Applied Physics 195 / Physics 195 — Assignment #8

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Due: **5pm SHARP (4:50pm + 10 min grace period)**, November 23rd, 2015; slide your work under through the door at Maxwell-Dworkin Room 131.

Problem 1 (40 pt; no collaboration): Dynamics of individual electrons in graphene

Calculate the effective mass tensor $(M^{-1})_{ij}$ for an individual graphene electron at state $\vec{k}$ near a Dirac point. Show that acceleration $\vec{a}$ 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 has been demonstrated to be $\sim 10^6$ m/s).

Problem 2 (200 pt): Tensors for conductivity and collective mass

In Lecture #17, in calculating the electrical conductivity and associated collective electron mass (a.k.a., plasmonic mass) of a conductor, we assumed that an electric field will produce a net overall current only along the direction of the field. This is certainly widely observed. Nonetheless, we do not have to assume $\vec{J}||\vec{E}$ *a priori*. We can calculate the general conductivity tensor σ_{ij} $(i, j = 1, 2, 3;$ subscripts 1, 2, and 3 represent x, y, and z) that relates electric field $\vec{E} = (E_1, E_2, E_3)$ and current density $\vec{J} = (J_1, J_2, J_3)$ via

$$J_i = \sum_{j=1}^{3} \sigma_{ij} E_j \quad (i = 1,\, 2,\, 3). \tag{1}$$

The associated collective mass (per electron) tensor $(M_p^{-1})_{ij}$ would then be given by

$$\sigma_{ij} = n_0 e^2 \tau (M_p^{-1})_{ij}, \tag{2}$$

where n_0 is the density of electrons in a given conduction band of concern with Fermi level ϵ_F and τ is the electron scattering time. If $\vec{J}||\vec{E}$, σ_{ij} and $(M_p^{-1})_{ij}$ will be diagonal with identical diagonal components, and can be expressed as

$$M_p^{-1} = \begin{pmatrix} 1/m_p & 0 & 0 \\ 0 & 1/m_p & 0 \\ 0 & 0 & 1/m_p \end{pmatrix} \tag{3}$$

$$\sigma = \begin{pmatrix} n_0 e^2 \tau / m_p & 0 & 0 \\ 0 & n_0 e^2 \tau / m_p & 0 \\ 0 & 0 & n_0 e^2 \tau / m_p \end{pmatrix}, \tag{4}$$

with which the collective mass per electron m_p (to be evaluated from the electronic band structure) is cleanly defined.

A conduction band can have valley degeneracy. Let $v = 1, 2, ..., g$ be the valley index (g: total number of valleys). Then the total conductivity tensor σ_{ij} above is the sum of all valley conductivity tensors σ_{ij}^v:

$$\sigma_{ij} = \sum_{v=1}^{g} \sigma_{ij}^v. \tag{5}$$

Each valley conductivity tensor is related to the valley collective mass tensor $(M_p^{-1})_{ij}^v$ via

$$\sigma_{ij}^v = n_0^v e^2 \tau (M_p^{-1})_{ij}^v, \tag{6}$$

where n_0^v is the electron density of the v-th valley with $n_0 = \sum_{v=1}^{g} n_0^v$. From Eqs. (2), (5), and (6), we can write

$$(M_p^{-1})_{ij} = \sum_{v=1}^{g} \frac{n_0^v}{n_0} (M_p^{-1})_{ij}^v \tag{7}$$

(a) Following the procedure of Lecture #17, but using general field and current density, $\vec{E} = (E_1, E_2, E_3)$ and $\vec{J} = (J_1, J_2, J_3)$, with no *a priori* directional relationship between them, prove that

$$\sigma_{ij}^v = e^2\tau \int_{1BZ} \frac{d^3\vec{k}}{4\pi^3}(M^{-1})_{ij}^v f(\epsilon^v(\vec{k})) \tag{8}$$

$$(M_p^{-1})_{ij}^v = \frac{1}{n_0^v} \int_{1BZ} \frac{d^3\vec{k}}{4\pi^3}(M^{-1})_{ij}^v f(\epsilon^v(\vec{k})) \tag{9}$$

where $(M^{-1})_{ij}^v = (1/\hbar^2)(\partial^2/\partial k_i \partial k_j)\epsilon^v(\vec{k})$ is the effective mass tensor in the v-th valley, $\epsilon^v(\vec{k})$ is the energy dispersion in the v-th valley, and $f(\epsilon^v(\vec{k}))$ is the FD distribution. Eq. (9) relates the effective mass tensor (individual electron effect) and the collective mass tensor in each valley. Argue that in the 2D case, $d^3\vec{k}/(4\pi^3)$ in the two integrations above can be replaced with $d^2\vec{k}/(2\pi^2)$.

(b) Gallium arsenide: GaAs has no valley degeneracy ($g = 1$) with a sole conduction band minimum lying at the center of the first Brillouin zone, with isotropic and quadratic dispersion $\epsilon(\vec{k}) = \hbar^2k^2/(2m^*)$; $m^* = 0.067m_0$.

- Show that

$$M_p^{-1} = M^{-1} = \begin{pmatrix} 1/m^* & 0 & 0 \\ 0 & 1/m^* & 0 \\ 0 & 0 & 1/m^* \end{pmatrix} \tag{10}$$

  and thus $m_p = m^*$.

- The identity between the effective mass tensor M^{-1} and the collective mass tensor M_p^{-1} is due to the quadratic energy dispersion. Individual electron effective mass m^* and collective electron mass m_p are identical.

- $\vec{J}||\vec{E}$ evidently.

(c) Graphene: Consider electron-doped graphene ($\epsilon_F > 0$). There are two conduction band valleys ($g = 2$) around the two Dirac points $\vec{K}$ and $\vec{K}'$ at two corners of the first Brillouin zone (Lecture #15; Homework #7). 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

$$(M_p^{-1})^{v=1} = (M_p^{-1})^{v=2} = M_p^{-1} = \begin{pmatrix} v_f^2/\epsilon_F & 0 \\ 0 & v_f^2/\epsilon_F \end{pmatrix}, \tag{11}$$

  thus, $m_p = \epsilon_F/v_F^2$. For simplicity, assume $\epsilon_F \gg k_BT$ and treat the Fermi-Dirac distribution function as a step function. Note that $\vec{J}^{v=1}||\vec{E}$, $\vec{J}^{v=2}||\vec{E}$, and $\vec{J}||\vec{E}$. 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.

- Show that

$$M_p^{-1} \neq M^{-1}. \tag{12}$$

  This difference between effective mass tensor M^{-1} and collective mass tensor M_p^{-1} arises because the energy dispersion is not quadratic. In this case, conductivity calculation must be based on the collective mass m_p, which is sharply distinguished from effective mass tensor components of individual electron.

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

$$\sigma = \frac{e^2\epsilon_F\tau}{\hbar^2\pi}; \tag{13}$$

$$\mu = \frac{e\epsilon_F\tau}{\hbar^2\pi n_0}. \tag{14}$$

(d) *Silicon*: Silicon has 6 conduction band minimum valleys along 6 {100} directions ($g = 6$) (Lecture #18). 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

$$\epsilon^{v=1}(\vec{k}) = \epsilon_c + \frac{\hbar^2(k_x - k_{x,0}^{v=1})^2}{2m_L^*} + \frac{\hbar^2(k_y - k_{y,0}^{v=1})^2}{2m_T^*} + \frac{\hbar^2(k_z - k_{z,0}^{v=1})^2}{2m_T^*}. \tag{15}$$

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 $(M_p^{-1})^v = (M^{-1})^v$ for each valley. This identity between the collective mass tensor and effective mass tensor for each valley is due to the quadratic energy dispersion at each valley.
- Show that $(M_p^{-1})^v$ is diagonal but with non-identical diagonal elements. This means that $\vec{J}^v \not\parallel \vec{E}$. This is due to the anisotropy in the energy dispersion in each valley.
- Show that (M_p^{-1}) is given by

$$M_p^{-1} = \begin{pmatrix} (1/3)(1/m_L^* + 2/m_T^*) & 0 & 0 \\ 0 & (1/3)(1/m_L^* + 2/m_T^*) & 0 \\ 0 & 0 & (1/3)(1/m_L^* + 2/m_T^*) \end{pmatrix}. \tag{16}$$

  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 $\vec{E}$. You may say (loosely) that taking all valleys together silicon recovers isotropy, more or less.

- Note that $m_p = [(1/3)(1/m_L^* + 2/m_T^*)]^{-1}$ is the mass you should use in the conductivity calculation for conduction electrons in silicon. Calculate this mass numerically.

[Remark] In this problem we have focused our attention to DC conductivity, but this does not compromise the generality of our treatment above. AC conductivity can be obtained by simply multiplying an extra factor $(1 + i\omega\tau)^{-1}$ to DC conductivity. The collective mass tensors as well as all the essential observations above remain the same whether we consider DC or AC conductivity. See Lecture #17.

Problem 3 (100 pt; no collaboration): 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

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{v}(\vec{k}) \times B_0\hat{z}, \tag{17}$$

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

$$v(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\epsilon(\vec{k}). \tag{18}$$

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[1] 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).

[1] We assume that the energy contour does not intersect with the boundary of the first Brillouin zone.

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

$$\omega_c = \frac{2\pi e B_0}{\hbar^2}\left[\frac{\partial A(\epsilon, k_{z,0})}{\partial \epsilon}|_{\epsilon=\epsilon_0}\right]^{-1} \tag{19}$$

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

$$m_c = \frac{\hbar^2}{2\pi}\frac{\partial A(\epsilon, k_{z,0})}{\partial \epsilon}|_{\epsilon=\epsilon_0} \tag{20}$$

(d) For

$$\epsilon(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + \frac{\hbar^2 k_z^2}{2m_3^*}, \tag{21}$$

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 k_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) Compare the result right above (*i.e.*, $m_c = \epsilon_F/v_F^2$ for a graphene electron at the Fermi level) with the graphene electron's collective or plasmonic mass, $m_p = \epsilon_F/v_F^2$ (Problem 2(c)), which was derived assuming[2] $T = 0$. You can see that $m_c|_{\epsilon=\epsilon_F} = m_p(T = 0)$ for graphene. This can be generalized. Prove that for a conductor (both 2D and 3D) with an isotropic electronic band $\epsilon(\vec{k}) = \epsilon(k)$, the plasmonic mass m_p at $T = 0$ is the same as the cyclotron mass at the Fermi surface.

Problem 4 (40 pt; no collaboration): Density of states for silicon conduction band

Considering all 6 valleys of silicon conduction band (Lecture #18) with the quadratic energy dispersion in each valley with transversal effective mass $m_T^* = 0.19m_0$ and longitudinal effective mass $m_L^* = 0.98m_0$, show that the density of states $D_n(\epsilon)$ near the conduction band minimum (minimum energy value: ϵ_c) taking into account all 6 valleys is given by

$$D_n(\epsilon) = g\frac{(m_L^* m_T^{*2})^{1/2}}{\hbar^3\pi^2} \times \sqrt{2(\epsilon - \epsilon_c)}, \tag{22}$$

where $g = 6$ is valley degeneracy. By comparing this to the density of states of the free electron Fermi gas, argue that the density-of-states effective mass for silicon conduction band can be expressed as

$$m_{DOS} = (g^2 m_L^* m_T^{*2})^{1/3} \tag{23}$$

Calculate the DOS effective mass for silicon conduction band.

[2] In Problem 2(c), we treated the FD distribution function as a step function assuming $\epsilon_F \gg k_B T$, which is equivalent to setting $T = 0$.