Physics 502 - Solutions for assignment 5

(Dated: December 6, 2023)

1. Thermally activated conductivity in a band insulator

a. The density of states can be calculated in the usual way for each band. For positive energies:

$$g(\epsilon) = 2\int \frac{d^2k}{(2\pi)^2}\delta(\epsilon - \Delta - \frac{\hbar^2k^2}{2m}) = \frac{1}{2\pi}\int d(k^2)\delta(\epsilon - \Delta - \frac{\hbar^2k^2}{2m}) = \frac{m}{\hbar^2\pi}\Theta(\epsilon - \Delta).$$

The delta function can only be satisfied if $\epsilon - \Delta > 0$ and hence the theta function. For negative energies we get the same coefficient with $\Theta(-\epsilon - \Delta)$ so altogether we have

$$g(\epsilon) = \frac{m}{\hbar^2\pi}[\Theta(\epsilon - \Delta) + \Theta(-\epsilon - \Delta)].$$

The occupation number at $T = 0$ and finite T is illustrated in the figure on the next page.

To show that the chemical potential is pinned at $\epsilon = 0$ note that at $T = 0$, at half filling the lower band is completely full and the upper band is completely empty. If the number of electrons is to stay fixed even at $T \neq 0$, the number of holes in the valence band should be equal to the number of electrons in the conduction band. Therefore:

$$\int_0^\infty g(\epsilon)f(\epsilon)d\epsilon = \int_{-\infty}^0 g(\epsilon)(1 - f(\epsilon))d\epsilon$$

where $f(\epsilon)$ is the Fermi-Dirac distribution of electrons and $1 - f(\epsilon)$ is the distribution of holes. Canceling the constant density of states from both sides we get:

$$\int_{-\infty}^{-\Delta} \frac{1}{1 + e^{\beta(\epsilon-\mu)}}d\epsilon = \int_\Delta^\infty [1 - \frac{1}{1 + e^{\beta(\epsilon-\mu)}}]d\epsilon.$$

The right hand side can be manipulated as follows

$$\int_\Delta^\infty [1 - \frac{1}{1 + e^{\beta(\epsilon-\mu)}}]d\epsilon = \int_\Delta^\infty \frac{1}{1 + e^{-\beta(\epsilon-\mu)}}d\epsilon = \int_{-\infty}^{-\Delta} \frac{1}{1 + e^{\beta(\epsilon+\mu)}}d\epsilon$$

where at the last step we have taken $\epsilon \to -\epsilon$. The equation can be satisfied only if

$$\frac{1}{1 + e^{\beta(\epsilon-\mu)}} = \frac{1}{1 + e^{\beta(\epsilon+\mu)}} \quad \Rightarrow \quad -\mu = \mu \quad \Rightarrow \quad \mu = 0$$

b. The specific heat is defined as:

$$c_v = \frac{d}{dT}\int \epsilon g(\epsilon)f(\epsilon)d\epsilon = \int \epsilon g(\epsilon)\left(\frac{\partial f(\epsilon)}{\partial T}\right)d\epsilon$$

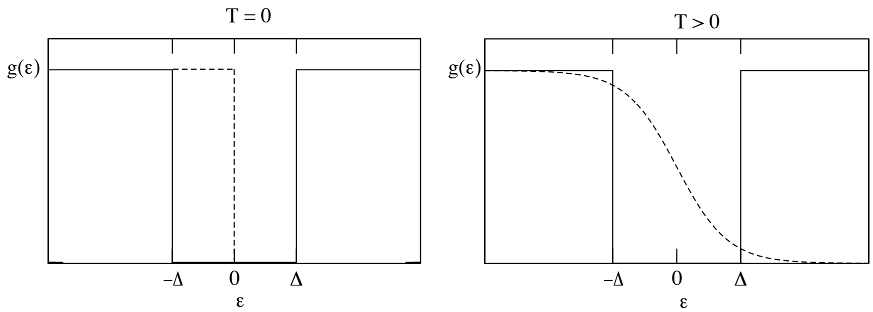

FIG. 1: At $T = 0$ the Fermi-Dirac distribution (dashed line, scaled by the coefficient of $g(\epsilon)$) is 1 for the valence band and 0 for the conduction band. At $T > 0$, some states in the top of the valence band are unoccupied and some states at the bottom of the conduction band are occupied.

$$\frac{\partial f(\epsilon)}{\partial T} = \frac{\epsilon}{k_B T^2} \frac{e^{\beta\epsilon}}{(1+e^{\beta\epsilon})^2} = \frac{\epsilon}{k_B T^2} \frac{1}{(e^{-\frac{\beta\epsilon}{2}}(1+e^{\beta\epsilon}))^2} = \frac{\epsilon}{k_B T^2} \frac{1}{(2\cosh(\frac{\beta\epsilon}{2}))^2}.$$

Inserting this into the specific heat we get

$$c_v = \frac{mk_B}{2\pi\hbar^2} \int_\Delta^\infty \frac{(\beta\epsilon)^2}{\cosh^2(\frac{\beta\epsilon}{2})} d\epsilon$$

where the factor of 2 was added to include the two bands. This gives $\mathcal{C}_1 = mk_B/2\pi\hbar^2$.

c. We can analyze the above integral in two limiting cases.

- At very low temperature $\beta\Delta \gg 1$ and therefore in all of the integration region $\beta\epsilon \gg 1$ and $\cosh(\frac{\beta\epsilon}{2}) \approx \frac{1}{2} e^{\frac{\beta\epsilon}{2}}$. In that case

$$c_v \simeq \frac{2mk_B}{\pi\hbar^2} \int_\Delta^\infty (\beta\epsilon)^2 e^{-\beta\epsilon} d\epsilon \propto \frac{e^{-\beta\Delta}}{\beta}((\beta\Delta)^2 + 2\beta\Delta + 2) \approx e^{-\beta\Delta}\Delta^2\beta.$$

Here the specific heat is exponentially activated due to the Boltzman like distribution of the electrons. This happens since Δ is much larger than the width of the Fermi-Dirac distribution and effectively we see only the exponential tail.

- At high temperature, $\beta\Delta \ll 1$.

$$c_v = \frac{mk_B}{2\pi\hbar^2} \int_\Delta^\infty \frac{(\beta\epsilon)^2}{\cosh^2(\frac{\beta\epsilon}{2})} d\epsilon = \frac{mk_B}{2\pi\hbar^2} \frac{1}{\beta} \left(\int_0^\infty \frac{x^2}{\cosh^2(\frac{x}{2})} dx - \int_0^{\beta\Delta} \frac{x^2}{\cosh^2(\frac{x}{2})} dx \right).$$

The first term gives contribution to c_v proportional to T and is what we would obtain in a 2D electron gas. In the second term we can replace the cosh by unity and the evaluation gives a term $\sim \Delta(\beta\Delta)^2$, negligible compared to the first term in the limit under consideration.

d. Within the relaxation time approximation the conductivity takes the form:

$$\sigma_{\mu\nu} = e^2 \int \frac{d^2k}{(2\pi)^2} \tau v_\mu v_\nu \left(-\frac{df(\epsilon)}{d\epsilon} \right) = e^2 \int \frac{d^2k}{(2\pi)^2} \tau \frac{\hbar k_\mu}{m} \frac{\hbar k_\nu}{m} \frac{\beta e^{\beta\epsilon}}{(1+e^{\beta\epsilon})^2}$$

For $\mu \neq \nu$ the integral vanishes so we can take $k_\mu k_\nu \to \delta_{\mu\nu}\frac{k^2}{2}$. We can then replace k^2 by $\epsilon - \Delta$ for positive energies and $-\epsilon - \Delta$ for negative energies (this just produces a factor of 2),

$$\sigma_{\mu\nu} = \delta_{\mu\nu} e^2 \tau \frac{\hbar^2}{2m} \int \frac{d^2k}{(2\pi)^2} \frac{\beta(\epsilon - \Delta)}{\cosh^2(\frac{\beta\epsilon}{2})} = \delta_{\mu\nu} \frac{e^2\tau}{2\hbar^2\pi} \int_\Delta^\infty \frac{\beta(\epsilon-\Delta)}{\cosh^2(\frac{\beta\epsilon}{2})} d\epsilon.$$

The constant $\mathcal{C}_2$ is $e^2\tau/2\hbar^2\pi$.

In the same way as before we can find the leading behaviour of the integral. For $\beta\Delta \gg 1$ the activation is exponential:

$$\sigma_{\mu\nu} \to \delta_{\mu\nu} \frac{4\mathcal{C}_2}{\beta} e^{-\beta\Delta} \propto T e^{-\beta\Delta}$$

and for $\beta\Delta \ll 1$ we recover the metallic behaviour:

$$\sigma_{\mu\nu} \to \delta_{\mu\nu} \frac{\mathcal{C}_2}{\beta} \int_0^\infty \frac{x}{\cosh^2(\frac{x}{2})} \propto T.$$

e. The thermal conductivity can be evaluated in a similar way (neglecting the thermo-electric effects):

$$\kappa_{\mu\nu} = \frac{\tau}{T} \int \frac{d^2k}{(2\pi)^2} (\epsilon(k))^2 v_\mu v_\nu \left(-\frac{df(\epsilon)}{d\epsilon}\right) = \frac{\mathcal{C}_2}{e^2 T} \delta_{\mu\nu} \int_\Delta^\infty \frac{\beta\epsilon^2(\epsilon-\Delta)}{\cosh^2(\frac{\beta\epsilon}{2})} d\epsilon$$

For $\beta\Delta \gg 1$ we have

$$\kappa_{\mu\nu} \to \frac{4\mathcal{C}_2}{e^2 T} \delta_{\mu\nu} \int_\Delta^\infty \beta\epsilon^2(\epsilon-\Delta) e^{-\beta\epsilon} d\epsilon \approx \frac{4k_B\mathcal{C}_2}{e^2} \Delta^2 e^{-\beta\Delta} \propto e^{-\beta\Delta}$$

And for $\beta\Delta \ll 1$

$$\kappa_{\mu\nu} \to \frac{\mathcal{C}_2 \delta_{\mu\nu}}{e^2} T^2 \int_0^\infty \frac{x^3 dx}{\cosh^2(\frac{x}{2})} \propto T^2$$

Parts (d) & (e) imply that the Wiedeman-Franz law is obeyed for high temperatures ($\beta\Delta \ll 1$) where the system behaves essentially like a metal, but is violated for the low temperatures where the band-gap is relevant and insulating behavior prevails. Note that the general derivation of the WF law given in the class was done for a metal so there is no reason to expect it to hold for an insulator.

2. e-ph interaction in 1D

Let us use the perturbation theory for e-ph interaction described in the text. We assume that the electronic energy changes significantly with $k \to k+q$ (where k is the electron momentum and q is the phonon momentum) relative to the phonon energy (i.e, $|\epsilon_k - \epsilon_{k+q}| \gg \hbar\omega_q$). This gives

$$\hbar\omega_q^{new} = \hbar\omega_q^{(0)} - 2M^2 \sum_k \frac{n_k(1-n_{k+q})}{\epsilon_{k+q} - \epsilon_k},$$

with $\hbar\omega_q^{(0)} = W\sin(qa/2)$. Going to a continuum limit and denoting the correction term $\delta\omega_q$, we find at $q = \pi/a$

$$\delta\omega_{\pi/a} = -2M^2 L \int_{-k_F}^{k_F} \frac{dk}{2\pi} \frac{1}{2A + 2B\cos 2ka}.$$

We assumed inter-band excitation since the numerator vanishes if both ϵ_k and ϵ_{k+q} are from the same band. This integral can be evaluated with ($k_F = \pi/2a$ at half filling), giving $\delta\omega_{\pi/a} = -\frac{M^2 L}{2a\sqrt{A^2 - B^2}}$. Using $M^2 = G/N$ and $L = Na$ we get $G = 2W\sqrt{A^2 - B^2}$ as the condition for vanishing phonon frequency at π/a.