Physics 195 / Applied Physics 195 — Assignment #6
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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:

$$V(x,y) = A\left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right)\right] \tag{1}$$

with $A > 0$.

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

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

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

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 $\epsilon(\vec{k}) = \hbar^2k^2/(2m^*)$ around this minimum point where $m^* = 0.067m_0$. Show that

$$m_{col}^{-1} = M^{-1} = \begin{pmatrix} 1/m^* & 0 & 0 \\ 0 & 1/m^* & 0 \\ 0 & 0 & 1/m^* \end{pmatrix}. \tag{3}$$

In this case, $\vec{J}||\vec{E}$ evidently ($\vec{J}$: current density; $\vec{E}$: 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 $\vec{K}$ and $\vec{K}'$ at two corners of the 1st Brillouin zone (Homework #5). In these valleys, we have isotropic but non-quadratic dispersions, $\epsilon_{v=1}(\vec{k}) = \hbar v_F|\vec{k}-\vec{K}|$ and $\epsilon_{v=2}(\vec{k}) = \hbar v_F|\vec{k}-\vec{K}'|$.

- Show that

$$(m_{col}^{-1})_{v=1} = (m_{col}^{-1})_{v=2} = \begin{pmatrix} v_F^2/\epsilon_F & 0 \\ 0 & v_F^2/\epsilon_F \end{pmatrix}, \tag{4}$$

  assuming $\epsilon_F \gg k_BT$ and treating the Fermi-Dirac distribution as a step function. Note that $\vec{J}_{v=1}||\vec{E}$, $\vec{J}_{v=2}||\vec{E}$, and $\vec{J}||\vec{E}$ (where $\vec{J} = \vec{J}_{v=1} + \vec{J}_{v=2}$). 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

$$(m_{col}^{-1})_v \neq (M^{-1})_v \tag{5}$$

for either $v = 1$ or $v = 2$.

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

$$\sigma = \frac{e^2 \epsilon_F \tau}{\hbar^2 \pi}; \tag{6}$$

$$\mu = \frac{e \epsilon_F \tau}{\hbar^2 \pi n_0}. \tag{7}$$

where n_0 is the density of conduction-band electrons and τ 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 $\sim 10^6$ 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

$$\epsilon_{v=1}(\vec{k}) = \epsilon_c + \frac{\hbar^2(k_x - k_{x,0}^{v=1})^2}{2m_L^*} + \frac{\hbar^2(k_y - k_{y,0}^{v=1})^2}{2m_T^*} + \frac{\hbar^2(k_z - k_{z,0}^{v=1})^2}{2m_T^*}. \tag{8}$$

where $(k_{x,0}^{v=1}, k_{y,0}^{v=1}, k_{z,0}^{v=1})$ is the center of this valley and ϵ_c is the valley energy minimum. Show that $(m_{col}^{-1})_v = (M^{-1})_v$ for each valley. Show that $(m_{col}^{-1})_v$ is diagonal but with non-identical diagonal elements. This means that $\vec{J}_v \not\parallel \vec{E}$. Show that *overall* m_{col}^{-1} that corresponds to the overall conductivity that takes into account all six conduction band valleys is given by

$$m_{col}^{-1} = \begin{pmatrix} (1/3)(1/m_L^* + 2/m_T^*) & 0 & 0 \\ 0 & (1/3)(1/m_L^* + 2/m_T^*) & 0 \\ 0 & 0 & (1/3)(1/m_L^* + 2/m_T^*) \end{pmatrix}. \tag{9}$$

This is diagonal with identical diagonal elements. Thus, $\vec{J}||\vec{E}$. 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

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{v}(\vec{k}) \times B_0\hat{z}, \tag{10}$$

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

$$v(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\epsilon(\vec{k}). \tag{11}$$

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 $\vec{F} = -e\vec{v}(\vec{k}) \times B_0\hat{z}$ 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

$$\omega_c = \frac{2\pi e B_0}{\hbar^2}\left[\frac{\partial A(\epsilon, k_{z,0})}{\partial \epsilon}|_{\epsilon=\epsilon_0}\right]^{-1} \tag{12}$$

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

$$m_c = \frac{\hbar^2}{2\pi}\frac{\partial A(\epsilon, k_{z,0})}{\partial \epsilon}|_{\epsilon=\epsilon_0} \tag{13}$$

(d) For

$$\epsilon(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + \frac{\hbar^2 k_z^2}{2m_3^*}, \tag{14}$$

show that the cyclotron mass is given by $m_c = \sqrt{m_1^* m_2^*}$ 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 $k_BT \ll \epsilon_F$. Show that this identity holds more generally for any conductor (either 2D and 3D) as far as the electronic band is isotropic, that is, $\epsilon(\vec{k}) = \epsilon(k)$.