

ECE 407: Homework 6 Solutions (By Farhan Rana)

Problem 6.1

An easy way to do this problem is to rotate the coordinate system such that the inverse effective mass matrix is diagonal in the new coordinate system. Let the appropriate rotation matrix and the resulting diagonal matrix be:

$$R.M^{-1}.R^{-1} = \begin{bmatrix} 1/m'_{xx} & 0 & 0 \\ 0 & 1/m'_{yy} & 0 \\ 0 & 0 & 1/m'_{zz} \end{bmatrix}$$

This implies that (just like in the case of Silicon) that the density of states effective mass is,

$$\begin{aligned} m_e &= (m'_{xx} m'_{yy} m'_{zz})^{1/3} = \frac{1}{\det(R.M^{-1}.R^{-1})^{1/3}} = \left[\frac{1}{\det(R). \det(M^{-1}) \det(R^{-1})} \right]^{1/3} \\ &= \left[\frac{\det(R)}{\det(R). \det(M^{-1})} \right]^{1/3} = \left[\frac{1}{\det(M^{-1})} \right]^{1/3} = [\det(M)]^{1/3} \end{aligned}$$

Problem 6.2

a) The answer follows from elementary vector calculus result that that the gradient of any function is perpendicular to the surface of constant value of the function. In the present case, the velocity is related to the gradient of the energy function,

$$\vec{v}_c(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} E(\vec{k})$$

And therefore the velocity must be perpendicular to the surfaces of constant energy.

Problem 6.3

a) First note that: $|\vec{k}_{||}| = \frac{\vec{B} \cdot \vec{k}}{|\vec{B}|}$

Now take the dot product on both sides of the crystal momentum equation with the magnetic field to get:

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

$$\Rightarrow \vec{B} \cdot \frac{d \hbar \vec{k}}{dt} = 0$$

$$\Rightarrow \frac{d \vec{B} \cdot \vec{k}}{dt} = 0$$

$$\Rightarrow \frac{d |\vec{k}_{||}|}{dt} = 0$$

$$b) \frac{dE_c(\vec{k}(t))}{dt} = \frac{1}{\hbar} \nabla_{\vec{k}} E_c(\vec{k}(t)) \cdot \frac{d\hbar \vec{k}(t)}{dt} = \vec{v}_c(\vec{k}(t)) \cdot \left[-e \left[\vec{v}_c(\vec{k}(t)) \times \vec{B} \right] \right] = 0$$

c) The complete argument follows in two steps:

- i) Since the energy of the electron remains unchanged and equal to its initial value E_0 , the motion in k-space of the electron must be confined to a constant energy surface corresponding to the initial energy E_0 of the electron.
- ii) Since the component of its crystal momentum parallel to the magnetic field also remains unchanged and equal to its initial value \vec{k}_{\parallel} , the motion in k-space of the electron must also be confined to the plane in k-space on which the components of all crystal momenta in the direction of the magnetic field is \vec{k}_{\parallel} (convince yourself that this later condition defines a plane in k-space that is perpendicular to the magnetic field).

Since both (i) and (ii) above must be true, the desired result follows.

d) One can always write the vector $\vec{r}(t)$ in terms of its components in two orthogonal directions: parallel and perpendicular to the magnetic field:

$$\vec{r}(t) = \vec{r}_{\perp}(t) + \vec{r}_{\parallel}(t)$$

But:

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

Therefore:

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

e) Start from,

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

Take the cross product on both sides with the magnetic field:

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

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

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

$$\text{Note: } \vec{A} \times (\vec{B} \times \vec{C}) = \vec{B} (\vec{A} \cdot \vec{C}) - \vec{C} (\vec{A} \cdot \vec{B})$$

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

Now integrate both sides from time 0 to t to get:

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

f) We have from lecture handouts:

$$M \cdot \frac{d\vec{v}_c(\vec{k})}{dt} = -e [\vec{v}_c(\vec{k}) \times \vec{B}_0 \hat{z}] = -e B_0 [\vec{v}_c(\vec{k}) \times \hat{z}]$$

$$\text{or: } \frac{d\vec{v}_c(\vec{k})}{dt} = -e B_0 M^{-1} \cdot [\vec{v}_c(\vec{k}) \times \hat{z}]$$

The above equation shows that the equations for the x- and y-components of the velocity depend only on the x- and y-components of the velocity – and not to the z-component of the velocity. Consequently, we can write the equations for only the x- and y-components as follows:

$$\frac{d}{dt} \begin{bmatrix} v_{cx} \\ v_{cy} \end{bmatrix} = -e B_0 \begin{bmatrix} 1/m_{xx} & 1/m_{xy} \\ 1/m_{yx} & 1/m_{yy} \end{bmatrix} \begin{bmatrix} v_{cy} \\ -v_{cx} \end{bmatrix}$$

We can now solve this simpler equation for the cyclotron frequency. The above are two coupled linear differential equations. One can take the derivative of the first and use the second to get a second order differential equation:

$$\begin{aligned} \frac{d^2 v_{cx}}{dt^2} &= -e^2 B_0^2 \left[\frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}} \right] v_{cx} \\ &= -e^2 B_0^2 \left[\frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}} \right] v_{cx} \end{aligned}$$

This implies the cyclotron frequency is:

$$\omega_c = \sqrt{e^2 B_0^2 \left[\frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}} \right]}$$

The term in the square brackets is the determinant of the upper-left 2x2 submatrix of the inverse effective mass tensor.

$$g) \frac{1}{m_e} = \sqrt{\frac{1}{m_{xx}} \frac{1}{m_{yy}} - \frac{1}{m_{xy}} \frac{1}{m_{yx}}}$$

h) In spherical coordinates the unit vector \hat{n} can be written as,

$$\hat{n} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}$$

If \hat{n} were in the \hat{z} direction, we would know the answer from part (f) above. So we perform a rotation of our coordinate system such that the z-axis of our rotated system is in the same direction as \hat{n} . This can be accomplished by a rotation matrix R :

$$R = \begin{bmatrix} \cos \phi \cos \theta & \sin \phi \cos \theta & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \cos \phi \sin \theta & \sin \phi \sin \theta & \cos \theta \end{bmatrix}$$

Note that, as wanted, $R.\hat{h} = \hat{z}$. The inverse effective mass matrix in the new co-ordinate system would be, $R.M^{-1}.R^{-1}$. The square of the inverse cyclotron effective mass is, from part (f), given by the determinant of the upper 2x2 matrix of the matrix $R.M^{-1}.R^{-1}$ and is as given in the homework set.

Problem 6.4 (Effective masses and momentum operator matrix elements)

a) The solution requires just a little algebra. Note that both the first order perturbation term and the second order perturbation term both contain terms that are of second order in $\Delta\vec{k}$.

b) Again the final answer follows by a simple use of the general result in part (a) to the specific case. Since the mass matrix is isotropic and diagonal, one can work with the “xx” component of the inverse effective mass tensor to get:

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

$$-\frac{1}{m_h} = \frac{1}{m} \left[1 - \frac{2}{m} \frac{\langle \psi_{c,\vec{k}=0} | \hat{P}_x | \psi_{v,\vec{k}=0} \rangle \langle \psi_{v,\vec{k}=0} | \hat{P}_x | \psi_{c,\vec{k}=0} \rangle}{E_g} \right]$$

Subtraction of the above two equations gives the desired result.