FYS3400 - Mandatory assignement III

Candidate number: 113

May 26, 2021

Ex1

The text of the exercise provides a basis for the honeycomb lattice related to a 2D graphene sheet that is

$$\mathbf{a}_1 = \frac{3a}{2}\,\mathbf{e}_x + \frac{\sqrt{3}a}{2}\,\mathbf{e}_y \qquad \mathbf{a}_2 = \frac{3a}{2}\,\mathbf{e}_x - \frac{\sqrt{3}a}{2}\,\mathbf{e}_y$$

where $a = 0.142\,\text{nm}$. In addition we know that the energy dispersion relation reads

$$E_{c,v}(\mathbf{k}) = \pm t \left[1 + 4\cos\frac{\sqrt{3}k_y a}{2}\cos\frac{3k_x a}{2} + 4\cos^2\frac{\sqrt{3}k_y a}{2} \right]^{1/2}$$

where the sign in front of t determines whether we are dealing with the valence band (sign "+") or the conduction band (sign "-").
A suitable choice for the basis $(\mathbf{b}_1, \mathbf{b}_2)$ in the reciprocal lattice can be obtained via the relation

$$a_i b_j = 2\pi \delta_{ij} \tag{1}$$

By writing $\mathbf{b}_1$ and $\mathbf{b}_2$ in a general form $\mathbf{b}_1 = c_1 \mathbf{e}'_x + c_2 \mathbf{e}'_y$, $\mathbf{b}_2 = c_1 \mathbf{e}'_x + c_2 \mathbf{e}'_y$ and substituting them into equation 1 one obtains 4 conditions

$$\begin{cases} c_1 \frac{3a}{2} + c_2 \frac{\sqrt{3}a}{2} = 2\pi \\ c'_1 \frac{a}{2} - c'_2 \frac{\sqrt{3}a}{2} = 2\pi \end{cases} \qquad \begin{cases} c'_1 \frac{3a}{2} + c'_2 \frac{\sqrt{3}a}{2} = 0 \\ c_1 \frac{a}{2} - c_2 \frac{\sqrt{3}a}{2} = 0 \end{cases}$$

that lead to

$$c_1 = \frac{2\pi}{3a} \quad c_2 = \frac{2\pi}{\sqrt{3}a} \quad c'_1 = \frac{2\pi}{3a} \quad c'_2 = -\frac{2\pi}{\sqrt{3}a}$$

The reciprocal lattis basis vectors are then

$$\mathbf{b}_1 = \frac{2\pi}{a}\left(\frac{1}{3}\mathbf{e}'_x + \frac{1}{\sqrt{3}}\mathbf{e}'_y\right) \qquad \mathbf{b}_2 = \frac{2\pi}{a}\left(\frac{1}{3}\mathbf{e}'_x - \frac{1}{\sqrt{3}}\mathbf{e}'_y\right)$$

The directions $[0,1], [1,0]$ and $[1,1]$ stand respectively for $\mathbf{b}_2, \mathbf{b}_1$ and $\mathbf{b}_1 + \mathbf{b}_2$.
Let us now introduce the electrons' effective mass in the following way.
If one thinks at the electrons as travelling wave packets, one can derive the group velocity as

$$\mathbf{v}_g = \vec{\nabla}_k\,\omega(\mathbf{k}) = \frac{1}{\hbar}\,\omega(\mathbf{k})$$

where I used the De Broglie relation $E = \hbar\omega$. The electrons' effetive mass m_e^* is such that

$$m_e^*\,\mathbf{v}_g = \mathbf{p} = \hbar\mathbf{k} \tag{2}$$

As can be seen in the last equation, the electrons' effective mass depends on the chosen direction. Hence at this point, one has to invert equation 2 for a precise direction to get the effective mass in that direction. This can be done by taking the scalar product of both members along the desired direction.
By denoting by $\mathbf{u}$ a general vector, the electrons' effective mass along $\mathbf{u}$ becomes

$$m_{e,\mathbf{u}}^* = \hbar^2\,\frac{\mathbf{u}\cdot\mathbf{k}}{\mathbf{u}\cdot\vec{\nabla}_k E(\mathbf{k})} \tag{3}$$

(a)

Figure 1 reports the energy function along $\mathbf{u}_1, \mathbf{u}_2$ and $\mathbf{u}_3$. The green line is the boundary of the conduction band, while the blue one represents the upper limit of the valence band. The energy gap between the conduction band and the valence band varies with k, reaching a minimum of $6\,\text{eV}$ and a maximum of $18\,\text{eV}$.
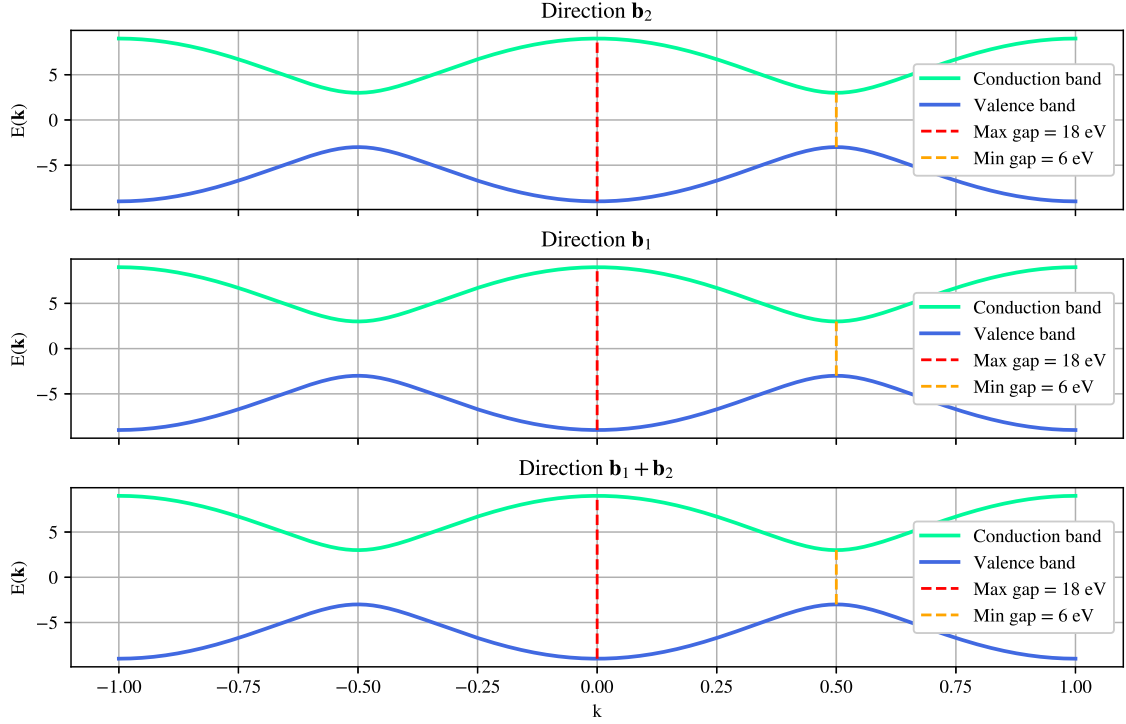
Figure 1: Energy dispersion relation function in a 2D graphene sheet. The first plot corresponds to the direction $\mathbf{b}_1$, the second to the direction $\mathbf{b}_2$ and the third to the direction $\mathbf{b}_1 + \mathbf{b}_2$.

(b)

The gradient of the energy is

$$\vec{\nabla}_k E(\mathbf{k}) = \left(-6a\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\sin\left(\frac{3k_x a}{2}\right), \; -2\sqrt{3}a\sin\left(\frac{\sqrt{3}k_y a}{2}\right) - 4\sqrt{3}a\cos\left(\frac{3k_x a}{2}\right)\sin\left(\frac{\sqrt{3}k_y a}{2}\right) \right)$$

hence by taking the scalar product with $\mathbf{b}_1 = \frac{2\pi}{a}\left(\frac{1}{3}, \frac{1}{\sqrt{3}}\right)$ and inserting into 3 one gets an expression for the mass along $\mathbf{b}_1$ which is plotted in figure 2. Let us take again expression 3 along k_x. In the limit $k_x, k_y \to 0$ the expression asymptotically approaches

$$m^*_{e,\mathbf{k}_x} \approx \hbar^2 \frac{2}{3a^2 t} = 0.839\, m_e$$

The result coincides with the one obtained via the second derivative

$$m^*_{e,\mathbf{k}_x} = \hbar^2 \left(\frac{\partial^2 E(\mathbf{k})}{\partial k_x^2}\right)^{-1} = \hbar^2 \left(\frac{\partial^2 E(\mathbf{k})}{\partial k_y^2}\right)^{-1}$$

Note, however, that this last expression holds only in a neighbourhood of the extremal point of the bands, while equation 3 is a more general expression.
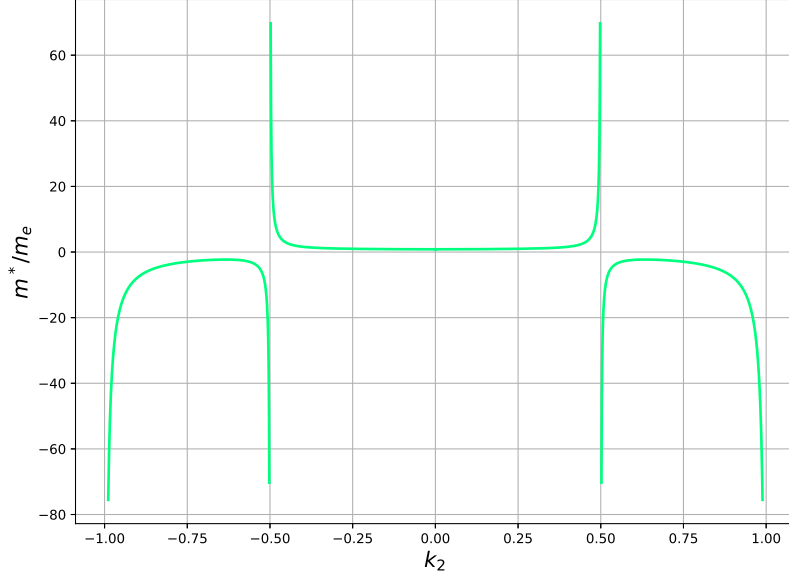Note also that at the edge of the Brillouin zone the mass diverges!

2

Figure 2: Effective electron mass in a 2D graphene sheet along direction [01] of the Brillouin zone

Ex2

The electrons' density of states in the conduction band is

$$D_e(\epsilon) = \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} (\epsilon - E_c)^{1/2}$$

hence the number of intrinsic carriers in the conduction band at temperature T can be calculated as

$$n(T) = \int_{E_C}^{+\infty} D_e(T) \ f_{FD}(T) \ d\epsilon =$$

$$= \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} \int_{E_C}^{+\infty} (\epsilon - E_c)^{1/2} \ \frac{1}{1 + \exp\left((\epsilon - E_f)/k_B T\right)} \ d\epsilon \approx$$

$$\approx \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2}\right)^{3/2} \int_{E_C}^{+\infty} (\epsilon - E_c)^{1/2} \ \exp\left((\epsilon - E_f)/k_B T\right) \ d\epsilon =$$

$$= 2 \left(\frac{m_e k_B T}{2\pi \hbar^2}\right)^{3/2} \exp\left(\frac{E_f - E_C}{k_B T}\right) \equiv N_C \exp\left(\frac{E_f - E_C}{k_B T}\right)$$

In a similar fashion the concentration of holes is

$$p(T) = \int_{E_C}^{+\infty} D_e(T) \ f_{FD}(T) \ d\epsilon =$$

$$= 2 \left(\frac{m_h k_B T}{2\pi \hbar^2}\right)^{3/2} \exp\left(\frac{E_V - E_f}{k_B T}\right) \equiv N_V \exp\left(\frac{E_V - E_f}{k_B T}\right)$$

and one can notice that

$$p(T)n(T) = N_C N_V \exp\left(\frac{E_V - E_C}{k_b T}\right) \equiv n_i^2(T)$$

For intrinsic carriers one has that $n(T) = p(T) = n_i(T)$, while in general

$$n(T) = n_i(T) \exp\left(\frac{E_f - E_i}{k_B T}\right) \tag{4}$$

$$p(T) = n_i(T) \exp\left(\frac{E_i - E_f}{k_B T}\right) \tag{5}$$

These expression give the number of conduction electrons as a function of temperature. To obtain the expression of the fermi energy it is convenient to make use of the *Mass-Action law*. In a doped

semiconductor the Mass-Action law estabilishes that

$$N_D^+ + p = N_A^- + n$$

or, in the case of $N_A^- = 0$ as in this case

$$N_D^+ + p = n \tag{6}$$

The number of ionized donors at temperature T is given by

$$N_D^+ = N_D \left(1 - \frac{1}{1 + \frac{1}{2} \exp\left(\frac{E_D - E_f}{k_B T}\right)} \right) = \frac{N_D}{1 + 2 \exp\left(\frac{E_f - E_D}{k_B T}\right)}$$

hence equation 6 becomes

$$n_i(T) \exp\left(\frac{E_f - E_i}{k_B T}\right) + \frac{N_D}{1 + 2 \exp\left(\frac{E_f - E_D}{k_B T}\right)} - n_i(T) \exp\left(\frac{E_i - E_f}{k_B T}\right) = 0$$

or

$$2\, n_i(T) \sinh\left(\frac{E_f - E_i}{k_B T}\right) + \frac{N_D}{1 + 2 \exp\left(\frac{E_f - E_D}{k_B T}\right)} = 0$$

This equation can be solved numerically for E_f, the value of which can be popped into 4 to obtain the concentration of conducting electrons. The energy E_i called the *intrinsic Fermi energy* is a function of the effective mass of the electrons and holes in the semiconductor. It can be easily calculated in the intrinsic case by imposing $n(T) = p(T)$. After some algebra one gets that

$$E_i = \frac{1}{2} E_g + \frac{3}{4} k_B T \log\left(\frac{m_h}{m_e}\right)$$

Approximation

Low temperature

In the regime of low temperature, in first approximation, all the electrons in the conduction band come from ionized impurities since they are higher in energy than the electrons in the valence band. Hence, for low T:

$$n(T) \approx N_D^+(T)$$

which means that equation 6 requests

$$N_D \left(1 - \frac{1}{1 + \exp\left((E_D - E_f)/k_B T\right)} \right) = 2 \left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{E_f - E_C}{k_B T}\right)$$

Medium temperature

For medium temperature all the impurities are ionized and only few electrons are excited from the valence band, hence

$$n(T) \approx N_D$$

High temperature

Finally, for high temperature, impurities and intrinsic donors both contribute to the number of electrons, but the number of intrinsic carries is normally way greater than the number of impurities addded, hence

$$n(T) \approx n_i(T)$$