NTNU

Institutt for fysikk

TFY4245/FY8917 Solid State Physics, Advanced Course

Problemset 3

Problem 1

If we apply a static electric field to a metal with free electrons, we would expect a dc electric current to flow. Let us examine this expectation from a quantum mechanical point of view.

In a metal, electrons move in a periodic potential set up by the crystal lattice. According to Bloch's theorem, we know that the solution of the Schrodinger equation with a periodic potential $V(\boldsymbol{r})$ are so-called Bloch states $\psi_{\boldsymbol{k}}$. These Bloch states are plane-waves modulated by a periodic function $u_{\boldsymbol{k}}$ that has the same periodicity as the potential, and are characterized by a wavevector $\boldsymbol{k}$:

$$\psi_k(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r}). \tag{1}$$

These are now eigenstates of the Hamiltonian $H_0 = \hat{\boldsymbol{p}}^2/2m + V(\boldsymbol{r})$ with eigenvalue $\varepsilon_{\boldsymbol{k}}$:

$$H_0|\psi_{\boldsymbol{k}}\rangle = \varepsilon_{\boldsymbol{k}}|\psi_{\boldsymbol{k}}\rangle. \tag{2}$$

(a) Compute an expression for the mean velocity

$$\boldsymbol{v}(\boldsymbol{k}) = \frac{\hbar}{m}\langle\psi_{\boldsymbol{k}}|\hat{\boldsymbol{p}}|\psi_{\boldsymbol{k}}\rangle \tag{3}$$

by first showing that

$$\lim_{\Delta\boldsymbol{k}\to 0} \varepsilon_{\boldsymbol{k}+\Delta\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}} = \langle u_{\boldsymbol{k}}|\Delta H_{\boldsymbol{k}}|u_{\boldsymbol{k}}\rangle \tag{4}$$

where you have to identify $\Delta H_{\boldsymbol{k}}$. Then, use that

$$\frac{1}{m}\langle u_{\boldsymbol{k}}|\hat{\boldsymbol{p}} + \hbar\boldsymbol{k}|u_{\boldsymbol{k}}\rangle = \frac{1}{m}\langle\psi_{\boldsymbol{k}}|\hat{\boldsymbol{p}}|\psi_{\boldsymbol{k}}\rangle. \tag{5}$$

(b) In the above problem, you should find that the mean velocity (group velocity) is determined by the dispersion relation $\varepsilon_{\boldsymbol{k}}$:

$$v(\boldsymbol{k}) = \frac{1}{\hbar}\frac{d\varepsilon_{\boldsymbol{k}}}{d\boldsymbol{k}}. \tag{6}$$

Imagine now that we add an electric field $\boldsymbol{E}$ to the system. The Hamiltonian will take the form $H = H_0 + \phi(\boldsymbol{r})$ where $-\nabla\phi = q\boldsymbol{E}$ where q is the charge. We then give a semiclassical argument: since energy must be conserved, the particle must move in such a way that the energy introduced by the potential $\phi(\boldsymbol{r}(t))$ from instant t to $t+dt$ into the system must corresponds to the variation of $\varepsilon_{\boldsymbol{k}(t)}$ in the same interval. Denoting the variation of ϕ and $\varepsilon_{\boldsymbol{k}}$ in this interval $d\phi$ and $d\varepsilon_{\boldsymbol{k}}$, respectively, we are effectively stating that:

$$d\varepsilon_{\boldsymbol{k}} - d\phi = 0. \tag{7}$$

Use this equation, and the result $\boldsymbol{v} = \frac{1}{\hbar} d\varepsilon_{\boldsymbol{k}}/d\boldsymbol{k}$ derived above, to derive that

$$\hbar\dot{\boldsymbol{k}} = -q\boldsymbol{E}. \tag{8}$$

(c) What is semiclassical about the procedure in (b)?

(d) Consider now a specific dispersion relation corresponding for simplicity to electrons moving in a lattice consisting of a 1D chain of equidistant atoms with periodic boundary conditions. Thus, $\varepsilon_k = -2w\cos ka$ where $ka = [-\pi, \pi)$ and we used w for the hopping element to avoid confusion with time t. Solve the system of equations

$$\hbar dk/dt = -qE,\ v_k = \frac{1}{\hbar} d\varepsilon_k/dk \tag{9}$$

to find $v(t)$. Integrate the expression you find to identify an expression for the position $x(t)$.

(e) What can we conclude about the motion of electrons in a periodic potential in a static electric field? This phenomenon is known as Bloch oscillations.

Hang on - are now stating that if we apply an electric field to a metal there should be no net current, only oscillations? While Bloch oscillations have been experimentally observed, they are very difficult to measure. Usually, one instead observes precisely a steady-state electric current. The reason for this is twofold.

One is due to impurities causing scattering of the above Bloch states. When impurities (non-periodic potential) are accounted for, one no longer observes an oscillatory motion of the electrons but instead a steady-state current. This can be understood from the fact that the period of the Bloch oscillations is inversely proportional to the electric field. Thus, for a small electric field the oscillations have a very long period, and the electrons will encounter an impurity to scatter on (changing their trajectory) long before an oscillation has been completed. In this case, one obtains instead a net current flow. We will give an argument for this later in this course when we discuss the so-called Drude conductivity.

The second reason is that even in a ballistic system free of impurities that is connected to two reservoirs with a potential difference, Bloch oscillations are destroyed by the finite size of the ballistic system as follows. The quantum mechanical eigenstates of electrons in a periodic potential *including also* an external electric field E are so-called Wannier-Stark states. These are localized states, unlike Bloch-states, with a localization length $\propto 1/E$. This means that if the ballistic system is long enough that there exists well-localized Wannier-Stark states inside the system, without touching or spilling over the edges into the reservoirs where the voltage has been applied, we should expect Bloch oscillations. This then requires a long system and/or a strong electric field E to localize the states. Instead, for a small electric field (small applied voltage), the states begin to extend, leading to more and more of them to effectively deform and 'escape' the sample into the reservoirs. It is in this regime that we recover our expectation of a constant electric current in the system: there exists delocalized, propagating states inside the ballistic system which can carry current between the reservoirs.

Problem 2

Derive the expression given in the lectures for the temperature-dependent density of electrons in the conduction band by completing the following steps.

(a) First, use that the number of electrons per unit volume in the conduction band is

$$n = \int dn = \int_{E_C}^{\infty} N(E) f(E) dE \tag{10}$$

where $N(E)$ is the density of states for electrons and $f(E)$ is the occupancy probability for energy E, in effect the Fermi-Dirac distribution function. Above, E_C is the minimum energy of the conduction band. First, identify the expressions for $N(E)$ and $f(E)$.

(b) Assume that $k_B T$ is much smaller than the distance from the Fermi level E_F to the conduction band energy and show that this approximation gives

$$n = \frac{4\pi}{h^3}(2m_e^*)^{3/2} \int_{E_C}^{\infty} \frac{(E-E_C)^{1/2} dE}{\mathrm{e}^{(E-E_F)/k_B T}}. \tag{11}$$

(c) Evaluate the above integral by using that

$$\int_0^{\infty} x^{1/2} \mathrm{e}^{-x/k_B T} dx = \frac{(k_B T)^{3/2} \pi^{1/2}}{2} \tag{12}$$

and show that this gives the result for n given in the lectures.