ECE 4070: Physics of Semiconductor and Nanostructures

Spring 2014

Homework 6 ` **Due on April 08, 2014 at 5:00 PM**

Suggested Readings:

a) Lecture notes
b) START EARLY – THIS IS A CHALLENGING HOMEWORK SET

Problem 6.1 (Effective mass tensor and density of states effective mass – the general case)

A solid has only one conduction band minimum at the Γ-point with an effective mass tensor given by:

$$M^{-1} = \begin{bmatrix} 1/m_{xx} & 1/m_{xy} & 1/m_{xz} \\ 1/m_{yx} & 1/m_{yy} & 1/m_{yz} \\ 1/m_{zx} & 1/m_{zy} & 1/m_{zz} \end{bmatrix}$$

The total electron density in the conduction band can be written as (assuming Maxwell Boltzmann approximation)

$$n = N_c \exp\left(\frac{E_f - E_c}{KT}\right)$$

where: $N_c = 2\left[\frac{m_e\ KT}{2\pi\ \hbar^2}\right]^{3/2}$

And m_e is the density of states effective mass for the conduction band. Show that:

$$m_e = [\ \det(M)\ ]^{1/3}.$$

Hint: This problem does not require any significant amount of algebra.

Problem 6.2 (Constant energy surfaces)

Consider a material with energy band dispersion given by:

$$E_c(\vec{k}) = E_c(\vec{k}_o) + \frac{\hbar^2}{2}(\vec{k} - \vec{k}_o)^T\ .\ M^{-1}\ .\ (\vec{k} - \vec{k}_o)$$

a) Show that for an electron with wavevector $\vec{k}$ the velocity in real space given by $\vec{v}_c(\vec{k})$ is always perpendicular to the constant energy surface that passes through $\vec{k}$.

Problem 6.3 (Band electrons in magnetic fields)

In homework 1 you looked at the problem of free electrons in a magnetic field. The electrons moved in circular orbits in real space with a frequency ω_c which was called the electron-cyclotron frequency. For free electrons,

$$\omega_c = \frac{eB_o}{m}$$

In this problem, you will look at electrons in the conduction band of a solid. Suppose the energy band dispersion near the conduction band minimum is given by:

$$E_c(\vec{k}) = E_c(\vec{k}_o) + \frac{\hbar^2}{2}(\vec{k} - \vec{k}_o)^T \, . \, M^{-1} \, . \, (\vec{k} - \vec{k}_o)$$

The motion of each electron in k-space is described by the equation:

$$\frac{d\,\hbar\vec{k}}{dt} = -e\left[\vec{v}_c(\vec{k}) \times \vec{B}\right]$$

And in real space by the equation:

$$\frac{d\,\vec{r}}{dt} = \vec{v}_c(\vec{k})$$

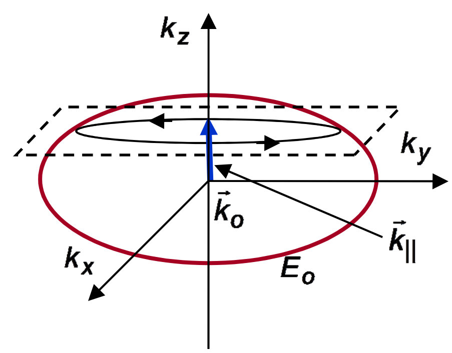
Needless the say, the motion of the electron is complicated both in k-space and in real space and the exploration of this motion is the purpose of this problem.

a) Show that the component of the crystal momentum of an electron parallel to the magnetic field is independent of time. We will call this component $\vec{k}_{||}$.

b) Show that the electron energy is independent of time.

c) Argue from results in (a) and (b) imply that in k-space the orbit of an electron with initial energy E_o is given by the intersection of the constant energy surface corresponding to energy E_o with a plane that passes through the point $\vec{k}_{||}$ and is perpendicular to the direction of the magnetic field (or perpendicular to $\vec{k}_{||}$). This shows that the motion of the electron in k-space is periodic.

Fig: The orbit in k-space of an electron in case where the energy band dispersion is anisotropic, the constant energy surfaces are ellipsoids, and the magnetic field is applied in the z-direction. All electrons with initial crystal momentum component in the z-direction given by $\vec{k}_{||}$ and energy E_o will have the orbit in k-space as shown.



d) In real space, the electron motion is described by the position vector $\vec{r}(t)$. The projection of the electron motion in a plane perpendicular to the magnetic field is given by $\vec{r}_\perp(t)$. Argue that,

$$\vec{r}_{\perp}(t) = \vec{r}(t) - \left[\frac{\vec{r}(t).\vec{B}}{|\vec{B}|^2}\right]\vec{B}$$

e) The orbit of the electron in k-space is given by the time-dependent vector $\vec{k}(t)$ and the projection of the electron orbit in real-space in a plane perpendicular to the magnetic field is given by $\vec{r}_{\perp}(t)$. Show that these two orbits are related by,

$$\vec{r}_{\perp}(t) - \vec{r}_{\perp}(t=0) = -\frac{\hbar}{e|\vec{B}|^2}\vec{B} \times \left[\vec{k}(t) - \vec{k}(t=0)\right]$$

Hint: start by taking the vector cross-product of an equation on both sides by $\vec{B}$ and then integrating. The above relation shows that the projection of the motion of the electron in real space in a plane perpendicular to the magnetic field will be periodic since the motion in k-space is periodic (as shown in part (c) earlier).

For parts (f) and (g) assume that the magnetic field is applied in the $\hat{z}$ direction and is given by $\vec{B} = B_o\hat{z}$. The inverse effective mass tensor is given by,

$$M^{-1} = \begin{bmatrix} 1/m_{xx} & 1/m_{xy} & 1/m_{xz} \\ 1/m_{yx} & 1/m_{yy} & 1/m_{yz} \\ 1/m_{zx} & 1/m_{zy} & 1/m_{zz} \end{bmatrix}$$

From part (e) it follows that the motion of the electrons in the x-y plane (and in k-space) is periodic and we suppose the period has a frequency ω_c.

f) Find an expression for ω_c in terms of the components of the inverse effective mass tensor.
Hint: The answer can be written in terms of the determinant of a sub-matrix of the inverse effective mass matrix. And this is not supposed to be an algebra-intensive problem - if you do it elegantly.

g) The frequency ω_c can be written as in the free electron case, $\omega_c = eB_o/m_e$, where m_e is now the cyclotron effective mass. Find an expression for the cyclotron effective mass. Note that the cyclotron effective mass depends on the direction in which the magnetic field has been applied.

NOTE: Measurement of cyclotron frequencies while applying the magnetic field in different directions is a commonly used and very effective experimental technique to determine the cyclotron effective masses and, from this knowledge, the effective mass tensor of a semiconductor.

For part (h) assume that the inverse effective mass tensor is diagonal and given by,

$$M^{-1} = \begin{bmatrix} 1/m_{xx} & 0 & 0 \\ 0 & 1/m_{yy} & 0 \\ 0 & 0 & 1/m_{zz} \end{bmatrix}$$

The magnetic field is applied in the direction of the unit vector $\hat{n} = (n_x, n_y, n_z)$ and is given by, $\vec{B} = B_o\hat{n}$. This last part could be challenging so if you get stuck, move on.

h) Show that now the cyclotron effective mass is given by the expression:

$$m_e = \sqrt{\frac{m_{xx}\ m_{yy}\ m_{zz}}{n_x^2\ m_{xx} + n_y^2\ m_{yy} + n_z^2\ m_{zz}}}$$

Hint: You might (or might not) want to use the result that,

$$\vec{B}\,.\,M\frac{d\,v_c\left(\vec{k}(t)\right)}{dt} = 0$$

$$\Rightarrow \vec{B}\,.\,M\,v_c\left(\vec{k}(t)\right) = \text{const.}$$

Problem 6.4 (Effective masses, momentum matrix elements, and the bandgap)

In lectures the following equation was derived for the periodic part of the Bloch function:

$$\left(\frac{\hat{\vec{P}}^2}{2m} + \frac{\hat{\vec{P}}}{m}.\,\hbar\vec{k} + \frac{\hbar^2 k^2}{2m} + V\left(\hat{\vec{r}}\right)\right) u_{n,\vec{k}}(\vec{r}) = E_n\left(\vec{k}\right) u_{n,\vec{k}}(\vec{r}) \quad \text{or} \quad \hat{H}_{\vec{k}} u_{n,\vec{k}}(\vec{r}) = E_n\left(\vec{k}\right) u_{n,\vec{k}}(\vec{r})$$

Suppose the above equation has been solved for a particular point $\vec{k}$ in the k-space and all band energies $E_n\left(\vec{k}\right)$ and corresponding functions $u_{n,\vec{k}}(\vec{r})$ have been obtained. Now we consider a close by point $\vec{k} + \Delta\vec{k}$ in k-space. The Hamiltonian is,

$$\hat{H}_{\vec{k}+\Delta\vec{k}} = \hat{H}_{\vec{k}} + \frac{\hat{\vec{P}}}{m}.\,\hbar\Delta\vec{k} + \frac{\hbar^2\left(2\vec{k}\,.\,\Delta\vec{k} + \Delta k^2\right)}{2m} = \hat{H}_{\vec{k}} + \Delta\hat{H}_{\vec{k}}$$

As in the lecture notes, we will treat $\Delta\hat{H}_{\vec{k}}$ as a small perturbation, and expand the new eigenfunction $u_{n,\vec{k}+\Delta\vec{k}}(\vec{r})$ in terms of the old eigenfunctions in the following form (just as we do in ordinary perturbation theory),

$$u_{n,\vec{k}+\Delta\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r}) + \sum_{m\neq n} c_m \quad u_{m,\vec{k}}(\vec{r})$$

As in the lecture notes, the first order correction to the energy is given by,

$$E_n\left(\vec{k}+\Delta\vec{k}\right) - E_n\left(\vec{k}\right) = \left\langle u_{n,\vec{k}}\left|\Delta\vec{H}_{\vec{k}}\right|u_{n,\vec{k}}\right\rangle$$

The second order correction to the energy would then be given by the second order perturbation theory,

$$E_n\left(\vec{k}+\Delta\vec{k}\right) - E_n\left(\vec{k}\right) = \left\langle u_{n,\vec{k}}\left|\Delta\vec{H}_{\vec{k}}\right|u_{n,\vec{k}}\right\rangle + \sum_{m\neq n}\frac{\left|\left\langle u_{n,\vec{k}}\left|\,\Delta\vec{H}_{\vec{k}}\,\right|u_{m,\vec{k}}\right\rangle\right|^2}{E_n\left(\vec{k}\right) - E_m\left(\vec{k}\right)}$$

If one expands the LHS to the second order in $\Delta\vec{k}$ one obtains (from Taylor series),

$$E_n\left(\vec{k}+\Delta\vec{k}\right) - E_n\left(\vec{k}\right) = \sum_{\alpha=x,y,z}\frac{\partial E_n\left(\vec{k}\right)}{\partial k_\alpha}\Delta k_\alpha \quad + \quad \frac{1}{2}\sum_{\substack{\alpha=x,y,z\\ \beta=x,y,z}}\frac{\partial^2 E_n\left(\vec{k}\right)}{\partial k_\alpha \partial k_\beta}\Delta k_\alpha \Delta k_\beta \quad + \quad \cdots$$

If one collects all terms that are of first order in $\Delta\vec{k}$ on the RHS and then equates the corresponding terms on the LHS and RHS then one obtains (as in the lecture notes),

$$\frac{1}{\hbar}\frac{\partial E_n\left(\vec{k}\right)}{\partial k_\alpha} = \left\langle u_{n,\vec{k}}\left|\frac{\left(\hat{P}_\alpha + \hbar k_\alpha\right)}{m}\right|u_{n,\vec{k}}\right\rangle = \left\langle \psi_{n,\vec{k}}\left|\frac{\hat{P}_\alpha}{m}\right|\psi_{n,\vec{k}}\right\rangle$$

which is the familiar relationship between the average velocity of the Bloch electron and the energy band gradient.

a) Collect all terms that are of second order in $\Delta\vec{k}$ on the RHS and then prove the following expression for the effective mass,

$$\frac{1}{m_{\alpha\beta}} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\vec{k})}{\partial k_\alpha \partial k_\beta}$$

$$= \frac{1}{m}\left[\delta_{\alpha\beta} + \frac{1}{m}\sum_{p\neq n}\frac{\langle\psi_{n,\vec{k}}|\hat{P}_\alpha|\psi_{p,\vec{k}}\rangle\langle\psi_{p,\vec{k}}|\hat{P}_\beta|\psi_{n,\vec{k}}\rangle + \langle\psi_{n,\vec{k}}|\hat{P}_\beta|\psi_{p,\vec{k}}\rangle\langle\psi_{p,\vec{k}}|\hat{P}_\alpha|\psi_{n,\vec{k}}\rangle}{E_n(\vec{k}) - E_p(\vec{k})}\right]$$

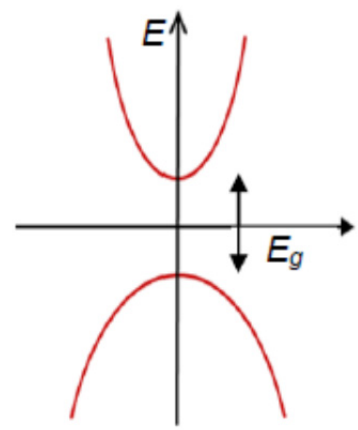
b) Consider a semiconductor with just two bands; a conduction band and a valence band with energy dispersions,

$$E_c(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m_e}$$

$$E_v(\vec{k}) = E_v - \frac{\hbar^2 k^2}{2m_h}$$

Show that the effective masses obey the relation:

$$\frac{1}{m_e} + \frac{1}{m_h} = \frac{4}{m}\frac{\left|\langle\psi_{c,\vec{k}=0}|\hat{P}_x|\psi_{v,\vec{k}=0}\rangle\right|^2}{E_g}$$



NOTE: This problem shows the important relationship between effective masses and momentum matrix elements between conduction and valence band Bloch states. It also shows that smaller bandgaps imply smaller effective masses and vice versa – something that we briefly mentioned in the lecture notes (see the plot in the lecture notes).