Exercise sheet 6.5 – Solutions
(24.11.22)

1. Estimate the density of “electron gas” in metals assuming that each atom contributes $Z$ electrons (usually 1 to 3), and the density of metals is about $1 \text{ g/cm}^3$. Compare with the density of a classical gas at normal temperature and pressure.

**Solution**

Let’s take $\rho$ as the mass density of a metal, $m_a$ as the relative atomic mass (e.g. 12.011 for Carbon). The density of electrons is then

$$n = \frac{Z \rho}{1.66 \cdot 10^{-27} \text{ kg} \times m_a}.$$ 

For $\rho = 1 \text{ g/cm}^3$

$$n \approx 0.6 \cdot 10^{24} \frac{Z}{m_a} \text{ cm}^{-3} \approx 1 \cdot 10^{22} \text{ cm}^{-3}.$$ 

The particle density of atmospheric air at 273.15 K at sea level is $2.7 \cdot 10^{19} \text{ cm}^{-3}$.

2. Use the equation $m \frac{dv}{dt} + \frac{mv}{\tau} = -eE$ to show that the complex Drude conductivity $\sigma(\omega)$ is

$$\sigma(\omega) = \sigma(0) \left[ \frac{1 + i\omega\tau}{1 + (\omega\tau)^2} \right],$$

where $\sigma(0) = n e^2 \tau / m$.

$\sigma(\omega)$ is defined as $\vec{j}(\omega) = \sigma(\omega) \vec{E}(\omega)$, $\vec{j}(t) = \text{Re} \left( j(\omega)e^{-i\omega t} \right)$, $E(t) = \text{Re} \left( E(\omega)e^{-i\omega t} \right)$.

**Solution**

From the equation one gets, using $E(t) = E(\omega)e^{-i\omega t}$, $v(t) = v(\omega)e^{-i\omega t}$

$$-i\omega mv(\omega) + \frac{mv(\omega)}{\tau} = -eE(\omega) \quad \Rightarrow \quad v(\omega) = \frac{-e\tau}{m(1 - i\omega\tau)} E(\omega).$$

The current density is as usual $\vec{j}(t) = -en\vec{v}(t)$, $\vec{j}(\omega) = -en\vec{v}(\omega)$, so that

$$j(\omega) = \frac{e^2 n \tau}{m(1 - i\omega\tau)} E(\omega) \quad \Rightarrow \quad \sigma(\omega) = \sigma(0) \left[ \frac{1}{1 - i\omega\tau} \right] = \sigma(0) \left[ \frac{1 + i\omega\tau}{1 + (\omega\tau)^2} \right].$$
3. Show that the chemical potential of a Fermi gas in two dimensions is given by

\[ \mu(T) = k_B T \ln[\exp(E_F/k_B T) - 1] = k_B T \ln[\exp(\pi n \hbar^2/m k_B T) - 1] \]

for \( n \) electrons per unit area. \( E_F = \pi n \hbar^2/m \) is defined at \( T = 0 \).

**Solution**

The 2D density of states with spin is

\[ D(E) = \frac{m}{\pi \hbar^2}. \]

Introducing the 2D electron density \( n = N/A \) (\( A \) is the area), one gets at \( T = 0 \)

\[ n = \frac{m}{\pi \hbar^2} E_F \quad \Rightarrow \quad E_F = \frac{\pi \hbar^2}{m} n. \]

On the other hand, \( n \) is defined by the Fermi-Dirac distribution

\[ n = \frac{1}{m} \int_0^\infty D(E) f(E) dE = \int_0^\infty \frac{D(E) dE}{\exp \left( \frac{E - \mu}{k_B T} \right) + 1}. \]

Substituting \( D(E) = \frac{m}{\pi \hbar^2} \), we have the implicit expression for \( \mu(T) \)

\[ E_F = \int_0^\infty \frac{dE}{\exp \left( \frac{E - \mu}{k_B T} \right) + 1}. \]

This integral is known function \( \exp \left( \frac{\mu - E}{k_B T} \right) \) and

\[ E_F = k_B T \ln \left[ \exp \left( \frac{\mu}{k_B T} \right) + 1 \right]. \]

Making simple transformation, finally

\[ \mu(T) = k_B T \ln \left[ \exp \left( \frac{E_F}{k_B T} \right) - 1 \right]. \]

At \( T \to 0: \mu \to E_F \).
4. Consider the Dirac-Kronig-Penney model

\[ U(x) = U_0 \sum_n \delta(x - an). \]

a) Find the equation for \( \epsilon_n(k) \).

b) Consider the limit \( \frac{mU_0 a}{\hbar^2} \gg 1 \) and find the lowest energy band \( \epsilon_1(k) \).

c) Consider the effective mass approximation near the bottom of the band.

d) Consider semi-classical dynamics of electrons in the constant electric field (Bloch oscillations).

**Solution**

a) **Find the equation for \( \epsilon_n(k) \).**

Consider two segments: \(-a < x < 0\) (I) and \(0 < x < a\) (II). Since the potential energy is equal to zero inside each of the segments, the corresponding wave functions are the linear combinations of two plane waves

\[ \psi_I = Ae^{iqx} + Be^{-iqx}, \]

\[ \psi_{II} = Ce^{iqx} + De^{-iqx}, \quad q = \frac{\sqrt{2mE}}{\hbar}. \]

The Bloch wave functions \( \psi_k(x) = u_k(x)e^{ikx} \) have the property

\[ \psi_k(x + a) = u_k(x + a)e^{ik(x+a)} = u_k(x)e^{ikx}e^{ika} = \psi_k(x)e^{ika}. \]

Assume that \(-a < x < 0\), then

\[ \psi_{II}(x + a) = \psi_I(x)e^{ika}, \]

or

\[ Ce^{iq(x+a)} + De^{-iq(x+a)} = (Ae^{iqx} + Be^{-iqx})e^{ika}. \]

The coefficients in front of the \( e^{\pm iqx} \) terms must match. This gives

\[ C = e^{-iqx}A, \quad D = e^{iqx}B. \]

and we can write

\[ \psi_{II} = e^{ika} \left( Ae^{iq(x-a)} + Be^{-iq(x-a)} \right). \]

Now we need boundary conditions at \( x = 0 \)

(1) the wavefunction is continuous

\[ \psi_I(0) = \psi_{II}(0) \Rightarrow A + B = e^{ika} \left( Ae^{-iqa} + Be^{iqa} \right). \]
(2) Let’s find the boundary condition for $\frac{\partial \psi(x)}{\partial x}$ at $x = 0$ integrating the Schrödinger equation between $x = -\varepsilon$ and $x = \varepsilon$ at $\varepsilon \to 0$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U_0 \delta(x) \psi(x) = E \psi(x)$$

$$-\frac{\hbar^2}{2m} \int_{-\varepsilon}^{\varepsilon} \frac{\partial^2 \psi(x)}{\partial x^2} dx + U_0 \int_{-\varepsilon}^{\varepsilon} \delta(x) \psi(x) dx = E \int_{-\varepsilon}^{\varepsilon} \psi(x) dx$$

$$-\frac{\hbar^2}{2m} \left( \frac{\partial \psi_1(x)}{\partial x} \bigg|_{x=0} - \frac{\partial \psi_1(x)}{\partial x} \bigg|_{x=0} \right) + U_0 \psi_I(0) = 0$$

Now calculate derivatives

$$\left. \frac{\partial \psi_I(x)}{\partial x} \right|_{x=0} = i q \left( A e^{i q x} - B e^{-i q x} \right) \bigg|_{x=0} = i q (A - B),$$

$$\left. \frac{\partial \psi_{II}(x)}{\partial x} \right|_{x=0} = i q e^{i k a} \left( A e^{i(q(x-a))} - B e^{-i(q(x-a))} \right) \bigg|_{x=0} = i q e^{i k a} \left( A e^{-i q a} - B e^{i q a} \right).$$

Finally, we have the system of two equations (1) and (2)

$$\begin{bmatrix} 1 - e^{i(k-q)a} & A + \left( 1 - e^{i(k+q)a} \right) B \end{bmatrix} = 0,$$

$$\begin{bmatrix} e^{i(k-q)a} - 1 - \frac{2mU_0}{i\hbar^2 q} & A + \left( -e^{i(k+q)a} + 1 - \frac{2mU_0}{i\hbar^2 q} \right) B \end{bmatrix} = 0.$$

This system has non-trivial solution if the determinant equals to zero

$$\begin{vmatrix} 1 - e^{i(k-q)a} & A + \left( 1 - e^{i(k+q)a} \right) B \end{vmatrix} = 0,$$

$$\begin{vmatrix} e^{i(k-q)a} - 1 - \frac{2mU_0}{i\hbar^2 q} & A + \left( -e^{i(k+q)a} + 1 - \frac{2mU_0}{i\hbar^2 q} \right) B \end{vmatrix} = 0.$$

Simplifying, one gets

$$\cos(ka) = \cos(qa) + \frac{mU_0 a \sin(qa)}{\hbar^2 qa},$$

$$q(k) + q = \frac{\sqrt{2mE}}{\hbar} \Rightarrow E = \frac{\hbar^2 q(k)^2}{2m}.$$

Fig.: Red: the RHS of Eq. (3) as a function of $qa$ for $\frac{mU_0 a}{\hbar^2} = 10$. Horizontal lines: bounds on $\cos(ka)$. 

$q a > \frac{1}{\hbar}$

$k a = qa$

$k = q$

$E = \frac{\hbar^2 k^2}{2m}$
b) Consider the limit \( \frac{mU_0a}{\hbar} \gg 1 \) and find the lowest energy band \( \epsilon_1(k) \).

Let’s expand the RHS near \( qa = \pi \) e.g. near the zeros of \( \frac{\sin(qa)}{qa} \)

\[
\cos(ka) = -1 + \frac{mU_0a}{\hbar^2 \pi} (\pi - qa),
\]

\[
q(k) = \frac{\pi}{a} \left[ 1 - \frac{\hbar^2}{mU_0a} [1 + \cos(ka)] \right],
\]

\[
\epsilon_1(k) = \frac{\hbar^2 q(k)^2}{2m} \approx E_0 + 2J [1 - \cos(ka)], \quad J = \frac{\pi^2 \hbar^4}{2m^2 a^3 U_0}.
\]

The constant term \( E_0 \) can always be chosen as the zero of energy and finally

\[
\epsilon_1(k) = 2J [1 - \cos(ka)].
\]

c) Consider the effective mass approximation near the bottom of the band.

Near the bottom of the band \( ka \ll 1 \) one gets

\[
\cos(ka) \approx 1 - \frac{(ka)^2}{2},
\]

\[
\epsilon_1(k) \approx J a^2 k^2 = \frac{\hbar^2 k^2}{2m^*}.
\]

The effective mass

\[
m^* = \left( \frac{maU_0}{\hbar^2} \right) \frac{m}{\pi^2} \gg m.
\]

d) Consider semi-classical dynamics of electrons in the constant electric field (Bloch oscillations).

\[
\hbar \frac{\partial k}{\partial t} = -eE \implies k(t) = k(0) + \frac{-eE t}{\hbar},
\]

\[
E(t) = E(k(t)) = 2J [1 - \cos(\phi_0 + \Omega_B t)] = 2J [1 - \cos(\phi_0 + \Omega_B t)].
\]

The energy oscillates with the \textit{Bloch frequency} \( \Omega_B = eEa/\hbar \).