ECE 4070: Physics of Semiconductor and Nanostructures

Spring 2014

Homework 7   **Due on April 15, 2014 at 5:00 PM**

Suggested Readings and Second Prelim:

a) Lecture notes
b) Date for second prelim: April 17

Problem 7.1 (Conductivity tensor of Germanium)

In germanium conduction band, there are 8 half electron pockets, or 4 full electron pockets, in the FBZ. Assume that the total electron density in all pockets is n and the scattering time is τ. Find the conductivity tensor of germanium and include contributions from all pockets.

Hint: To find the answer you will have to figure out the individual conductivity tensors for all the pockets separately in the un-rotated standard x,y,z co-ordinate system and then add them up. This can be tricky and simple symmetry considerations can help. We know that the inverse effective mass tensor for the pocket located at $(\pi/a, \pi/a, \pi/a)$ is as given in the handout,

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

And for this pocket,

$$
\begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} = \frac{n}{4} e^2 \tau\, M^{-1} \cdot \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}
$$

Assume 4 full pockets in the FBZ. Now suppose, I need to find the tensor for the pocket located at $(-\pi/a, -\pi/a, \pi/a)$. I argue that if I let E_x become $-E_x$ and E_y become $-E_y$ then in the current density contributed from the pocket at $(-\pi/a, -\pi/a, \pi/a)$ I should see J_x become $-J_x$ and J_y become $-J_y$ but J_z should remain J_z (these arguments follow from the symmetry of the two pockets with respect to the *xyz* co-ordinate system). This can only happen if the inverse mass tensor for the pocket at $(-\pi/a, -\pi/a, \pi/a)$ is,

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

You need to use similar symmetry arguments and find the conductivity (or inverse effective mass) tensors for all pockets and then add them up to find the conductivity tensor for germanium.

Problem 7.2: (Graphene: Statistics and current for non-parabolic bands)

Expressions for the conductivity in semiconductors with non-parabolic bands can take unfamiliar forms. In this problem we will look at graphene.

Graphene has six conduction band minima in the FBZ (refer to the handout on graphene bandstructure and the diagram below). That means it has 6 electron pockets. However, 1/3 of each pocket is inside the FBZ and 2/3 is outside the FBZ. So graphene has only 2 complete pockets in the FBZ. This situation is somewhat similar to that in Germanium.
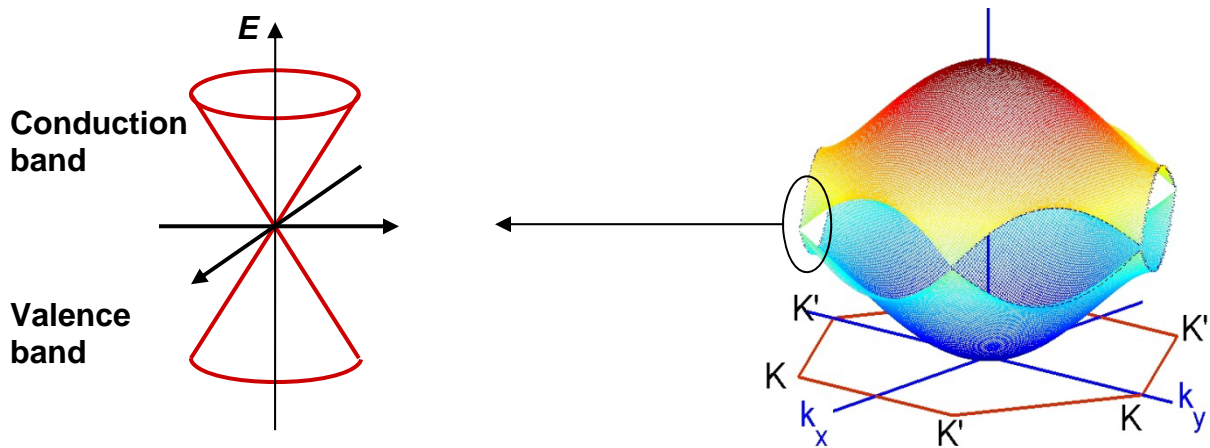
Near the conduction band minima in graphene the dispersion relation cannot be Taylor expanded but can still be written in a simple form (assuming the zero of energy is chosen such that the band edge energy is zero, i.e. $E_p = 0$).

$$E(\vec{k}) = \hbar \, v \left| \vec{k} - \vec{k}_o \right| = \hbar \, v \sqrt{(k_x - k_{ox})^2 + (k_y - k_{oy})^2}$$

The value of the parameter v is 10^6 m/s. You can see that the energy dispersion in non-analytic right at the band edge.

NOTE: It might be beneficial for you to redefine the k-space coordinate system such that the zero wavevector is where the band minimum is located when doing integrals.

a) Find an expression for the electron velocity vector $\vec{v}(\vec{k})$ in graphene near the band edge. What is the magnitude of $\vec{v}(\vec{k})$?

b) Write an expression for the total electron density in graphene in the form:

$$n = \int_0^\infty dE \, g(E) \, f(E - E_f)$$

and be sure to include contributions from all valleys (pockets) and spin. What is the density of states function $g(E)$?

c) Now suppose an E-field $\vec{E}$ is applied to graphene. The scattering time is τ. You need to find an expression for the current density $\vec{J}$. In general, the current density for non-parabolic bands is not linearly related to the electric field $\vec{E}$. **However, for small electric fields one can keep the terms that are of first order in the electric field.** In this small-field limit, show that:

$$\vec{J} = \sigma \, \vec{E}$$

and

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

Hint: The dynamical equation for the crystal momentum still holds. Be sure to include contributions from all valleys and spin. Be sure to CAREFULLY select and keep terms that are of first order in the electric field. Your answer will be correct if you get all factors of 2, π, etc. correct.

d) Argue that the conductivity in graphene is not directly proportional to the electron density as is the case in most other semiconductors that have parabolic energy dispersions near the band edges.

e) If you did part (a) correctly, you would have found that $\left|\vec{v}(\vec{k})\right|$ for all electrons in graphene is the same and equals v irrespective of the wavevector. So all electrons in graphene always move with the same speed. Therefore, an externally applied field can never change the speed of the carriers. Explain then how is the field able to generate current in graphene?

Problem 7.3 (Bloch Oscillations in GaAs)

Consider a GaAs crystal with a lattice constant of 5.65 Angstroms. Suppose an electric field, $\vec{E} = E_x \hat{x}$, is applied from outside.

a) Assuming no scattering, what is the frequency ω_B of Bloch oscillations? Caution: don't blindly copy the 1D formula from notes. Consider carefully the dimensions of the FBZ of GaAs and figure out what is happening.

b) Assuming a typical scattering time of 100 fs and a maximum electric field of 5e7 V/m that one can apply in GaAs without breaking it, find if electrons can or can not complete one period of a Bloch oscillation before they scatter.

Problem 7.4: (Phonons in a 1D crystal)
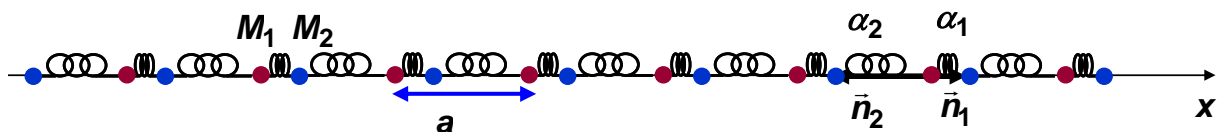
Consider a 1D crystal with two atoms in the primitive cell. The mass M_1 equals 2×10^{-26} kg. The nearest neighbor vectors are:

$$\vec{n}_1 = \frac{a}{4}\,\hat{x} \qquad \vec{n}_2 = -\frac{3\,a}{4}\,\hat{x}$$

The force constants are:

$$\alpha_1 = 600 \text{ N/m} \qquad \alpha_2 = 200 \text{ N/m}$$

And the size of the primitive cell is:

$$a = 3 \text{ Angstroms}$$

Case I: Assume $M_2 = M_1$.

a) Calculate and plot (using Matlab or Mathematica) the optical and acoustic phonon bands in the entire FBZ (i.e. $-\pi \le q_x a \le \pi$).

b) What is the velocity of sound in the crystal in m/s?

Case II: Assume $M_2 = 10\, M_1$.

c) Calculate and plot (using Matlab or Mathematica) the optical and acoustic phonon bands in the entire FBZ (i.e. $-\pi \le q_x a \le \pi$).

d) What is the velocity of sound in the crystal in m/s?

Case III: Now assume $\alpha_1 = \alpha_2 = 400$ N/m and $M_2 = M_1 = 2 \times 10^{-26}$ kg.

e) Calculate and plot (using Matlab or Mathematica) the optical and acoustic phonon bands in the entire FBZ (i.e. $-\pi \le q_x a \le \pi$). Do you see any major qualitative difference compared to parts (a) and (c)?

f) If you did part (e) correctly, you should have seen zero bandgap between the optical and acoustic bands Can you explain physically why the bandgap is zero?