Condensed Matter - HW1 :: Fermi gas

PHSX 545

Problem 1

Calculate the specific heat of a semiconductor under the assumption $k_B T \ll E_g$ where E_g is the gap between valence and conduction bands. Show that it is given by an ideal gas-like part $(3/2)n(T)k_B$ plus a correction, where $n(T)$ is the number of excitations. Is this correction small or large?

Hint: First, approximate the dispersion of both the conduction and the valence band parabolically, with the two effective masses m_v and m_c. Determine the density of states for the two bands in 3D case. Then, calculate the chemical potential μ from the condition, that the number of electrons in the conduction band $n_e(T)$ must be equal to the number of holes in the valence band $n_h(T)$, under condition $k_B T \ll \mu, E_g - \mu$.

Problem 2

A quasiparticle wave packet is given by a superposition of plane waves

$$\psi_{\mathbf{p}}(\mathbf{r}, t) = \sum_{\mathbf{k}} A_{\mathbf{p}}(\mathbf{k}) e^{i(\mathbf{k}\mathbf{r} - \epsilon(\mathbf{k})t)}$$

with Gaussian weight around momentum $\mathbf{p}$:

$$A_{\mathbf{p}}(\mathbf{k}) = C \exp\left(-\frac{(\mathbf{k} - \mathbf{p})^2}{2\Delta k^2}\right)$$

The spread of the wavepacket in momentum space is Δk.
- Find the normalization constant C for 3-dimensional case from $\int d^3\mathbf{r} |\psi_{\mathbf{p}}(\mathbf{r}, t)|^2 = 1$.
- Find the behavior of this wavepacket in real space (how it propagates and its shape), and from it estimate the lifetime of the quasiparticle.

Hint: You may assume that the energy $\epsilon(\mathbf{k})$ does not change drastically on the scale of the wavepacket, and you can use Taylor expansion around $\mathbf{p}$. Take $\partial^2 \epsilon_{\mathbf{p}} / \partial p_i \partial p_j \propto \delta_{ij}$.

Answer of exercise 1

For $T \ll E_g$ only the band edges are important, so we can approximate the energy

$$\varepsilon_e = E_g + \frac{k^2}{2m_c} \qquad \varepsilon_h = -\frac{k^2}{2m_v}$$

We start again by finding the dependence $\mu(T)$ of chemical potential on temperature. At zero temperature it is in the middle of the gap. For non-zero temperature it shifts. To determine $\mu(T)$ we consider again the fixed density of particles, i.e.

$$\int \frac{d^3k}{(2\pi)^3} n(\varepsilon_e(k)) = \int \frac{d^3k}{(2\pi)^3} [1 - n(\varepsilon_h(k))]$$

$$\int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(\varepsilon_e(k)-\mu)} + 1} = \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{-\beta(\varepsilon_h(k)-\mu)} + 1}$$

If we assume that $T \ll \mu$ and $T \ll E_g - \mu$, then we can neglect the $+1$ in the Fermi-Dirac distribution function and the previous equation simplifies to

$$\int \frac{d^3k}{(2\pi)^3} e^{-\beta(\varepsilon_e(k)-\mu)} = \int \frac{d^3k}{(2\pi)^3} e^{\beta(\varepsilon_h(k)-\mu)}$$

Note that this corresponds to using Maxwell-Boltzmann statistics as for the ideal gas, rather than the Fermi-Dirac statistics.

To proceed, we define density of states in the valence and conduction bands analogous to free fermion gas:

$$N_c(\varepsilon) = 2 \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_e(\mathbf{k})) = \frac{2}{8\pi^3\hbar^3} \int\limits_{surface\ \varepsilon_e(\mathbf{k})=\varepsilon} \frac{d^2p}{|v_e(\mathbf{k})|} = \theta(\varepsilon - E_g) \frac{p(\varepsilon)m_c}{\pi^2\hbar^3} = \theta(\varepsilon - E_g) \frac{\sqrt{2m_c^3}}{\pi^2\hbar^3} \sqrt{\varepsilon - E_g}$$

$$N_v(\varepsilon) = 2 \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_h(\mathbf{k})) = \frac{2}{8\pi^3\hbar^3} \int\limits_{surface\ \varepsilon_h(\mathbf{k})=\varepsilon} \frac{d^2p}{|v_h(\mathbf{k})|} = \theta(-\varepsilon) \frac{\sqrt{2m_v^3}}{\pi^2\hbar^3} \sqrt{-\varepsilon}$$

With these we can change integration over momenta to integration over energies

$$\int\limits_{-\infty}^{+\infty} d\varepsilon N_c(\varepsilon) e^{-\beta(\varepsilon-\mu)} = \int\limits_{-\infty}^{+\infty} d\varepsilon N_v(\varepsilon) e^{\beta(\varepsilon-\mu)}$$

that give

$$\sqrt{m_e^3} \int\limits_{E_g}^{+\infty} d\varepsilon \sqrt{\varepsilon - E_g} e^{-\beta(\varepsilon-\mu)} = \sqrt{m_h^3} \int\limits_{-\infty}^{0} d\varepsilon \sqrt{-\varepsilon} e^{\beta(\varepsilon-\mu)} \qquad \sqrt{m_e^3} e^{-\beta(E_g-\mu)} \frac{\sqrt{\pi}}{2} T^{3/2} = \sqrt{m_h^3} e^{-\beta(\mu)} \frac{\sqrt{\pi}}{2} T^{3/2}$$

From this it follows that

$$\mu(T) = \frac{E_g}{2} + \frac{3T}{4} \ln \frac{m_h}{m_e}$$

and the electron and hole numbers are

$$n_e(T) = n_h(T) = \int\limits_{E_g}^{+\infty} d\varepsilon \frac{\sqrt{2m_c^3}}{\pi^2\hbar^3} \sqrt{\varepsilon - E_g} e^{-\beta(\varepsilon-\mu)} = \frac{\sqrt{2m_c^3}}{\pi^2\hbar^3} e^{-\beta(E_g-\mu)} \frac{\sqrt{\pi}}{2} T^{3/2} = \frac{(m_c m_v)^{3/4}}{\sqrt{2}} e^{-E_g/2T} \left(\frac{T}{\pi\hbar^2} \right)^{3/2}$$

We finally find the energy of the system at finite temperature.

$$E(T) = 2 \int \frac{d^3k}{(2\pi)^3} \varepsilon_e(k) n(\varepsilon_e(k)) + 2 \int \frac{d^3k}{(2\pi)^3} [-\varepsilon_h(k)][1 - n(\varepsilon_h(k))]$$

$$E(T) = \frac{\sqrt{2m_c^3}}{\pi^2\hbar^3} \int\limits_{E_g}^{+\infty} d\varepsilon \sqrt{\varepsilon - E_g}\, \varepsilon e^{-\beta(\varepsilon-\mu)} + \frac{\sqrt{2m_v^3}}{\pi^2\hbar^3} \int\limits_{-\infty}^{0} d\varepsilon \sqrt{-\varepsilon}\, [-\varepsilon] e^{\beta(\varepsilon-\mu)}$$

$$= E_g n_e(T) + \left(\frac{\sqrt{2m_c^3}}{\pi^2\hbar^3} e^{-\beta(E_g-\mu)} + \frac{\sqrt{2m_v^3}}{\pi^2\hbar^3} e^{\beta(\mu)} \right) \int\limits_0^{+\infty} d\varepsilon\, \varepsilon^{3/2} \varepsilon e^{-\beta\varepsilon}$$

$$= E_g n_e(T) + \frac{3}{2}T(n_e(T) + n_h(T)) = \left[\frac{E_g}{2} + \frac{3}{2}T \right] n(T)$$

where we defined the total carrier density $n(T) = n_e(T) + n_h(T)$. The specific heat is

$$C_V = \frac{\partial E}{\partial T} = \frac{3}{2}n(T) + \left[\frac{E_g}{2} + \frac{3}{2}T \right] \frac{\partial n(T)}{\partial T}$$

We see that the specific heat of a semiconductor is given by a contribution similar to the specific heat of an ideal gas of excitations that are already present in the system due to thermal excitation, plus an additional contribution originating from the excitation of new particle hole pairs $\sim \dfrac{\partial n(T)}{\partial T}$. Using number of particles derived earlier, we can rewrite the derivative

$$\frac{\partial n(T)}{\partial T} = \frac{3}{2}\frac{n}{T} + \frac{E_g}{2T^2}n = \left[\frac{3}{2} + \frac{E_g}{2T} \right] \frac{n}{T}$$

and this term dominates over the ideal gas-like part for small temperatures!

Answer of exercise 2

From normalization condition

$$1 = \int d^3r |\psi_{\mathbf{p}}(\mathbf{r},t)|^2 = \sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{p}}(\mathbf{k})A_{\mathbf{p}}(\mathbf{k}')^* \int d^3r e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}} e^{-i(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})t} = \sum_{\mathbf{k},\mathbf{k}'} A_{\mathbf{p}}(\mathbf{k})A_{\mathbf{p}}(\mathbf{k}')^* V\delta_{\mathbf{k},\mathbf{k}'}$$

$$= V \sum_{\mathbf{k}} |A_{\mathbf{p}}(\mathbf{k})|^2 = V^2|C|^2 \int \frac{d^3k}{(2\pi\hbar)^3} e^{-(\mathbf{k}-\mathbf{p})^2/\Delta k^2} = V^2|C|^2 \frac{(\pi\Delta k^2)^{3/2}}{(2\pi\hbar)^3}$$

(The product of 3 Gaussian integrals.) So for the coefficient we have

$$|C| = \frac{1}{V} \frac{(2\pi\hbar)^{3/2}}{(\pi\Delta k^2)^{3/4}}$$

We next expand the energy around $\mathbf{p}$:

$$\varepsilon(\mathbf{k}) = \varepsilon_{\mathbf{p}} + (\boldsymbol{\nabla}_{\mathbf{p}}\varepsilon_{\mathbf{p}})(\mathbf{k} - \mathbf{p}) + \frac{1}{2}\varepsilon''_{ij}(\mathbf{k}-\mathbf{p})_i(\mathbf{k}-\mathbf{p})_j$$

where $\varepsilon''_{ij} = \partial^2\epsilon_{\mathbf{p}}/\partial p_i\partial p_j$.

The wavepacket function then can be expressed as a function of $\delta\mathbf{k} = \mathbf{k} - \mathbf{p}$:

$$\psi_{\mathbf{p}}(\mathbf{r},t) = e^{i(\mathbf{p}\mathbf{r}-\varepsilon_{\mathbf{p}}t)} \sum_{\delta\mathbf{k}} C e^{-\delta\mathbf{k}^2/2\Delta k^2} e^{i(\mathbf{r}-\mathbf{v}_{\mathbf{p}}t)\delta\mathbf{k} - i\frac{1}{2}\varepsilon''\delta\mathbf{k}^2 t}$$

and we write it as a Gaussian integral:

$$\psi_{\mathbf{p}}(\mathbf{r},t) = e^{i(\mathbf{p}\mathbf{r}-\varepsilon_{\mathbf{p}}t)} CV \int \frac{d^3k}{(2\pi\hbar)^3} e^{-\frac{1}{2}(1/\Delta k^2 + i\varepsilon'' t)\delta\mathbf{k}^2} e^{i(\mathbf{r}-\mathbf{v}_{\mathbf{p}}t)\delta\mathbf{k}}$$

$$\psi_{\mathbf{p}}(\mathbf{r}, t) = CVe^{i(\mathbf{p}\mathbf{r}-\varepsilon_{\mathbf{p}}t)} \frac{1}{(2\pi\hbar)^3} \left[2\pi\left(1/\Delta k^2 + i\varepsilon''t\right)^{-1}\right]^{3/2} \exp\left[-\frac{(\mathbf{r}-\mathbf{v_p}t)^2}{2(1/\Delta k^2 + i\varepsilon''t)}\right]$$

This wavepacket propagates $(\mathbf{r} - \mathbf{v_p}t)$ with group velocity

$$\mathbf{v_p} = \frac{\partial \varepsilon_{\mathbf{p}}}{\partial \mathbf{p}}$$

and the width of the packet grows with time

$$width^2 \sim \left|\frac{1}{\Delta k^2} + i\varepsilon''t\right|$$

We may say that the time it takes for the width to double is the lifetime of the quasiparticle:

$$\tau \approx \frac{1}{\varepsilon'' \Delta k^2}$$