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Suggested solution for spring 2025 exam TFY4245: Solid State Physics, Advanced Course

NOTE: The solutions below are meant as guidelines for how the problems may be solved and do not necessarily contain all the detailed steps of the calculations.

PROBLEM 1

(a) Graphene has a hexagonal lattice structure with a two-atom basis. Recall that the crystal is made up out of all atomic sites, and that this is equal to a lattice + basis. The Wigner-Seitz cell is constructed from the lattice, i.e. by considering one type of atom alone in graphene. By drawing lines from any given A sublattice point to all neighboring A sublattice points, intersecting the midpoint of each line, and then shading the enclosed area, one obtains exactly the same unit cell as shown in the figure, only shifted a distance $d/2$ to the left. The figure thus already shows the Wigner-Seitz cell as the gray area: the position of the cell does not matter, only its shape and size.

(b) The formulas for constructing reciprocal lattice vectors are shown in the formula sheet of the exam. Since we consider a 2D system, we set the third lattice vector a_3 to $\hat{\mathbf{z}}$ to consider a stacked system in the z-direction. Then, the first BZ in the xy-plane is given solely by the first and second reciprocal lattice vectors b_1 and b_2. Using the equation in the formula sheet gives:

$$b_1 = \frac{2\pi}{d}(\frac{1}{\sqrt{3}}, 1),\ b_2 = \frac{2\pi}{d}(-\frac{1}{\sqrt{3}}, 1). \tag{1}$$

It is straightforward to check that these satisfy $a_i \cdot b_j = 2\pi\delta_{ij}$. The reciprocal lattice now consists of lattice points located at any linear combinations of b_1 and b_2.

(c) ARPES is based on the photoelectric effect. An incoming photon of sufficient energy ejects an electron from the surface of a material. By directly measuring the kinetic energy and emission angle distributions of the emitted photoelectrons, one determines the relation between energy and (in-plane) momentum of the state in the material that the electron was ejected out of. By measuring the freed electron's kinetic energy, its velocity and momentum magnitude can be calculated. By measuring the emission angle with respect to the surface normal, ARPES can also determine the two in-plane components of momentum that are preserved in the photoemission process. In this way, one maps the electronic band structure.

PROBLEM 2

(a)

- The ground-state at $T = 0$ will consist of every single valence band electron state being filled. Thus,

$$|GS\rangle = \prod_{k,s} c^{\dagger}_{V,k,s}|0\rangle \tag{2}$$

  where $c^{\dagger}_{V,k,s}$ creates a valence band electron state and $|0\rangle$ is the vacuum state with no filled electron states.

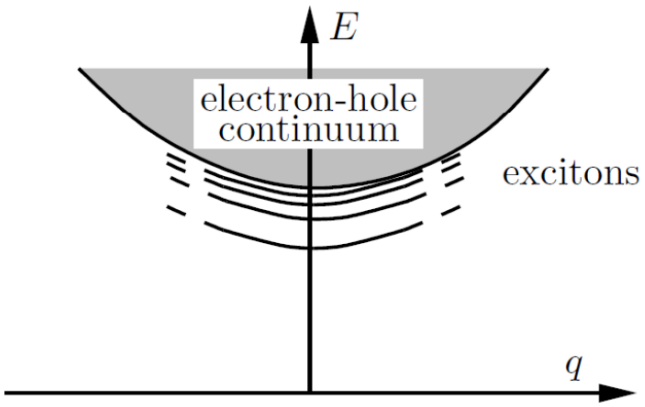
- The ground-state energy is

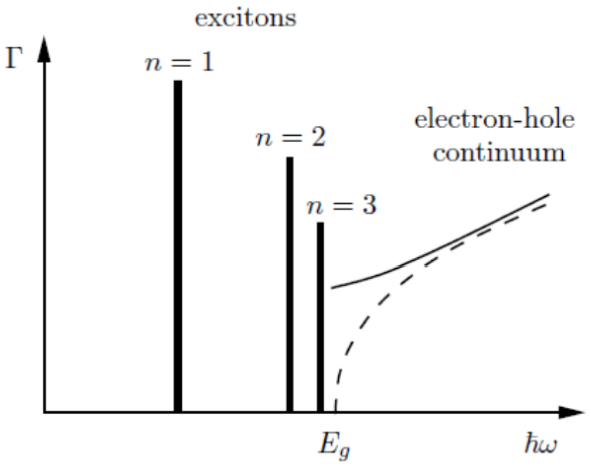
$$E_0 = 2\sum_k \varepsilon_{V,k} \tag{3}$$

  where the factor 2 is due to spin degeneracy.

(b)

- The electron excitation in the conduction band and a hole excitation in the valence band of a semiconductor can interact through the Coulomb interaction. This gives rise to a bound state called an exciton, which has slightly less energy than the lowest state in the conduction band. This is shown in the figure below.
- The absorption rate Γ including the exciton states for a direct-gap semiconductor is shown in the figure below. The exciton states, labelled by their principal quantum number n, appear as sharp lines, due to their discrete nature, below the e-h continuum starting at $\hbar\omega = E_g$ where E_g is the semiconductor gap.





(c)

- We cannot affect the past. This statement of causality means that any response function $\chi(\tau)$, where $\tau = t - t'$ is relative time, should satisfy

$$\chi(\tau) = 0 \text{ for all } \tau < 0. \tag{4}$$

  Thus, σ has to obey this criterion.

- Using that

$$f(\omega) = \int dt e^{i\omega t} f(t) \text{ and } f(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} f(\omega), \tag{5}$$

and taking the Fourier-transformation of

$$\langle \hat{J}(t) \rangle = \int_{-\infty}^{\infty} \sigma(t-t')E(t')dt' \tag{6}$$

gives

$$\begin{aligned} \langle \hat{J}(\omega) \rangle &= \int dt' \int dt e^{i\omega t} \sigma(t-t')E(t') \\ &= \int dt' \int dt e^{i\omega(t-t')} \sigma(t-t') e^{i\omega t'} E(t') \qquad (7) \\ &= \sigma(\omega)E(\omega). \qquad (8) \end{aligned}$$

We see that the linear response is local in frequency space: if you shake something a frequency ω, it responds at frequency ω. Anything beyond this lies within the domain of nonlinear response.

PROBLEM 3

(a) Since the problem text specifies that the Heisenberg model under consideration is ferromagnetic, we have $J = -|J|$. Inserting the linearized HP transformation gives

$$H = -|J|NS^2 z/2 - |J|S \sum_{i,\delta} [a^\dagger_{i+\delta} a_i + a^\dagger_i a_{i+\delta} - a^\dagger_i a_i - a^\dagger_{i+\delta} a_{i+\delta}] \tag{9}$$

(b) Inserting the expression for a_i given in the problem text, one obtains

$$H = E_0 + \sum_k \omega_k a^\dagger_k a_k, \tag{10}$$

where

$$E_0 = -|J|NS^2 z/2, \; \omega_k = 2|J|S \sum_\delta (1 - \cos k \cdot \delta). \tag{11}$$

By using periodic boundary conditions, we impose specific values that k can take. Such boundary conditions imply that for instance $a_i = a_{i+N_x \hat{x}}$ where N_x is the number of sites in the x-direction. This is satisfied if $e^{ik_x N_x} = 1$, so that $k_x = 2\pi n_x / N_x$ where n_x is an integer. It is customary to choose n_x to take N_x successive values

$$-\frac{N_x}{2}, -\frac{N_x}{2} + 1, \ldots \frac{N_x}{2} - 1. \tag{12}$$

For simplicity, we assumed here that N_x is even so that $N_x/2$ is in fact an integer, but one can choose such a series of values even if N_x is odd. Then, k_x takes values in the interval $[-\pi, \pi\rangle$. The same analysis holds for k_y.

(c) The first term E_0 is the classical ground-state energy of having all spins parallel with an energy gain of $|J|/2$ per pair. The second term describes excitations above the ground-state: magnons, which are quantized spin-waves that act to reduce the magnetization of the $T = 0$ ground-state.

(d) Inserting the linearized HP transformation to S^z_i, and using that,

$$\sum_i a^\dagger_i a_i = \sum_k a^\dagger_k a_k, \tag{13}$$

we get

$$\begin{aligned} M &= \frac{1}{N} \sum_i \langle S^z_i \rangle \\ &= S - \frac{1}{N} \sum_k \langle \hat{n}_k \rangle \qquad (14) \\ &= S - \frac{1}{N} \sum_k \frac{1}{e^{\beta\omega_k} - 1}. \qquad (15) \end{aligned}$$

where $\beta = 1/k_B T$.

PROBLEM 4

(a) Spontaneously breaking a U(1) symmetry means that the free energy (and Hamiltonian/Lagrangian) of the system is invariant under a U(1) transformation of the superconducting order parameter $\psi \to \psi e^{i\theta}$, whereas the ground-state itself is not invariant under a U(1) transformation.

(b) A linear term is present if the order parameter couples to an external field. This allows for a non-zero value of the order parameter even for temperatures above the critical temperature of the phase transition from the disordered to ordered phase, due to the presence of an external field. This happens for instance in a ferromagnet in the presence of an external magnetic field or a ferroelectric material in the presence of an external electric field.

(c) Noncentrosymmetric: the unit cell has an arrangement of atoms which lacks inversion symmetry. Polar: the unit cell lacks inversion symmetry and has a net electric dipole moment.

(d) Consider a stable crystal structure, call it A, which at zero temperature has the lowest accessible internal energy of all possible ways the atoms in the crystal can arrange themselves. Consider next a different crystal structure B, consisting of the same atoms as in A, but which has a softer frequency phonon spectrum than a crystal structure A (meaning the phonons are more easily excited).

As temperature is increased, the phonons in B will be more easily excited (higher thermal average occupancy) than the phonons in A. The entropy, or the disorder of the system, tends to be lower when it is in its ground state as opposed to having many excited phonon states. This is because when an a phonon is excited, there are more energy levels and configurations it can occupy compared to the ground-state. The entropy increases with the number of ways that the phonon states can be occupied for a given temperature.

Since entropy increases with the occupancy, the entropy of B will become higher than the entropy of A as T increases. Then it is possible for the stable structure to transform from A to B with increasing temperature. This is because the most stable structure at any given, constant temperature T and volume V is determined by the minimum of the Helmholtz free energy $F = U - TS$. Thus, a transition from structure A to B will take if a temperature T_c exists (below the melting point of the material) such that $F_A(T_c) = F_B(T_c)$ even if $F_A(T = 0) < F_B(T = 0)$.

(e) Due to the large speed of light compared to the speed of sound, the photon has a much steeper dispersion relation as a function of momentum k compared to a phonon. The dashed red line is the photon and the blue line is the optical phonon, which looks almost dispersionless (constant) compared to the photon. Near the crossing point of the photon and phonon, these modes hybridize and create a hybrid excitation called a phonon polariton. These are the purple lines and come in two branches: as one moves away from the crossing point, each branch becomes either photon- or phonon-like.

A gap in the polariton dispersion relation is seen to arise in the figure due to the avoided crossing of the original photon and phonon dispersions. As a consequence, light will reflect more efficiently for frequencies inside the gap, since there are no available modes present in the material. Therefore, polaritons may be observed experimentally by measuring the reflectance as a function of the frequency and angle of incidence (which alters the momentum direction) of the incident photons.