EE 207 [Spring 24-25] ***HW-3 Solutions***

1. The effective mass tensor is defined as $\overleftrightarrow{M}_{ij}^{-1} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_j \partial k_i}$.

(a) Calculate it for electrons in a 2D material with the following dispersion relation. $E = E_C + \frac{\hbar^2 k_x^2}{2m_{11}} + \frac{\hbar^2 k_y^2}{2m_{22}} + \frac{\hbar^2 k_x k_y}{m_{12}}$

(b) Calculate the electron acceleration for an external electric field parallel to the X-axis. Explain in physical terms, any peculiarity you observe in the result.

(a) $\overleftrightarrow{M}^{-1} = \begin{bmatrix} 1/m_{11} & 1/m_{12} \\ 1/m_{12} & 1/m_{22} \end{bmatrix}$

(b) $\vec{F} = \overleftrightarrow{M}\vec{a} \Rightarrow \vec{a} = \overleftrightarrow{M}^{-1}\vec{F} = -e\overleftrightarrow{M}^{-1}\vec{E}$

$$\vec{a} = -e\begin{bmatrix} 1/m_{11} & 1/m_{12} \\ 1/m_{12} & 1/m_{22} \end{bmatrix}\begin{bmatrix} E \\ 0 \end{bmatrix} = \begin{bmatrix} -eE/m_{11} \\ -eE/m_{12} \end{bmatrix}$$

The peculiarity is a Y-component of acceleration even though there is no Y-component of field/force, just an X-component. This mixing happens because of the cross term in the dispersion relation that mixes up the X and Y response.

2. The dispersion relation for band electrons in a 2D material is given by: $E = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2}$.

(a) What is the equal energy surface? What will be the radius of a circle of equal area?

(b) Show that the density of states (DOS) can still be written in the form $g = m^*/\pi\hbar^2$ which was derived for a spherical dispersion relation. m^* is called the 'density of states effective mass'. It is some average of m_1 and m_2 that must give you the correct DOS. Write down m^* in terms of m_1 and m_2 (hint: consider the second part of 3a).

(a) For a fixed energy ε, the surface in k-space is an ellipse given by:

$$\frac{k_x^2}{2m_1\varepsilon/\hbar^2} + \frac{k_y^2}{2m_2\varepsilon/\hbar^2} = 1$$

$$\frac{k_x^2}{k_1^2} + \frac{k_y^2}{k_2^2} = 1$$

With axes k_1 and k_2. The area of the ellipse is $\pi k_1 k_2$. Ergo, the circle of equal area in k-space is one with radius $k_{eff} : \pi k_{eff}^2 = \pi k_1 k_2$.

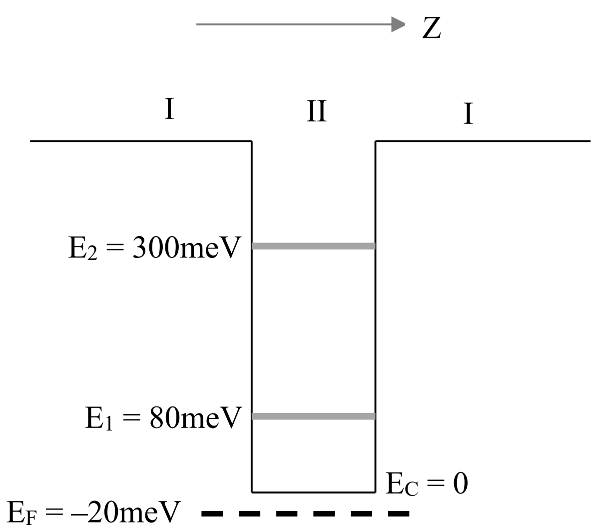
(b) If we consider the circle of equal area in k-space, we will have the same number of k-states therein, and therefore we will arrive at the same DOS. Thus, the DOS effective mass may be obtained from:

$$\pi k_{eff}^2 = \pi k_1 k_2 \Rightarrow k_{eff}^2 = k_1 k_2$$

$$\Rightarrow 2m_{eff}\varepsilon/\hbar^2 = \sqrt{2m_1\varepsilon/\hbar^2}\cdot\sqrt{2m_2\varepsilon/\hbar^2}$$

$$\Rightarrow m_{eff} = \sqrt{m_1 m_2}$$

3. Consider the quantum well for electrons formed in the heterostructure shown below. It has two bound states as shown below. Assuming a constant, isotropic effective mass everywhere, the 2D density of states is given by $g = m^*/\pi\hbar^2$. Take $g = 2\times10^{14}\,cm^{-2}eV^{-1}$. Then calculate the 2D carrier density at 300K. State clearly and justify any assumptions you make.



(a) The 2D carrier density will be given by:

$$n_{2D} = \int_{E_1}^{\infty} g_{2D}(\varepsilon) f_{FD}(\varepsilon)\,d\varepsilon + \int_{E_2}^{\infty} g_{2D}(\varepsilon) f_{FD}(\varepsilon)\,d\varepsilon \qquad f_{FD}(\varepsilon) = \frac{1}{e^{(\varepsilon-\varepsilon_F/k_B T)}+1}$$

Since $(E_1 - \varepsilon_F) >> k_B T$, we may apply the Boltzmann approximation to the FD distribution function: $f_{FD}(\varepsilon) \rightarrow f_{MB}(\varepsilon) = e^{-(\varepsilon-\varepsilon_F/k_B T)}$

Further, given this now exponential distribution, we may drop the second integral (since it will be negligible compared to the first) and approximate the first integral in the 2D carrier density to give:

$$n_{2D} \approx \int_{E_1}^{\infty} g_{2D}(\varepsilon) e^{-(\varepsilon-\varepsilon_F)/k_BT} d\varepsilon$$

$$\Rightarrow n_{2D} = \frac{m^* k_B T}{\pi\hbar^2} \int_{(E_1-\varepsilon_F)/k_BT}^{\infty} e^{-x} dx = \frac{m^* k_B T}{\pi\hbar^2} e^{-(E_1-\varepsilon_F)/k_BT}$$

[Note that we would have had another term like this from the second integral, which would be smaller by a factor of $e^{(E_2-E_1)/k_BT} \approx 4729$.]

Substituting the numerical values:

$$n_{2D} = 2\times10^{14} cm^{-2} eV^{-1} \times 0.026 eV \times \exp\left(-\frac{0.1}{0.026}\right)$$

$$\Rightarrow n_{2D} = 1.1\times10^{11} cm^{-2}$$

4. Consider particles in 3D, with dispersion relation $E = \hbar c|k|$.

(a) Calculate the density of states.

(b) Assume these are bosons. Write down the energy density as a function of wavelength $\lambda = 2\pi/k$. Comment on the result.

(a) The DOS calculation proceeds per the usual prescription. First, the no. of states in a given k-space volume is given by:

$$\Delta N = \frac{\Delta k}{\delta k} \times 2 = \left(\frac{L}{2\pi}\right)^3 \Delta k \times 2$$

The dispersion relation being anisotropic (spherically symmetric), we calculate the no. of states in incremental k-space volume $4\pi k^2 dk$ as $dN = \frac{L^3}{4\pi^3} 4\pi k^2 dk$. Then, the no. of states per unit real space volume (including 2 possible polarizations) is:

$$dn = \frac{2}{8\pi^3} 4\pi k^2 dk = \frac{1}{\pi^2} k^2 dk$$

Then, we can find the density of states as $g = \frac{dn}{dE} = \frac{dn}{dk}\frac{dk}{dE}$. Using the given dispersion relation, we find:

$$g = \frac{k^2}{\pi^2}\frac{1}{\hbar c} = \frac{E^2}{\pi^2 (\hbar c)^3} = \frac{8\pi E^2}{(hc)^3}$$

[Note the difference in the E-dependence of the 3D DOS here vis a vis electrons due to the dispersion relation.]

(b) Now, the average number of particles in these states is given by the Bose-Einstein distribution:

$$f = \frac{1}{e^{E/k_B T} - 1}$$

Putting this together with the DOS, we can find the density of particles as usual:

$$n = \frac{8\pi E^2}{(hc)^3} \frac{1}{e^{E/k_B T} - 1}$$

The dispersion relation gives the energy of each particle. Using this, the energy density is obtained as:

$$u(E) = n \cdot E = \frac{8\pi E^3}{(hc)^3} \frac{1}{e^{E/k_B T} - 1}$$

Now, $u(\lambda) = -u(E) \cdot (dE/d\lambda)$ with $E = hc/\lambda$.

$$\Rightarrow u(\lambda) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda k_B T} - 1}$$

[This is the Planck Blackbody Radiation formula.] ?

5. Consider the free electron Fermi gas in three dimensions (3D). The 3D density-of-states (DOS) for this case is given by $g_{3D}(E) = \frac{1}{2\pi^2}\left(\frac{2m_0}{\hbar^2}\right)^{3/2} E^{1/2}$. Assume $T = 0K$. Suppose $k_F = \sqrt{2m_0 E_F/\hbar^2}$ is the Fermi wavevector and $2a_0$ is the average distance between electrons. Show that $k_F a_0 \square 1$. Provide a physical interpretation for this result.

The standard derivation for $g_{3D}(E)$ gives (see previous)

$$dn = \frac{k^2}{\pi^2} dk$$

At $T = 0K$, all states up to the Fermi vector k_F are occupied, and higher ones are empty. Therefore we can calculate the electron density by integrating up to k_F.

$$n_e = \int_0^{k_F} \frac{k^2}{\pi} dk = \frac{k_F^3}{3\pi^2}$$

Now, if the 'average radius of an electron' is a_0, its volume $v = 4\pi a_0^3/3$.

But, $n_e \sim \frac{1}{v \Rightarrow} n \sim \frac{3a_0^{-3}}{4\pi}$

Therefore, $\frac{k_F^3}{3\pi^2} \sim \frac{3a_0^{-3}}{4\pi} \Rightarrow k_F a_0 \sim 1$

[Note: This says that when we try to confine electrons (or fermion in general) in a smaller volume, their momentum increases. Therefore the pressure of the Fermi gas increases and it exerts a so-called degeneracy pressure to resist confinement. (You could also write down the last equation from the Heisenberg Uncertainty Principle.)]