ECE 4070: Homework 7 solutions (By Farhan Rana)

Problem 7.1 (Conductivity tensor of germanium)

For the pocket at $(\pi/a, \pi/a, \pi/a)$ we have:

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t & 1/3m_\ell - 1/3m_t \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

This pocket's inverse effective mass tensor will serve as the reference. Now, for the pocket at $(-\pi/a, -\pi/a, \pi/a)$ it was shown that:

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t & -(1/3m_\ell - 1/3m_t) \\ 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) \\ -(1/3m_\ell - 1/3m_t) & -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

Now we look at the pocket at $(-\pi/a, \pi/a, \pi/a)$. If we let E_x become $-E_x$ then in the current density contributed from the pocket at $(-\pi/a, \pi/a, \pi/a)$ we should see J_x become $-J_x$ and J_y and J_z should remain the same. This can only happen if the inverse mass tensor for the pocket at $(-\pi/a, \pi/a, \pi/a)$ is,

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) & -(1/3m_\ell - 1/3m_t) \\ -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t & 1/3m_\ell - 1/3m_t \\ -(1/3m_\ell - 1/3m_t) & 1/3m_\ell - 1/3m_t & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

Now we look at the pocket at $(\pi/a, -\pi/a, \pi/a)$. If we let E_y become $-E_y$ then in the current density contributed from the pocket at $(\pi/a, -\pi/a, \pi/a)$ we should see J_y become $-J_y$ and J_x and J_z should remain the same. This can only happen if the inverse mass tensor for the pocket at $(\pi/a, -\pi/a, \pi/a)$ is,

$$M^{-1} = \begin{bmatrix} 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) & 1/3m_\ell - 1/3m_t \\ -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t & -(1/3m_\ell - 1/3m_t) \\ 1/3m_\ell - 1/3m_t & -(1/3m_\ell - 1/3m_t) & 1/3m_\ell + 2/3m_t \end{bmatrix}$$

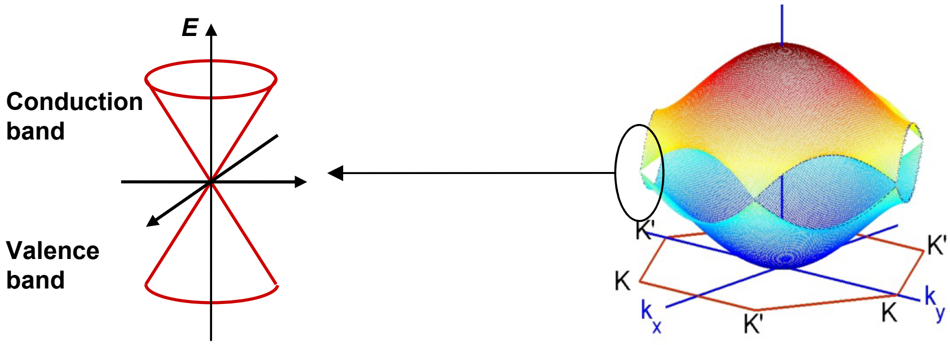
Now we add contributions from all pockets to get the expression for the total current density:

$$\begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} = \overline{\overline{\sigma}} \cdot \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

$$\overline{\overline{\sigma}} = n\, e^2\, \tau \begin{bmatrix} 1/3\, m_\ell + 2/3\, m_t & 0 & 0 \\ 0 & 1/3\, m_\ell + 2/3\, m_t & 0 \\ 0 & 0 & 1/3\, m_\ell + 2/3\, m_t \end{bmatrix}$$

Conductivity tensor is diagonal and isotropic!! This is the case for all materials with cubic symmetry (which includes FCC, BCC, SC).

Problem 7.2:



a) $\vec{v}(\vec{k}) = \frac{1}{\hbar}\nabla_{\vec{k}} E(\vec{k}) = v \, \frac{\vec{k}-\vec{k}_o}{\left|\vec{k}-\vec{k}_o\right|}$

b)

$$n = 2\times 2\times \int_{\text{near } \vec{k}_o} \frac{d^2\vec{k}}{(2\pi)^2} \, f\left(E(\vec{k}) - E_f\right)$$

$$\textbf{Let:} \quad \vec{q} = \vec{k} - \vec{k}_o \quad \Rightarrow \quad E(\vec{q}) = \hbar \, v \, q$$

$$n = 2\times 2\times \int_{\text{near } \vec{q}=0} \frac{d^2\vec{q}}{(2\pi)^2} \, f\left(E(\vec{q}) - E_f\right) = \frac{2}{\pi}\int_0^\infty q\, dq \;\; f\left(E(\vec{q}) - E_f\right)$$

$$= \frac{2}{\pi}\int_0^\infty q \left|\frac{dq}{dE}\right| dE \; f(E - E_f) = \frac{2}{\pi \, (\hbar v_o)^2}\int_0^\infty E \, dE \; f(E - E_f)$$

$$\Rightarrow g(E) = \frac{2\,E}{\pi \, (\hbar v)^2}$$

In the factor of 2x2, one factor of 2 comes from the spin and one factor of 2 comes from the 2 full electron pockets in the FBZ.

c) PTO

$$\vec{J} = -e \times 2 \times 2 \times \int_{\text{near } \vec{k}_o} \frac{d^2\vec{k}}{(2\pi)^2} \; f\left(\vec{k} + \frac{e\tau\,\vec{E}}{\hbar}\right) \vec{v}(\vec{k})$$

$$\text{Let :} \quad \vec{q} = \vec{k} - \vec{k}_o \quad \Rightarrow \quad E(\vec{q}) = \hbar\, v\, q \quad \Rightarrow \quad \vec{v}(\vec{q}) = v\,\hat{q} = v\,\frac{\vec{q}}{[\vec{q}]}$$

$$\vec{J} = -4e \times \int_{\text{near } \vec{q}=0} \frac{d^2\vec{q}}{(2\pi)^2} \; f\left(\vec{q} + \frac{e\tau\,\vec{E}}{\hbar}\right) \vec{v}(\vec{q})$$

$$= -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\,\vec{v}\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)$$

$$= -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)}{\left|\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right|} = -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)}{\sqrt{\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right) . \left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)}}$$

$$\approx -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)}{\sqrt{q^2 - 2\frac{e\tau\,\vec{q}\,.\,\vec{E}}{\hbar}}} = -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)}{q\left(1 - \frac{e\tau\,\vec{q}\,.\,\vec{E}}{q^2\hbar}\right)}$$

$$\vec{J} = -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(\vec{q} - \frac{e\tau\,\vec{E}}{\hbar}\right)\left(1 + \frac{e\tau\,\vec{q}\,.\,\vec{E}}{q^2\hbar}\right)}{q}$$

$$= -4e \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(-\frac{e\tau\,\vec{E}}{\hbar} + \frac{e\tau\,\vec{q}\left[\vec{q}\,.\,\vec{E}\right]}{q^2\hbar}\right)}{q}$$

$$= \frac{4e^2\tau}{\hbar} \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q})\, v \frac{\left(\vec{E} - \frac{\vec{q}\left[\vec{q}\,.\,\vec{E}\right]}{q^2}\right)}{q}$$

There is something interesting about the expression above. It tells us that only those electrons who have a q-vector component perpendicular to the electric field contribute to the current density. The easiest way to proceed from here is to assume that the electric field is the x-direction (without loosing generalization – since current density the response will be isotropic).

$$\vec{J} = \frac{4e^2\tau}{\hbar} \times \int \frac{d^2\vec{q}}{(2\pi)^2} \; f(\vec{q}) \frac{v}{q} \left(\vec{E} - \frac{\vec{q}\,[\vec{q} \,.\, \vec{E}]}{q^2} \right)$$

$$= \frac{4e^2\tau}{\hbar} \times \int \frac{q\, d\theta\, dq}{(2\pi)^2} \; f(\vec{q}) \frac{v}{q} \left(1 - \cos^2\theta\right) E_x \hat{x}$$

$$= \frac{e^2\tau}{\pi\,\hbar} \times \int_0^\infty \left|\frac{dq}{dE}\right| dE\, f(E - E_f) \; v\, E_x \hat{x}$$

$$= \frac{e^2\tau}{\pi\,\hbar^2} \times \int_0^\infty dE\, f(E - E_f) \; E_x \hat{x} = \sigma\, E_x \hat{x}$$

$$\Rightarrow \quad \sigma = \frac{e^2\tau}{\pi\,\hbar^2} \times \int_0^\infty dE\, f(E - E_f)$$

d) Comparing the result in (b) with that in (c) it is seen from the energy integrals that the current density is not directly proportional to the electron density.

e) In response to an electric field the electrons in graphene change their direction of motion (but not their speed). This is also why the electrons that had a larger component of their initial velocity perpendicular to the electric field contributed the most to the conductivity.

Problem 7.3

a) $\omega_B = \dfrac{2\pi}{T}$

The time period T is the time taken by the electron moving in k-space in the negative x-direction to traverse the FBZ (from the X-point $(2\pi/a, 0, 0)$ to the X-point $(-2\pi/a, 0, 0)$ covering a total distance of $4\pi/a$ in k-space. This will take time equal to: $4\pi\,\hbar/a\,e\,E_x$.

$$\omega_B = \frac{2\pi}{T} = \frac{a\,e\,E_x}{2\,\hbar}$$

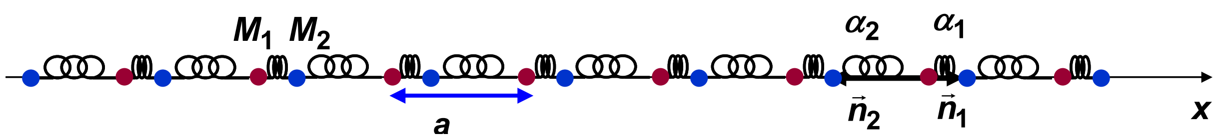
b) We have,

$$\omega_B = \frac{2\pi}{T} = \frac{a\,e\,E_x}{2\,\hbar} = 2.14 \times 10^{13} \text{ rad/s}$$

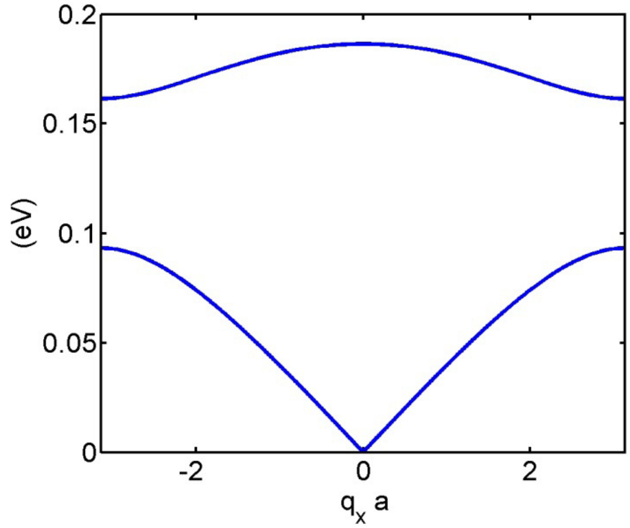
$T = 294$ fs.

Therefore, electrons will not complete even a single period before they are scattered.

Problem 7.4:

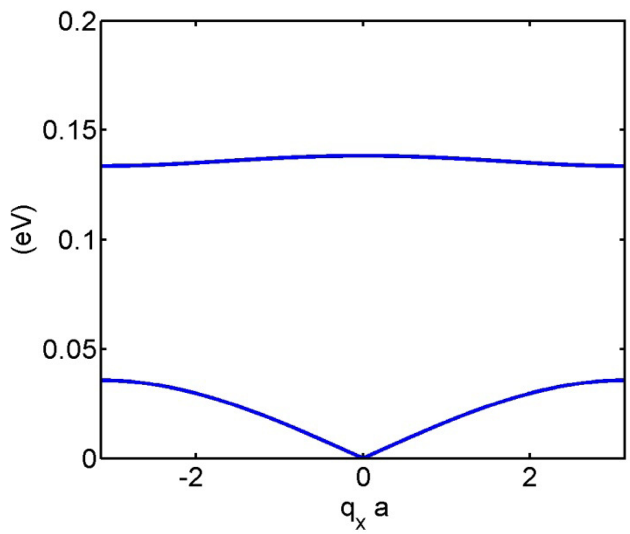


a)



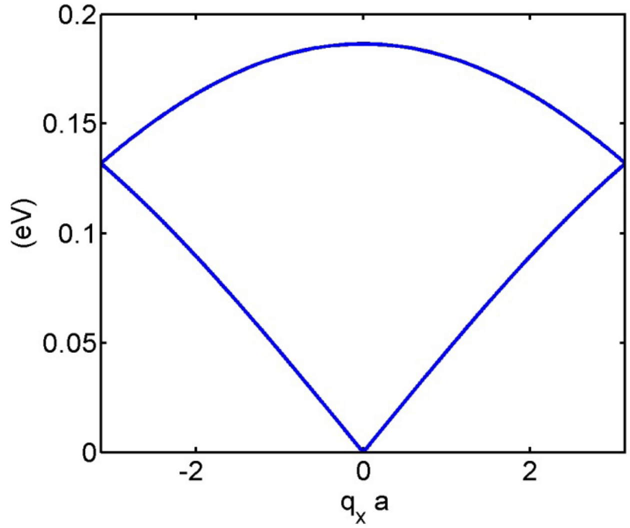
b) Sound velocity is 18.37 km/s.

c)



d) The sound velocity is 7.83 km/s.

e)



There is no gap between the acoustic and optical phonon modes.

f) For $\alpha_1 = \alpha_2$ **and** $M_2 = M_1$ the crystal can be thought of as one with a monoatomic basis but with a primitive cell that is half the size and a FBZ that is double the size. This crystal will only have one acoustic phonon band. What you are seeing in the figure above as an optical phonon band is in fact that one acoustic phonon band folded over in the smaller BZ and so there is no gap.