PHYS-E0421 Solid-State Physics (5cr), Spring 2019
Exercise session 2
Model solutions

1. **The electric conductivity of a metal**

   a) For free electron gas, energy dispersion is

$$E(k) = \frac{\hbar^2 k^2}{2m}. \tag{1}$$

States are filled up to the Fermi-energy E_F, leading to spherical Fermi-surface in k-space at Fermi wave vector k_F, with a total surface area $S_F = 4\pi k_F^2$.
In the expression for the conductivity of a metal,

$$\sigma = \frac{e^2}{4\pi^3\hbar}\int_{E=E_F}\frac{v_x^2(\mathbf{k})}{v(\mathbf{k})}\tau(\mathbf{k})dS_E,$$

we need the velocity at k_F. For free electron gas $v(k_F) = \frac{1}{\hbar}\frac{\partial E}{\partial k}\big|_{k=k_F} = \frac{\hbar k_F}{m}$. Moreover, in a system with a cubic symmetry (such as spherical system)

$$\begin{aligned}\int v^2(k)f(k)dS &= \int v_x^2(k)f(k)dS + \int v_y^2(k)f(k)dS + \int v_z^2(k)f(k)dS &(2)\\ &= 3\int v_x^2(k)f(k)dS. &(3)\end{aligned}$$

Putting all of the above together

$$\begin{aligned}\sigma &= \frac{e^2}{4\pi^3\hbar}\int_{E=E_F}\frac{v_x^2(\mathbf{k})}{v(\mathbf{k})}\tau(\mathbf{k})dS_E &(4)\\ &= \frac{e^2}{4\pi^3\hbar}\int_{E=E_F}\frac{1}{3}v(\mathbf{k})\tau(\mathbf{k})dS_E &(5)\\ &= \frac{e^2}{4\pi^3\hbar}\frac{1}{3}v(k_F)\tau S_F &(6)\\ &= \frac{e^2}{4\pi^3\hbar}\frac{\hbar k_F}{3m}\tau 4\pi k_F^2 &(7)\\ &= \frac{e^2}{m}\frac{k_F^3}{3\pi^2}\tau &(8)\end{aligned}$$

where we have assumed $\tau(k_F)$ is constant (or marked it's average over the sphere surface with τ). The number of particles can be related to Fermi wave vector through

$$k_F^3 = 3\pi^2 n \tag{9}$$

to finally obtain

$$\sigma = \frac{ne^2\tau}{m}. \tag{10}$$

   b) After again assuming cubic symmetry, the conductivity is

$$\sigma = \frac{e^2}{4\pi^3\hbar}\int_{E=E_F}\frac{1}{3}v(\mathbf{k})\tau(\mathbf{k})dS_E. \tag{11}$$

By denoting the average of mean free path $\lambda = v\tau$ over the surface S_E (with total area S_F) as

$$\Lambda = \frac{1}{S_F}\int v(\mathbf{k})\tau(\mathbf{k})dS_E \tag{12}$$

the conductivity can be written immediately as

$$\sigma = \frac{e^2}{12\pi^3\hbar}\Lambda S_F. \tag{13}$$

2. **Mean free path**

a) Mean free path $\lambda = v_F\tau$, where v_F is the Fermi velocity and τ the average time between electron collisions (electron relaxation time).
The Fermi velocity for a free electron gas ($E(k) = \hbar^2k^2/2m$) is given by

$$v_F = \frac{1}{\hbar}\frac{\partial E}{\partial k}\bigg|_{k=k_F} = \frac{\hbar k_F}{m}.$$

Relaxation time can be calculated from the resistivity

$$\frac{1}{\rho} = \sigma = \frac{ne^2\tau}{m}$$
$$\Rightarrow \tau = \frac{m}{\rho n e^2}$$

Only unknown quantity is the electron concentration n. In the case of free electon gas, the electron concentration can be calculated from the number of occupied states (from zero to Fermi energy) and yields

$$k_F^3 = 3\pi^2 n$$

The final result for the mean free path is then

$$\lambda = v_F\tau = \frac{\hbar k_F}{\rho n e^2}$$
$$= \frac{3\pi^2\hbar}{\rho k_F^2 e^2}$$

Inserting the numerical values for ρ and k_F we obtain $\lambda = 34$ nm. Comparing to the lattice constant of silver ($= 4.08$ Å), the mean free path is equivalent to roughly 100 lattice constants.

b) On the basis of the previous exercise, the mean free path is found to be inversely proportional to the resistivity

$$\lambda(T) \sim \tau(T) \sim \frac{1}{\rho(T)} \tag{14}$$

so that

$$\frac{\lambda(4\text{ K})}{\lambda(293\text{ K})} = \frac{\rho(293\text{ K})}{\rho(4\text{ K})} = 10^2 \tag{15}$$

The mean free path becomes $\lambda(4\text{ K}) = 10^2\lambda(290\text{ K}) = 3.4$ µm.

3. **Thermopower**

PHYS-E0421, Homework 2, Per Kennett Aschan 21470A

3. (a)

For free electrons we have

$$\varepsilon = \frac{\hbar^2 k^2}{2m_e}$$

from which we get

$$k = \frac{1}{\hbar}\sqrt{2m_e\varepsilon}$$

$$\frac{d\varepsilon}{dk} = \frac{\hbar^2 k}{m_e}$$

The energy density of states is

$$g(\varepsilon) = 2\frac{V}{(2\pi)^3} 4\pi k^2 \frac{dk}{d\varepsilon} = 2\frac{V}{(2\pi)^3} 4\pi k^2 \frac{m_e}{\hbar^2 k}$$

$$= \frac{V}{\pi^2}\frac{m_e}{\hbar^2} k = \frac{V}{\pi^2}\frac{m_e}{\hbar^3}\sqrt{2m_e\varepsilon}$$

The Fermi-Dirac distribution is

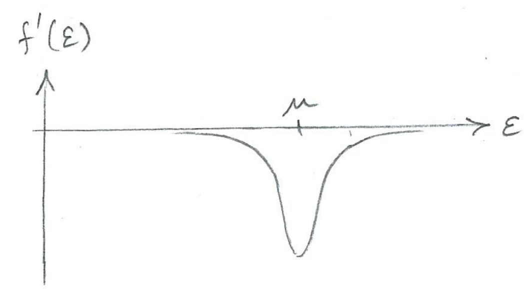
$$f(\varepsilon) = \frac{1}{\exp[(\varepsilon-\mu)/k_BT]+1}$$

We find that

$$f'(\varepsilon) = -\frac{1}{k_BT}\frac{\exp[(\varepsilon-\mu)/k_BT]}{\{\exp[(\varepsilon-\mu)/k_BT]+1\}^2}$$

$$= -\frac{1}{k_BT}\frac{\exp[-(\varepsilon-\mu)/k_BT]}{\{1+\exp[-(\varepsilon-\mu)/k_BT]+1\}^2}$$

$$= f'(\mu-(\varepsilon-\mu))$$



3. (a) cont.

The number of electrons is

$$N = \int_0^\infty d\varepsilon\, g(\varepsilon) f(\varepsilon) = \int_0^\infty d\varepsilon\, \Gamma'(\varepsilon) f(\varepsilon)$$

$$= \left[\Gamma(\varepsilon) f(\varepsilon)\right]_0^\infty - \int_0^\infty d\varepsilon\, \Gamma(\varepsilon) f'(\varepsilon)$$

$$= -\int_0^\infty d\varepsilon\, \Gamma(\varepsilon) f'(\varepsilon)$$

We approximate $\Gamma(\varepsilon)$ with a Taylor series:

$$\Gamma(\varepsilon) = \Gamma(\varepsilon_F) + \frac{\Gamma'(\varepsilon_F)}{1!}(\varepsilon - \varepsilon_F) + \frac{\Gamma''(\varepsilon_F)}{2!}(\varepsilon - \varepsilon_F)^2$$

$$= \Gamma(\varepsilon_F) + \Gamma'(\varepsilon_F)\left[(\varepsilon-\mu) + (\mu - \varepsilon_F)\right]$$
$$+ \tfrac{1}{2}\Gamma''(\varepsilon_F)\left[(\varepsilon-\mu)^2 + 2(\varepsilon-\mu)(\mu-\varepsilon_F) + (\mu-\varepsilon_F)^2\right]$$

Then

$$N \approx -\Gamma(\varepsilon_F)\int_0^\infty d\varepsilon\, f'(\varepsilon) - \Gamma'(\varepsilon_F)\int_0^\infty d\varepsilon\left[(\varepsilon-\mu) + (\mu-\varepsilon_F)\right] f'(\varepsilon)$$
$$- \tfrac{1}{2}\Gamma''(\varepsilon_F)\int_0^\infty d\varepsilon\left[(\varepsilon-\mu)^2 + 2(\varepsilon-\mu)(\mu-\varepsilon_F) + (\mu-\varepsilon_F)^2\right] f'(\varepsilon)$$

We have

$$\int_0^\infty d\varepsilon\, f'(\varepsilon) \approx \int_{-\infty}^\infty d\varepsilon\, f'(\varepsilon) = \left[f(\varepsilon)\right]_{-\infty}^\infty = -1$$

$$\int_0^\infty d\varepsilon\, (\varepsilon-\mu) f'(\varepsilon) \approx \int_{-\infty}^\infty d\varepsilon\, (\varepsilon-\mu) f'(\varepsilon) = 0$$

$$\int_0^\infty d\varepsilon\, (\varepsilon-\mu)^2 f'(\varepsilon) \approx \int_{-\infty}^\infty d\varepsilon\, (\varepsilon-\mu)^2 f'(\varepsilon)$$

$$\approx (k_B T)^2 \int_{-\infty}^\infty dx\, \frac{-x^2 e^x}{(e^x+1)^2} = (k_B T)^2\left(-\frac{\pi^2}{3}\right)$$

3. (a) cont.

Therefore

$$N \approx \Gamma(\varepsilon_F) + \Gamma'(\varepsilon_F)(\mu - \varepsilon_F) + \frac{1}{2}\Gamma''(\varepsilon_F)\left[(k_B T)\frac{\pi^2}{3} + (\mu - \varepsilon_F)^2\right]$$

Since N does not depend on temperature, we must have

$$\Gamma'(\varepsilon_F)(\mu - \varepsilon_F) + \frac{1}{2}\Gamma''(\varepsilon_F)\left[(k_B T)^2\frac{\pi^2}{3} + (\mu - \varepsilon_F)^2\right] = 0$$

If we assume that $k_B T \gg |\mu - \varepsilon_F|$, then we have

$$\Gamma'(\varepsilon_F)(\mu - \varepsilon_F) + \frac{1}{2}\Gamma''(\varepsilon_F)(k_B T)^2\frac{\pi^2}{3} = 0$$

When we solve this for μ, we get

$$\mu = \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2\frac{\Gamma''(\varepsilon_F)}{\Gamma'(\varepsilon_F)} = \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2\frac{g'(\varepsilon_F)}{g(\varepsilon_F)}$$

$$= \varepsilon_F - \frac{\pi^2}{6}(k_B T)^2\frac{1}{2\varepsilon_F} = \varepsilon_F - \frac{\pi^2}{12}\frac{(k_B T)^2}{\varepsilon_F}$$

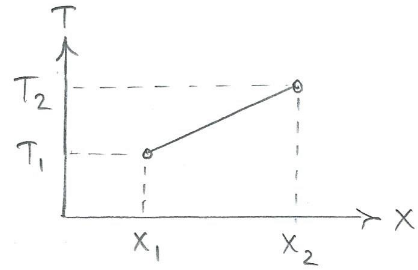
3. (b)

From the previous problem we have

$$\mu = \varepsilon_F - \frac{\pi^2}{12} \frac{(k_B T)^2}{\varepsilon_F}$$

Let the coordinates of the sample endpoints be x_1 and x_2. Let the corresponding temperatures be T_1 and T_2. Since the temperature gradient is constant, we have

$$\frac{dT}{dx} = \frac{T_2 - T_1}{x_2 - x_1}$$



Also

$$\frac{d\phi}{dx} = -E$$

$$\frac{d\mu}{dx} = \frac{d\mu}{dT}\frac{dT}{dx} = \left(-\frac{\pi^2}{6}\frac{k_B^2}{\varepsilon_F} T\right)\frac{T_2 - T_1}{x_2 - x_1}$$

The Seebeck coefficient is

$$S_T = -\frac{\pi^2 k_B^2 T}{3 e \varepsilon_F}$$

By definition

$$\frac{d}{dx}\left(\frac{\eta}{e}\right) = S_T \frac{dT}{dx}, \quad \eta = \mu - e\phi$$

Thus we have

$$\frac{1}{e}\left(-\frac{\pi^2}{6}\frac{k_B^2}{\varepsilon_F} T\right)\frac{T_2 - T_1}{x_2 - x_1} + E = -\frac{\pi^2 k_B^2 T}{3 e \varepsilon_F}\frac{T_2 - T_1}{x_2 - x_1},$$

from which we get

$$E = -\frac{\pi^2 k_B^2 T}{6 e \varepsilon_F}\frac{T_2 - T_1}{x_2 - x_1} = -\frac{d\phi}{dT}\frac{dT}{dx}$$

$$\phi = \frac{\pi^2}{12}\frac{(k_B T)^2}{e \varepsilon_F}, \quad \eta = \mu - e\phi = \varepsilon_F - \frac{\pi^2}{6}\frac{(k_B T)^2}{\varepsilon_F}$$