boundary conditions (for instance, in the SOC-case).

Above, we have a mix of g_0 and g terms where 0 means that it is the Green function satisfying the Dyson equation without the tunneling term. Instead of using an isotropization zone argument, we proceed as follows. When we solve the Usadel equation on either side of the interface, we solve it without any explicit tunneling self-energy term in it. This corresponds to solving for g_0 . Then, we supplement the Usadel equation with boundary conditions, which should then be boundary conditions for g_0 .

Our strategy here is to derive an expression for current that depends on the GFs on both sides of the interface. Then, matching that with the $g_0 \nabla g_0$ for current derived on a single side of the material, we get a boundary condition for the GF g_0 .

However, if we now restrict our attention to lowest order in tunneling, then we have $g \simeq g_0$ since the difference between them is that g satisfies an Usadel equation with an additional tunneling self-energy term. Therefore, we can replace g with g_0 and then drop all subscripts 0, keeping in mind that the equation of motion for the GF g_0 is an equation of motion without any explicit tunneling term in it. This is the standard treatment and is equivalent to the argument made right under eq. 2.8 in <https://arxiv.org/pdf/1211.0870>.

We then end up with

$$I = \frac{V^3 T^2}{2(2\pi)^3} \int \frac{dE}{2\pi} \text{Tr} \left\{ \rho_3 [g_L^R(E) g_R^K(E) + g_L^K(E) g_R^A(E)] - \rho_3 [g_R^R(E) g_L^K(E) + g_R^K(E) g_L^A(E)] \right\} \quad (28.409)$$

which can be written more compactly as

$$I = \frac{V^3 T^2}{2(2\pi)^3} \int \frac{dE}{2\pi} \text{Tr} \left\{ \rho_3 [\check{g}_L, \check{g}_R]^K \right\} \quad (28.410)$$

where we defined

$$\check{g} = \begin{pmatrix} g^R & g^K \\ 0 & g^A \end{pmatrix}. \quad (28.411)$$

Comparing this with the quasiclassical expression for the current at the interface (or more precisely, at the beginning of the isotropization zone):

$$I_T \propto \int dE \text{Tr} \{ \rho_3 (\check{g}_L \partial_x \check{g}_L)^K \}, \quad (28.412)$$

we see that the following equation is consistent with the above expressions (by equating the integrands):

$$\check{g}_L \partial_x \check{g}_L \propto T^2 [\check{g}_L, \check{g}_R]. \quad (28.413)$$

This reproduces the KL boundary conditions.

Several comments are in order here. First of all, we have strictly speaking only shown that (dropping a overall constant of proportionality):

$$\text{Tr} \{ \rho_3 (\check{g}_L \partial_x \check{g}_L)^K \} = \text{Tr} \left\{ \rho_3 [\check{g}_L, \check{g}_R]^K \right\}. \quad (28.414)$$

The first step is to try to remove the Tr-operation. This can be justified by noting that if we repeated the analysis above for the spin-current, rather than charge-current, we would have found

$$\text{Tr} \{ \rho_3 \hat{\sigma} (\check{g}_L \partial_x \check{g}_L)^K \} = \text{Tr} \left\{ \rho_3 \hat{\sigma} [\check{g}_L, \check{g}_R]^K \right\}. \quad (28.415)$$

We see that a different spin-dependent matrix appears inside the trace compared to the charge-current case. Similarly, one can find expressions for spin-energy and energy currents with yet a different ρ and/or σ matrix inside the trace. The point is then that although we in each of these cases only show that the traces are supposed to be equal, it is reasonable to assume that the stricter requirement

$$(\check{g}_L \partial_x \check{g}_L)^K = ([\check{g}_L, \check{g}_R])^K \quad (28.416)$$

holds since this would ensure that the equations with traces above are valid for all the different combinations of ρ and/or σ matrices.

The last step required to justify Eq. (28.413) is to show that Eq. (28.416) also holds for the retarded and advanced components. Interestingly, this can be seen to follow by considering the Keldysh component of the boundary condition, namely Eq. (28.416). First, we use that generally one has $g^K = g^R h - h g^A$ where h is the distribution function matrix. Now insert this into Eq. (28.416) and consider two cases.

The first case is when the retarded and advanced (R and A) part of the Usadel equation does not contain any self-energies that depend on h , such as the superconducting gap. This is then true *e.g.* for normal metals with spin-splitting and/or spin-orbit interactions, including also the possibility of spin-flip and spin-orbit impurity scattering. Since the R and A components of the Usadel equation is independent on h , then g^R and g^A must be independent on h . Therefore, any statement we can make about the boundary conditions for g^R and g^A from Eq. (28.416) at a given h must be true for *any* h . Based on this, consider the case of h being a constant throughout the system, so on both sides of the interface. It does not have to be its equilibrium value, but it must be spatially homogeneous so that $\partial_x h = 0$. In that case, Eq. (28.416) reduces to

$$\left[(\check{g}_L \partial_x \check{g}_L)^R - ([\check{g}_L, \check{g}_R])^R \right] h - h \left[(\check{g}_L \partial_x \check{g}_L)^A - ([\check{g}_L, \check{g}_R])^A \right] = 0. \quad (28.417)$$

For this to be true for an arbitrary constant h , the terms in $[\dots]$ must vanish, and thus we find that Eq. (28.416) with $K \rightarrow R, A$ holds for *any* h (including spatially inhomogeneous ones).

The second case is when the retarded and advanced (R and A) part of the Usadel equation *does* contain self-energies that depend on h , such as Δ (through its self-consistency equation). In this case, g^R and g^A depend on h through the self-energy terms which depend on h . Therefore, we cannot immediately conclude that if Eq. (28.416) holds when $K \rightarrow R, A$ for one particular h , it must hold for every h . However, using the same argument as in the first case above when h is a constant which may or may not be out of equilibrium, we see that Eq. (28.416) for $K \rightarrow R, A$ still holds in this case. For the case of a spatially inhomogeneous h , I am not aware of any argument which allows us to conclude that Eq. (28.416) for $K \rightarrow R, A$ still holds using this particular derivation of the boundary conditions (it can be shown mathematically using the much more complicated approach of Eschrig and Cottet).

The summary is therefore that it follows mathematically from Eq. (28.416) that

$$(\check{g}_L \partial_x \check{g}_L)^{R,A} = ([\check{g}_L, \check{g}_R])^{R,A} \quad (28.418)$$

holds for both normal and superconducting systems with any spatially homogeneous h , and it in fact also holds for a normal system with arbitrary h . We will assume that it also holds for superconducting systems with arbitrary h (which has been shown using different methodology in previous papers by Eschrig and Cottet).

Arbitrary tunneling matrix elements

Now that we have seen how the derivation works, we generalize it to arbitrary tunneling matrix. In this case, we shall find use for Langreth rules for products of more than two matrices, such that if

$$D = \int_c ABC \quad (28.419)$$

where $\int_c$ is an integral along the Keldysh-contour, then for instance

$$\begin{aligned} D^< &= \int_t (A^R B^R C^< + A^R B^< C^A + A^< B^A C^A), \\ D^R &= \int_t A^R B^R C^R, \end{aligned} \quad (28.420)$$

where $\int_t$ is along the real time axis.

The derivation now starts from the expression

$$\begin{aligned} \langle \dot{N} \rangle &= \frac{1}{2} \sum_{pp'} \langle A_p^\dagger(t) \mathcal{H}_L^\dagger A_p(t) \delta_{pp'} + B_{p'}^\dagger(t) \tilde{\Gamma}_{p'p} A_p(t) - A_p^\dagger(t) \mathcal{H}_L A_p(t) \delta_{pp'} - A_p^\dagger(t) \Gamma_{pp'} B_{p'}(t) \rangle \\ &= \frac{i}{2} \sum_{pp'} \text{Tr} \{ C_L^<(p, t; p', t) - C_R^<(p, t; p', t) \}. \end{aligned} \quad (28.421)$$

Since Γ and $\tilde{\Gamma}$ are now matrices, we have defined

$$\begin{aligned} C_L^<(p, t; p', t') &= i \langle \left[\left(\tilde{\Gamma}_{p'p}^{\text{tr}} B_{p'}^\dagger(t') \right)^{\text{tr}} \left(A_p(t) \right)^{\text{tr}} \right]^{\text{tr}} \rangle, \\ C_R^<(p, t; p', t') &= i \langle \left[\left(\Gamma_{p'p}^{\text{tr}} A_p^\dagger(t') \right)^{\text{tr}} \left(B_p(t) \right)^{\text{tr}} \right]^{\text{tr}} \rangle. \end{aligned} \quad (28.422)$$

In the above summation, we also used that

$$\sum_{pp'} C_R^<(p', t; p, t) = \sum_{pp'} C_R^<(p, t; p', t) \quad (28.423)$$

which follows simply from renaming indices. Moreover, instead of using a specific $\mathcal{H}_L$ which contains ξ_p and Δ , we do not have to specify $\mathcal{H}_L$ and instead keep it arbitrary in order to avoid assumptions like homogeneous L and R materials. At first glance, this means we write $\sum_{p'} \mathcal{H}_{L,p'} A_{p'}$ instead of $\mathcal{H}_L A_p$ in the Heisenberg equation of motion for the operator-spinor A_p , and similarly for B_p .

We here make some clarifying remarks and corrections to the result derived in Phys. Rev. B **105**, 064506 (2022). First, the term $-d\mathbf{A}^2$ in eq. (53) and the equations following should not be there. This has no consequence for the final result, as the term drops out of the linearized equations.

Secondly, we comment on the transition between eq. (41) and (42) and the accompanying assumptions.

Consider the last line of eq. (41). There are only contributions from the products $p_i q_k$ and $p'_i q'_k$, since the other combinations are averaged to zero when we only take into account the isotropic part of the Green function (since we drop terms that are higher than first order in derivatives). Consider the $p_i q_k$ term. We need to evaluate:

$$\int \int d\mathbf{p} d\mathbf{q} [t\mathbf{p}] G(\mathbf{p}, \mathbf{q}) [t \cdot \mathbf{q}]. \quad (28.424)$$

Introduce CoM and relative coordinates $\mathbf{P} = (\mathbf{p} + \mathbf{q})/2$ and $\mathbf{k} = \mathbf{p} - \mathbf{q}$. If we assume that $G(\mathbf{P}, \mathbf{q})$ is strongly peaked at the Fermi level, which we know to be the case for small perturbations away from the Fermi level for a free electron gas (weak potentials), we can set $\mathbf{p} \rightarrow \mathbf{p}_F$ and $\mathbf{q} \rightarrow \mathbf{q}_F$. For instance, consider a free homogeneous electron gas where the Green function does not depend on CoM coordinate $\mathbf{R}$:

$$G(\mathbf{P}, \mathbf{k}) = \int d\mathbf{R} e^{i\mathbf{k} \cdot \mathbf{R}} G(\mathbf{P}, \mathbf{R}) = \int d\mathbf{R} e^{i\mathbf{k} \cdot \mathbf{R}} G(\mathbf{P}) \propto \delta(\mathbf{k}), \quad (28.425)$$

which shows that the $G(\mathbf{P}, \mathbf{k})$ is peaked at $\mathbf{k} = 0$.

The main contribution to the integrals come from $\mathbf{P} \simeq \mathbf{p}_F$ and $\mathbf{k} \simeq 0$. Switching to CoM and relative coordinate variables in the integral (Jacobian for this transformation is unity), we may write:

$$\int \int d\mathbf{P} d\mathbf{k} [t \cdot \mathbf{P}_F] G(\mathbf{P}, \mathbf{k}) [t \cdot \mathbf{P}_F]. \quad (28.426)$$

We can replace both p and q with $\mathbf{p}_F$ since both are close to the Fermi level like the CoM coordinate, since G ensures that the integrand is largest there.

As we now perform the angular part of the $\int d\mathbf{P}$ integral, we obtain an extra factor $p_F^2/3$ which is not present in the PRB.

28.6.7 Prefactor in KL boundary conditions

The KL boundary condition is derived in detail by Raimondi in these lecture notes <https://citeseerx.ist.psu.edu/document?repid=rep1&type=pdf&doi=454719d38c80426c5bbc24fdf6d1e37a800b2df0> Gyldighet KL-grensebetingelse for liten γ -parameter. Den fundamentale antakelsen som blir gjort n  r man utleder KL grensebetingelser er at transmisjonssannsynligheten gjennom interface er lav. Dvs vi er i tunneling limit. I likningen 63 tilsv  rer alts   tunneling limit $T/R \ll 1$ hvor T og R er transmisjons og refleksjonssannsynlighet. Den antisymmetriske delen (p-wave) av Green funksjonen

som kalles g_a i likning 63 er relatert til den deriverte av s-wave delen av Green funksjonen som vist i likningen nederst på siden. Dette er helt ekvivalent med likningen du kanskje husker fra utledningen av Usadel:

$$g_p = -l_m f p * g s d x g s \quad (28.427)$$

hvor $l_m f p = v F * \tau$ er mean free path i systemet. I artikkelen ovenfor er $\mu = \cos \theta$ hvor θ er innfallsvinkel til elektronene relativt interface, så la oss bare for enkelhets skyld sette $\mu=1$ for et 1D system. La oss normalisere x på ξ , slik at $\tilde{x} = x/\xi$ er dimensjonsløs. Da får vi følgende KL grensebetingelse

$$\gamma * g * d g / d \tilde{x} = [g_1, g_2] \quad (28.428)$$

hvor $\gamma = (R/T) * (l_m f p / \xi)$

Vi vet at $R/T \ll 1$ for at KL skal være gyldig. Men γ -parameteren, slik boundary condition er skrevet ovenfor, kan i prinsippet likevel være ~ 1 dersom $l_m f p / \xi \ll 1$.

Med andre ord: jo mer diffusiv superlederen er, jo mindre er $l_m f p / \xi$, og i prinsippet kan $(R/T) * (l_m f p / \xi)$ være ~ 1 selv om KL krever at $(R/T) \gg 1$.

28.7 Magnetism and RKKY interaction in quasiclassical theory

One has to be careful when considering quantities in quasiclassical theory that have a finite value even in the normal-state. Consider for instance magnetization or RKKY interaction. If one computes the magnetization of a bulk spin-split superconductor to linear response in h , one finds a finite value even at $T = 0$. However, the spin susceptibility of a superconductor at $T = 0$ should be zero since there are no quasiparticles present. Another problem arises if we compute the magnetization of a normal metal with an exchange field quasiclassically: one obtains zero at any temperature.

Therefore, quasiclassical theory in fact only computes the change in magnetization that occurs in the superconducting state. To get the total magnetization, one has to add a Pauli paramagnetic term that has a contribution from states far away from the Fermi level. This can be computed using the exact Green function. There should be no magnetism in a homogeneous and magnetic impurity-free superconductor at $T = 0$ at $h < \Delta$, but for $h > \Delta$ (which is achievable close to T_c) the gap in the spectrum closes and a finite magnetization $\propto \sqrt{h^2 - \Delta^2}$ should appear.

One also has to consider the fact that in some cases, it may not be sufficient to simply add the normal-state result to the result obtained for a physical quantity using quasiclassical theory. To see this, consider the RKKY interaction in an FSF junction. If we evaluate the equilibrium supercurrent quasiclassically in an FNF junction, we get zero. This is wrong since we know that there should exist an RKKY interaction. Since this oscillates on a scale k_F^{-1} , quasiclassical theory does not capture this contribution. If we compute the RKKY current in an FSF junction, we do obtain a finite value. This is the superconducting contribution to the RKKY current which decays exponentially over ξ and favors and antiferromagnetic coupling. Now, we might be tempted to think that we simply have to add the normal-state contribution (oscillating) to the RKKY current to get the total RKKY current in the FSF case. However, this is not entirely correct. The normal-state oscillating RKKY interaction is in fact renormalized in the superconducting case: it also acquires an exponential damping factor over a length ξ .

Similarly, the quasiclassically computed proximity-induced magnetization in the S of an S/F structure contains only the *quasiclassically* allowed change in magnetization that occurs in the superconducting state compared to the normal state. Any rapidly oscillating induced magnetization in the normal-state is not captured, and such a term can also potentially be renormalized in the superconducting state.

RKKY interaction mediated by a superconductor

The effect of superconductivity on RKKY interactions is well established at lowest-order perturbation theory (Born approximation) in the exchange interaction between the localized and itinerant spins. In particular, the suppressed spin susceptibility in the superconducting ground state modifies the inter-impurity interaction to become purely anti-ferromagnetic when the separation between the impurities exceeds the superconducting coherence length; at such distances however, the strength of this antiferromagnetic exchange is exponentially small in the separation r . On the other hand, for impurities separated by distances $r < \xi$ conventional RKKY dominates the effective interaction and superconductivity yields only a weak antiferromagnetic correction. Crucially, this perturbative treatment neglects the formation of so-called Yu-ShibaRusinov (YSR) bound states—localized electronic states that arise near a magnetic impurity. It has been shown that if such states are tuned to an energy close to the middle of the superconducting gap, the superconducting contribution to RKKY becomes much stronger.

The RKKY current through a superconductor in general thus has two terms: an oscillating one, which exists also in the normal state, and an exponentially decaying one, which exists only in the superconducting state [60]. Quasiclassical theory can be used to compute the purely superconducting contribution to the RKKY interaction which does not exist in the normal state. However, one should be careful to conclude that the superconducting contribution is the dominant one for large separation distances between the F electrodes. This is tempting since in the ballistic case the normal-state RKKY current decays as $(k_F L)^{-d}$ where d is the dimension of the normal metal, whereas the superconducting contribution decays as $(k_F L)^{-d+1} e^{-L/\xi}$ as shown in [61]. However, the superconducting term also has an additional prefactor Δ/E_F which is very small for conventional low- T_c superconductors (higher for high- T_c ones). In the limit $T \rightarrow 0$, homogeneous spin susceptibility $\chi(\mathbf{q} = 0) = \int d\mathbf{r} \chi(\mathbf{r})$ should vanish. This does not mean that the RKKY current vanishes at $T = 0$ in a superconductor since other $\mathbf{q}$ modes can contribute when the superconductor has a finite length.

In the diffusive limit, the normal metal contribution acquires an exponentially damping factor $e^{-L/l_{\text{mfp}}}$ if one averages over different impurity configurations. If one does not average over impurity configurations, i.e. consider one specific configuration, no such factor appears and the oscillations are instead just phase-shifted. However, one should average over different impurity configurations for a macroscopic sample $L \gg l_{\text{mfp}}$ because ... On the other hand, the superconducting contribution has a longer range because it is cut off by an exponential $e^{-L/\xi}$ instead. Therefore, quasiclassical theory can appropriately describe the RKKY interaction of a diffusive FSF structure for $L \geq \xi$ since the oscillating contribution is completely suppressed by then since $l_{\text{mfp}} \ll \xi$.

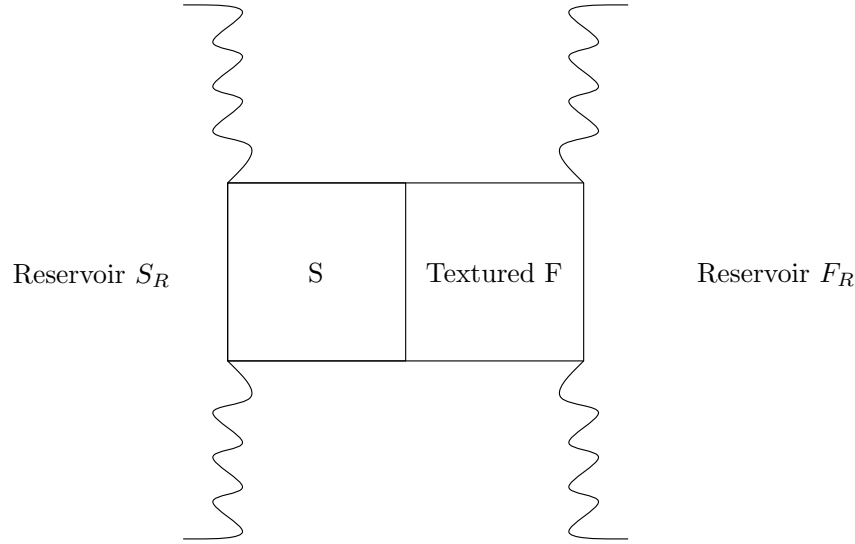


Figure 28.12: (Color online) Generic setup for study of non-equilibrium properties: a mesoscopic ferromagnet/superconductor bilayer is connected to respective reservoirs in each end. We shall allow for an arbitrary spin-texture in the ferromagnet, thus accounting for triplet correlations and the resulting spin accumulation properties.

28.8 Non-equilibrium effects

28.8.1 Kinetic equations

To illustrate how non-equilibrium effects may be captured in the quasiclassical theory, we consider a quite general type of structure shown in Fig. 28.12: a non-superconducting reservoir F_R is connected to a mesoscopic metal F , which may be ferromagnetic. In turn, this metal is in contact to a mesoscopic superconductor S which finally is terminated by a superconducting reservoir S_R . The reservoirs are mainly present to provide suitable boundary conditions at the edges of the mesoscopic samples, in particular for the distribution functions.

To study the full non-equilibrium properties of this system, accounting for all possible types of superconducting pairing correlations, we will use the Ricatti-parametrization for the Green's function. The starting point is the Usadel equation and the Kupriyanov-Lukichev boundary conditions for the 8×8 Green's function $\check{g}$ in Keldysh-Nambu space. The Usadel equation reads:

$$D_F \partial_x (\check{g} \partial_x \check{g}) + i[\varepsilon \hat{\rho}_3 + \hat{\Delta} + \hat{M} - \check{\sigma}_{sf}, \check{g}] = 0, \quad (28.429)$$

whereas the boundary conditions are:

$$2L_j \gamma_j \check{g}_j \partial_x \check{g}_j = [\check{g}_1, \check{g}_2], \quad j \in 1, 2. \quad (28.430)$$

Here, $\check{g}_j$ is the Green's function in region j with $j = 1$ being S and $j = 2$ being F whereas L_j and γ_j represent the width of region j and the ratio between interface barrier and bulk resistance of the region j , respectively (i.e. $\gamma_j = R_B/R_j$). In Ref. Matthias PRL 13, spin-dependent boundary

conditions valid for an arbitrary polarization in the tunneling limit were derived. They read:

$$\begin{aligned}
2d\gamma_l\check{g}_l\partial_x\check{g}_l &= [\check{g}_l, \check{g}_r] + \frac{G_{MR}}{G_T}[\check{g}_l, \{\check{A}, \check{g}_r\}] + \frac{iG_\phi^l}{G_T}[\check{g}_l, \check{A}] + \frac{iG_\chi^l}{G_T}[\check{g}_l, \check{g}_r\check{g}_l\check{A} + \check{A}\check{g}_l\check{g}_r] \\
&\quad + \frac{iG_\chi^r}{G_T}[\check{g}_l, \check{g}_r[\check{A}, \check{g}_r]] + \frac{G'}{G_T}[\check{g}_l, \check{A}\check{g}_r\check{A}], \\
2d\gamma_r\check{g}_r\partial_x\check{g}_r &= [\check{g}_l, \check{g}_r] - \frac{G_{MR}}{G_T}[\check{g}_r, \{\check{A}, \check{g}_l\}] - \frac{iG_\phi^r}{G_T}[\check{g}_r, \check{A}] - \frac{iG_\chi^r}{G_T}[\check{g}_r, \check{g}_l\check{g}_r\check{A} + \check{A}\check{g}_r\check{g}_l] \\
&\quad - \frac{iG_\chi^l}{G_T}[\check{g}_r, \check{g}_l[\check{A}, \check{g}_l]] - \frac{G'}{G_T}[\check{g}_r, \check{A}\check{g}_l\check{A}],
\end{aligned} \tag{28.431}$$

All quantities are microscopically defined as follows:

$$\begin{aligned}
G_T &= G_q \sum_n T_n (1 + \sqrt{1 - P_n^2}), \\
G' &= G_q \sum_n T_n (1 - \sqrt{1 - P_n^2}), \\
G_{MR} &= G_q \sum_n T_n P_n, \\
G_\chi^j &= G_q \sum_n T_n d\phi_n^j / 2, \\
G_\phi^j &= -2G_q \sum_n d\phi_n^j \\
\gamma_j &= \frac{A}{LG_T \rho_j} = \frac{R_B}{R_j}
\end{aligned} \tag{28.432}$$

Above, $G_q = e^2/h$ is the quantum of conductance, A is the interface area, d is the width of the junction, ρ_j is the resistivity of the material on the j 'th side ($j = l, r$), T_n is the transmission probability for channel n , P_n is the polarization of channel n , while $d\phi_n^j$ is the spin-dependent phase-shifts occuring on side j . Note that these reduce to Eq. (28.430) in the non-magnetic limit $\{P_n, d\phi_n\} \rightarrow 0$. We defined $\hat{A} = \text{diag}(\hat{A}, \hat{A})$.

$$\hat{A} = \begin{pmatrix} \mathbf{m} \cdot \boldsymbol{\sigma} & 0 \\ 0 & \mathbf{m} \cdot \boldsymbol{\sigma}^* \end{pmatrix} \tag{28.433}$$

where $\mathbf{m}$ is the unit magnetization vector at the interface. These boundary conditions are valid for any P_n in the range 0 to 1.

The self-energy spin-flip term has the structure

$$\check{\sigma}_{\text{sf}} = \begin{pmatrix} \hat{\sigma}^R & \hat{\sigma}^K \\ 0 & \hat{\sigma}^A \end{pmatrix} \tag{28.434}$$

in general. If we now insert our $\check{g}$ into the Usadel equation, we obtain the standard Usadel equation for the retarded and advanced component of the Green's function:

$$D_F \partial_x (\hat{g}^{R,A} \partial_x \hat{g}^{R,A}) + i[\hat{P}^{R,A}, \hat{g}^{R,A}] = 0, \tag{28.435}$$

where we have defined

$$\hat{P}^{R,A} = \varepsilon \hat{\rho}_3 + \hat{\Delta} + \hat{M} - \hat{\sigma}^{R,A}. \tag{28.436}$$

From the definition of the Green's function, one may derive that $\hat{g}^A = -(\hat{\rho}_3 \hat{g}^R \hat{\rho}_3)^\dagger$ holds both in and out of equilibrium, meaning that it is sufficient to compute $\hat{g}^R$. To solve the equation for $\hat{g}^R$, it is convenient to parametrize it in Ricatti-style, where we introduce the two matrices γ and $\tilde{\gamma}$:

$$\hat{g}^R = \begin{pmatrix} N(1 + \gamma\tilde{\gamma}) & 2N\gamma \\ -2\tilde{N}\tilde{\gamma} & -\tilde{N}(1 + \tilde{\gamma}\gamma) \end{pmatrix} \quad (28.437)$$

with the normalization matrices $N = (1 - \gamma\tilde{\gamma})^{-1}$ and $\tilde{N} = (1 - \tilde{\gamma}\gamma)^{-1}$. It is useful to note the following properties:

$$N\gamma = \gamma\tilde{N}, \quad \tilde{N}\tilde{\gamma} = \tilde{\gamma}N, \quad \partial_x N = NDN, \quad \partial_x \tilde{N} = \tilde{N}\tilde{D}\tilde{N}, \quad (28.438)$$

with $D = (\partial_x \gamma)\tilde{\gamma} + \gamma(\partial_x \tilde{\gamma})$ and $\tilde{D} = (\partial_x \tilde{\gamma})\gamma + \tilde{\gamma}(\partial_x \gamma)$.

$$\begin{aligned} D_F[\partial_x^2 \gamma + 2(\partial_x \gamma)\tilde{N}\tilde{\gamma}(\partial_x \gamma)] + 2i\varepsilon\gamma + i\mathbf{h} \cdot (\boldsymbol{\sigma}\gamma - \gamma\boldsymbol{\sigma}^*) + \Delta(\sigma_y - \gamma\sigma_y\gamma) &= 0, \\ D_F[\partial_x^2 \tilde{\gamma} + 2(\partial_x \tilde{\gamma})N\gamma(\partial_x \tilde{\gamma})] + 2i\varepsilon\tilde{\gamma} + i\mathbf{h} \cdot (\tilde{\gamma}\boldsymbol{\sigma} - \boldsymbol{\sigma}^*\tilde{\gamma}) - \Delta(\sigma_y - \tilde{\gamma}\sigma_y\tilde{\gamma}) &= 0. \end{aligned} \quad (28.439)$$

The order parameters $\mathbf{h}$ and Δ should be put to zero in the S and F regions, respectively. For a bulk superconductor in equilibrium, one has:

$$\hat{g}_{\text{BCS}} = \begin{pmatrix} c\mathbb{1} & s i\sigma_y \\ s i\sigma_y & -c\mathbb{1} \end{pmatrix}, \quad s \equiv \sinh(\theta), c \equiv \cosh(\theta), \theta = \text{atanh}(\Delta/\varepsilon). \quad (28.440)$$

Comparison with the parametrization of the Green's function in Eq. (28.437) gives:

$$\gamma = s i\sigma_y / (1 + c), \quad \tilde{\gamma} = -s i\sigma_y / (1 + c). \quad (28.441)$$

For a bulk homogeneous ferromagnet, the solution is simply $\gamma = \tilde{\gamma} = 0$. Note that it might look like we have the symmetry $f_s(\varepsilon) = -f_s(-\varepsilon)^*$ for singlet correlations from the above Green's function [and one might think this generalizes to $f_t(\varepsilon) = f_t(-\varepsilon)^*$ for triplet ones], but this is only the case because we have set the superconducting phase to zero. In a bilayer setup, where the SC phase plays no role, we should thus have this symmetry for the proximity-induced anomalous Green's function. In a Josephson junction, however, we cannot assume that this is the case. Note that what defines if superconducting correlations are even- or odd-frequency is the relation between the retarded and advanced part of the Green's function:

$$\text{Even-frequency: } f^R(\varepsilon) = f^A(-\varepsilon), \quad (28.442)$$

$$\text{Odd-frequency: } f^R(\varepsilon) = -f^A(-\varepsilon). \quad (28.443)$$

Distribution function matrix and fluctuation-dissipation theorem

For the Keldysh part (upper right 4×4 block of the Usadel equation), we obtain:

$$D_F \partial_x (\hat{g}^R \partial_x \hat{g}^K + \hat{g}^K \partial_x \hat{g}^A) + i(\hat{P}^R \hat{g}^K - \hat{\sigma}^K \hat{g}^A) - i(\hat{g}^K \hat{P}^A - \hat{g}^R \hat{\sigma}^K) = 0. \quad (28.444)$$

We know that the following properties hold in general:

$$(\hat{g}^R)^2 = (\hat{g}^A)^2 = \hat{1}, \quad \hat{g}^R \hat{g}^K + \hat{g}^K \hat{g}^A = 0. \quad (28.445)$$

From the latter property, one can infer that $\hat{g}^K$ may always be written as

$$\hat{g}^K = \hat{g}^R \hat{h} - \hat{h} \hat{g}^A \quad (28.446)$$

where $\hat{h}$ is any matrix. To be precise, however, $\hat{h}$ needs to have a specific symmetry structure which one may verify directly from Eq. (28.356) and the symmetry structure of $\hat{g}^K$:

$$\hat{h} = \begin{pmatrix} \mathcal{X} & \mathcal{Y} \\ -\tilde{\mathcal{Y}} & -\tilde{\mathcal{X}} \end{pmatrix}. \quad (28.447)$$

An important observation is that $\hat{h}$ is not uniquely defined from the last equation in Eq. (28.445). This can be seen by noting that if you add an arbitrary matrix $\hat{y}$ so that $\hat{h} \rightarrow \hat{h} + \hat{g}^R \hat{y} + \hat{y} \hat{g}^A$, then the equation is still satisfied. This gives us some freedom in terms of choosing $\hat{h}$ in a form that is convenient for us, depending on if we would like to do analytical or numerical calculations. A common choice is to let $\hat{h}$ be diagonal, which we shall also use here: $\hat{h} = \text{diag}(\mathcal{X}, -\tilde{\mathcal{X}})$. To determine the content of $\hat{h}$, we need an equation of motion for it. This is obtained from the Keldysh part of the Usadel equation, Eq. (28.444). Inserting for $\hat{g}^K$, we obtain:

$$\begin{aligned} [D_F \partial_x^2 \hat{h} + (\hat{g}^R \partial_x \hat{g}^R)(\partial_x \hat{h}) - (\partial_x \hat{h})(\hat{g}^A \partial_x \hat{g}^A) - \partial_x(\hat{g}^R(\partial_x \hat{h})\hat{g}^A)] \\ + i\hat{g}^R(\hat{P}^R \hat{h} - \hat{h} \hat{P}^A) - i(\hat{P}^R \hat{h} \hat{g}^A - \hat{h} \hat{P}^A \hat{g}^A) + i(\hat{g}^R \hat{\sigma}^K - \hat{\sigma}^K \hat{g}^A) = 0. \end{aligned} \quad (28.448)$$

At this point, it is useful to motivate the interpretation of $\hat{h}$ as the distribution function matrix from a mathematical viewpoint. In what follows, let us for simplicity work with scalar Green functions without spin indices. The arguments are straightforward to generalize to matrix form.

Firstly, consider the non-quasiclassical Gor'kov Green functions $G^R, G^A, G^K, G^<, G^>$. For instance, the Keldysh Green function is $G^K(\mathbf{r}, \mathbf{r}', t, t') = -i\langle[\psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t')]\rangle$. The two latter are the lesser and greater Green functions which are for fermions defined as:

$$\begin{aligned} G^<(\mathbf{r}, \mathbf{r}', t, t') &= i\langle\psi^\dagger(\mathbf{r}', t')\psi(\mathbf{r}, t)\rangle, \\ G^>(\mathbf{r}, \mathbf{r}', t, t') &= -i\langle\psi(\mathbf{r}, t)\psi^\dagger(\mathbf{r}', t')\rangle. \end{aligned} \quad (28.449)$$

Consider now thermal equilibrium. The correlation functions (Green functions) are then subject to a boundary condition in imaginary time which is related to the fluctuation-dissipation theorem. Namely, in a grand canonical ensemble, one verifies that

$$\langle\psi(\mathbf{r}, t - i\beta)\psi^\dagger(\mathbf{r}', t')\rangle = \langle\psi^\dagger(\mathbf{r}', t')\psi(\mathbf{r}, t)\rangle \quad (28.450)$$

by using that

$$\begin{aligned} \psi(\mathbf{r}, t) &= e^{i(H - \mu N)t} \psi(\mathbf{r}) e^{-i(H - \mu N)t}, \\ \langle \dots \rangle &= \text{Tr} \left(\frac{e^{-(H - \mu N)\beta}}{\text{Tr}\{e^{-(H - \mu N)\beta}\}} \dots \right) \end{aligned} \quad (28.451)$$

and the cyclic property of trace. For the Green functions, the same procedure gives

$$G^<(t, t') = -G^>(t - i\beta, t') \quad (28.452)$$

where we omitted spatial indices for simplicity. Fourier-transforming via $\int d\tau e^{iE\tau}$ with $\tau \equiv t - t'$, we get the equilibrium relation

$$G^<(E) = -G^>(E)e^{-\beta E} \quad (28.453)$$

This relation can now be used to derive a general relation between the retarded, advanced, and Keldysh Green function in equilibrium. Namely, the following relations are valid (not only in equilibrium):

$$G^K = G^> + G^<, \quad G^R - G^A = G^> - G^<. \quad (28.454)$$

Therefore, in equilibrium we may insert Eq. (28.453) to get

$$G^R - G^A = G^K \frac{1 + e^{-\beta E}}{1 - e^{-\beta E}}. \quad (28.455)$$

Rearranging the energy-dependent factor, this shows that in equilibrium we have generally

$$G^K = (G^R - G^A) \tanh(\beta E/2). \quad (28.456)$$

We note that $\tanh(\beta E/2) = 1 - 2f(E)$ where $f(E)$ is the Fermi-Dirac distribution function. A key message is thus that in thermal equilibrium, all Green's functions can thus be specified once a *single* of them is known, say the retarded Green's functions, and the quantum statistics of the particles is then reflected in relations governed by the fluctuation-dissipation type relationship given by the energy-dependent factor above. For instance, in the case of bosons in equilibrium at temperature T , the fluctuation-dissipation relation instead reads

$$G^K = (G^R - G^A) \coth(\beta E/2). \quad (28.457)$$

Formally, the fluctuation-dissipation theorem expresses a relationship between a commutator and anti-commutator equilibrium average. This is also the case for the relation $G^K = (G^R - G^A) \tanh(\beta E/2)$ since the Green functions are given by commutators and anti-commutators, respectively. Another application of the fluctuation-dissipation theorem is a relationship the imaginary part of a linear response function (governing the dissipation in a system) and the equilibrium fluctuations.

Next, we note that the number of particles at $(\mathbf{r}, t)$ is

$$n_e(\mathbf{r}, t) = \langle \psi^\dagger(\mathbf{r}, t) \psi(\mathbf{r}, t) \rangle. \quad (28.458)$$

From their definitions, we then have generally [see *e.g.* Sci. Rep. **9**, 12731 (2019)]

$$n_e(\mathbf{r}, t) = \frac{i}{2} [G^R(\mathbf{r}, \mathbf{r}, t, t) - G^A(\mathbf{r}, \mathbf{r}, t, t) - G^K(\mathbf{r}, \mathbf{r}, t, t)]. \quad (28.459)$$

Since $G(t, t) = \int dE G(E)$ for a stationary situation where the Green function depends only on relative time, we get that the particle number n_e must be time-independent and thus

$$n_e = \frac{i}{2} \int dE [G^R(E) - G^A(E) - G^K(E)] \quad (28.460)$$

In equilibrium, we derived above that $G^K = (G^R - G^A) \tanh(\beta E/2)$ so that

$$n_e = i \int dE (G^R - G^A) f(E) \quad (28.461)$$

From their definitions, we have generally in a stationary situation that $G^A(E) = [G^R(E)]^*$. Therefore, the above equation reduces to

$$n_e = - \int dE \text{Im}\{G^R\} f(E). \quad (28.462)$$

It is clear that $-\text{Im}\{G^R(E)\}$ has to be the energy-resolved density of states $D(E)$: the integral over the density of states D times the occupation of states f has to be the total number of states n_e .

Now we can finally see why h in the Usadel equation (diffusive limit) is related to quasiparticle occupation. Namely, if we use a non-equilibrium relation *ansatz* $G^K = (G^R - G^A)h(E)$ instead, which is consistent with the quasiclassical relation $g^K = (g^R - g^A)h$ in the diffusive limit (the defining equation for h), we get

$$n_e = - \int dE \text{Im}\{G^R\}[1 - h(E)]/2. \quad (28.463)$$

The DOS $D(E) = -\text{Im}\{G^R(E)\}$ is the same, but the occupation of quasiparticle states might differ from Fermi-Dirac. Therefore, $f(E)$ is replaced by $(1 - h)/2$ where h must be solved for by kinetic equations. The quantity $(1 - h)/2$ then describes the occupation for electrons in a general non-equilibrium situation. We may write such an occupation function as $f_{\text{noneq}}(E)$. It follows that $h = 1 - 2f_{\text{noneq}}(E)$.

28.8.2 Convenient matrix form of kinetic equations

Just as we obtain equations of motion for the Ricatti-matrices γ and $\tilde{\gamma}$ from the retarded and advanced components of the Green's function, we here seek an equation of motion for the distribution functions $\mathcal{X}$ and $\tilde{\mathcal{X}}$. Here, we wish to rewrite the equation in a form where the second derivative of $\hat{h}$ is expressed as a function of all other matrices, including the first derivatives of $\hat{h}$. This is particularly convenient in terms of numerical implementation in *e.g.* MATLAB. To do so, we first rewrite the Keldysh part of the Usadel equation as:

$$D_F[\partial_x^2 \hat{h} - (\hat{g}^R(\partial_x^2 \hat{h})\hat{g}^A)] = \hat{T} \quad (28.464)$$

where the matrix $\hat{T} = \hat{T}(\hat{g}^R, \hat{g}^A, \hat{P}^R, \hat{P}^A, \hat{h}, \partial_x \hat{h})$ can be identified from Eq. (28.448). By considering the $_{11}$ and $_{12}$ components of Eq. (28.464) and combining them to eliminate $\partial_x^2 \tilde{\mathcal{X}}$ in favor of $\partial_x^2 \mathcal{X}$, one eventually finds an expression of the form:

$$D_F \partial_x^2 \mathcal{X} + \hat{\mathcal{C}}(\partial_x^2 \mathcal{X})\hat{\mathcal{D}} = \hat{\mathcal{E}} \quad (28.465)$$

where we have defined the matrices:

$$\begin{aligned} \hat{\mathcal{C}} &= D_F N(1 + \gamma\tilde{\gamma}), \\ \hat{\mathcal{D}} &= (1 + \tilde{\gamma}^\dagger \gamma^\dagger)N^\dagger - 4\tilde{\gamma}^\dagger(1 + \gamma^\dagger \tilde{\gamma}^\dagger)^{-1}\gamma^\dagger N^\dagger, \\ \hat{\mathcal{E}} &= T_{11} - 2T_{12}(\tilde{N}^\dagger)^{-1}(1 + \gamma^\dagger \tilde{\gamma}^\dagger)^{-1}\gamma^\dagger N^\dagger. \end{aligned} \quad (28.466)$$

The above equation constitutes a linear system of equations for the components of $\partial_x^2 \mathcal{X}$, which thus may be solved in the form:

$$\begin{pmatrix} \partial_x^2 \mathcal{X}_{11} \\ \partial_x^2 \mathcal{X}_{12} \\ \partial_x^2 \mathcal{X}_{21} \\ \partial_x^2 \mathcal{X}_{22} \end{pmatrix} = \hat{A}^{-1} \begin{pmatrix} \mathcal{E}_{11} \\ \mathcal{E}_{12} \\ \mathcal{E}_{21} \\ \mathcal{E}_{22} \end{pmatrix} \quad (28.467)$$

with

$$\hat{A} = \begin{pmatrix} D_F + \mathcal{C}_{11}\mathcal{D}_{11} & \mathcal{C}_{11}\mathcal{D}_{21} & \mathcal{C}_{12}\mathcal{D}_{11} & \mathcal{C}_{12}\mathcal{D}_{21} \\ \mathcal{C}_{11}\mathcal{D}_{12} & D_F + \mathcal{C}_{11}\mathcal{D}_{22} & \mathcal{C}_{12}\mathcal{D}_{12} & \mathcal{C}_{12}\mathcal{D}_{22} \\ \mathcal{C}_{21}\mathcal{D}_{11} & \mathcal{C}_{21}\mathcal{D}_{21} & D_F + \mathcal{C}_{22}\mathcal{D}_{11} & \mathcal{C}_{22}\mathcal{D}_{21} \\ \mathcal{C}_{21}\mathcal{D}_{12} & \mathcal{C}_{21}\mathcal{D}_{22} & \mathcal{C}_{22}\mathcal{D}_{12} & D_F + \mathcal{C}_{22}\mathcal{D}_{22} \end{pmatrix} \quad (28.468)$$

By performing the $\tilde{\cdot}$ operation on the equation, we get the corresponding equation for $\partial_x^2 \tilde{\mathcal{X}}$. Summarizing so far, Eqs. (??) and (28.467) must be solved to determine $\{\gamma, \tilde{\gamma}, \mathcal{X}, \tilde{\mathcal{X}}\}$. Since these are coupled differential equations, we have to supply boundary conditions. We here restrict our attention to the experimentally most relevant form of the boundary conditions with a relatively low interface transparency due to Kupriyanov and Lukichev. For a bilayer with region 1 to the left and region 2 to the right side of the interface, these read:

$$2L_j \zeta_j \check{g}_j \partial_x \check{g}_j = [\check{g}_1, \check{g}_2] \text{ with } j = 1, 2 \quad (28.469)$$

with $\zeta_j \equiv R_B/R_j$ characterizing the interface resistance. These boundary conditions are thus applicable for $\zeta_i \gg 1$ although it may be noted that they also give the correct result in the limit of perfect interface transparency, in which case the Green's function and its derivative are both continuous across the interface. The boundary conditions for $\hat{g}^R$ take identical form as Eq. (28.469) with the substitution $\check{g} \rightarrow \hat{g}^R$. From the Keldysh part of Eq. (28.469), we obtain:

$$2L_j \zeta_j [\partial_x \hat{h}_j - \hat{g}_j^R (\partial_x \hat{h}_j) \hat{g}_j^A] = \hat{T}_j' \text{ with } j = 1, 2 \quad (28.470)$$

where we have defined the matrix:

$$\hat{T}_j' = [\check{g}_1, \check{g}_2]^K - 2L_j \zeta_j [\hat{g}_j^R (\partial_x \hat{g}_j^R) \hat{h}_j - \hat{g}_j^R \hat{h}_j (\partial_x \hat{g}_j^A) + (\hat{g}_j^R \hat{h}_j - \hat{h}_j \hat{g}_j^A) \partial_x \hat{g}_j^A]. \quad (28.471)$$

Equation (28.470) has exactly the same form as Eq. (28.464) upon the substitution $\partial_x^2 \hat{h} \rightarrow \partial_x \hat{h}$ and $D_F \rightarrow p_j \equiv 2L_j \zeta_j$. Thus, we can immediately write down the boundary conditions:

$$\begin{pmatrix} \partial_x (\mathcal{X}_{11})_j \\ \partial_x (\mathcal{X}_{12})_j \\ \partial_x (\mathcal{X}_{21})_j \\ \partial_x (\mathcal{X}_{22})_j \end{pmatrix} = \hat{A}_j^{-1} \begin{pmatrix} \mathcal{E}'_{11} \\ \mathcal{E}'_{12} \\ \mathcal{E}'_{21} \\ \mathcal{E}'_{22} \end{pmatrix}, \quad (28.472)$$

with:

$$\hat{A}_j = \begin{pmatrix} p_j + (\mathcal{C}'_{11})_j (\mathcal{D}'_{11})_j & (\mathcal{C}'_{11})_j (\mathcal{D}'_{21})_j & (\mathcal{C}'_{12})_j (\mathcal{D}'_{11})_j & (\mathcal{C}'_{12})_j (\mathcal{D}'_{21})_j \\ (\mathcal{C}'_{11})_j (\mathcal{D}'_{12})_j & p_j + (\mathcal{C}'_{11})_j (\mathcal{D}'_{22})_j & ((\mathcal{C}'_{12})_j (\mathcal{D}'_{12})_j & (\mathcal{C}'_{12})_j (\mathcal{D}'_{22})_j \\ (\mathcal{C}'_{21})_j (\mathcal{D}'_{11})_j & (\mathcal{C}'_{21})_j (\mathcal{D}'_{21})_j & p_j + (\mathcal{C}'_{22})_j (\mathcal{D}'_{11})_j & (\mathcal{C}'_{22})_j (\mathcal{D}'_{21})_j \\ (\mathcal{C}'_{21})_j (\mathcal{D}'_{12})_j & (\mathcal{C}'_{21})_j (\mathcal{D}'_{22})_j & (\mathcal{C}'_{22})_j (\mathcal{D}'_{12})_j & p_j + (\mathcal{C}'_{22})_j (\mathcal{D}'_{22})_j \end{pmatrix} \quad (28.473)$$

where we have defined the matrices:

$$\begin{aligned} \hat{\mathcal{C}}_j' &= p_j N_j (1 + \gamma_j \tilde{\gamma}_j), \\ \hat{\mathcal{D}}_j' &= (1 + \tilde{\gamma}_j^\dagger \gamma_j^\dagger) N_j^\dagger - 2\tilde{\gamma}_j^\dagger (1 + \gamma_j^\dagger \tilde{\gamma}_j^\dagger)^{-1} \gamma_j^\dagger N_j^\dagger, \\ \hat{\mathcal{E}}_j' &= (T'_{11})_j - 2(T'_{12})_j (\tilde{N}_j^\dagger)^{-1} (1 + \gamma_j^\dagger \tilde{\gamma}_j^\dagger)^{-1} \gamma_j^\dagger N_j^\dagger. \end{aligned} \quad (28.474)$$

There is also an alternative, and in hindsight actually better, way to write down the kinetic equations. Ali has derived this in his thesis and is shown in detail in some of the later papers. The expressions for the total charge and spin currents flowing in the system are (in the absence of any gauge-potential)

$$\begin{aligned} I_Q &= \frac{N_0 e D A}{16} \int d\varepsilon \text{Tr} \{ \rho_3 (\check{g} \partial_x \check{g})^K \}, \\ I_{S,j} &= \frac{N_0 \hbar D A}{8} \int d\varepsilon \text{Tr} \{ \rho_3 \tau_j (\check{g} \partial_x \check{g})^K \}, \end{aligned} \quad (28.475)$$

where $\tau_j = \text{diag}(\sigma_j, \sigma_j^*)$. Note that one may prove that the charge-current is conserved by performing the operation $\text{Tr}\{\rho_3 \dots\}$ on the Keldysh part of the Usadel equation (this procedure will reveal if there is some term that should cause charge-current to not be conserved, which is not the case in typical proximity structures). The spin-current will in general not be conserved. However, it can be shown from the fundamental symmetries of the Green's function that it must be purely real for all components. In particular, this is clearly seen in the weak proximity effect regime.

28.8.3 Self-energy terminology for skew scattering and side jump

Hei Lina,

nÅr tror jeg at jeg har fått mer klarhet i bakgrunnen for terminologien sidejump/skew scattering for selvenneriene. Figurene i litteraturen som viser bevegelsesbanen til elektronene for disse (f.eks. figur 3b,c i <https://arxiv.org/pdf/0904.4154.pdf>), antyder jo at disse leddene har ulik påvirkning på hvordan elektronene beveger seg som følge av spredningen på urenheten med spinn-bane kobling. Dette er ikke så lett å se fra selvenneriene, men det går derimot an å se hvis man går kvantemekanisk spredningsteori - på samme måte som vi gjorde i kvantemekanikk 2, hvis du husker det ;)

Man skriver da bølgefunksjonen som en innkommende planbølge og en spredt del, dvs $\psi = \exp(ik \cdot r) + f(\theta, \phi) \exp(ikr)/r$, og beregner spredningsamplituden $f(\theta, \phi)$. Denne gir blant annet diff. scatt. cross section via $d\sigma/d\Omega = |f|^2$. Når man har funnet spredningsamplituden, kan vi si noe om hvordan elektronet beveger seg siden vi vet hvordan bølgefunksjonen ser ut i real-space. Da kan man identifisere baner som vist i figur 3b,c.

Spørsmålet er da hvordan vi finner amplituden f . I kvante2, viste vi hvordan den kunne beregnes i Born-approximasjon eller via partial wave method. Side-jump mekanismen (dvs. som gir en spredningsamplitude som tilsvarer en elektronbane som vist figur 3b) kan beregnes som vist her:

<https://arxiv.org/pdf/1211.2372.pdf>

Se equation 1. Den inneholder impurity potential i uperturbert H-operator, og SOC impurity potential i perturbasjonen. På den måten blir side-jump mekanismen første orden i impurity og første orden i SOC. Dermed burde selvennerien som vi beregner i kvasiklassisk teori som er første orden i impurity og første orden i SOC tilsvare nettopp denne side-jump mekanismen.

På samme vis kan man beregne skew scattering bidraget i kvantemekanisk spredningsteori. Dette krever tydeligvis en tredje ordens Born approximasjon, se seksjon 3.2 her <https://arxiv.org/pdf/cond-mat/0603306.pdf>. Det er igjen konsistent med at skew-scattering selfenergien i Camilla sin artikkel er tredje orden totalt i impurity og SOC-potensialet.

Med andre ord: navnet sidejump og skew scattering kommer av hvordan den spredte bølgefunksjonen blir seende ut når man går kvantemekanisk spredningsteori. De to effektene opptrer til ulik orden i impurity potential og SOC potential, og dermed er det naturlig å kalle selvenneriene til tilsvarende orden i impurity potential og SOC potential for hhv sidejump og skew scattering.

Kan forøvrig nevne at navnet "spin swapping" kommer av at dette selvenneri-leddet konverterer en innkommende spinnstrøm med en gitt spinnpolariseringsretning til en transversal spinnstrøm med en annen spinnpolariseringsretning. Denne effekten kan man beregne direkte via kvasiklassisk teori, hvilket da rettferdiggjør navnet. Det er mulig at man også kan vise at noe slikt skjer i kvantemekanisk spredningsteori (dvs man sender inn en spinnpolarisert bølge og finner spredning perpendikulært med en annen spinnpolarisering, men det vet jeg ikke sikkert).

28.8.4 Charge imbalance and charge neutrality

Following <https://arxiv.org/pdf/1810.08623.pdf>, we know that the electron and hole densities are given by

$$\begin{aligned} n_{e\sigma}(\mathbf{r}, t) &= \langle \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma}(\mathbf{r}, t) \rangle, \\ n_{h\sigma}(\mathbf{r}, t) &= \langle \psi_{\sigma}^{\dagger}(\mathbf{r}, t) \psi_{\sigma}(\mathbf{r}, t) \rangle. \end{aligned} \quad (28.476)$$

Using the definitions for the different Green functions, such as

$$G_{\sigma\sigma'}^K(\mathbf{r}, t; \mathbf{r}', t') = -i \langle [\psi_{\sigma}(\mathbf{r}, t), \psi_{\sigma'}^{\dagger}(\mathbf{r}', t')] \rangle, \quad (28.477)$$

it follows that

$$\begin{aligned} n_{e,\sigma} &= \frac{i}{2} (G_{\sigma\sigma}^R - G_{\sigma\sigma}^A - G_{\sigma\sigma}^K), \\ n_{h\sigma} &= \frac{i}{2} (G_{\sigma\sigma}^R - G_{\sigma\sigma}^A + G_{\sigma\sigma}^K). \end{aligned} \quad (28.478)$$

Since holes carry opposite charge and spin compared to electrons, these densities enter with opposite signs when determining the charge of quasiparticles in the system. Let us examine the electron density closer. The electron charge density

$$\rho_{\text{electron}} = \sum_{\sigma} n_{e,\sigma} \quad (28.479)$$

can then be written (assuming a time-independent situation for simplicity):

$$\rho_{\text{electron}} \propto \sum_{\sigma} \int A_{\sigma}(E) f_{\sigma}(E) \quad (28.480)$$

where $A_{\sigma}(E)$ is the spectral function for electrons σ and $f_{\sigma}(E)$ is the distribution function for such electrons (not necessarily Fermi-Dirac). This can be seen as follows. The field operators used to evaluate ρ_e are taken at equal times. This means that relative time $t \rightarrow 0$. Generally, we have

$$G^K(t) = \int dE e^{iEt} G^K(E) \quad (28.481)$$

so

$$\begin{aligned} G^K(t \rightarrow 0) &\equiv G^K = \int dE G^K(E) \\ &= \int dE [G^R(E) - G^A(E)] h(E). \end{aligned} \quad (28.482)$$

where the Green functions and distribution function matrix entry $h(E)$ should be understood as for a single spin species σ . Since the spectral function is defined as

$$A(E) = \frac{i}{2\pi} (G^R - G^A), \quad (28.483)$$

we obtain from Eq. (28.479)

$$\rho_{\text{electron}} = \sum_{\sigma} 2\pi \int dE A(E) [1 - h(E)] \quad (28.484)$$

Generally, $h(E) = 1 - 2f(E)$ where $f(E)$ is a non-equilibrium distribution function. Thus, inserting this $h(E)$ lands us at Eq. (28.480).

Now, Chandrasekhar writes that G^R and G^A only depend on equilibrium properties of the system and do not contribute to non-equilibrium charge accumulation. This is only partially true, since G^R and G^A depend on self-energies which, in turn, can depend on non-equilibrium distribution functions (such as the superconducting gap). Based on this, he concludes that the contribution to the non-equilibrium charge $\delta\rho_{\text{electron}}$ comes only from the Keldysh part, so that

$$\delta\rho_{\text{electron}} = -\sum_{\sigma} \frac{i}{2} G_{\sigma\sigma}^K. \quad (28.485)$$

In all of this, we have not considered the charge coming from the background of positive ions. The above considerations only regard the electron charge.

Consider now a non-equilibrium situation where, in general, the number of electron- and hole-excitations can differ from each other. If so, this creates a *charge imbalance* (also known as charge accumulation). This can be quantified by defining the charge imbalance $\delta\rho$:

$$\delta\rho = \frac{e}{2}[n_{e\uparrow} + n_{e\downarrow} - n_{h\uparrow} - n_{h\downarrow}]. \quad (28.486)$$

The factor $1/2$ is explained in Ali's paper. Note how this takes into account both electron and hole excitations. It can be written compactly as

$$\delta\rho = -\frac{i}{2} e \text{Tr}\{G^K(t=0)\}. \quad (28.487)$$

In equilibrium, this quantity is zero. If an electron below the Fermi level is moved to an unoccupied state above the Fermi level due to a thermal excitation, we have created both an electron and hole excitation and there is no change in $\delta\rho$.

However, it is possible to have a charge imbalance and still maintain charge neutrality, meaning that $\delta\rho$ is still zero. This can be seen by noting that our expression Eq. (??) is not written in a gauge-invariant form. A gauge-invariant expression for the charge deviation from equilibrium $\delta\rho$ can be derived as follows.

We saw that $\delta\rho = \text{Tr}[G^K(t=0)]$. Generally, we have

$$G^K = G^R \circ h - h \circ G^A \quad (28.488)$$

where h is a matrix. Perform a gauge-transformation

$$\phi \rightarrow \phi' = \phi + \partial\lambda/\partial T \quad (28.489)$$

and the Green function is transformed according to

$$G^K \rightarrow G^{K'} = e^{-ie\rho_3\lambda(T+t/2)} G^K e^{ie\rho_3\lambda(T-t/2)}. \quad (28.490)$$

We then see that

$$\begin{aligned} \lim_{t \rightarrow 0} \text{Tr}\{G^{K'}\} &= \lim_{t \rightarrow 0} \text{Tr}\{e^{-ie\rho_3[\lambda(T+t/2)-\lambda(T-t/2)]} G^K\} \\ &= \lim_{t \rightarrow 0} \left[\text{Tr}\{G^K\} - \text{Tr}\{ie\rho_3 \frac{\partial\lambda}{\partial t} t G^K\} \right]. \end{aligned} \quad (28.491)$$

At this point, it is useful to note that the distribution function matrix at small times goes like $1/t$ and is proportional to the identity matrix. This can be seen as follows. Generally, we have

$$h(t) = \int dE e^{iEt} h(E). \quad (28.492)$$

Any dependence on center-of-mass-time T is suppressed notationwise. Do a partial integration to obtain

$$h(t) = \frac{1}{it} e^{iEt} \frac{dh(E)}{dE} \Big|_{E=-\infty}^{E=\infty} - \frac{1}{it} \int_{-\infty}^{\infty} e^{iEt} \frac{dh(E)}{dE} dE. \quad (28.493)$$

We note that $h(E)$ is in general a non-equilibrium distribution function matrix and thus not proportional to the identity matrix. However, we still know that h has to attain its equilibrium value at sufficiently large energies, $\tanh(\beta E/2)$, and this equilibrium value is proportional to the identity matrix. Therefore, the surface term in the partial integration goes to zero at $E \rightarrow \pm\infty$ since the derivative of the tanh vanishes. If we now let $t \rightarrow 0$ in the remaining term, we can set $e^{iEt} \rightarrow 1$ and obtain

$$\begin{aligned} \lim_{t \rightarrow 0} h(t) &= -\frac{1}{it} \int_{-\infty}^{\infty} h'(E) dE \\ &= -\frac{1}{it} [h(\infty) - h(-\infty)] \\ &= -\frac{2}{it}. \end{aligned} \quad (28.494)$$

In practice, we just have to integrate up to energies that are large, but such that the product $\lim_{t \rightarrow 0} Et$ still goes to zero, so that we may set $e^{iEt} \rightarrow 1$ for all energies in the integral.

Using this, we obtain

$$\lim_{t \rightarrow 0} \text{Tr}\{G^{K'}\} = \text{Tr}\{G^K\}|_{t=0} - 4e\phi' \quad (28.495)$$

which completes the proof, namely that

$$\delta\rho = \text{Tr}\{G^K\}|_{t=0} - 4e\phi \quad (28.496)$$

in general. Defining the charge accumulation

$$\mu = -\text{Tr}\{G^K\}|_{t=0} \propto -\int dE \text{Tr}\{g^K\} \quad (28.497)$$

where g^K is the Keldysh quasiclassical Green function, we then see that when charge neutrality is maintained (as it is in metals over length scales that are large compared to the Thomas-Fermi screening length), we have

$$\mu = -4e\phi \quad (28.498)$$

and thus a finite gradient in the charge accumulation μ implies the presence of a static electric field $\nabla\phi$.

Finally, note that if one wants to use the expression for $\delta\rho$ above as the charge in Maxwell's equations, one must assume that the total charge in the system in equilibrium is zero. The reason for this is that it is the total charge ρ which enters Maxwell's equations, and thus the total charge is only equal to $\delta\rho$ if the equilibrium charge is zero. Summarizing, using a gauge $\phi = 0$, the total electron charge is given by $G^K - (G^R - G^A)$ whereas the electron-charge out of equilibrium is given by G^K . If one says that $\delta\rho$ is the charge of the system, we are implicitly assuming that the electron-charge in equilibrium [given by $G^R - G^A$] is cancelled by the positive ion background.

We close by remarking on some points that can cause confusion regarding notation and terminology.

- The charge imbalance μ is not the same as the chemical potential in general.
- In fact, the quantity which is often referred to as the chemical potential in the Fermi-Dirac distribution function is more precisely the *electrochemical potential*: it includes both the particle chemical potential and any electrostatic potential shifts.
- When the system is driven out of equilibrium and the distribution function becomes non-thermal (non-Fermi Dirac), the electrochemical potential and temperature is not well-defined. However, one can still define an effective electrochemical potential and temperature based on integrating moments of the non-thermal distribution function and equating to the integral over a thermal distribution which gives the same total particle number and energy.
- The models for spin-accumulation as spin-dependent chemical potentials are thus a simplification for a non-equilibrium situation where one assumes that the spin-species are described by Fermi-Dirac functions with spin-dependent chemical potentials. The spin accumulation computed quasiclassically is generally different from $\mu_\uparrow - \mu_\downarrow$, since the quasiclassical distribution function can be strongly non-thermal.
- Both in the phenomenological treatment with quasiparticle and Cooper pair chemical potential *and* in the rigorous quasiclassical treatment, one finds that the charge imbalance is proportional to the electric potential. In the latter case, it follows from charge neutrality. In the former case, it follows from having a stationary situation with non-accelerated Cooper pairs. In the phenomenological theory, the electric field force on the Cooper pairs is balanced by the gradient in Cooper pair chemical potential. In the quasiclassical theory, the gradient in charge imbalance (which gives an electric field) and the gradient of the magnitude of the superconducting order parameter (which should affect the Cooper pair chemical potential) near an interface balance each other so that the net supercurrent is stationary and gradually builds up by converting resistive current.

28.8.5 Relaxation time approximation for inelastic scattering in Usadel equation

Inelastic scattering such as e-e or e-phonon scattering does not conserve energy, and affects both the lifetime/broadening of the retarded Green function and the kinetic distribution functions. In the Usadel equation

$$D\nabla(g\nabla g) + i[\epsilon + \Sigma, g] = 0 \quad (28.499)$$

inelastic scattering can be included in the simplest form by a relaxation time approximation term, which models energy-independent inelastic scattering:

$$\Sigma = \begin{pmatrix} i\delta\rho_3 & 2i\delta\rho_3 h_0 \\ 0 & -i\delta \end{pmatrix}. \quad (28.500)$$

The appearance of such a term can be motivated on physical grounds. Inelastic scattering can be modelled as a coupling between the system and an infinite reservoir/bath, allowing for energy-transfer. We can include such a coupling in the Usadel equation by considering the system being in contact with such a reservoir. Consider a normal metal:

$$D\nabla(g\nabla g) + i[\epsilon, g] = 0 \quad (28.501)$$

Assume for concreteness a normal metal in the xy -plane where we couple a fictitious reservoir to it on top of the normal metal (say $y = L$). We have vacuum at $y = 0$. Assuming that L is small, we can integrate the Usadel equation over the y -direction and use that g remains approximately constant along this direction due to the smallness of L . We then get

$$DL\partial_x(g\partial_x g) + iL[\epsilon, g] + D(g\partial_y g) \Big|_{y=0}^{y=L} = 0. \quad (28.502)$$

Now, we can use KL boundary conditions at $y = L$ and $y = 0$. At $y = 0$, the extra term vanishes, but at the interface to the fictitious reservoir we have:

$$g\partial_y g = T[g, g_{\text{res}}]. \quad (28.503)$$

where T is a constant characterizing the coupling strength to the reservoir and g_{res} is an infinite normal metal reservoir with Keldysh structure:

$$g_{\text{res}} = \begin{pmatrix} \rho_3 & 2\rho_3 h_0 \\ 0 & -\rho_3 \end{pmatrix} \quad (28.504)$$

with $h_0 = \tanh(\beta E/2)$. Therefore, the Usadel equation now takes the form:

$$D\partial_x(g\partial_x g) + i[\epsilon, g] + DT[g, g_{\text{res}}]/L = 0 \quad (28.505)$$

which we can write as

$$D\partial_x(g\partial_x g) + i[\epsilon + \Sigma, g] = 0 \quad (28.506)$$

with

$$\Sigma = \frac{iDT}{L} g_{\text{res}} \quad (28.507)$$

We see that this is consistent with Eq. (28.500) by identifying $DT/L = \delta$. The stronger coupling T to the reservoir, the stronger the effect δ of the inelastic scattering.

Thus, the relaxation time approximation self-energy can be understood physically as coupling the system to a reservoir in equilibrium: it is equivalent mathematically.

An important point is nevertheless the following: when inelastic scattering is modelled in the manner above, it will cause *every* distribution mode (including charge and spin) to relax toward equilibrium (in the case of charge and spin, to zero). This causes charge and spin currents to not be conserved. Inelastic scattering via e-e and e-phonon collisions should not have this effect: they should only cause loss of the energy mode.

Therefore, it is possible to revise the above self-energy slightly so that the inelastic scattering only causes decay of the energy mode?

Using the method above, the kinetic equation for a normal metal takes the form

$$D\partial_x^2\check{h} - 2\delta[\check{h} - h_0] = 0. \quad (28.508)$$

We see that regardless of which matrix we multiply with and then take trace of the equation for, we will always get a decay of the corresponding mode due to the $\delta\check{h}$ term. However, by adjusting this equation slightly to

$$D\partial_x^2\check{h} - 2\delta[h_L - h_0] = 0, \quad (28.509)$$

only the energy-mode will be affected by the inelastic scattering parameter δ . This is because the δ term vanishes when taking the trace after multiplying with any matrix other than unity, the latter giving precisely the energy mode. This modified equation then corresponds physically to a material coupled to a reservoir which forces the energy-mode to relax toward equilibrium h_0 (which is the distribution function in the reservoir), but leaves all other modes (like charge and spin) alone. This "reservoir" then corresponds to e-e and e-phonon collisions. This is in contrast to the original model above where the reservoir attempts to cause all modes (including charge and spin) to relax toward equilibrium.

28.8.6 Spin injection and lifetimes in superconductors

Let us first distinguish a bit more carefully between spin-lifetimes for different types of quantities. For a single quasiparticle, we call this the spin-flip time τ_{sf} . This quantity is different in the normal and superconducting state, being much larger in the SC state for energies near the gap $E = \Delta$. At the same time, the group velocity of quasiparticles at $E \rightarrow \Delta$ is very small, meaning that the net spin-flip length l_{sf} is actually the same as in the normal state. The spins live longer, but move slower, and thus the length it takes for them to randomize is the same for a single quasiparticle.

The above holds when the spin-flip mechanism is due to spin-orbit scattering on non-magnetic impurities and was analyzed by Takahashi and Maekawa (PRB 2002). Now, we may also talk about the spin relaxation time of a macroscopic, non-equilibrium spin density S which is obtained by integrating over the distribution functions for spin- $\uparrow$ and spin- $\downarrow$ particles over the entire energy range from $E = \Delta$ and upwards. Unlike the spin-flip time, this quantity is energy-independent (since we integrate over energy) and instead depends on temperature. One may refer to both the spin-flip and the spin-relaxation time as spin-lifetimes since both refer to how long a spin keeps its direction, but it is to be understood that we are talking about different objects then: quasiparticles and macroscopic spin densities, respectively.

The situation changes when the origin of spin-flip changes from spin-orbit scattering on non-magnetic impurities to spin-flip scattering due to magnetic impurities. In this case, the spin relaxation length decreases compared to the normal-state. A simplified picture of the reason for this is that slowly moving quasiparticles will now be exposed to a magnetic impurity causing spin-precession for a longer time, which increases the spin relaxation rate (inverse spin lifetime).

28.9 Useful tricks and approximations in q.c. theory

28.9.1 Computation of supercurrent from asymptotic Green function

Consider an S_{eff}/F bilayer where each region is semi-infinite. Here, S_{eff} is an effective superconducting region (for instance a bilayer of its own) which we assume is such that it generates long-range triplet components in the F layer. An example could be that S_{eff} is an S/F' layer on its own, where

the F' is misaligned with the F . Since the $x > 0$ region where F resides is semi-infinite, we can now compute the supercurrent that flows in this region when a second S_{eff} layer is added on the right side at a distance L if we assume that $L \gg \xi_F$. In such a case, only the LRTC can contribute to the supercurrent. The strategy is explained on page 16 in the arXiv-version of RMP 2005 Bergeret *et al.* and goes as follows.

We first compute the LRTC $f_1(x)$ in the S_{eff}/F bilayer by getting rid off the exponentially increasing part of the solution for $x \rightarrow \infty$. Then we can compute the LRTC $f_2(x)$ in the F/S_{eff} bilayer in the same way, by discarding the exponentially increasing part for $x \rightarrow -\infty$. The two solutions should be related by the substitutions $x \rightarrow (-x)$ and $\phi \rightarrow (-\phi)$, assuming that the two superconductors have phase $\pm\phi$. Now we can say that the general solution for the LRTC in the $S_{\text{eff}}/F/S_{\text{eff}}$ case is just a superposition of the two LRTC obtained above, assuming that the large separation of the superconductors causes the proximity-induced condensates from them individually to have little overlap in the F region. In other words,

$$f = f_1(x + L/2) + f_2(x - L/2) \quad (28.510)$$

if the two interfaces are located at $x = -L/2$ and $x = L/2$. Note how we had to shift the spatial argument to obtain the correct "starting point" for the Green function solutions. With the solution f in hand, we can now compute the supercurrent in the Josephson setup (carried by the LRTC) using the standard formula.

Chapter 29

Bose-Einstein Condensates

29.1 Optical lattice and neutral atoms

The reason that the electric field from the lasers setting up the optical lattice affects the overall neutral atoms is that although they are neutral and on their own have no net dipole moment (although molecules such as water can have that), the electric field can induce a finite atomic dipole moment by disturbing the electron distribution around the core. This dipole moment will then interact with the electric field in the usual way $V = -\mathbf{d} \cdot \mathbf{E}$.

The induced dipole field $\mathbf{d}$ will be proportional to $\mathbf{E}$:

$$\mathbf{d} = \alpha \mathbf{E} \quad (29.1)$$

and so whether or not the atoms experience a negative or positive potential energy V will be determined by the constant of proportionality α . In a simple model, one finds that $\text{sign}(\alpha)$ is determined by the *detuning parameter* $\delta = \omega - \omega_0$. Here, ω is the frequency of the electric field $\mathbf{E}(\mathbf{r})e^{-i\omega t} + (\text{h.c.})$ while ω_0 is the separation between the the ground state $|g\rangle$ and excited state $|e\rangle$ in a two-level atom. Thus, depending on the detuning, a given region $\mathbf{r}$ where the electric field exists will be positive or negative depending on the sign of δ and $V \propto \alpha \mathbf{E}^2$ effectively creates a potential landscape the atoms can move through since $\mathbf{E}^2$ varies in magnitude across space $\mathbf{r}$.

29.2 Van Der Waals force

In discussing the interaction between atoms in a BEC, we need to introduce the concept of a van der Waals force.

This is a weakly attractive force that occurs between electrically neutral atoms (or molecules) which collide with each other or at least move in each others vicinity. The origin of the van der Waals force is electric in nature, despite the fact that the overall objects are neutral. In general, it is caused by the attraction between an electron-rich region of an atom and an electron-poor region of another atom. The attraction causes a weak chemical bond, and van der Waals forces are indeed the forces that cause molecules and atoms to cohere in liquid and solid states of matter.

The above explanation requires that the electron distribution around the atom core is not spherically symmetry, at least not at all times. Van der Waals forces are usually classified to occur in three possible ways, depending on which mechanism that causes this deviation from spherical symmetry:

- *Orientation*: If the molecules are permanent electric dipoles, this causes a dipole-dipole interaction between different molecules. This is not relevant for atoms which are not permanent electric dipoles. On the other hand, if an external electric field $\mathbf{E}$ induces an electric dipole moment in an atom, then there can be atomic dipole-dipole interactions.
- *Induction*: If molecules with permanent electric dipoles exist, this also distorts the electron charge in other nearby atoms or molecules (both polar and nonpolar) and causes further polarization. This in turn causes an additional attractive force from the interaction between a permanent dipole with the induced dipole moment in a neighboring atom or molecule.
- *Dispersion*: More relevant for the atomic case, even if there exists no permanent dipole moment, a force of attraction can still exist between the atoms or molecules. This accounts for the condensation into the liquid state at sufficiently low temperatures. The nature of this attractive force is quantum mechanical in nature: it is caused by *fluctuations* of the electron charge distribution around the atom core which makes the atoms time-varying dipoles. The average of the polarization over a given time period may be zero and such time-varying dipoles cannot align themselves spontaneously in a macroscopic fashion, but they do induce temporary polarization in adjacent atoms or molecules. This results in a net attractive force. Such forces coming from temporary electron fluctuations are known as London forces. It is known as a dispersive force as it originates from variation of a quantity with frequency/time (the fluctuation of electron density).

29.3 Interactions between atoms

In a Bose-Hubbard model one includes an interaction between the neutral atoms. But what is this interaction *physically*? A common model is to treat a stable neutral atom with a hard core that is short-ranged (a few Angstrom) and thus strongly repulsive. This repulsion can be understood as Coulomb repulsion between the positive cores of atoms. On the other hand, at longer distances of several hundred Angstrom the atoms can attract each other due to the *van der Waals force*.

Therefore, when two atoms collide they will generally experience both of these forces and the net force will be determined by how close the atoms approach each other. The range of the net interaction is determined by how much kinetic energy the atoms have (which affects how close they can get to each other) and the specific van der Waals potential for the atomic species in question. For instance, the net force is typically repulsive for ^1H , ^{23}Na , and ^{87}Rb whereas it is attractive for ^7Li , precisely because of this balance between the kinetic energy and VdW force.

Moreover, since BECs occur at so low temperatures that the de Broglie wavelength $\lambda = h/p$ of each atom is much larger than the interaction range (ballpark $\sim \text{nm}$), the scattering of atoms is very close to spherically symmetric. If the atomic gas additionally is highly dilute (low density), each atom rarely encounters a different atom within its range of interaction. If the net interaction is repulsive, this justifies using a theoretical framework of weakly interacting bosons (such as Bogoliubov theory).

29.4 Feshbach resonance

A neat opportunity exists in the experimental study of BECs, namely that the strength and even the sign of the atomic interaction can be tuned by an external magnetic field. This phenomenon is

an example of a Feshbach resonance. Very simply put, such a resonance occurs when a pair of atoms collide at an energy E in a particular reaction channel and this energy is in resonance with (equal to) the bound-state energy available in a closed (forbidden) channel. The magnetic field tunes the bound-state energy in the closed channel and can thus be used to match its energy to the energy E of the colliding atoms. When this occurs, a mixing occurs between the open (available) and closed channels which results in a new effective interaction strength.

29.5 Critical superfluid velocity

The Landau criterion for when superfluid motion is degraded to viscous motion is related to how the energy of an excitation transforms when looking at it from a moving frame. To be concrete, consider a superfluid at rest with an impurity moving through it with velocity $\mathbf{v}$. In practice, this impurity need not be an actual massive object, but can also be a general time-dependent potential as realized experimentally by moving a laser beam through the condensate REF. We may write the Hamiltonian describing the superfluid as:

$$\hat{H}_0 = \sum_i \frac{\mathbf{p}_i^2}{2m} + H_{\text{int}}, \quad (29.2)$$

where H_{int} contains all the interaction terms. In the rest frame of the impurity, the superfluid is moving with a velocity $-\mathbf{v}$. Performing a Galilean boost on the Hamiltonian, we obtain the Hamiltonian in the rest frame of the impurity:

$$\hat{H}'_0 = \sum_i \frac{(\mathbf{p}_i - m\mathbf{v})^2}{2m} + H_{\text{int}} = H_0 - \mathbf{v} \sum_i \mathbf{p}_i + \frac{1}{2}v^2 \sum_i m = H_0 - \mathbf{v}\mathbf{P} + \frac{1}{2}Nmv^2, \quad (29.3)$$

where N is the number of particles and $\mathbf{P}$ is the total momentum of the superfluid system. In the ground-state of a superfluid at rest, we have $\mathbf{P} = 0$ so that the Hamiltonian of the superfluid as seen from the moving frame is simply $H_0 + \frac{1}{2}Nmv^2$.

Now consider what happens if we allow for the presence of an excitation $\epsilon(\mathbf{p})$ with momentum $\mathbf{p}$ in the superfluid. The total momentum of the superfluid is now $\mathbf{p}$, and according to Eq. (29.3) the energy of the superfluid with the excitation as seen from the moving frame is now:

$$\hat{H}'_0 = H_0 + \epsilon(\mathbf{p}) - \mathbf{v}\mathbf{p} + \frac{1}{2}Nmv^2, \quad (29.4)$$

By comparison with the case without an excitation, it is clear that the energy of the excitation as seen from the moving frame is:

$$\epsilon'(\mathbf{p}) = \epsilon(\mathbf{p}) - \mathbf{v}\mathbf{p} \quad (29.5)$$

If there exists a velocity vector $\mathbf{v}$ which renders $\epsilon'(\mathbf{p}) < 0$, the system can spontaneously lower its energy by creating excitations and hence superfluidity would be lost as the motion of the condensate would be degraded. The minimal velocity v_c at which it is possible to create excitations is seen to be:

$$v_c = \min\{\epsilon(\mathbf{p})/|\mathbf{p}|\} \quad (29.6)$$

which occurs when $\mathbf{v}$ and $\mathbf{p}$ are parallel. If their directions are opposite, ϵ' is always positive and the superfluid state is stable. This observation is of particular importance when the quasiparticle

dispersion is anisotropic in $\mathbf{p}$ -space such that the critical velocity v_c will depend on which direction the motion occurs in. Eq. (29.6) is the Landau criterion for the energetic instability of superfluid flow. If the long wave-length excitations are phonons, $\epsilon = c|\mathbf{p}|$ for $\mathbf{p} \rightarrow 0$, the critical velocity is simply the sound velocity c of the excitations in the Bose-Einstein condensate.

It should be mentioned that we have in the above discussion have assumed that the excitations of the superfluid generated by moving an impurity through the condensate are the same as the elementary excitations of the superfluid without any impurity. In practice, non-ideal effects such as the influence of the impurity-potential on the excitation-spectrum would contribute to getting a better fit to experimental results.

How does the Landau criterion change when the Bose-Einstein condensate is loaded onto an optical lattice? The most transparent physics emerges in the combined limit of long-wavelength for the excitations (small $\mathbf{p}$) and small lattice-constant a , in which case we may approximate the lowest Bloch energy-band by a free-particle spectrum with an effective mass m^* : $E(\mathbf{p}) \simeq \mathbf{p}^2/2m^*$. Assuming that the lattice is moving with a velocity v and generates excitations in the superfluid, as realized experimentally in Refs. XX, the same analysis as above may be undertaken and resulting in:

$$\epsilon'(\mathbf{p}) = \epsilon(\mathbf{p}) - m\mathbf{v}\mathbf{p}/m^*. \quad (29.7)$$

Here, ϵ' is the energy of the excitation in the moving frame (where the lattice is at rest) and ϵ is the excitation energy in the superfluid rest frame. It is seen that the critical velocity is then modified by a prefactor containing the ratio of the bare and effective mass of the particles, the latter depending on factors such as the lattice depth and the hopping strength:

$$v_c = m^* c/m. \quad (29.8)$$

With the realization of spin-orbit coupled Bose-Einstein condensates, it is of interest to discuss the differences arising in the above reasoning due to the presence of SOC.

29.6 Bose-Hubbard model: superfluid and Mott insulating state

Creating an optical lattice where atoms can reside is an interesting manifestation of the Bose-Hubbard model. In its simplest form, it looks like:

$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \sum_i \epsilon_i b_i^\dagger b_i + U \sum_i b_i^\dagger b_i^\dagger b_i b_i. \quad (29.9)$$

Here, $\{b_i\}$ are boson operators, t is the hopping matrix element, ϵ_i is the local onsite energy shift (*e.g.* from interaction with a harmonic potential confining the atoms), and U is the onsite interaction term. This model is capable of describing both a superfluid and Mott insulating ground state.

29.7 Superfluid case

In the superfluid case, we expect that the phase should be sharply defined so that the atoms are coherent. In turn, the number of atoms per lattice site should be ill-defined since the phase and the number of atoms are canonical conjugate variables. More heuristically, if atoms flow around in the condensate without friction, we should not expect the number of atoms per site to be sharply defined. The superfluid phase occurs if $t \gg U$.

According to the above argument, the ground-state in the superfluid phase has the form (which one also can show formally):

$$|\Psi\rangle_{\text{SF}} \propto \left(\sum_{i=1}^M a_i^\dagger \right)^N |0\rangle \quad (29.10)$$

Here, M is the number of lattice sites and N is the number of atoms. This means that the ground-state is a superposition of states which all have a different number of atoms at a given site. Such a delocalized state makes sense since a large hopping energy means that the energy of the system will be minimized by spreading out the atoms across the entire lattice.

In the Bose-Hubbard treatment, we can describe the condensation of a macroscopic amount of bosons into the lowest single-particle state by stating that $b_{k=0}^\dagger b_{k=0} = N_0 \gg 1$. Here, b_k is the Fourier-transformed boson operators and N_0 is the number of condensed bosons. According to boson commutation rules, we know that $bb^\dagger - b^\dagger b = 1$ so that:

$$b_{k=0}^\dagger b_{k=0} \simeq b_{k=0} b_{k=0}^\dagger \quad (29.11)$$

in this case. If this is true, it means that $b_{k=0}$ and $b_{k=0}^\dagger$ commute just like scalars and, if they can be treated like scalars, warrants to set $b_{k=0} = b_{k=0}^\dagger = \sqrt{N_0}$. This is the effective mean-field approximation in the superfluid phase.

29.8 Mott insulating case

If instead interactions dominate, $U \gg t$, it becomes very expensive energetically to have several atoms at a given lattice site i . Therefore, the ground-state will consist of a fixed number of atoms per site which minimize the interaction energy. In effect, the ground-state will be a product of local Fock states (eigenstates for the number operator) for each lattice site:

$$|\Psi\rangle_{\text{MI}} \propto \prod_{i=1}^M (a_i^\dagger)^{N/M} |0\rangle. \quad (29.12)$$

In this case, since the number of atoms N/M per site is sharply defined, the phase of the wavefunction cannot be sharply defined. Thus, no phase coherence is present and the Mott insulating state cannot be described by a macroscopic quantum mechanical wavefunction as in the superfluid phase.

Chapter 30

Quantized radiation theory

In a fully quantum theory treating both matter and light, we have to treat not only the matter wavefunction ψ quantum mechanically, but also the scalar ϕ and vector potential $\mathbf{A}$ providing the electric and magnetic fields.

Write about quantization of $\mathbf{A}$...

An interesting observation is that $\langle n | \mathbf{E} | n \rangle = 0$. This shows that the expectation value for the electric field of a Fock photon state (definite number of photons, such as $n = 1$) is zero. However, $\langle n | \mathbf{E}^2 | n \rangle \neq 0$ which means that the standard deviation $\Delta \mathbf{E} \neq 0$. This tells us that the electric field of a single photon is not identically zero, but it *fluctuates with an average value of zero*.

Chapter 31

Metamaterials

31.1 Some preliminaries regarding the treatment of EM fields in hybrid structures

Boundary conditions include that the tangential component of the electric field is always continuous across an interface. The tangential component of the H -field can be discontinuous if there exists a free current, in which case the difference between $H_{\perp}$ on each side is given by $\mathbf{J} = \sigma \mathbf{E}$. Here, $\sigma = \sigma(\omega)$ is the optical conductivity. The meaning of the dependence on ω is the following. In the static limit, $\omega \rightarrow 0$, one typically has that σ is purely real and proportional to the relaxation time τ_{rel} . Thus, for a constant electric field giving a voltage bias the dc conductivity is directly proportional to the relaxation time which, in turn, says something about how long time it takes between scattering events for the charge-carriers (either due to lattice imperfections, impurities, phonons, et.c.). The larger time between such events, the more ballistic the conduction and the larger σ , as is reasonable. However, if we instead apply an ac $\mathbf{E}$ field with a frequency ω , the resulting relation between current and field is given by the ac conductivity $\sigma(\omega)$. For large enough frequencies, this σ becomes complex which means that there will be a phase-lag between the $\mathbf{E}$ field and the current $\mathbf{J}$.

31.2 How to make metamaterials

Metamaterials derive their properties not from the atoms of the material itself, but rather how the atoms are arranged. They are typically created by using several composite materials, such as metals or plastics, which are arranged in a repeated pattern. The scale at which these composite material structures are tailored is smaller than the wavelength of the phenomena they influence. The exact shape, geometry, orientation, and arrangement of the composite materials that make up the metamaterial is what endows them with their unusual characteristics regarding manipulation of EM waves. Metamaterials can block, enhance, absorb, and bend EM waves in a manner that is not possible with conventional "pure" materials.

31.2.1 Negative permittivity metamaterials

There are many different types of metamaterials that have attracted much interest. One is the negative index metamaterials, which display negative index of refraction for certain desired wavelengths. It is interesting to note that negative permittivity also occurs in natural materials, such as gold, but then only for frequencies exceeding the plasma frequency ω_p . Let us elaborate a bit on

this.

For sufficiently high frequencies, the electric response of a metal is that of a plasma. In this case, there exists a resonance frequency ω_p which distinguishes two regimes. Below ω_p , the EM waves oscillate slowly enough in order for the electrons to manage to follow them. The material then acts as a good conductor. However, for $\omega > \omega_p$, the fact that electrons have inertia prevents them from responding fast enough to follow the ac electric field with the same phase. The result is that the EM wave now goes through the metal as if it was a dispersive and lossy vacuum. Typically, one can write:

$$\epsilon = \epsilon_0 \left(1 - \omega_p^2 / \omega^2\right) \quad (31.1)$$

for the electric permittivity. Plasma oscillations, also known as "Langmuir waves" (after Irving Langmuir), are fast oscillations of the electron density in conducting media such as plasmas or metals. The oscillations can be described as an instability in the dielectric function of a free electron gas. The frequency only depends weakly on the wavelength of the oscillation. The quasiparticle resulting from the quantization of these oscillations is the plasmon.

31.2.2 Epsilon-near-zero metamaterials

One can envision at least three ways in which to achieve a material with a near-zero permittivity ϵ :

1. It can occur in natural materials by using ac fields with frequency $\omega \rightarrow \omega_p$, see equation (31.1). However, since we cannot exert much control over the value of ω_p in a natural material, it is desirable to find alternative ways where one can achieve $\epsilon \rightarrow 0$ for any or a broader range of wavelengths.
2. By mixing materials that have negative and positive permittivities in the correct amount, it is possible to tailor an effective zero permittivity response at the desirable frequency. This is done in metamaterials.
3. A final option is to use waveguides clad with metals.

31.3 Guided waves, leaky waves, and perfect absorption

When considering a light plane-wave incident on a material, different types of excited waves can arise. We here provide a classification of such waves and also comment on the relation between perfect absorption and fast-wave modes as determined by the zeros and special poles of the reflection coefficient, respectively.

Consider a model system as shown in Fig. 31.1: this corresponds to the scenario considered by Linder and Halterman [17]. Let $k_0 = \omega/c$ be the wavevector in the air region for a plane-wave. Due to translational symmetry, k_x has to be conserved in the system. By setting up incoming, reflected, and transmitted waves in the various regions, one can solve for the coefficients associated with each of these types of waves. The coefficient r for reflecting the incident wave back into the air region is of particular interest since it determines the absorption of the material. If the entire structure, as shown in the figure, is backed by a perfect electric conductor (PEC) there can be no transmitted waves through the structure. This is because the electric field inside a PEC must be zero (otherwise

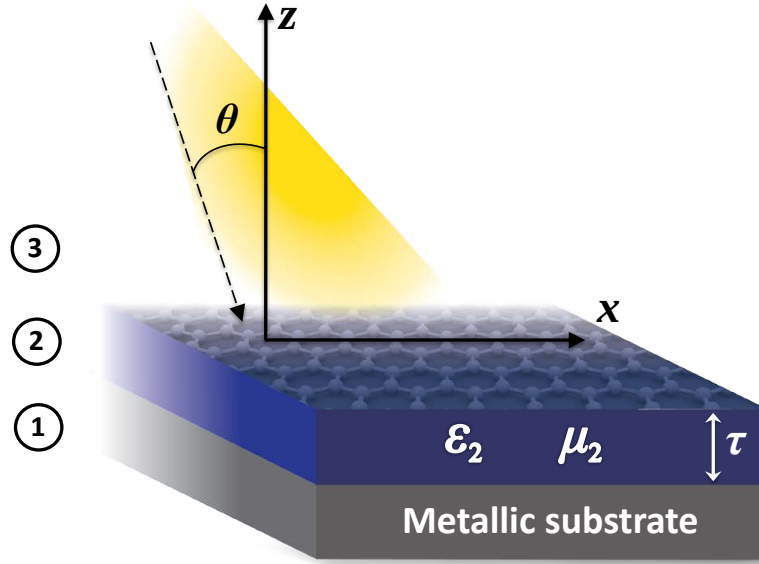


Figure 31.1: (Color online) Model setup to illustrate the excitations produced by a light-wave.

charges would move to the surface). In this case, only reflection or absorption can take place. Thus, the absorption probability $\mathcal{A}$ is given by:

$$\mathcal{A} = 1 - |r|^2. \quad (31.2)$$

If $r = 0$ for an incident wave with a given wavenumber k_z , perfect absorption takes place. What is the physical mechanism allowing for perfect absorption? To answer this question, it becomes crucial to consider what kind of excited waves that can exist in the structure. To find such states, one should in general solve Maxwell's equations for the EM fields *in the absence of an incident field*. In effect, which types of intrinsic modes can exist in the structure even in the absence of an incident field? This amounts to finding the poles of the reflection coefficient r which describes such states. Physically, a pole in r means that there can exist a reflected (outgoing) wave even without an incident wave, i.e. stemming from an intrinsic mode in the system. This is conceptually similar to the calculation of Andreev bound states in SNS junctions where there is no incident wave and still waves reflected from the SN and NS interfaces due to Andreev bound-state propagation in the N part. Thus, such modes can be found also by eliminating incident waves and setting up an additional boundary condition in the air region.

Finding poles in r means identifying the parameters that causes r to diverge. Depending on the character of the wavenumber, various classifications of modes can be identified. If $\text{Im}(k_x) \neq 0$, we have a so-called *leaky wave* which decays (or grows) as it propagates along the interface of the structure. If $k_x/k_0 > 0$, it necessarily means that k_z must be complex in the air region so that it consequently decays there. We then have a *guided wave*.

However, there exists a third type of wave which turns out to be closely related to the criterion of perfect absorption of an incident plane-wave. This is a so-called *fast-wave* which satisfies $k_x/k_0 < 1$ and $\text{Im}(k_x) = 0$. These types of waves can be excited by an incident wave hitting the material at

just the right angle. The connection to perfect absorption is made clear by the following central relation [18, 19]:

$$r(k_z) = r^{-1}(-k_z). \quad (31.3)$$

In effect, an incident plane-wave with wavenumber k_z can couple perfectly to a fast-wave with wavenumber $-k_z$ when $r(k_z) = 0$ since this also corresponds to a pole at $-k_z$. It is not problematic that k_z changes sign, since k_z does not have to be conserved during scattering (just look at the reflected wave which also has opposite k_z compared to the incident one). Fast-waves are modes that propagate without loss along the surface since they have no imaginary part of the wavenumber.

Let us consider this more carefully. The relation $1/r(k_z) = 0$ means that the reflected wave (given as $e^{ik_z z}$ when the z -axis points away from the interface) can exist even without any incident wave, i.e. it is related to an intrinsic EM mode of the system. In the same way, if $1/r(-k_z) = 0$, it means that a wave $e^{-ik_z z}$ is the extension of the intrinsic mode in the air region. But $e^{-ik_z z}$ is precisely described by an incident wave, so that if we have

$$r(k_z) = 0 \quad (31.4)$$

and

$$1/r(-k_z) = 0 \quad (31.5)$$

simultaneously it means precisely that the incident wave is perfectly phase-matched to the intrinsic mode of the system: both of them are described by $e^{-ik_z z}$ at the angle of incidence which causes the above equations to be fulfilled. Since this occurs at $k_x/k_0 < 1$ with $\text{Im}(k_x) = 0$, it is a fast-wave mode of the system propagating without loss along the ENZ/graphene boundary.

It might seem paradoxical to say that the fast-wave is allowed to exist without an incident wave when its manifestation in the air region is precisely that of an incident wave. This is a very special case of the pole of the reflection coefficient: perhaps it is more general to say that the poles of the reflection coefficient provide the intrinsic modes of the system without specifying the "without an incident wave part". Although the latter is true for *e.g.* guided wave modes, it is not true for fast-waves since the intrinsic mode is identical to an incident wave in the air region: it must be excited by one and thus requires the existence of a plane-wave in air in the first place.

It seems like a plane-wave is the only way to excite the fast-wave, although bound-states are usually thought of as being independent on the source of excitation. The reason is that the manifestation of the fast-wave in air is that of an incident plane-wave and it doesn't make sense to consider a bound-state giving rise to a wave propagating toward the interface by itself (unlike a guided wave that can give rise to a decay wave propagating outwards).

Note that there can exist many solutions to the pole equation $r^{-1} = 0$ with longitudinal wavenumbers k_x that may or may not be complex. Since k_x is conserved in the structure, we're only looking for fast-wave modes in the scenario of an incident light-wave since these modes are the only ones that can couple to an incident wave with $k_x/k_0 < 1$ and $\text{Im}(k_x) = 0$. If perfect absorption occurs at k_z and Eq. (31.3) holds, it means that we have excited a fast-wave at $-k_z$, and we disregard any other solutions of $r^{-1} = 0$ that do not satisfy $k_x/k_0 < 1$ and $\text{Im}(k_x) = 0$ since these are unrelated to perfect absorption in the present case.

Summarizing, finding the poles of the reflection coefficients identifies the intrinsic modes of the system. Depending on the wavenumbers that are associated with these poles, the modes are classified differently: guided waves, leaky waves, and fast-waves.

31.4 Cloaking of EM and matter waves

31.5 Anisotropic and chiral metamaterials

Chapter 32

Topological order

32.1 Definition of topological order and some example systems

From a macroscopic perspective, a state with topological order is characterized by a ground state degeneracy [22] that is robust against any weak perturbations. Two states that have different topological order must undergo a phase transition in order to change into each other. Precisely which quantity that the ground-state energy is degenerate in depends on which system one considers. For instance, in the quantum Hall state the degeneracy is the number of plane-wave wave vectors k_x that fit into the area of the sample $L_x \times L_y$ since the Landau energy levels are massively degenerate in k_x (using a convenient gauge-choice). The topological degeneracy depends on the topology of space, *e.g.* if one considers a torus or other type of geometry. From a microscopic perspective, topological order is equivalent to patterns of long-range quantum entanglement [21] between quantum states in the system.

Several physical systems show topological order, such as the quantum Hall state and spin liquids. A common property of topologically ordered states is that they feature protected boundary states, which in many cases even conduct electricity or spin without any resistance.

32.2 Topological insulators: symmetry-protected topological order

Topological insulators feature gapless edge or surface states, but differ from true topologically ordered states as their properties only remain invariant under weak perturbations that respect time-reversal and $U(1)$ symmetries. In contrast, true topological order and the corresponding boundary states are invariant under any weak perturbations, regardless of their symmetry. Therefore, topological insulators are an example of *symmetry-protected topological order*. As a consequence, on a microscopic level, they also only have short-ranged entanglement.

Chapter 33

Basic theory: second quantization and Hamiltonians

33.1 Introductory remarks and key results

First quantization. The original form of quantum mechanics where physical quantities such as position and momentum are converted into operators. A typical first quantized Hamiltonian could then look like:

$$\hat{H} = \sum_{i=1}^N \left(-\frac{\hbar^2 \nabla_i^2}{2m} + U(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j), \quad (33.1)$$

where U is the single-particle potential whereas V contains the interactions between particles at various positions.

Second quantization. Also known as *canonical quantization* in quantum field theory, one here upgrades the fields in the first quantization formalism to field operators. Second quantization is expressed via creation and annihilation operators in such a way that the matrix elements (expectation values of operators) remains the same both in the first and second quantized formalisms, as they have to since matrix elements may correspond to physical observables. To be concrete, one converts from first to second quantization as follows. For single-particle operators, we have:

$$\hat{H} = \sum_{i=1}^N \hat{h}(\mathbf{r}_i) \rightarrow \hat{H} = \sum_{\alpha, \beta} \langle \alpha | \hat{h} | \beta \rangle c_{\alpha}^{\dagger} c_{\beta}, \quad (33.2)$$

where we defined the matrix element:

$$\langle \alpha | \hat{h} | \beta \rangle = \int d\mathbf{r} \phi_{\alpha}^*(\mathbf{r}) \hat{h}(\mathbf{r}) \phi_{\beta}(\mathbf{r}). \quad (33.3)$$

For two-particle operators, we have:

$$\hat{H} = \frac{1}{2} \sum_{i \neq j} \hat{v}(\mathbf{r}_i, \mathbf{r}_j) \rightarrow \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} \langle \alpha \beta | \hat{v} | \gamma \delta \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma},$$

where $\langle \alpha \beta | \hat{v} | \gamma \delta \rangle = \int \int d\mathbf{r} d\mathbf{r}' \phi_{\alpha}^*(\mathbf{r}) \phi_{\beta}^*(\mathbf{r}') \hat{v}(\mathbf{r}, \mathbf{r}') \phi_{\gamma}(\mathbf{r}) \phi_{\delta}(\mathbf{r}').$ (33.4)

This procedure holds for both fermions and bosons. The equivalence between the Hamiltonians may be verified by computing matrix elements $\langle \Psi_a | \hat{O} | \Psi_b \rangle$ for some operator $\hat{O}$ between any basis states $|\Psi_a\rangle$ and $|\Psi_b\rangle$ and see that the same element is obtained with both Hamiltonians. In the first quantization case, the basis states are Slater determinants (wavefunctions) whereas the basis states in the second quantization are of the type $|n\rangle = |n_1, n_2, \dots\rangle$ (there is a unique state of this type for each Slater determinant).

Note that one can also use real-space *field operators* instead of creation and annihilation operators to formulate second quantization. In this case, one considers the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ expressed via creation/annihilation operators in some other basis $\{|\gamma\rangle\}$ as:

$$\begin{aligned}\hat{\psi}_\sigma^\dagger(\mathbf{r}) &= \sum_\gamma \langle \gamma | \mathbf{r}, \sigma \rangle c_\gamma^\dagger = \sum_\gamma \phi_{\gamma,\sigma}^*(\mathbf{r}) c_\gamma^\dagger, \\ \hat{\psi}_\sigma(\mathbf{r}) &= \sum_\gamma \langle \mathbf{r}, \sigma | \gamma \rangle c_\gamma = \sum_\gamma \phi_{\gamma,\sigma}(\mathbf{r}) c_\gamma.\end{aligned}\tag{33.5}$$

These field operators create and annihilate a particle at the position $\mathbf{r}$ with spin σ . The quantity $\phi_{\gamma,\sigma}$ is the single-particle wavefunction that emerges from the overlap between the single-particle ket $|\gamma\rangle$ and the position-spin eigenstate $|\mathbf{r}, \sigma\rangle$.

33.2 Derivation of second quantization

We now proceed to give a detailed derivation of the above results. The following notes are based on the lecture notes in the course "Quantum theory for many-particle systems" taught by J. O. Fjaerestad at NTNU, 2014.

33.2.1 Systems of identical particles

Since quantum mechanics introduces the concept of *identical particles*, unlike classical physics where particle trajectories can in principle always be distinguished, we know that there is a constraint on the many-particle wavefunction describing a system of many identical particles (such as electrons). Let $\Psi(x_1, x_2, x_3, \dots)$ be this wavefunction where we let $x_i = (\mathbf{r}_i, s_i)$ denote the position and spin coordinates of particle i . Since the probability density must be invariant under an exchange of two identical particles:

$$|\Psi(x_1, \dots, x_j, \dots, x_k, \dots, x_N)|^2 = |\Psi(x_1, \dots, x_k, \dots, x_j, \dots, x_N)|^2,\tag{33.6}$$

we are left with only two possibilities in 3D systems (we exclude here consideration of *anyons* which may exist in 2D):

$$\Psi \rightarrow +\Psi \text{ or } \Psi \rightarrow -\Psi.\tag{33.7}$$

This is the bosonic and fermionic case we have treated earlier, and this symmetry property has profound implications for the physical behavior of an ensemble of such particles at low temperatures. The energy distribution of such particles are in the non-interacting case described by the Bose-Einstein and Fermi-Dirac distribution, respectively.

33.2.2 Many-particle wavefunctions

Just like single-particle wavefunctions satisfying the SE are usually expanded in some complete basis, we can do the same for many-particle wavefunctions. An additional aspect to take into consideration compared to the single-particle case is, however, that the many-particle wavefunction basis set must have the appropriate symmetries under particle exchange as discussed above.

We start by considering a very general Hamiltonian of the type

$$\hat{H} = \hat{H}_0 + \hat{H}_I \quad (33.8)$$

where we defined

$$\hat{H}_0 = \sum_i \hat{h}(x_i), \quad \hat{h}(x_i) = -\frac{\hbar^2}{2m} \nabla_i^2 + U(x_i) \quad (33.9)$$

and x_i is the coordinate and spin of particle i . This is a sum over the single-particle kinetic energy and potential energy $U(x_i)$ and an interaction part which will be a sum of terms that involve coordinates of multiple particles (such as Coulomb-interaction).

Our strategy will now be to set up a basis set where the many-particle wavefunctions in this basis set are eigenfunctions of a single-particle operator, such as $\hat{h}(x_i)$. Assume then that these are known:

$$\hat{h}(x)\phi_\nu(x) = \epsilon_\nu\phi_\nu(x). \quad (33.10)$$

The index ν describes a set of quantum number (assumed to be discrete for concreteness) which characterize the single-particle states ϕ_ν . These states are taken to form an orthonormal and complete set. We thus have for instance

$$\sum_\nu \phi_\nu^*(x)\phi_\nu(x') = \delta(x - x') = \delta(\mathbf{r} - \mathbf{r}')\delta_{s,s'}. \quad (33.11)$$

We will use the notation

$$\int dx \equiv \sum_s \int d\mathbf{r}. \quad (33.12)$$

Using these single-particle wavefunctions, we can now construct a many-particle wavefunction which is correctly symmetrized. For bosons, we have

$$\Phi^{\text{boson}}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!} \sqrt{\prod_\nu (n_\nu!)}} \sum_{P \in S_N} P \phi_{\nu_1}(x_1) \phi_{\nu_2}(x_2) \dots \phi_{\nu_N}(x_N). \quad (33.13)$$

The sum goes over all permutations P of the N coordinates $\{x_i\}$ while S_N is the set of these permutations. In total, there are $N!$ permutations. The prefactor ensures that the state is normalized to 1. Since bosons have no restriction regarding how many particles that can be in the same single-particle state, Φ^{boson} can in general be non-zero even if two indices ν_j are the same. For instance, if $\nu_7 = \nu_9$ there are two bosons in the single-particle state ν_7 so that $n_{\nu_7} = 2$.

For fermions, we instead have:

$$\Phi^{\text{fermion}}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} \text{sgn}(P) \cdot P \phi_{\nu_1}(x_1) \dots \phi_{\nu_N}(x_N). \quad (33.14)$$

The dependence on $n_\nu!$ is gone, compared to the bosonic case, since for fermions n_ν is 0 or 1, in which case $n_\nu! = 1$. Moreover, there is a sign factor accounting for the antisymmetric property under exchange of two fermions. The sign of P is defined in the following manner. A permutation has a positive sign if it can be arrived at by an even number of two-particle permutations. It has a negative sign if one requires an odd number of two-particle permutations.

As expected, we can also write the fermionic many-body wavefunction as a *Slater determinant*

$$\Phi^{\text{fermion}} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \dots & \phi_{\nu_1}(x_N) \\ \vdots & \ddots & \vdots \\ \phi_{\nu_N}(x_1) & \dots & \phi_{\nu_N}(x_N) \end{vmatrix}. \quad (33.15)$$

The Pauli exclusion principle discussed earlier is manifested in that the determinant, and thus wavefunction, vanishes if $\nu_i = \nu_j$ for some $i \neq j$. It is not possible to put more than one fermion into a specific single-particle state.

Both in the fermionic and bosonic case, the many-particle wavefunctions $\Phi^{\text{fermion/boson}}$ are eigenfunctions of the non-interacting part $\hat{H}$ of our Hamiltonian. Their eigenvalues are

$$E = \sum_{\nu} \epsilon_{\nu} n_{\nu} \quad (33.16)$$

where n_{ν} is the number of particles that reside in quantum state ν . The point is now that we can use these wavefunctions Φ as a complete, orthonormal basis set for the wavefunctions Ψ that solve the *interacting* problem:

$$\Psi(x_1, \dots, x_N) = \sum_a f_a \Phi_a(x_1, \dots, x_N) \quad (33.17)$$

where f_a are expansion coefficients and the wavefunctions satisfy

$$\int d^N x \Phi_a^* \Phi_b = \delta_{a,b}. \quad (33.18)$$

33.2.3 Second quantization (*aka* occupation-number formalism)

The wavefunction formalism we have discussed in the preceding sections is known as *first quantization*. Although we can in principle make use of the above treatment in order to deal with many-particle basis wavefunctions, there exists a more elegant and practical formalism. This is the *second quantization procedure* also known as the *occupation-number representation*. The essence of this formalism is that the many-body state can be described in a very succinct manner, as the relevant information consists of only two parts:

- The occupation number for each single-particle state (0 or 1 for fermions).
- The symmetry or antisymmetry of the state under an exchange of particles.

33.2.4 Fermionic case

To describe second quantization for fermions, we shall make use of creation and annihilation operators $c^\dagger$ and c which act on specified single-particle states. The antisymmetry property of fermions

will then be taken care of via the anti-commutation relations that these operators satisfy.

The many-particle basis states that we used previously were Slater determinants. Now, we shall use products of creation operators acting on the "vacuum" state (with no fermions) as our many-particle basis state which then automatically has the correct anti-symmetry property under exchange of particles. Let us consider an example consisting of a 3-particle state where the single-particle states 2, 4, and 6 are occupied whereas the rest are empty. The analogue of the unique Slater determinant for this state (once we have agreed upon an ordering of the states 2,4,6) in the *occupation number representation* (rather than the position-space representation) is then:

$$|0, 1, 0, 1, 0, 1, 0, 0, 0, \dots\rangle \quad (33.19)$$

which states that there 0 particles in single-particle state 1, 1 particle in state 2, and so forth. An arbitrary many-particle basis state can then be written as

$$|n_1, n_2, n_3, \dots\rangle. \quad (33.20)$$

The creation operator $c_\nu^\dagger$, where ν labels the single-particle state, is defined as

$$c_\nu^\dagger |n_1, n_2, \dots, n_\nu, \dots\rangle = (-1)^{\sum_{\mu < \nu} n_\mu} (1 - n_\nu) |n_1, n_2, \dots, 1_\nu, \dots\rangle. \quad (33.21)$$

Here, $\theta_\nu \equiv (-1)^{\sum_{\mu < \nu} n_\mu}$ is a phase factor equal to +1 or -1 which ensures the correct antisymmetric property of the state vector. To see this, we first realize that the phase factor depends on whether the total number of fermions in single-particle states with labels less than ν is even or odd. If we start with the vacuum state $|0\rangle = |0, 0, 0, \dots\rangle$ and first create a fermion in state 1, we get

$$c_1^\dagger |0\rangle = |1, 0, 0, \dots\rangle. \quad (33.22)$$

If we subsequently create a fermion in state 2, the final state is:

$$c_2^\dagger c_1^\dagger |0\rangle = -|1, 1, 0, \dots\rangle \quad (33.23)$$

where the minus sign came from the phase factor $(-1)^{\sum_{\mu < \nu} n_\mu}$. But if we instead had created the fermions in the opposite order (first state 2, then state 1), we would have obtained

$$c_1^\dagger c_2^\dagger |0\rangle = |1, 1, 0, \dots\rangle. \quad (33.24)$$

Thus, the creation operators *anticommute* which ensures the antisymmetry property of the state vector: $\{c_i^\dagger, c_j^\dagger\} = 0$. An arbitrary many-particle basis state which has the correct antisymmetry property under exchange of particles may then generally be written as

$$|n_1, n_2, n_3, \dots\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \dots |0\rangle. \quad (33.25)$$

Moreover, the factor $(1 - n_\nu)$ ensures that if a fermion already exists in state ν , then acting with $c_\nu^\dagger$ gives 0 due to the Pauli principle.

The *annihilation operator* is defined in a similar manner

$$c_\nu |n_1, n_2, \dots, n_\nu, \dots\rangle = (-1)^{\sum_{\mu < \nu} n_\mu} n_\nu |n_1, \dots, 0_\nu, \dots\rangle. \quad (33.26)$$

The result is non-zero only if there already existed a fermion in state ν due to the prefactor n_ν . This is reasonable as we cannot annihilate a fermion that does not exist in the first place.

Fock space

If we let $|\psi_N\rangle$ be a state with N fermions, then $c_\nu^\dagger|\psi_N\rangle$ and $c_\nu|\psi_N\rangle$ are states with $N+1$ and $N-1$ fermions, respectively. We can thus say that c_ν and $c_\nu^\dagger$ are mappings between fixed particle-number fermionic Hilbert spaces $\mathcal{H}_N$ whose particle numbers are different by 1:

$$\begin{aligned} c_\nu : \mathcal{H}_N &\rightarrow \mathcal{H}_{N-1}, \\ c_\nu^\dagger : \mathcal{H}_N &\rightarrow \mathcal{H}_{N+1}. \end{aligned} \quad (33.27)$$

These mappings hold for any value N and the collection (direct sum) of all these fixed particle-number fermionic Hilbert spaces $\{\mathcal{H}_N\}$ ($N = 0, 1, 2, \dots$) are referred to as *the Fock space* $\mathcal{F}$. It is therefore common to see many-particle states being referred to as Fock states in the literature and that they reside in Fock space. The operators c_ν and $c_\nu^\dagger$ are thus operators which map between states in Fock space.

From the way we defined the creation and annihilation operators in Eq. (33.21) and (33.26), we can prove that the operators satisfy the following anticommutation relations:

$$\begin{aligned} \{c_\mu, c_\nu\} &= 0, \\ \{c_\mu^\dagger, c_\nu^\dagger\} &= 0, \\ \{c_\mu^\dagger, c_\nu\} &= \delta_{\mu\nu}. \end{aligned} \quad (33.28)$$

Another useful and commonly encountered operator is the *number operator* $\hat{n}_\nu \equiv c_\nu^\dagger c_\nu$. To see why it earns its name, consider that

$$\begin{aligned} c_\nu^\dagger c_\nu |\dots, n_\nu, \dots\rangle &= \theta_\nu n_\nu c_\nu^\dagger |\dots, 0_\nu, \dots\rangle = \theta_\nu^2 n_\nu (1-0) |\dots, 1_\nu, \dots\rangle \\ &= n_\nu |\dots, n_\nu, \dots\rangle \end{aligned} \quad (33.29)$$

since $\theta_\nu^2 = 1$. Therefore, a basis state $|n\rangle$ is an eigenstate of $\hat{n}_\nu$ with eigenvalue n_ν : the operator $\hat{n}_\nu$ counts the number of fermions in the single-particle state ν . The total number operator is then:

$$\hat{N} = \sum_\nu \hat{n}_\nu \quad (33.30)$$

so that

$$\hat{N}|n\rangle = \sum_\nu n_\nu |n\rangle = N|n\rangle. \quad (33.31)$$

33.2.5 Second-quantized representation of operators

The next step is to figure out how operators in general are expressed in our newly formulated second-quantized language. We here confine our attention to the two most common and important types of operators: single-particle and two-particle operators.

Single-particle operators, such as the Hamiltonian $\hat{H}_0$ for a collection of free particles, can be written as a sum of terms and each term only involves the coordinates of a single particle. On the other hand, two-particle operators can be written as a sum of terms which each involve the coordinates of two particles. An example of the latter is the Coulomb interaction between electrons. We summarized the procedures for how to convert first-quantized operators to second-quantized operators initially in this chapter:

- Single-particle operators:

$$\hat{H}_0 = \sum_{i=1}^N \hat{h}(x_i) \implies \sum_{\alpha\beta} \langle \alpha | \hat{h} | \beta \rangle c_{\alpha}^{\dagger} c_{\beta} \quad (33.32)$$

where we defined

$$\langle \alpha | \hat{h} | \beta \rangle = \int dx \phi_{\alpha}^*(x) \hat{h}(x) \phi_{\beta}(x). \quad (33.33)$$

- Two-particle operators:

$$\hat{H}_I = \frac{1}{2} \sum_{i \neq j} \hat{v}(x_i, x_j) \implies \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma}, \quad (33.34)$$

where we defined

$$\langle \alpha\beta | \hat{v} | \gamma\delta \rangle = \int \int dx dx' \phi_{\alpha}^*(x) \phi_{\beta}^*(x') \hat{v}(x, x') \phi_{\gamma}(x) \phi_{\delta}(x'). \quad (33.35)$$

However, we not only wish to state this, but let us now *prove this*. The equivalence of the first- and second-quantized formalisms can be proven by considering matrix elements since these correspond to physically observable quantities (expectation values). The key point is that matrix elements of the type

$$\langle \Phi_a | \hat{O} | \Phi_b \rangle \quad (33.36)$$

for an operator $\hat{O}$ and two basis states $|\Phi_a\rangle$ and $|\Phi_b\rangle$ should yield the same value *regardless of which formalism (first or second quantization)* that is used to calculate it. We know that in the first quantized formalism, the basis states are Slater determinant wavefunctions. In the second quantized formalism, the basis states are the Fock states $|n\rangle = |n_1, n_2, \dots\rangle$. There exists a unique correspondence between each Fock state and each Slater determinant.

It is clear from the outset that a matrix element involving a single-particle operator will be zero if the two Slater determinants differ in the occupation of more than two single-particle states (since such states are orthogonal). This can be seen easily in the second quantized version, where a single-particle operator is in general a sum of terms which each only changes (at most) the occupation of two single-particle states. For instance, $c_{\alpha}^{\dagger} c_{\beta}$ transfers a fermion from state β to state α . In the same way, a matrix element for two-particle operators if the occupation between the two states differ with more than four single-particle states.

Before proving the above correspondence between first- and second-quantized operators, let us briefly go through the second quantization procedure for *bosons*.

33.2.6 Second quantization for bosons

Whereas the fundamental (anti)commutation relations for fermions were discussed above, bosonic operators b satisfy $[b, b^{\dagger}] = 1$. In the occupation-number representation, many-particle basis states for bosons read

$$|n\rangle = |n_1, n_2, \dots\rangle. \quad (33.37)$$

Unlike fermions, bosons can have an occupancy of a particular single-particle state that exceeds 1. In fact, n_ν can be any nonnegative integer. Just like there was a unique correspondence between fermionic Slater determinants and fermionic many-particle basis states in the occupation number representation, the same one-to-one correspondence exists between Eq. (33.13) and states of the type shown in Eq. (33.37). The bosonic creation and annihilation operators are defined by

$$\begin{aligned} b_\nu^\dagger |\dots, n_\nu, \dots\rangle &= \sqrt{n_\nu + 1} |\dots, n_\nu + 1, \dots\rangle, \\ b_\nu |\dots, n_\nu, \dots\rangle &= \sqrt{n_\nu} |\dots, n_\nu - 1, \dots\rangle. \end{aligned} \quad (33.38)$$

The bosonic number operator for state ν is $\hat{n}_\nu = b_\nu^\dagger b_\nu$. An arbitrary and properly normalized many-particle basis state can now be written as

$$|n_1, n_2, n_3, \dots\rangle = \prod_\nu \frac{(b_\nu^\dagger)^{n_\nu}}{\sqrt{n_\nu!}} |0\rangle \quad (33.39)$$

where $|0\rangle$ as before is the vacuum state with no bosons. The operators satisfy

$$\begin{aligned} [b_\mu, b_\nu] &= 0, \\ [b_\mu^\dagger, b_\nu^\dagger] &= 0, \\ [b_\mu, b_\nu^\dagger] &= \delta_{\mu,\nu}. \end{aligned} \quad (33.40)$$

The conversion between first- and second-quantized single and two-particle operators for bosons is identical to that of fermions shown in the previous section.

33.2.7 Basis transformations

We need one final piece of the puzzle before we can prove the equivalence of first and second-quantization, namely how to do basis transformations. We have thus far only used a particular basis set $\{\phi_\alpha(x)\}$ of single-particle wavefunctions, but let us now investigate how to proceed if we wish to use some different single-particle basis set.

We let $|\alpha\rangle$ be the single-particle ket whose overlap with the position-spin eigenstate $|x\rangle$ is the wavefunction $\phi_\alpha(x)$ we've been using:

$$\phi_\alpha(x) \equiv \langle x | \alpha \rangle. \quad (33.41)$$

Both in the bosonic and fermion case we may write

$$|\alpha\rangle = a_\alpha^\dagger |0\rangle \quad (33.42)$$

where $a_\alpha^\dagger$ is the creation operator for a particle in single-particle state α . Consider now a different single-particle basis set $\{\psi_{\tilde{\alpha}}(x)\}$ whose associated single-particle kets are denoted $|\tilde{\alpha}\rangle$:

$$\psi_{\tilde{\alpha}}(x) = \langle x | \tilde{\alpha} \rangle, \quad |\tilde{\alpha}\rangle = a_{\tilde{\alpha}}^\dagger |0\rangle. \quad (33.43)$$

Here, $a_{\tilde{\alpha}}^\dagger$ is the creation operator for a particle in the single-particle state characterized by quantum number(s) $\tilde{\alpha}$. For instance, $\{|\alpha\rangle\}$ could be the set of eigenstates for the kinetic energy operator $\hat{p}^2/(2m)$ whereas $\{|\tilde{\alpha}\rangle\}$ could be the set of eigenstates for the total Hamilton operator $\hat{p}^2/(2m) + U(\hat{x})$.

If we want to transform between the two single-particle basis sets, we make use of the completeness relation in single-particle Hilbert space:

$$1 = \sum_{\alpha} |\alpha\rangle\langle\alpha| = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|. \quad (33.44)$$

It follows that

$$a_{\alpha}^{\dagger}|0\rangle = |\alpha\rangle = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle\langle\tilde{\alpha}|\alpha\rangle = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle a_{\tilde{\alpha}}^{\dagger}|0\rangle. \quad (33.45)$$

By comparing the leftmost and rightmost side of the above equation, we see that

$$a_{\alpha}^{\dagger} = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle a_{\tilde{\alpha}}^{\dagger}. \quad (33.46)$$

Taking the adjoint produces the relation for how to transform annihilation operators:

$$a_{\alpha} = \sum_{\tilde{\alpha}} \langle\alpha|\tilde{\alpha}\rangle a_{\tilde{\alpha}}. \quad (33.47)$$

Using these transformation rules, it is straightforward to show that the wavefunction $\phi_{\alpha}(x) = \langle x|\alpha\rangle$ transforms as:

$$\phi_{\alpha}(x) = \sum_{\tilde{\alpha}} \langle\tilde{\alpha}|\alpha\rangle \zeta_{\tilde{\alpha}}(x) \quad (33.48)$$

where $\zeta_{\tilde{\alpha}}(x) = \langle x|\tilde{\alpha}\rangle$. Such basis transformations as above are *unitary transformations*. This can be proven by defining the matrix D which have elements $D_{\tilde{\alpha}\alpha} \equiv \langle\tilde{\alpha}|\alpha\rangle$. If D is unitary, we must have $DD^{\dagger} = 1$ so that $(DD^{\dagger})_{\alpha\beta} = \delta_{\alpha\beta}$. We obtain:

$$\begin{aligned} \delta_{\alpha\beta} &= \langle\alpha|\beta\rangle = \sum_{\gamma} \langle\alpha|\gamma\rangle\langle\gamma|\beta\rangle = \sum_{\gamma} \langle\alpha|\gamma\rangle\langle\beta|\gamma\rangle^{*} \\ &= \sum_{\gamma} D_{\alpha\gamma} D_{\beta\gamma}^{*} = \sum_{\gamma} D_{\alpha\gamma} (D^{\dagger})_{\gamma\beta} = (DD^{\dagger})_{\alpha\beta}. \end{aligned} \quad (33.49)$$

which shows the unitarity. It is also important to note that basis transformations preserve anti-commutation and commutation relations: the new creation/annihilation operators satisfy the same kind of relations as the ones in the old basis.

33.2.8 Proof of the second-quantized representation of single-particle operators

Finally, we are ready to give the proof for how to second-quantize single-particle operators. The proof for two-particle operators is performed analogously.

Consider an arbitrary single-particle operator

$$\hat{O} = \sum_{i=1}^N \hat{o}_i. \quad (33.50)$$

We choose the set $\{|\tilde{\alpha}\rangle\}$ to be the single-particle basis of eigenstates of $\hat{o}$, meaning that

$$\hat{o}|\tilde{\alpha}\rangle = o_{\tilde{\alpha}}|\tilde{\alpha}\rangle. \quad (33.51)$$

Thus, $o_{\tilde{\alpha}}$ is the eigenvalue of $\hat{o}$ associated with the eigenstate $|\tilde{\alpha}\rangle$.

Our first claim is that the second-quantized representation of $\hat{O}$ can be expressed as

$$\hat{O} = \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} \hat{n}_{\tilde{\alpha}} \quad (33.52)$$

where $\tilde{\alpha} = a_{\tilde{\alpha}}^{\dagger} a_{\tilde{\alpha}}$ is the number operator for the state $|\tilde{\alpha}\rangle$. To show this, we compute the matrix element of $\hat{O}$ in both the first- and second-quantized formalism and show that the result is identical. We use a many-particle basis that is built from single-particle basis $\{|\tilde{\alpha}\rangle\}$.

Consider the matrix element $\langle \Phi' | \hat{O} | \Phi \rangle$ where $|\Phi\rangle$ and $|\Phi'\rangle$ are two arbitrary basis states in this many-particle basis set. We obtain

$$\begin{aligned} \langle \Phi' | \hat{O} | \Phi \rangle &= \langle n'_{\tilde{\alpha}_1}, n'_{\tilde{\alpha}_2}, \dots | \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} \hat{n}_{\tilde{\alpha}} | n_{\tilde{\alpha}_1}, n_{\tilde{\alpha}_2}, \dots \rangle \\ &= \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}} \langle n'_{\tilde{\alpha}_1}, n'_{\tilde{\alpha}_2}, \dots | n_{\tilde{\alpha}_1}, n_{\tilde{\alpha}_2}, \dots \rangle \\ &= \delta_{\Phi, \Phi'} \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}}. \end{aligned} \quad (33.53)$$

If we instead compute the expectation value using first quantization, we obtain:

$$\begin{aligned} \langle \Phi' | \hat{O} | \Phi \rangle &= \int d^N x \Phi'^*(x_1, \dots, x_N) \sum_{i=1}^N \hat{o}(x_i) \Phi(x_1, \dots, x_N) \\ &= \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}} \int d^N x \Phi'^*(x_1, \dots, x_N) \Phi(x_1, \dots, x_N) \\ &= \delta_{\Phi, \Phi'} \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} n_{\tilde{\alpha}}. \end{aligned} \quad (33.54)$$

where we made use of Eq. (33.16). This *proves that we get exactly the same result* when computing the expectation value both in first- and second-quantization for this particular basis choice.

We should in fairness state that we used a particular single-particle basis here, namely that one that diagonalizes $\hat{o}$. The expression Eq. (33.52) is therefore not valid for an arbitrary basis. However, we can start from that expression we can use the basis transformations considered in the previous subsection to derive an expression for the operator $\hat{O}$ that *is valid* in an arbitrary basis:

$$\begin{aligned} \hat{O} &= \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} a_{\tilde{\alpha}}^{\dagger} a_{\tilde{\alpha}} = \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} \left(\sum_{\alpha} \langle \alpha | \tilde{\alpha} \rangle a_{\alpha}^{\dagger} \right) \left(\sum_{\beta} \langle \tilde{\alpha} | \beta \rangle a_{\beta} \right) \\ &= \sum_{\alpha, \beta} \langle \alpha | \left(\sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle o_{\tilde{\alpha}} \langle \tilde{\alpha}| \right) | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} = \sum_{\alpha, \beta} \langle \alpha | \hat{o} | \beta \rangle a_{\alpha}^{\dagger} a_{\beta}. \end{aligned} \quad (33.55)$$

Above, we used that

$$\hat{o} = \hat{o} \cdot 1 = \hat{o} \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle \langle \tilde{\alpha}| = \sum_{\tilde{\alpha}} o_{\tilde{\alpha}} |\tilde{\alpha}\rangle \langle \tilde{\alpha}| = \sum_{\tilde{\alpha}} |\tilde{\alpha}\rangle o_{\tilde{\alpha}} \langle \tilde{\alpha}|. \quad (33.56)$$

The matrix element $\langle \alpha | \hat{o} | \beta \rangle$ is

$$\langle \alpha | \hat{o} | \beta \rangle = \int \int dx dx' \langle \alpha | x \rangle \langle x | \hat{o} | x' \rangle \langle x' | \beta \rangle = \int dx \langle \alpha | x \rangle \hat{o}(x) \langle x | \beta \rangle = \int dx \phi_\alpha^*(x) \hat{o}(x) \phi_\beta(x), \quad (33.57)$$

where we used that $\langle x | \hat{o} | x' \rangle = \hat{o}(x) \delta(x - x')$. We know from the calculation above, using the $|\alpha\rangle$ -basis, that $\hat{O}$ gives exactly the same expectation value as the first-quantized formalism, and therefore we have now derived a general prescription for how to second-quantize an operator in an arbitrary basis.

This framework provides a great flexibility in that any complete set of basis vectors can be used to second-quantize the Hamiltonian. The corresponding general eigenstates are then Fock-type state vectors which are characterized by the number of particles for each possible eigenvalue. However, it is worth noting that some basis choices are definitely more convenient than others in terms of evaluating what the expectation value $\langle \alpha | \hat{o} | \beta \rangle$ actually is. In the diagonal basis, as we saw initially, it is trivial. We can choose any other basis set, even a basis set which does not appear physically reasonable for the given system at hand, but the evaluation of this expectation value will then be much more cumbersome.

33.2.9 Field operators

Finally, we consider creation and annihilation operators in the single-particle basis consisting of the states $|x\rangle$ where $x = (\mathbf{r}, s)$ as before. In this basis, rather than the occupation number basis considered above, the creation and annihilation operators are referred to as *field operators* and denoted $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$. Note how we have put the state label as an argument rather than as a subscript (this is just notation). We know how to transform operators from one basis to another, so we can immediately write down

$$\begin{aligned} \hat{\psi}^\dagger(x) &= \sum_\alpha \langle \alpha | x \rangle a_\alpha^\dagger = \sum_\alpha \phi_\alpha^*(x) a_\alpha^\dagger, \\ \hat{\psi}(x) &= \sum_\alpha \langle x | \alpha \rangle a_\alpha = \sum_\alpha \phi_\alpha(x) a_\alpha. \end{aligned} \quad (33.58)$$

The field operators create and annihilate a particle at space-spin coordinate x and obey the proper (anti-)commutation relations:

$$\begin{aligned} [\hat{\psi}(x), \hat{\psi}(x')]_\mp &= [\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')]_\mp = 0, \\ [\hat{\psi}(x), \hat{\psi}^\dagger(x')]_\mp &= \delta(x - x'). \end{aligned} \quad (33.59)$$

Here, $\mp$ refers to bosons/fermions. The above relations follow immediately from the commutation relations of the second quantized operators $\{a_\alpha, a_\alpha^\dagger\}$. The Dirac-delta function comes from $\langle x | x' \rangle$ which cannot be normalized to 1 since x is continuous. Using the $\{|x\rangle\}$ basis, the second-quantized representation of single- and two-particle operators is

$$\begin{aligned} \hat{H}_0 &= \int dx \hat{\psi}^\dagger(x) \hat{h}(x) \hat{\psi}(x), \\ \hat{H}_I &= \frac{1}{2} \int \int dx dx' \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \hat{v}(x, x') \hat{\psi}(x') \hat{\psi}(x). \end{aligned} \quad (33.60)$$

This can be verified by inserting Eq. (33.58) into Eq. (33.60) and observing that this reproduces the general second-quantized form of operators mentioned earlier in the occupation number basis.

Alternatively, one can insert the inverse transformations

$$a_\alpha = \int dx \phi_\alpha^*(x) \psi(x), \quad a_\alpha^\dagger = \int dx \phi_\alpha(x) \psi^\dagger(x) \quad (33.61)$$

into the previously obtained expression

$$H = \sum_{\alpha\beta} \langle \alpha | h | \beta \rangle a_\alpha^\dagger a_\beta \quad (33.62)$$

which gives

$$H = \int \int dx dx' \sum_{\alpha\beta} \langle \alpha | h | \beta \rangle \langle x | \alpha \rangle \psi^\dagger(x) \langle \beta | x' \rangle \psi(x'). \quad (33.63)$$

Now, all the expectation values are scalars and commute with the operators. Specifically, $\phi_\alpha(x)$ and $\psi^\dagger(x)$ commute just like a wavefunction $u_{\mathbf{k}}$ and operator $c_{\mathbf{k}}^\dagger$ commute since $c_{\mathbf{k}}^\dagger$ acts on the Fock states $|n_{\mathbf{k}}\rangle$ while $\psi^\dagger(x)$ acts on the states $|x\rangle$. Therefore, we move terms inside the integral to obtain:

$$H = \int \int dx dx' \sum_{\alpha\beta} \psi^\dagger(x) \langle x | \alpha \rangle \langle \alpha | h | \beta \rangle \langle \beta | x' \rangle \psi(x'). \quad (33.64)$$

Using now the completeness relations for $|\alpha\rangle$ and $|\beta\rangle$, we obtain

$$H = \int \int dx dx' \psi^\dagger(x) \langle x | h | x' \rangle \psi(x'). \quad (33.65)$$

But as shown *e.g.* in the QM II lecture notes, we have

$$\langle x | h | x' \rangle = \hat{h}(x') \delta(x - x'). \quad (33.66)$$

Therefore, we end up with

$$H = \int \int dx \psi^\dagger(x) \hat{h}(x) \psi(x). \quad (33.67)$$

33.3 The importance of ensuring Hermiticity of H

In the wavemechanics representation where ψ and ϕ are scalar wavefunctions, the adjoint $\hat{A}^\dagger$ of an operator $\hat{A}$ is defined from the equation

$$\int dx \phi^* \hat{A} \psi = \int dx (\hat{A}^\dagger \phi)^* \psi. \quad (33.68)$$

Any operator corresponding to a physical observable, such as momentum $\hat{p}$ or position $\hat{x}$, must be a hermitian operator. A hermitian operator satisfies $\hat{A} = \hat{A}^\dagger$ and is guaranteed to have real expectation values (as a physical observable should). Let us show how $\hat{p}$ is hermitian:

$$\int dx \phi^* \hat{p} \psi = \frac{\hbar}{i} [\phi^* \psi]_{\text{boundary}} - \int dx (\hat{p} \phi^*) \psi \quad (33.69)$$

$$= \int dx (\hat{p} \phi)^* \psi. \quad (33.70)$$

From the definition of the adjoint operator, we see that $\hat{p} = \hat{p}^\dagger$. The boundary term vanishes since we assume that the wavefunction must go to zero at infinity. Note that even if $\hat{p} = \frac{\hbar}{i}\partial_x$, we have $\hat{p}^\dagger = \hat{p}$ since the dagger operation not only complex conjugates scalars, but also reverses the sign of ∂_x for the operator.

In the context of second quantized Hamiltonians, we know that the Hamilton-operator itself is written in a different way than considered above. For instance, using the position eigenvectors as basis-vectors in the second quantized formalism, the kinetic energy reads:

$$H = \int dx \psi^\dagger(x) \left(-\frac{\hbar^2 \nabla^2}{2m} - \mu \right) \psi(x), \quad (33.71)$$

so that we have a sandwich between field operators $\psi(x)$ and $\psi^\dagger(x)$. In order to correspond to physically observable quantities, we need the first-quantized operators inside the integral of H to be hermitian. We here wish to illustrate an important point regarding hermiticity in junctions and the spin index is not important. For instance, imagine that we have a junction between a normal metal with SOC and a superconductor. In other words, the SOC coefficient is non-zero only on the normal metal side. In particular, if the Hamiltonian depends on the component of momentum that is perpendicular to the junction we have to be careful. To see why, consider the expectation value of a first-quantized Hamiltonian describing antisymmetric spin-orbit interactions, $H_{\text{SOC}} = \alpha(x)\hat{p}_x$. We see that:

$$\begin{aligned} \int dx \psi^*(x) H_{\text{SOC}} \psi(x) &= \int dx \psi^*(x) \left[\alpha(x) \hat{p}_x \right] \psi(x) \\ &= \int dx \psi^*(x) \left[\alpha(x) \frac{\hbar}{i} \partial_x \right] \psi(x). \end{aligned} \quad (33.72)$$

Here, ψ are scalar wavefunctions and the SOC operator corresponds to the scenario described above: the SOC is non-zero for $x < 0$ and zero when $\alpha(x) = \alpha_0 \Theta(x)$. However, this Hamilton-operator is not hermitian. We see this via:

$$\begin{aligned} \int dx \psi^*(x) \left[\alpha(x) \frac{\hbar}{i} \partial_x \right] \psi(x) &= [\dots]_{\text{boundary}} - \int dx \frac{\hbar}{i} \partial_x [\psi^*(x) \alpha(x)] \psi(x) \\ &= \int dx \left\{ \left(\frac{\hbar}{i} \partial_x \right)^* [\psi^*(x) \alpha(x)] \right\} \psi(x) \\ &\neq \int dx [H_{\text{SOC}} \psi(x)]^* \psi(x). \end{aligned} \quad (33.73)$$

The point is that the derivative operator in the last term also acts on $\alpha(x)$ and produces a δ -function. However, this problem is remedied by *symmetrizing* the SOC Hamiltonian from the outset. If we define:

$$H_{\text{SOC}} = \alpha(x) \hat{p}_x + \hat{p}_x \alpha(x), \quad (33.74)$$

then we see that (by doing a partial integration on each term and collecting all the boundary terms):

$$\begin{aligned}
\int dx \psi^*(x) H_{\text{SOC}} \psi(x) &= \int dx \psi^*(x) [\alpha(x) \hat{p}_x + \hat{p}_x \alpha(x)] \psi(x) \\
&= \text{Boundary terms} - \int dx \hat{p}_x [\psi^*(x) \alpha(x)] \psi(x) - \int dx [\hat{p}_x \psi^*(x)] \alpha(x) \psi(x) \\
&= \int dx \left[(\hat{p}_x^* \alpha(x) + \alpha(x) \hat{p}_x^*) \psi^*(x) \right] \psi(x) \\
&= \int dx [H_{\text{SOC}} \psi(x)]^* \psi(x).
\end{aligned} \tag{33.75}$$

which proves that the Hamiltonian is hermitian according to Eq. (33.68). We can apply the same logic to a problem where the effective mass is different on the two sides of the interface, i.e. the mass m is a step-function. In order to make the Hamiltonian hermitian, instead of

$$H = \int dx \psi^\dagger(x) \left(\frac{\hat{p}_x^2}{2m(x)} - \mu \right) \psi(x), \tag{33.76}$$

we can write:

$$H = \int dx \psi^\dagger(x) \left(\hat{p}_x \frac{1}{2m(x)} \hat{p}_x - \mu \right) \psi(x). \tag{33.77}$$

Note that there are in fact several ways in which one can make the Hamiltonian Hermitian when the mass is position-dependent. See equation 1 in <https://arxiv.org/pdf/2303.02507.pdf>. The Hamilton-operator above corresponds to the case $a = b = 0$.

Choosing representation of differential operators in lattice-Hamiltonian

In an analysis in May 2023, Ali pointed out that when a central difference method is used to represent derivatives ∂_x when going to the second-quantized H , one obtains a special treatment of the lattice sites closest to the interface (as originally shown by K. Svalland and L. Johnsen in the appendix of PRL 2020 Inversion Symmetry). The starting point always has to be the symmetrized version in the continuum. However, an important point is that even when this is the starting point, one can obtain a Hamilton-operator on the lattice which has no special treatment at the interfacial points *depending* on how one represents ∂_x . For instance, preliminary calculations by Ali shows that using a forward difference method, the Hamilton-operator on the lattice does not distinguish the points at the interface (modifying the hopping by $1/2$) and still remains Hermitian.

Chapter 34

Basic theory for Hilbert space

34.0.1 Not as abstract as one might think - just a linear vector space

A Hilbert space is a linear vector space which can be thought of as a generalization of Euclidean space (such as normal 3D space) to any finite or infinite number of dimensions. Hilbert space thus possesses the structure of an inner product, allowing a generalized length and angle to be measured, and is complete. Hilbert spaces are relevant in the general formulation of quantum mechanics, but let us first briefly remind ourselves of some familiar properties from linear algebra.

An N -dimensional vector space is spanned by N basis vectors and any vector $\mathbf{v}$ in that space can be expressed as a unique linear combination of the basis vectors $\mathbf{e}_i$:

$$\mathbf{v} = \sum_i c_i \mathbf{e}_i \quad (34.1)$$

Here, c_i is the projection of $\mathbf{v}$ on $\mathbf{e}_i$. These basis vectors form a complete set.

All of these statements have an analogue in Hilbert space where $|\Psi\rangle$ takes the role of the vector $\mathbf{v}$. The object $|\Psi\rangle$ which describes the state of a quantum system is a Hilbert space vector. Hilbert space is thus spanned by all the possible state vectors that the system can be in. Let us denote these $|\psi_n\rangle$ where n is the quantum number associated with eigenvalue E_n . A general vector in this Hilbert space can thus be written $|\Psi\rangle = \sum_n c_n |\psi_n\rangle$. The dimension of a Hilbert space can therefore be infinite. This is the case especially for state vectors associated with continuous variables, such as position, since there are infinitely many states the system can be in (infinitely many positions). The eigenstates of a *Hermitian operator* in quantum mechanics generally form a complete basis.

The coefficients c_n represent the projection of $|\Psi\rangle$ onto a specific basis. Just as for a normal vector $\mathbf{v}$, we can't know much about it unless we choose a coordinate system where $\mathbf{v}$ exists. Only then can we say what its components are. The same is true about $|\Psi\rangle$: if we choose a position representation, the wavefunction $\psi(x) = \langle x|\Psi\rangle$ plays the equivalent role of vector components c_i in Eq. (34.1). Note that we certainly *don't have to* choose a position representation, just as little as we have to choose a Cartesian coordinate system. The position wavefunction representation taught in introductory QM courses is thus the equivalent of just staying in a Cartesian coordinate system all the time.

34.0.2 Distinguishing eigenstates associated with discrete and continuous eigenvalues

It follows from the above that a basis in a finite-dimensional Hilbert space can only be used to define a ket corresponding that has a discrete eigenvalue spectrum. For example, you could use a two-dimensional basis for a system describing the spin of a $s = \frac{1}{2}$ particle, with two basis kets $|\uparrow\rangle$ and $|\downarrow\rangle$ that have corresponding eigenvalues $+1$ and -1 .

But an observable like position is continuous – we can ask what's the probability that the position is 0.6, or 0.601, and so forth. Since there are infinite possible values of position, we need infinitely many eigenvectors, and an infinite-dimensional Hilbert space. Having stated this, there are some points which we should keep in mind.

- **Continuous eigenstates strictly speaking are not appropriate as a basis and do not exist in a Hilbert-state (unlike discrete eigenstates), but in practice they can be used anyway.**

In short, the problem lies in that the norm of continuous eigenstates is infinite. We have for instance $\langle x'|x\rangle = \delta(x - x')$. Since such eigenstates cannot be normalized to a finite number (unity), they cannot strictly speaking represent possible physical states of a system. Moreover, Hilbert spaces in quantum mechanics have to be separable. Mathematically, a complex Hilbert space does not have to be separable, but a Hilbert space where a state vector describing a physical system exists has to be. Practically speaking, this means that a countable basis is used in the infinite-dimensional case: $|0\rangle, |1\rangle, \dots$. This is distinct from an uncountable basis of infinite dimension, such as position eigenvectors, where the states are labelled by a continuous number. Note that a countable basis can still be infinite-dimensional, which *e.g.* is the case for the harmonic oscillator energy eigenstates.

Let us elaborate a bit. As in any vector space, a basis is a set of linearly independent vectors that span the entire space, and the number of such vectors is the dimension of the space. This is a familiar concept in finite dimensions. In an infinite-dimensional space, we obviously need an infinite number of basis vectors, but is the basis countably or uncountably infinite? That is, can we label the basis vectors with a discrete index, or do we need continuous indices as well?

As it turns out, it is one the mathematical properties of Hilbert spaces that they always possess a countable basis, that is, a set of linearly independent, normalizable vectors that span the space and can be indexed $n = 1, 2, 3, \dots$, or by some other such discrete indexing scheme. This does not mean that every basis we encounter will be labeled by a discrete index, only that such bases always exist.

In fact, in practice in quantum mechanics we frequently encounter "bases" with continuous indices as well. However, as we have stated above, the basis vectors of the continuum are not normalizable to unity and do not belong to Hilbert space. The eigenfunctions that result in this case are nevertheless orthonormal and complete in a certain sense - for instance, we can δ -function normalize them. We obtain an orthonormal basis, but it consists of vectors that lie outside Hilbert space. Formally, they exist in something called a "rigged Hilbert space". The strict mathematical derivation which justifies that we can use continuous eigenvectors as

a basis for a Hilbert space in quantum mechanics is beyond the scope of this text, but the interested reader can check out a link on the course webpage.

This means that we can expand state vectors in position eigenvectors after all. In practice, just think of the continuous eigenstates as a limiting case of a set of discrete eigenstates (for instance position eigenvalue discretized on a lattice with a distance $a \rightarrow 0$). As they obey certain orthonormality and completeness conditions they are referred to as "continuous bases".

For example, the one dimensional harmonic oscillator has a countable basis of energy eigenstates but an uncountable basis of position eigenstates (whose wave functions are delta functions). The continuous "bases" do not belong to the respective Hilbert space themselves. However, they are useful mathematical tools to expand any states actually belonging to the Hilbert space.

- **Which basis we should use to expand a state-vector in a Hilbert space depends on the dimension of the Hilbert space.**

For a finite dimension, it is clear that the basis is countable, the basis vectors are normalizable to unity and everything is fine. For an infinite dimension, we can choose between a countable and uncountable basis (*e.g.* harmonic oscillator eigenstates or position eigenstates). In effect, we could in principle expand $|\Psi\rangle$ for the harmonic oscillator in position eigenstates, because these also constitute an infinitely-dimensional basis. We could, however, not expand $|\Psi\rangle$ in spinor eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$, because these only span a 2D Hilbert space.

When we're given a Hamiltonian, we can't necessarily immediately know what the dimension of the Hilbert space is. If it is infinite, however, it shouldn't matter in principle if we expand in a countable or uncountable basis. If it is finite, the basis is always countable. For instance, for a free particle we know that the eigenstates of the Hamiltonian constitute an uncountable basis in an infinite-dimensional Hilbert space (but can still be used, as mentioned above).

Thus, if we have an infinitely dimensional Hilbert space, it is possible to choose a discrete basis of normalizable vectors that span this space - however, it may be convenient in practice to choose other types of bases, such as a continuous basis, consisting of unnormalizable vectors outside Hilbert space, or a mixed basis, or other possibilities. For a finite-dimensional Hilbert space, for instance describing a spin in a magnetic field with the Hamilton-operator

$$\hat{H} = -\mu_B \mathbf{B} \cdot \hat{\mathbf{S}}, \quad (34.2)$$

requires a 2D basis such as spin- $\uparrow$ and spin- $\downarrow$ spinors.

Chapter 35

Some useful mathematical tools

35.1 Fourier transformation and Fourier series

A periodic function can be written as a Fourier series, where the function is represented as a superposition of sine and cosine waves having different wavenumbers and with belonging coefficients for each wavenumber. Let the periodicity of the function be L . A Fourier transformation is the generalization of a Fourier series into complex values in the limit $L \rightarrow \infty$. Thus, *any function*, not necessarily periodic, can be Fourier transformed.

Chapter 36

Experimental techniques

In this chapter, we give a qualitative discussion on the principles behind some of the most important experimental techniques used in modern condensed matter physics.

36.0.1 Scanning tunneling microscopy (STM)

36.0.2 Scanning electron microscopy (SEM)

36.0.3 Transmission electron microscopy (TEM)

36.0.4 Atomic force microscopy (AFM)

36.0.5 Angle-resolved photoemission spectroscopy (ARPES)

The following text from <https://arxiv.org/pdf/1303.1438.pdf>.

Angle-resolved photoemission spectroscopy (ARPES) is one of the most direct methods of studying the electronic structure of solids. By measuring the kinetic energy and angular distribution of the electrons photoemitted from a sample illuminated with sufficiently high-energy radiation, one can gain information on both the energy and momentum of the electrons propagating inside a material. This is of vital importance in elucidating the connection between electronic, magnetic, and chemical structure of solids, in particular for those complex systems which cannot be appropriately described within the independent-particle picture. Among the various classes of complex systems, of great interest are the transition metal oxides, which have been at the center stage in condensed matter physics for the last four decades.

Photoelectron spectroscopy is a general term that refers to all those techniques based on the application of the photoelectric effect originally observed by Hertz and later explained as a manifestation of the quantum nature of light by Einstein, who recognized that when light is incident on a sample an electron can absorb a photon and escape from the material with a maximum kinetic energy $E_{\text{kin}} = h\nu - \phi$ (where ν is the photon frequency and ϕ , the material work function, is a measure of the potential barrier at the surface that prevents the valence electrons from escaping, and is typically 4- 5 eV in metals).

Due to the complexity of the photoemission process in solids the quantitative analysis of the experimental data is often performed under the assumption of the independent-particle picture and of the sudden approximation (i.e., disregarding the many-body interactions as well as the relaxation of the system during the photoemission itself). The problem is further simplified within the so-called three-step model in Fig. 36.1, in which the photoemission event is decomposed in three independent steps: optical excitation between the initial and final bulk Bloch eigenstates, travel of the excited electron to the surface, and escape of the photoelectron into vacuum after transmission through the

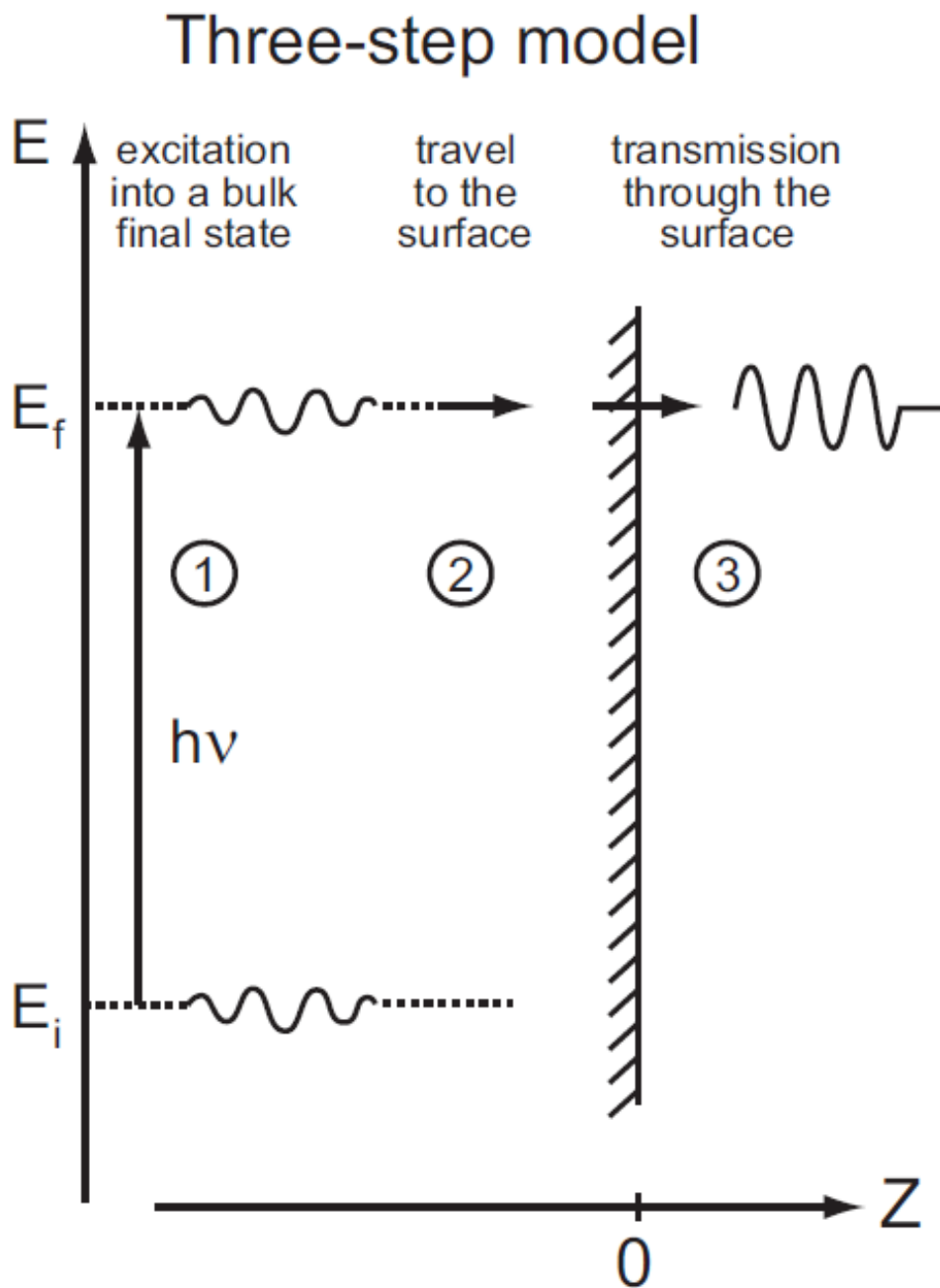


Figure 36.1: (Color online) ...

surface potential barrier. This is the most common approach, in particular when photoemission spectroscopy is used as a tool to map the electronic band structure of solids.

The energetics and kinematics of the photoemission process are shown in Fig. 36.3. Recall that the energy difference between Fermi energy and vacuum level corresponds to the work function (ϕ). The work function corresponds to the minimum amount of energy needed to remove an electron from the metal. In metals, work function and ionization energy are the same.

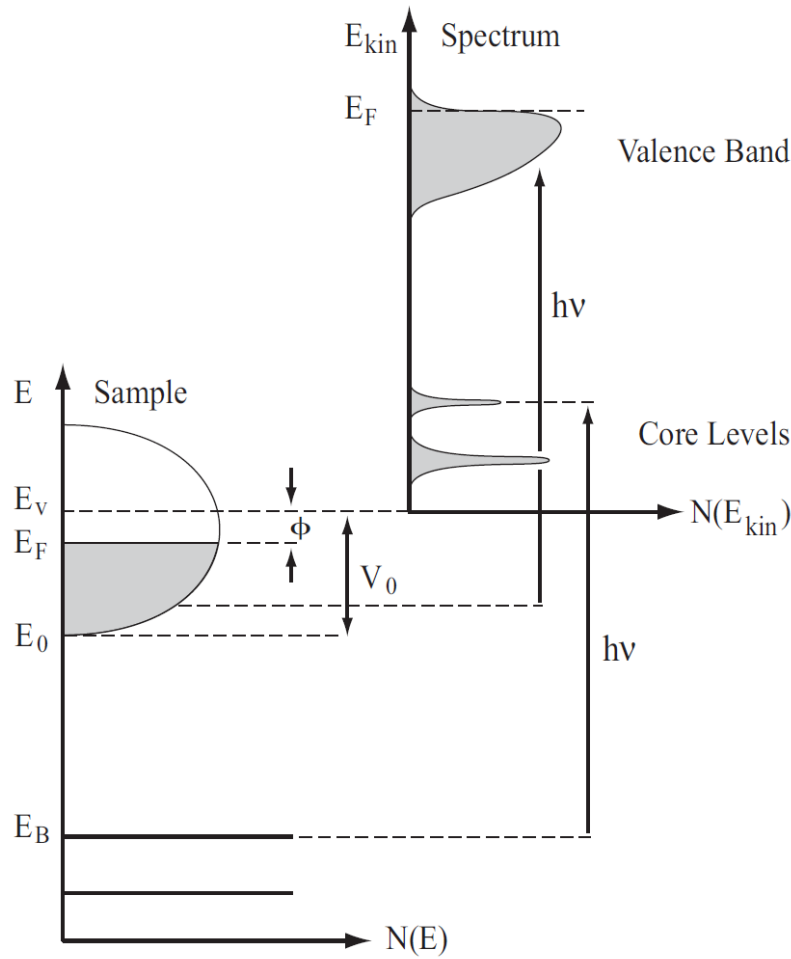


Figure 36.2: (Color online) Energetics of the photoemission process (from Ref. [22]). The electron energy distribution produced by the incoming photons, and measured as a function of the kinetic energy E_{kin} of the photoelectrons (right), is more conveniently expressed in terms of the binding energy E_B (left) when one refers to the density of states in the solid ($E_B = 0$ at E_F).

The geometry of an ARPES experiment is sketched in can be understood as follows. A beam of monochromatized radiation supplied either by a gasdischarge lamp, a UV laser, or a synchrotron beamline is incident on a sample (which has to be a properly aligned single crystal in order to perform angle- or, equivalently, momentum-resolved measurements). As a result, electrons are emitted by photoelectric effect and escape into the vacuum in all directions. By collecting the photoelectrons with an electron energy analyzer characterized by a finite acceptance angle, one measures their kinetic energy E_{kin} for a given emission direction. This way, the wave vector or momentum $\mathbf{K} = \mathbf{p}/\hbar$ of the photoelectrons in vacuum is also completely determined: its modulus is given by $K = \sqrt{2mE_{kin}}/\hbar$. The goal is then to deduce the electronic dispersion relation $E(\mathbf{k})$ in solid left behind, i.e. the relation between energy and momentum $\mathbf{k}$ for the electrons propagating *inside* the solid, starting from the measured E_{kin} and $\mathbf{K}$ *in vacuum*. To do so, one has to exploit the total energy and momentum conservation laws for the electron and photon. In a non-interacting

electron picture, it is particularly straightforward to take advantage of the energy conservation law:

$$E_{\text{kin}} = h\nu - \phi - |E_B| \quad (36.1)$$

where E_B is the binding energy of the electron ($E_B = 0$ at the Fermi level). Note that while $|\mathbf{k}_{\parallel}| = |\mathbf{K}_{\parallel}|$ for the component parallel to the surface, whereas $\mathbf{k}_{\perp}$ is not conserved.

Three-step model and sudden approximation

To develop a formal description of the photoemission process, one has to calculate the transition probability w_{fi} for an optical excitation between the N -electron ground-state Ψ_i^N and one of the possible final states Ψ_f^N . This can be done by using Fermi's golden rule:

$$w_{fi} = \frac{2\pi}{\hbar} |\langle \Psi_f^N | H_{\text{int}} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu) \quad (36.2)$$

where $E_i^N = E_i^{N-1} - E_B^{\mathbf{k}}$ and $E_f^N = E_f^{N-1} + E_{\text{kin}}$ are the initial and the final-state energies of the N -particle system. Here, $E_B^{\mathbf{k}}$ is the binding energy of the photoelectron with kinetic energy E_{kin} and momentum $\mathbf{k}$. The interaction with the photon is treated as a perturbation given by

$$H_{\text{int}} = \frac{e}{2mc} (\mathbf{A} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{A}) \quad (36.3)$$

in a gauge where the electrostatic potential is zero and we dropped quadratic terms in $\mathbf{A}$ which is permissible in the linear optical regime. The matrix element can then be computed using the unperturbed states.

As mentioned above, it is useful to use a phenomenological three-step model which has proven rather successful. Within this approach, the photoemission process is subdivided into three independent and sequential steps:

- Optical excitation of the electron in the bulk
- Travel of the excited electron to the surface
- Escape of the photoelectron into vacuum

The total photoemission intensity is then given by the product of three independent terms: the total probability for the optical transition, the scattering probability for the travelling electrons, and the transmission probability through the surface potential barrier. Step (i) contains all the information about the intrinsic electronic structure of the material and will be discussed in detail below. Step (ii) can be described in terms of an effective mean free path, proportional to the probability that the excited electron will reach the surface without scattering (i.e., with no change in energy and momentum). The inelastic scattering processes, which determine the surface sensitivity of photoemission, give rise to a continuous background in the spectra which is usually ignored or subtracted. Step (iii) is described by a transmission probability through the surface, which depends on the energy of the excited electron and the material work function ϕ .

To evaluate step (i) and the photoemission intensity in terms of the transition probability w_{fi} , it is convenient to factorize the wavefunctions above into photoelectron and $(N-1)$ -electron terms. The final state ψ_f^N becomes

$$\psi_f^N = \mathcal{A} \phi_f^{\mathbf{k}} \psi_f^{N-1} \quad (36.4)$$

where $\mathcal{A}$ is an antisymmetric operator that properly antisymmetrizes the N -electron wavefunction so that the Pauli principle is satisfied, while $\phi_f^{\mathbf{k}}$ is the wavefunction of the $(N-1)$ -electron system left behind. The latter is an excited state with eigenfunction ψ_m^{N-1} and energy E_m^{N-1} . The total transition probability is then given by the sum over all possible excited states m . This derivation, which originated from writing the transition probability using Fermi's golden rule implicitly assumes the validity of the so-called sudden approximation, which is extensively used in many-body calculations of the photoemission spectra from interacting electron systems, and is in principle applicable only to high kinetic-energy electrons. In this limit, the photoemission process is assumed to be sudden, with no post-collisional interaction between the photoelectron and the system left behind (in other words, an electron is instantaneously removed and the effective potential of the system changes discontinuously at that instant)⁴. Note, however, that the sudden approximation is inappropriate for low kinetic energy photoelectrons, which may need longer than the system response time to escape into vacuum. In this case, the so-called adiabatic limit, one can no longer use the instantaneous transition amplitudes $w_{f,i}$ and the detailed screening of photoelectron and photohole has to be taken into account [66]. For the initial state, let us first assume for simplicity that ψ_i^{N-1} is a single Slater determinant, so that we can write it as a product of one-electron orbit $\phi_i^{\mathbf{k}}$ and an $(N-1)$ particle term

$$\Psi_i^N = \mathcal{A}\phi_i^{\mathbf{k}}\Psi_i^{N-1}. \quad (36.5)$$

More generally, however, Ψ_i^{N-1} should be expressed as $\Psi_i^{N-1} = c_{\mathbf{k}}\Psi_i^N$ where $c_{\mathbf{k}}$ is an annihilation operator for an electron with momentum $\mathbf{k}$. The different matrix elements in Eq. (36.2) can now be written

$$\langle \Psi_f^N | H_{\text{int}} | \Psi_i^N \rangle = \langle \phi_f^{\mathbf{k}} | H_{\text{int}} | \phi_i^{\mathbf{k}} \rangle \langle \Psi_m^{N-1} | \Psi_i^{N-1} \rangle. \quad (36.6)$$

Here, we replaced Ψ_f^{N-1} with an eigenstate Ψ_m^{N-1} as discussed above. The total photoemission intensity measured as a function of E_{kin} at a momentum $\mathbf{k}$, namely

$$I(\mathbf{k}, E_{\text{kin}}) = \sum_{f,i} w_{f,i} \quad (36.7)$$

is then proportional to

$$\sum_{f,i} |M_{f,i}^{\mathbf{k}}|^2 \sum_m |c_{m,i}|^2 \delta(E_{\text{kin}} + E_m^{N-1} - E_i^N - h\nu) \quad (36.8)$$

where $|c_{m,i}|^2 = |\langle \Psi_m^{N-1} | \Psi_i^{N-1} \rangle|^2$ is the probability that the removal of an electron from state i will leave the $(N-1)$ particle system in the excited state m .

From here, we see that if $\Psi_i^{N-1} = \Psi_{m_0}^{N-1}$ for one particular $m = m_0$, the corresponding $|c_{m_0,i}|^2$ will be unity and all the others $c_{m,i}$ zero. In this case, if also $M_{f,i}^{\mathbf{k}} \neq 0$, the ARPES spectra will be given by a delta-function, as shown in Fig. ??(b) in the non-interacting particle picture.

In strongly correlated systems, however, many of the $|c_{m,i}|^2$ terms will be non-zero because the removal of the photoelectron results in a strong change of the system effective potential. In turn, ψ_i^{N-1} will have an overlap with many of the eigenstates Ψ_m^{N-1} . Therefore, the ARPES spectra will not consist of single δ -functions, but will show a main line and several satellites according to the number of excited states m created in the process [Fig. ??(c)].

Treatment via spectral function

In the discussion of photoemission on solids, and in particular on the correlated electron systems in which many $|c_{m,i}|^2$ in the above equations are different from zero, the most powerful and commonly used approach is based on the Green's function formalism. In this context, the propagation of a single electron in a many-body system is described by the time-ordered one-electron Green's function $G(\mathbf{k}, t - t')$ which is related to the probability amplitude that an electron added to the system in a Bloch state with momentum $\mathbf{k}$ at a time zero will still be in the same state after a time $t - t'$. After a Fourier-transformation, we obtain

$$G(\mathbf{k}, \omega) = G^+(\mathbf{k}, \omega) + G^-(\mathbf{k}, \omega) \quad (36.9)$$

where $G^\pm$ are the one-electron addition and removal Green's function. At $T = 0$, one finds

$$G^\pm(\mathbf{k}, \omega) = \sum_m \frac{|\langle \Psi_m^{N\pm 1} | c_{\mathbf{k}}^\pm | \Psi_i^N \rangle|^2}{\omega - E_m^{N\pm 1} + E_i^N \pm i\eta} \quad (36.10)$$

where the operator $c_{\mathbf{k}}^+ = c_{\mathbf{k}\sigma}^\dagger$ ($c_{\mathbf{k}}^- = c_{\mathbf{k}\sigma}$) creates (annihilates) an electron with energy ω , momentum $\mathbf{k}$, and spin σ in the N -particle initial state Ψ_i^N . The summation over m runs over all possible $(N \pm 1)$ particle eigenstates $\Psi_m^{N\pm 1}$ with eigenvalues $E_m^{N\pm 1}$ and η is a positive infinitesimal (inverse lifetime).

In the limit $\eta \rightarrow 0^+$, we can use that

$$\text{Im} \frac{1}{x + i\eta} = -\frac{\eta}{x^2 + \eta^2} = -\pi \delta(x) \quad (36.11)$$

so that the one-particle spectral function

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G(\mathbf{k}, \omega) \quad (36.12)$$

reads $A = A^+ + A^-$ where

$$A^\pm(\mathbf{k}, \omega) = \sum_m |\langle \Psi_m^{N\pm 1} | c_{\mathbf{k}}^\pm | \Psi_i^N \rangle|^2 \delta(\omega - E_m^{N\pm 1} + E_i^N). \quad (36.13)$$

Above, $G = G^R$ is actually the retarded Green function.

The spectral function satisfies an important sum rule and has a physical interpretation. In general, one can write the retarded Green function in the Lehmann representation:

$$G^R(\mathbf{k}, \omega) = \frac{1}{Z} \sum_{nm} \frac{|\langle m | c_{\mathbf{k}}^\dagger | n \rangle|^2}{\omega + E_n - E_m + i\eta} (e^{-\beta E_m} + e^{-\beta E_n}). \quad (36.14)$$

From this, we can prove that the spectral function $A(\mathbf{k}, \omega)$ satisfies

$$\int_{-\infty}^{\infty} d\omega A(\mathbf{k}, \omega) = 1. \quad (36.15)$$

The proof goes like this:

$$\begin{aligned}
\int_{-\infty}^{\infty} A(\mathbf{k}, \omega) d\omega &= \frac{1}{Z} \sum_{mn} |\langle m | c_{\mathbf{k}}^{\dagger} | n \rangle|^2 (e^{-\beta E_n} + e^{-\beta E_m}) \int_{-\infty}^{\infty} d\omega \delta(\omega + E_n - E_m) \\
&= \frac{1}{Z} \sum_{mn} |\langle m | c_{\mathbf{k}}^{\dagger} | n \rangle|^2 (e^{-\beta E_n} + e^{-\beta E_m}) \\
&= \frac{1}{Z} \sum_{mn} \langle m | c_{\mathbf{k}}^{\dagger} | n \rangle \langle c_{\mathbf{k}} | m \rangle (e^{-\beta E_n} + e^{-\beta E_m}) \\
&= \frac{1}{Z} \sum_{mn} \left[e^{-\beta E_n} \langle n | c_{\mathbf{k}} | m \rangle \langle m | c_{\mathbf{k}}^{\dagger} | n \rangle + e^{-\beta E_m} \langle m | c_{\mathbf{k}}^{\dagger} | n \rangle \langle n | c_{\mathbf{k}} | m \rangle \right] \\
&= \frac{1}{Z} \left[\sum_n e^{-\beta E_n} \langle n | c_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} | n \rangle + \sum_m e^{-\beta E_m} \langle m | c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} | m \rangle \right] \\
&= \frac{1}{Z} \sum_n e^{-\beta E_n} = 1.
\end{aligned} \tag{36.16}$$

This sum rule is an exact result for the energy integral of the spectral functions. In actual calculations for real systems, however, one is usually only able to get approximate results for such quantities, which may not satisfy the sum rule exactly. In such cases, the extent to which the sum rule is approximately satisfied can be a measure of the quality of the approximations made.

The sum rule and Eq. (36.13) [which shows that $A(\mathbf{k}, \omega) \geq 0$] suggests that A can be interpreted as a probability density: $A(\mathbf{k}, \omega) d\omega$ is the probability density that a fermion with momentum $\mathbf{k}$ has an energy in an infinitesimal energy window $d\omega$ around ω .

For non-interacting fermions, one can insert the known form of G^R to obtain

$$A(\mathbf{k}, \omega) = \delta(\omega - \xi_{\mathbf{k}}). \tag{36.17}$$

The energy of the particle is thus known with certainty if the momentum is given. In the more general case of interacting fermions, a large class of systems with such fermions are Fermi liquids in which case the spectral function can be written

$$A(\mathbf{k}, \omega) \simeq \frac{Z_{\mathbf{k}}}{\pi} \frac{(1/2\tau_{\mathbf{k}})}{(\omega - \xi_{\mathbf{k}}^*)^2 + (1/2\tau_{\mathbf{k}})^2} + A_{\text{incoherent}}(\mathbf{k}, \omega) \tag{36.18}$$

Here, $\tau_{\mathbf{k}}$ is the lifetime for the excitation $(\mathbf{k}, \omega)$, $\xi_{\mathbf{k}}^*$ is the renormalized energy, and $Z_{\mathbf{k}}$ is the residue which is a positive number between 0 and 1. Compared to the non-interacting δ -function case, there is still a peak in the spectral function represented by the first term above. However, the peak is now a Lorentzian instead of a delta function. Also, the width of the peak has broadened, the area under the peak has decreased (from 1 to $Z_{\mathbf{k}}$), and the single-particle energies are renormalized. There is also an additional term $A_{\text{incoherent}}$ representing a continuum (not a peak) which must be there if $Z_{\mathbf{k}} \neq 1$ in order for the sum rule for $A(\mathbf{k}, \omega)$ to be satisfied. The entities having energy $\xi_{\mathbf{k}}^*$ and lifetime $\tau_{\mathbf{k}}$ are quasiparticles which can be thought of as dressed electrons.

Finite temperature effects can be taken into account by extending the Green function formalism either to Matsubara or Keldysh framework. If $T \neq 0$, the intensity measured in an ARPES experiment can generally be written [as seen from Eqs. (36.7) and (36.8)]

$$I(\mathbf{k}, \omega) = I_0(\mathbf{k}, \nu, \mathbf{A}) f(\omega) A(\mathbf{k}, \omega) \tag{36.19}$$

where $\mathbf{k} = \mathbf{k}_{\parallel}$ is the in-plane electron momentum, ω is the electron energy with respect to the Fermi level, and $I_0(\mathbf{k}, \nu, \mathbf{A})$ is proportional to the squared one-electron matrix element $|M_{f,i}^{\mathbf{k}}|^2$ which depends on the electron momentum as well as the energy and polarization of the incoming photon. We also introduced the Fermi function $f(\omega) = (e^{\omega/k_B T} + 1)^{-1}$, which accounts for the fact that direct photoemission probes only the occupied electronic states. Note that we neglected the presence of any extrinsic background and the broadening due to the energy and momentum resolution, which however have to be carefully considered when performing a quantitative analysis of the ARPES spectra.

The corrections to the Green function due to interactions and e-e correlations can be conveniently expressed in terms of the self-energy (proper and 1PI-irreducible)

$$\Sigma(\mathbf{k}, \omega) = \Sigma'(\mathbf{k}, \omega) + i\Sigma''(\mathbf{k}, \omega). \quad (36.20)$$

The real and imaginary parts contain all the information on the energy renormalization and lifetime, respectively, of an electron with band energy $\epsilon_{\mathbf{k}}$ and momentum $\mathbf{k}$ propagating in a manybody system. The retarded Green's and spectral functions expressed in terms of the self energy are then given by:

$$\begin{aligned} G^R(\mathbf{k}, \omega) &= \frac{1}{\omega - \xi_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)}, \\ A(\mathbf{k}, \omega) &= -\frac{1}{\pi} \frac{\Sigma''(\mathbf{k})}{[\omega - \xi_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + [\Sigma''(\mathbf{k}, \omega)]^2}. \end{aligned} \quad (36.21)$$

Since $G^R(t, t')$ is response function to an external perturbation, the real and imaginary parts of its Fourier transform $G^R(\mathbf{k}, \omega)$ have to satisfy causality and thus Kramers-Kronig relations. This implies that if the full $A(\mathbf{k}, \omega) \propto \text{Im}G^R$ is available from photoemission, one can calculate $\text{Re}G^R$ and then obtain both the real and imaginary parts of the self-energy from the above equations.

Generally speaking, the exact calculation of $\Sigma(\mathbf{k}, \omega)$ and $A(\mathbf{k}, \omega)$ is a very challenging task. We illustrate this using the interacting Fermi liquid case. Start from the trivial non-interacting case with $\Sigma(\mathbf{k}, \omega) = 0$. The N -particle eigenfunction Ψ^N is a single Slater determinant and we have $G(\mathbf{k}, \omega) = 1/(\omega - \xi_{\mathbf{k}} + i\eta)$ with only one pole for each $\mathbf{k}$. Moreover, $A(\mathbf{k}, \omega) = \delta(\omega - \xi_{\mathbf{k}})$ consists of a single line at the band energy $\xi_{\mathbf{k}}$. In this case, the occupation numbers $n_{\mathbf{k}\sigma} = c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$ are good quantum numbers and for a metallic system the momentum distribution $n(\mathbf{k}) = \langle n_{\mathbf{k}\sigma} \rangle$ is characterized by a sudden drop from 1 to 0 at $\mathbf{k} = \mathbf{k}_F$. This defines a sharp Fermi surface.

If we now switch on electron-electron correlations adiabatically, so that the system remains at equilibrium at all times, any particle added into a Bloch state has a certain probability of being scattered out of it by a collision with another electron, leaving the system in an excited state where electron-hole pairs have been created. The momentum distribution will therefore show a discontinuity smaller than 1 at $\mathbf{k}_F$ and a finite occupation probability for $\mathbf{k} > \mathbf{k}_F$ even at $T = 0$. As long as $n(\mathbf{k})$ shows a finite discontinuity $Z_{\mathbf{k}} > 0$ at $\mathbf{k} = \mathbf{k}_F$, we can describe the correlated Fermi sea in terms of well defined quasiparticles. There are electrons dressed with a manifold of excited states, characterized by a pole structure similar to the one of the non-interacting system but with a renormalized energy $\xi_{\mathbf{k}}^*$, mass m^* , and a finite lifetime $\tau_{\mathbf{k}} = 1/\Gamma_{\mathbf{k}}$. Since Fermi liquids are metals, $\xi_{\mathbf{k}}^*$ has to be gapless and thus vanish at some $\mathbf{k}$. The $\mathbf{k}$ -values where $\xi_{\mathbf{k}}^*$ vanishes are thus used to define the Fermi surface of the system.

We note in passing that the quantity $Z(\omega, \mathbf{k})$ in Eliashberg theory is related to the residue $Z_{\mathbf{k}}$ above, but not identical. The quantity $Z(\omega, \mathbf{k})$ in the normal-state of Eliashberg theory enters the Green function as

$$G^R(\mathbf{k}, \omega) = \frac{1/Z(\omega, \mathbf{k})}{E + \beta\delta - \xi_{\mathbf{k}}/Z(\omega, \mathbf{k})}. \quad (36.22)$$

Thus, $1/Z(\omega, \mathbf{k})$ renormalizes the quantum field in the Green function (i.e. the second-quantized field operators that enter the expectation value that is G^R), but also the dispersion relation $\epsilon_{\mathbf{k}}$ and thus the DOS.

In other words, the properties of a Fermi liquid are similar to those of a free electron gas with damped quasiparticles that have a finite lifetime. The bare-electron character of the quasiparticle (the electron propagator which takes into account self-energy effects) is $Z_{\mathbf{k}} < 1$ and the total spectral weight must be conserved. Starting from Eq. (36.21) and following https://www.lptmc.jussieu.fr/files/chap_fl.pdf, one derives that the Green function and spectral weight consist of a coherent part with a pole (sharp peak) and an incoherent smooth part without poles:

$$\begin{aligned} G(\mathbf{k}, \omega) &= \frac{Z_{\mathbf{k}}}{\omega - \xi_{\mathbf{k}}^* + i\Gamma_{\mathbf{k}}} + G_{\text{incoh}}, \\ A(\mathbf{k}, \omega) &= Z_{\mathbf{k}} \frac{\Gamma_{\mathbf{k}}/\pi}{(\omega - \xi_{\mathbf{k}}^*)^2 + \Gamma_{\mathbf{k}}^2} + A_{\text{incoh}}. \end{aligned} \quad (36.23)$$

Here, we defined

$$\begin{aligned} Z_{\mathbf{k}} &= \left(1 - \frac{\partial \Sigma'}{\partial \omega}\right)^{-1}, \\ \xi_{\mathbf{k}}^* &= Z_{\mathbf{k}}(\xi_{\mathbf{k}} + \Sigma'), \\ \Gamma_{\mathbf{k}} &= Z_{\mathbf{k}}|\Sigma''|. \end{aligned} \quad (36.24)$$

The self-energy and its derivatives are understood to be evaluated at $\omega = \epsilon_{\mathbf{k}}^*$. It should be emphasized that the Fermi liquid description is valid only in proximity to the Fermi surface and rests on the condition

$$\xi_{\mathbf{k}}^* \gg |\Sigma''| \quad (36.25)$$

close to the Fermi level, i.e. $\omega \simeq \mu$ and $\mathbf{k} \simeq \mathbf{k}_F$. Furthermore, one has

$$\Gamma_{\mathbf{k}} \propto [(\pi k_B T)^2 + \xi_{ve} c k^2] \quad (36.26)$$

for a Fermi liquid system in two or more dimensions (with additional logarithmic corrections in the 2D case).

The coherent and incoherent part of $A(\mathbf{k}, \omega)$ represent the main line and satellite structure shown in Fig. 36.3(c). Note that the peak position is also shifted with respect to the bare band energy $\xi_{\mathbf{k}}$ due to Σ' .

Among the general properties of the spectral function, there are several sum rules. A fundamental one which is exact is that

$$\int d\omega A(\omega, \mathbf{k}) = 1. \quad (36.27)$$

In terms of the coherent and incoherent part, one finds

$$\begin{aligned}\int d\omega A_{\text{coh}} &= Z_{\mathbf{k}}, \\ \int d\omega A_{\text{incoh}} &= 1 - Z_{\mathbf{k}}.\end{aligned}\tag{36.28}$$

A useful sum rule in ARPES is

$$\int_{-\infty}^{\infty} d\omega f(\omega) A(\mathbf{k}, \omega) = n(\mathbf{k})\tag{36.29}$$

which relates one-electron removal part of the spectral weight (A^-) to the momentum distribution $n(\mathbf{k})$, since the weight-factor $f(\omega)$ ensures that only A^- gives a contribution.

36.0.6 Neutron-scattering

36.0.7 Brillouin light scattering

36.0.8 Synchrotrons

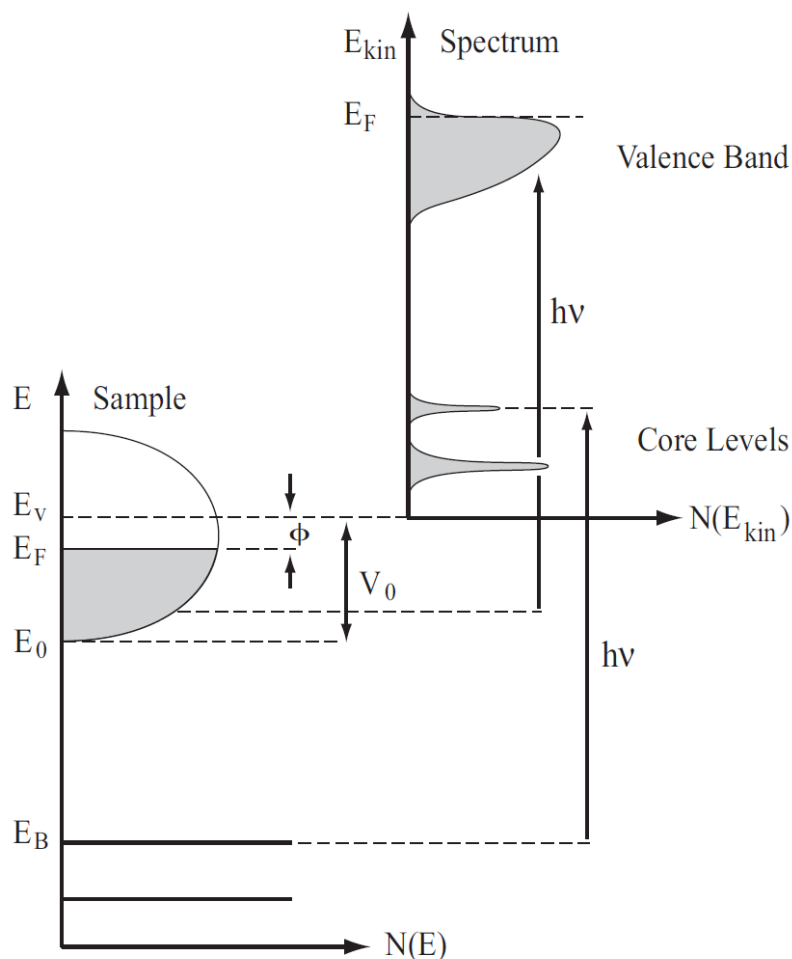


Figure 36.3: (Color online) (a) Geometry of an ARPES experiment; the emission direction of the photoelectron is specified by the polar and azimuthal angles. Momentum resolved one-electron removal and addition spectra for: (b) a non-interacting electron system (with a single energy band dispersing across the Fermi level); (c) an interacting Fermi liquid system. The corresponding ground-state ($T = 0$ K) momentum distribution function $n(k)$ is also shown. (c) Bottom right: photoelectron spectrum of gaseous hydrogen (black) and the ARPES spectrum of solid hydrogen developed from the gaseous one (red).

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