<u>Problem Set #3</u> (Parts III.3 & IV.1-3) November 1, 2016
(Due date: November 15, 2012)

1. Degenerate k • p perturbation theory for a Γ_{15}^{-} level

For a cubic crystal it is common to have triply-degenerate energy bands at the zone center **k** = 0. These bands are of great importance to the transport properties of such semiconductors as silicon, germanium, and the III-V compounds. Here we consider how this degeneracy is lifted as we move away from **k** = 0 for an energy band of the Γ_{15}^{-} symmetry representation. From group theory (to be discussed further in Part V), we know that the allowed symmetry representations for the intermediate states in the second-order perturbation theory for the Γ_{15}^{-} level are Γ_{1}^{+}, Γ_{15}^{+} and Γ_{25}^{+}. The basis functions of these symmetries in the O_h point group operation are given below:

$$\begin{aligned}
&\Gamma_1^{+} : 1 \\
&\Gamma_{15}^{-} : x, y, z \\
&\Gamma_{12}^{+} : f_1 = x^2 + \omega y^2 + \omega^2 z^2,\ f_2 = x^2 + \omega^2 y^2 + \omega z^2,\ \omega \equiv e^{i2\pi/3} \\
&\Gamma_{15}^{+} : yz\left(z^2 - y^2\right), zx\left(z^2 - x^2\right), xy\left(x^2 - y^2\right) \\
&\Gamma_{25}^{+} : yz, zx, xy
\end{aligned} \tag{P3.1}$$

(a) Show that the first-order **k • p** perturbation terms vanish.

(b) Show that the second-order secular equation for the **k** = 0 point in the Γ_{15}^{-} level is given by the following:

$$\begin{vmatrix}
Lk_x^2 + M\left(k_y^2 + k_z^2\right) - E(\mathbf{k}) & Nk_x k_y & Nk_x k_z \\
Nk_y k_x & Lk_y^2 + M\left(k_z^2 + k_x^2\right) - E(\mathbf{k}) & Nk_y k_z \\
Nk_z k_x & Nk_z k_y & Lk_z^2 + M\left(k_x^2 + k_y^2\right) - E(\mathbf{k})
\end{vmatrix} = 0, \tag{P3.2}$$

where $L \equiv (F+2G)$, $M \equiv (H_1+H_2)$, $N \equiv (F-G+H_1-H_2)$, and

$$F \equiv \frac{\hbar^2}{m^2} \sum_{n',\Gamma_1^+} \frac{\left|\langle x | p_x | 1 \rangle\right|^2}{E_n^{\left(\Gamma_{15}^-\right)}(0) - E_{n'}^{\left(\Gamma_1^+\right)}(0)}, \tag{P3.3}$$

$$G \equiv \frac{\hbar^2}{m^2} \sum_{n',\Gamma_{12}^+} \frac{\left|\langle x | p_x | f_1 \rangle\right|^2}{E_n^{\left(\Gamma_{15}^-\right)}(0) - E_{n'}^{\left(\Gamma_{12}^+\right)}(0)}, \tag{P3.4}$$

$$H_1 \equiv \frac{\hbar^2}{m^2} \sum_{n',\Gamma_{25}^+} \frac{\left|\langle x | p_y | xy \rangle\right|^2}{E_n^{\left(\Gamma_{15}^-\right)}(0) - E_{n'}^{\left(\Gamma_{25}^+\right)}(0)}, \tag{P3.5}$$

$$H_2 \equiv \frac{\hbar^2}{m^2} \sum_{n',\Gamma_{15}^+} \frac{\left|\langle x | p_y \left| xy\left(x^2 - y^2\right)\right\rangle\right|^2}{E_n^{\left(\Gamma_{15}^-\right)}(0) - E_{n'}^{\left(\Gamma_{15}^+\right)}(0)}. \tag{P3.6}$$

Here m denotes the free electron mass. In general the quantities L, M, N and the bandstructures can be determined by carrying out the cyclotron resonance experiments along various high symmetry directions.

(c) Find the dispersion relations $E(\mathbf{k})$ for $\mathbf{k}$ along the [100] and [111] axes.

2. The effective mass tensor and mean velocity of band electrons

We have discussed in class that the effective mass tensor of a band electron is defined as

$$\left(\frac{1}{m^*}\right)_{\mu\nu} \equiv \left(\frac{1}{\hbar^2}\right)\frac{\partial^2 E_{\mathbf{k}}}{\partial k_\mu \partial k_\nu}, \tag{III.70}$$

where μ and ν represent the polarization indices. Now consider the wave equation in EQ. (III.61):

$$\mathcal{H}\varphi_{\mathbf{k}}(\mathbf{r}) = \left[\frac{p^2}{2m} + \mathcal{V}(\mathbf{r})\right]\varphi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\varphi_{\mathbf{k}}(\mathbf{r}), \tag{III.61}$$

where $\mathcal{V}(\mathbf{r})$ is the periodic potential of the lattice, $\varphi_{\mathbf{k}}(\mathbf{r})$ denotes the solutions, and for simplicity we have assumed the absence of spin-orbit interactions. In the following we want to find an alternative expression for the effective mass tensor and the velocity of band electrons in terms of the reciprocal lattice vectors.

(a) Let's consider a specific Bloch form for the solutions $\varphi_{\mathbf{k}}(\mathbf{r})$, similar to the nearly-free-electron model:

$$\varphi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{\mathbf{G}} f_{\mathbf{G}}(\mathbf{k})e^{i\mathbf{G}\cdot\mathbf{r}}, \tag{P3-7}$$

where $f_{\mathbf{G}}(\mathbf{k})$ represents c-numbers, and $\mathbf{G}$ denotes the reciprocal lattice vectors. Using EQ. (P3-7) and EQ. (III.61), show that the expectation value of the band electron velocity $\langle v_{\mathbf{k}}\rangle$ has the following form:

$$\langle \mathbf{v}_{\mathbf{k}}\rangle \equiv \langle \mathbf{k}|\mathbf{v}|\mathbf{k}\rangle = \langle \mathbf{k}|(\mathbf{p}/m)|\mathbf{k}\rangle = \frac{\hbar}{m}\sum_{\mathbf{G}}(\mathbf{k}+\mathbf{G})\left|f_{\mathbf{G}}(\mathbf{k})\right|^2 = \frac{1}{\hbar}\nabla_{\mathbf{k}}E_{\mathbf{k}}. \tag{P3-8}$$

(b) Using EQs. (III.61), (III.70) and (P3-7), show that the effective mass tensor can be expressed as follows:

$$\left(\frac{m}{m^*}\right)_{\mu\nu} = \delta_{\mu\nu} + \sum_{\mathbf{G}} G_\mu \frac{\partial}{\partial k_\nu}\left|f_{\mathbf{G}}(\mathbf{k})\right|^2. \tag{P3-9}$$

3. Fermi statistics of carriers in doped semiconductors

Consider a two-band semiconductor with an energy gap E_G separating the minimum of the conduction band $E_c(\mathbf{k})$ and the maximum of the valence band $E_v(\mathbf{k})$, where $E_c(\mathbf{k})$ and $E_v(\mathbf{k})$ are given in terms of the anisotropic effective masses as follows:

$$E_c(\mathbf{k}) = E_G + \frac{\hbar^2 k_1^2}{2m_{e1}} + \frac{\hbar^2 k_2^2}{2m_{e2}} + \frac{\hbar^2 k_3^2}{2m_{e3}}, \qquad E_v(\mathbf{k}) = \frac{\hbar^2 k_1^2}{2m_{h1}} + \frac{\hbar^2 k_2^2}{2m_{h2}} + \frac{\hbar^2 k_3^2}{2m_{h3}}, \tag{P3-10}$$

where $k_{1,2,3}$ represent the wave-vector components along the three principal axes. Assume that the semiconductor is heavily doped with electrons so that the Fermi level is near the bottom of the conduction band. We further denote the donor atoms per unit volume by N_{donor} so that $N_{donor} = n_e - n_h$ where n_e and n_h are the electron and hole carrier densities per unit volume and $n_e >> n_h$.

(a) Show that the density of states for the conduction band $\mathcal{N}(E_c)$ and that for the valence band $\mathcal{N}(E_v)$ are given respectively by

$$\mathcal{N}\left(E_c\right)=\frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}E_c^{1/2}, \qquad \mathcal{N}\left(E_v\right)=\frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}E_v^{1/2}, \tag{P3-11}$$

where $m_e \equiv \left(m_{e1}m_{e2}m_{e3}\right)^{1/3}$ and $m_h \equiv \left(m_{h1}m_{h2}m_{h3}\right)^{1/3}$.

(b) At sufficiently low temperature where $E_G >> k_BT$, express the temperature dependent chemical potential $\zeta_e(T)$ of the heavily doped semiconductor below the bottom of the conduction band in terms of N_{donor} and m_e.

(c) Find the hole carrier density n_h in this heavily doped n-type semiconductor.

4. Static dielectric constant ε(q,0) and the effective screening length λ^{-1}(q)

We have shown in class that the momentum (**q**) and frequency (ω) dependent dielectric constant $\varepsilon(\mathbf{q},\omega)$ is given by the following expression

$$\varepsilon\left(\mathbf{q},\omega\right)=1+\frac{4\pi e^2}{q^2}\lim_{\alpha\to 0+}\sum_{\mathbf{k}}\frac{f^0\left(\mathbf{k}\right)-f^0\left(\mathbf{k}+\mathbf{q}\right)}{E\left(\mathbf{k}+\mathbf{q}\right)-E\left(\mathbf{k}\right)-\hbar\omega+i\hbar\alpha}, \tag{P3-12}$$

where $f^0(\mathbf{k})$ denotes the Fermi-Dirac distribution function for an electronic state $|\mathbf{k}\rangle$, and the sum is made over all possible $|\mathbf{k}\rangle$ states.

(a) Using EQ. (P3-12), show that the static dielectric constant is given by

$$\varepsilon\left(\mathbf{q},0\right)=1+\frac{4\pi e^2}{q^2}\mathcal{N}\left(E_F\right)\left\{\frac{1}{2}+\frac{4k_F^2-q^2}{8k_Fq}\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right\}. \tag{P3-13}$$

(b) The effective screening length $\lambda^{-1}(q)$ is defined by the static dielectric constant via the following relation:

$$\varepsilon\left(\mathbf{q},0\right)=1+\left[\frac{\lambda(q)}{q}\right]^2. \tag{P3-14}$$

Using EQs. (P3-13) and (P3-14), find the asymptotic expressions for $\lambda^2(q<<2k_F)$ and $\lambda^2(q>>2k_F)$. Sketch $\lambda^2(q)$-vs.-q and show that there is a singularity in the derivative of $\lambda^2(q)$ relative to q at $q = 2k_F$. This anomaly associated with $q = 2k_F$ is responsible for the so-called *Kohn effect* in the lattice spectrum, where the ions interact under a screened potential proportional to $1/\varepsilon(\mathbf{q})$ due to the presence of conduction electrons. In other words, the anomaly in the dielectric constant $\varepsilon(\mathbf{q})$ due to conduction electrons is actually reflected in the phonon spectrum because of the electron-phonon interaction.