ECE-606 Homework No. 4 Assigned: Sept. 11 Due: Sept.18

1) The effective mass equation with ellipsoidal energy surfaces is given by

$$E = \frac{\hbar^2}{2m_x}k_x^2 + \frac{\hbar^2}{2m_y}k_y^2 + \frac{\hbar^2}{2m_z}k_z^2$$

Using this dispersion, solve the questions below for the density-of-state mass and cyclotron mass.

a) Derive an expression for the density of states. Work out the density of state mass.

Recall: an ellipsoid is described by $1 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}$ with volume given by

$$V = \frac{4}{3}\pi abc$$

b) The two equations governing the dynamics of electrons in solids are:

$$\frac{d\vec{k}}{dt} = -\frac{e}{\hbar}\vec{v}\times\vec{B} \qquad \text{and} \qquad v_j = \frac{1}{\hbar}\frac{\partial E}{\partial k_j}$$

Suppose we have a magnetic field in the z direction and that the cyclotron mass m_c is defined as $m_c = \frac{eB}{\omega_c}$ where ω_c is the cyclotron frequency. Express m_c in terms of m_x, m_y, m_z. Hint: Use the two dynamics equations to obtain $k_x = \exp(i\omega_c t)$, where ω_c is to be determined.

c) Show that the cyclotron mass in the presence of a B field $\vec{B} = B(\alpha, \beta, \gamma)$ is given by $\frac{1}{m_c} = \sqrt{\frac{m_x\alpha^2 + m_y\beta^2 + m_z\gamma^2}{m_x m_y m_z}}$

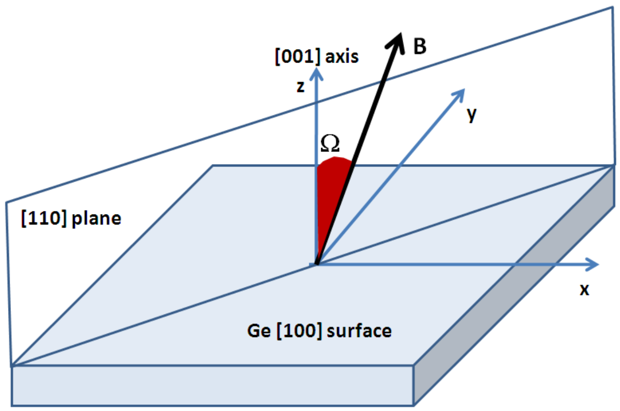
Hint: By using the two dynamics equations and knowing that the solution is $\vec{k} = \exp(i\omega_c t)$, you would be able to get the following,

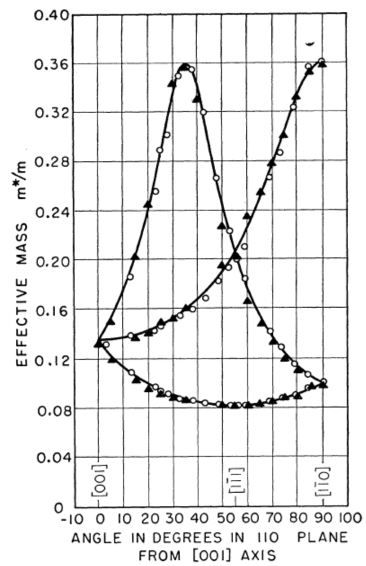
$$[A]\begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix} = 0$$ where [A] is a 3x3 matrix. Existence of solution requires det[A]=0

d) Let us consider the material Germanium. It has four ellipsoids each described by a longitudinal and transverse effective mass $\boldsymbol{m_l}$ and $\boldsymbol{m_t}$ respectively. Prove that in the presence of a $\boldsymbol{B}$ field making an angle θ with the longitudinal axis of an ellipsoid, the cyclotron mass of this ellipsoid is given by:

$$\frac{1}{m_c} = \sqrt{\frac{\cos^2\theta}{m_t^2} + \frac{\sin^2\theta}{m_t m_l}}$$

In 1955, Dresselhaus and co-workers performed an experiment as shown below,





The B field is rotated within the [110] plane. The right plot is the measured cyclotron mass when the B field angle is being swept from -90^o to 90^o. The various curves are due to the 4 ellipsoids, where 2 of them yield the same curve. Assuming $m_l = 1.59$ and $m_t = 0.082$, reproduce these experimental curves theoretically.

2) Solve ASF 4.14

3) Solve ASF 4.16

4) Compute the mean kinetic energy of free electrons in a metal. Assume Maxwell-Boltzmann statistics. Do you expect to get the same result when applying Fermi-Dirac statistics? Explain the difference if any.

Answer the following sub-questions.

- It is generally more convenient to use the Maxwell-Boltzmann distribution, rather than quantum statistics. Under what conditions can quantum systems be described by a classical approximation?

- How far must the energy be above the Fermi-level at T=300K for the appropriate Maxwell-Boltzmann distribution to result in an error of less than 5% in the occupation probability? Assume **$E\text{-}E_f > 4kT$**.

- Give two examples where a Fermi system occurs.

5) This question makes use of Band Structure Lab on nanohub. It is designed to give you more practice with band structure concepts.

Launch BS Lab:

- Choose Si as the material. As you did in Hw # 3 simulate the band structure of bulk Si. From the plot measure and write down the band gap.
- Now perform a similar calculation, but instead of bulk choose for the structure a rectangular nanowire. Under the dimensions tab, set the height and width to be 3nm. Plot and display both the conduction and valence bands.
- Obtain the band gap from the plot and note it down.
- Repeat the above sub question but with the dimensions now set to 4nm. What difference do you observe in the band gap?
- Give a physical argument as to why the band gap changes when the dimensions of the wire is altered.
- What physical parameters would you expect to change from the values you computed for the bulk material? List at least three of them.
- Can you reconcile your answers with simple expressions for energy states for a particle in a box that you have learnt earlier?
- When would you expect the energy states for the nanowire to be close to the bulk values?

Bonus Question

In class you saw how the simple particle in a box problem uses some of the elementary results of quantum mechanics to arrive at a simple expression for the eigenstates of a confined particle. The box where the particle was confined was rectangular in shape with infinite potential barriers.

Now assume that the rectangular box has been replaced by a cylindrical well. The potential is zero inside the cylindrical well and infinite outside. Set up the Schrödinger equation for an electron of mass ***m*** that is confined in this cylindrical well. You do not have to explicitly compute the eigenstates for this problem.

Please do not google to find an answer. Try to construct simple mathematical steps that can lead you to a possible solution.