Physics 195 / Applied Physics 195 — Assignment #6  
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Date: Oct. 25, 2017  
Due: 12:45pm + 10 min grace period, Nov. 3, 2017 at the dropbox outside Maxwell-Dworkin Room 131.

**Problem 1 (130 pt): Nearly free electron model**

Consider a 2D square lattice crystal with a lattice constant $a$ (one atom per unit cell). Let the periodic potential energy for an electron propagating in this crystal be given by:

$$V(x, y) = A \left[ \cos \left( \frac{2\pi x}{a} \right) + \cos \left( \frac{2\pi y}{a} \right) \right]$$

with $A > 0$.

(a) Draw the 1st, 2nd, 3rd, and 4th Brillouin zones in the Bloch $\mathbf{k}$-space.

(b) By using the nearly free electron approximation, calculate all single-electron energy eigenvalues at the mid point of each edge of the 1st Brillouin zone boundary to the first non-vanishing order. What is the band gap at these points?

(c) Again resorting to the nearly free electron approximation, evaluate all single-electron energy eigenvalues at each corner of the 1st Brillouin zone boundary to the first non-vanishing order.

(d) Assume that this 2D crystal is made out of divalent atoms (two valence electrons per atom). This 2D crystal can be a metal or an insulator depending on whether bands overlap or not. Show that the condition for this crystal to be a metal is given by

$$A < \frac{\hbar^2 \pi^2}{3ma^2}$$

where $m$ is the intrinsic electron mass. Assume that $A < h^2 \pi^2/(ma^2)$.

**Problem 2 (130 pt): Effective mass tensor $M^{-1}$ and collective mass tensor $m_{col}^{-1}$**

(a) Gallium arsenide (GaAs) has a sole conduction band minimum lying at the center of the 1st Brillouin zone (no valley degeneracy) with isotropic quadratic dispersion $\epsilon(\mathbf{k}) = \hbar^2 k^2/(2m^*)$ around this minimum point where $m^* = 0.067m_0$. Show that

$$m_{col}^{-1} = M^{-1} = \begin{pmatrix} 1/m^* & 0 & 0 \\ 0 & 1/m^* & 0 \\ 0 & 0 & 1/m^* \end{pmatrix}.$$  

In this case, $\mathbf{J}||\mathbf{E}$ evidently ($\mathbf{J}$: current density; $\mathbf{E}$: electric field applied).

(b) Consider electron-doped graphene ($\epsilon_F > 0$). There are two conduction band valleys (valley indices: $v = 1$ and $2$) around the two Dirac points $\mathbf{K}$ and $\mathbf{K}'$ at two corners of the 1st Brillouin zone (Homework #5). In these valleys, we have isotropic but non-quadratic dispersions, $\epsilon_{v=1}(\mathbf{k}) = \hbar v_F |\mathbf{k} - \mathbf{K}|$ and $\epsilon_{v=2}(\mathbf{k}) = \hbar v_F |\mathbf{k} - \mathbf{K}'|$. 

- Show that

$$(m_{col}^{-1})_{v=1} = (m_{col}^{-1})_{v=2} = \begin{pmatrix} v_F^2/\epsilon_F & 0 \\ 0 & v_F^2/\epsilon_F \end{pmatrix},$$

assuming $\epsilon_F \gg k_B T$ and treating the Fermi-Dirac distribution as a step function. Note that $\mathbf{J}_{v=1}||\mathbf{E}$, $\mathbf{J}_{v=2}||\mathbf{E}$, and $\mathbf{J}||\mathbf{E}$ (where $\mathbf{J} = \mathbf{J}_{v=1} + \mathbf{J}_{v=2}$). That is, each valley current is parallel to the applied field, and so is the total current. This is because each valley’s energy dispersion is isotropic.
• Calculate the effective mass tensor \((M^{-1})_v\) at each valley and check that

\[
(m_{\text{col}}^{-1})_v \neq (M^{-1})_v
\]

for either \(v = 1\) or \(v = 2\).

• Show that the conductivity and mobility of graphene are given by

\[
\sigma = \frac{e^2 \epsilon_F \tau}{\hbar^2 \pi}, \quad \mu = \frac{e \epsilon_F \tau}{\hbar^2 \pi n_0}
\]

where \(n_0\) is the density of conduction-band electrons and \(\tau\) is the electron scattering time.

• Show that acceleration \(\vec{a}\) of an individual electron due to an external force \(\vec{F}\) is either zero or perpendicular to the electron velocity \(\vec{v}\). From this, argue that the magnitude of the individual graphene electron velocity is maintained at a constant value of \(v_F\) (which is \(\sim 10^6 \text{ m/s}\)).

(c) Silicon has six conduction band minimum valleys along six \{100\} directions (We will see this in detail in Lecture #14). In each valley, the electron energy dispersion is quadratic, but anisotropic with transversal effective mass \(m_T^* = 0.19m_0\) and longitudinal effective mass \(m_L^* = 0.98m_0\). Take an example of the valley lying along the positive (100) direction (say \(v = 1\)); the energy dispersion there is given by

\[
\epsilon_{v=1}(\vec{k}) = \epsilon_c + \frac{\hbar^2 (k_x - k_{x,0})^2}{2m_L^*} + \frac{\hbar^2 (k_y - k_{y,0})^2}{2m_T^*} + \frac{\hbar^2 (k_z - k_{z,0})^2}{2m_T^*}.
\]

where \((k_{x,0}, k_{y,0}, k_{z,0})\) is the center of this valley and \(\epsilon_c\) is the valley energy minimum. Show that \((m_{\text{col}}^{-1})_v = (M^{-1})_v\) for each valley. Show that \((m_{\text{col}}^{-1})_v\) is diagonal but with non-identical diagonal elements. This means that \(\vec{J}_v \parallel \vec{E}\). Show that overall \(m_{\text{col}}^{-1}\) that corresponds to the overall conductivity that takes into account all six conduction band valleys is given by

\[
m_{\text{col}}^{-1} = \begin{pmatrix}
(1/3)(1/m_L^* + 2/m_T^*) & 0 & 0 \\
0 & (1/3)(1/m_L^* + 2/m_T^*) & 0 \\
0 & 0 & (1/3)(1/m_L^* + 2/m_T^*)
\end{pmatrix}.
\]

This is diagonal with identical diagonal elements. Thus, \(\vec{J} \parallel \vec{E}\). So the valley currents, each of which is not parallel to \(\vec{E}\), add up to create a total current that is parallel to \(\vec{E}\). Note that \([(1/3)(1/m_L^* + 2/m_T^*)]^{-1}\) is the mass you should use in the conductivity calculation for conduction electrons in silicon. Calculate this mass numerically.

Problem 3 (140 pt): Cyclotron resonance of Bloch electrons

The semiclassical motion of a Bloch electron subjected to a static magnetic field \(\vec{B} = B_0 \hat{z}\) is described by

\[
\hbar \frac{d\vec{k}}{dt} = -e\vec{v}(\vec{k}) \times B_0 \hat{z},
\]

where \(\vec{k}\) is the Bloch wave vector and \(\vec{v}(\vec{k})\)—the electron velocity—is given by

\[
\vec{v}(\vec{k}) = \frac{1}{\hbar} \vec{\nabla}_k \epsilon(\vec{k}).
\]

Here \(\epsilon(\vec{k})\) is the electron energy dispersion in a band of concern.

(a) Prove that \(k_z\) and \(\epsilon(\vec{k})\) are constants of motion. Thus \(\vec{k}(t)\) of the Bloch electron with \(k_z(t = 0) = k_{z,0}\) and \(\epsilon(t = 0) = \epsilon_0\) will lie on the closed-loop curve \(C\) that is the intersection of energy contour \(\epsilon(\vec{k}) = \epsilon_0\) and
plane \( k_z = k_{z,0} \).

(b) Show that the Lorentz force \( \vec{F} = -e\vec{v}(\vec{k}) \times \vec{B}_0 \hat{z} \) is always tangential to the curve \( C \) and \( \vec{k}(t) \) traces \( C \) in the counter-clockwise direction (when viewed down from the \( k_z = +\infty \) point).

(c) Show that the angular frequency of rotation (cyclotron resonance frequency) of \( \vec{k}(t) \) around \( C \) is

\[
\omega_c = \frac{2\pi e B_0}{\hbar^2} \left[ \frac{\partial A(\epsilon, k_{z,0})}{\partial \epsilon} \right]_{\epsilon = \epsilon_0}^{-1}
\]

where \( A(\epsilon_0, k_{z,0}) \) is the area encircled by the curve \( C \). By comparing this to the cyclotron resonance frequency of a free electron, argue that the cyclotron effective mass can be defined as

\[
m_c = \frac{\hbar^2}{2\pi} \left[ \frac{\partial A(\epsilon, k_{z,0})}{\partial \epsilon} \right]_{\epsilon = \epsilon_0}
\]

(d) For

\[
\epsilon(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2} + \frac{\hbar^2 k_z^2}{2m_3},
\]

show that the cyclotron mass is given by \( m_c = \sqrt{m_1^3 m_2^3} \) for \( \vec{B} = B_0 \hat{z} \).

(e) Let a static magnetic field \( B_0 = 0.1 \) T be applied to a silicon sample along the \( z \) direction. Calculate all possible cyclotron resonance frequencies due to conduction electrons.

(f) For a graphene electron exhibiting the cyclotron resonance at the energy contour at the Fermi level \( \epsilon_F > 0 \) (electron-doped graphene) near the Dirac point \( \vec{K} \) with the dispersion relation \( \epsilon(\vec{k}) = \hbar v_F |\vec{k} - \vec{K}| \), show that \( m_c = \epsilon_F / v_F^2 \).

(g) From Parts 3(f) and part 2(b), notice that in graphene \( m_c \) at the Fermi level is the same as the inverse of any identical diagonal element of the collective mass tensor \( m_{col}^{-1} \) derived under \( k_B T \ll \epsilon_F \). Show that this identity holds more generally for any conductor (either 2D and 3D) as far as the electronic band is isotropic, that is, \( \epsilon(\vec{k}) = \epsilon(k) \).