PHYS4450 Solid State Physics Problem Set 5 Due: 15 April 2013 (Monday)
All problem sets should be handed in not later than 5pm on the due date. Drop your assignment in the Box in Rm.213.
Please work out the steps of the calculations in detail.

5.0 *Reading Assignment:* Kittel's Chapters 7-9 cover band theory, including semiconductor band structures. Class notes Chapter XII covers Electron Dynamics (discussed in Kittel's Chapter 8). Class notes Chapter XIII discuss some semiconductor physics. Kittel's Chapter 8 treated some basic semiconductor physics (see also Chapter 15 for discussion on Wannier excitons).

5.1 **Electron Dynamics.** Consider a rectangular lattice formed by $\mathbf{a}_1 = a\hat{x}$ and $\mathbf{a}_2 = b\hat{y}$ with $b < a$. Construct the corresponding reciprocal lattice and identify the first Brillouin zone.

(a) First, show (or illustrate by selecting a few points) that a point on the edge of the 1st BZ is related to another point on the edge of the 1st BZ by a reciprocal lattice vector $\mathbf{G}$.

(b) Let's start with a $\mathbf{k}$-value inside the 1st BZ. Let's say there is no phonon scattering and no impurities, etc. There is an external static electric field applied at an arbitrary direction. [Note: Don't take some simple direction like $\hat{x}$ or $\hat{y}$, take an arbitrary direction.] This field provides a $\mathbf{F}_{ext}$. Under this $\mathbf{F}_{ext}$, $\mathbf{k}$ must change according to the equation governing electron dynamics.
Discuss how $\mathbf{k}$ changes by drawing lines in the 1st BZ to indicate the $\mathbf{k}$ values covered as time evolves.

(c) Similar to (a), but now don't restrict to show $\mathbf{k}$-values within the 1st BZ, instead allow $\mathbf{k}$ to change in the whole reciprocal space. Indicate how $\mathbf{k}$ changes and discuss how the figure here is related to that in (b).

5.2 **Forming a tight-binding band and find electron effective mass.**

(a) Review the tight-binding model of energy bands. Consider a (monatomic) crystal taking on the *bcc* lattice and there is one atom per primitive cell. The cube edge is a. Assume wave functions can be constructed from, say, s atomic orbitals and that only the nearest neighbour overlap is important in $A(\mathbf{R})$. Assume that $A(\mathbf{0})$ and the nearest neighour hopping (overlap) integral t are positive and that t is the same for all nearest neighbours. Choose the parameters so that the bottom of the band is at the zone center $\mathbf{k} = 0$. [Remark: There is a sum over the nearest neighbors and it is a sum in real space. The $\mathbf{k}$ in the expression is a wave vector $\mathbf{k}$ in the first Brillouin zone corresponding to a fcc direct lattice.]

(b) Show that the effective mass is isotropic near $\mathbf{k} = 0$ and find its value.

(c) Using the tight-binding band, construct the reciprocal effective mass tensor for an arbitrary $\mathbf{k}$ in the 1st BZ.

(d) Look up a picture for the 1st BZ of a *bcc* lattice. Besides the zone center, there are other special points corresponding to points at the edge of the 1st BZ. They are usually labelled the H point (along [100]), the N point (along [110]) and the P point (along [111]). Find the reciprocal effective mass tensor mid-way from $\mathbf{k} = 0$ to these points.

(e) Find the electron effective mass at the top of the band.

5.3 **Silicon Band Structure.** Take a look at the band structure of silicon. It is an indirect gap semiconductor.

Let's consider the conduction band. The vicinity of the bottom of the conduction band corresponds to six patches near the X-points in the 1st B.Z. The constant energy surfaces near the bottom of the band are cigar-shaped. From the bottom of the band, it looks parabolic in every direction, but in each direction there is a different curvature. Consider one of the patches or pockets. Let's not worry about the band minimum being at some finite value of $\mathbf{k}_{min}$ near the X-point. Sitting at the band minimum and looking around, data books give two effective masses, usually called m_t (transverse effective mass) and m_l (longitudinal effective mass), to describe the energy band near the minimum. Referring to the pictures in Kittel's Chapter 8, explain why it is necessary to use two different masses.

(b) **(See SQ22.)** Let's assume that the conduction band energies for silicon near the conduction band minimum (and some other semiconductors) can be described by

$$\epsilon(\mathbf{k}) = \hbar^2[\frac{k_x^2}{2m_1} + \frac{k_y^2}{2m_2} + \frac{k_z^2}{2m_3}],$$

where m_1, m_2, m_3 could be different effective masses. [In silicon, we have two of the masses being equal and $\mathbf{k}$ measured from $\mathbf{k}_{min}$.] The band structure around the minimum is therefore **anisotropic**, but it still goes like k^2. For such a model band structure, find the density of states. Hence, find the density of states for the case of $m_1 = m_2 \neq m_3$, as in silicon.

(c) (Basically, if we take the electron picture, then a band that curves upward has a positive electron mass near the bottom of the band. A band that curves downward has a **negative electron mass** near the top of the band. However, if one switches to a hole picture, then for an electron band that curves downward, the hole band curves upward and thus corresponding to a **positive hole mass**. Details are discussed in Chapter XIII.)

Next, let's look at the valence bands of silicon. The top of the bands is at $\mathbf{k} = 0$. Formally, there are three valence bands, called light hole (LH) band, heavy hole (HH) band, and split-off band. All these electron bands curve downward. The LH and HH bands touch at $\mathbf{k} = 0$. Let's focus on the LH and HH bands. [They are similar to the valence bands shown in Fig. 13 of Chapter 8 in Kittel.] Mathematically, these two bands can be described by

$$E_{1,2}(\mathbf{k}) = E_V - \frac{\hbar^2}{2m}\left(Ak^2 \pm \sqrt{B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)}\right)$$

where m is the bare electron mass, k is the magnitude of $\mathbf{k}$, and E_V is the energy of the top of the valence band (which can be taken as zero). For silicon, the parameters are $A = 4.0$, $B = 1.1$ and $C = 4.1$.

(i) Consider $\mathbf{k}$ that goes from the 1st BZ center along $(k, 0, 0)$ direction (i.e., towards X-point). Derive the expressions for the LH and HH valence bands. Sketch these electron valence bands. Identify which band is LH and which is HH.

(ii) Hence, find the light-hole effective mass and heavy-hole effective mass at the top of the two bands.

(iii) If we switch to the hole picture, sketch the two HOLE BANDS.

(iv) Now, if $\mathbf{k}$ goes along the line from 1st BZ center to the face of a hexagon in the zone edge (i.e., along a diagonal), derive expressions for the LH and HH effective masses at $\mathbf{k} = 0$ and evaluate their values.

5.4 A key equation for carrier densities in semiconductors is

$$np = 4\left(\frac{kT}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{3/2} \exp\left(-\frac{E_g}{kT}\right).$$

(a) The key point is that product np is a constant at a given temperature. In semiconductor books and literature, this constant is written as n_i^2. For silicon, $m_e^* = 0.26m_0$ and $m_h^* = 0.49m_0$, where m_0 is the bare electron mass. Calculate n_i^2 at $T = 300K$. Give your answer in units of cm^{-6}.

(b) Let's say in an n-doped silicon, we have the concentration of donors $N_d = 10^{16}\ cm^{-3}$. These donor impurities will be ionized at $300K$ and dominate the electron density. Hence, estimate the minority carrier (i.e., hole) concentration at 300 K. This is usually referred to as p_{n0} in semiconductor literature.

(c) An experimentalist prepared a sample of pure silicon crystal. It is found that the ratio of charge carries at $300K$ and $330K$ is 0.125. Determine the band gap of the crystal.

(d) When Sb (a donor) is doped into silicon, the impurity states have an ionization energy of 0.043 eV. Find the electron effective mass.

Important: For every PHYS4450 Problem Set, you must attach a SIGNED copy of the academic honesty declaration form given below. It is a university policy. Homework without a signed declaration form will NOT be graded and thus will carry zero mark.

I declare that the assignment here submitted is original except for source material explicitly acknowledged, and that the same or related material has not been previously submitted for another course. I also acknowledge that I am aware of University policy and regulations on honesty in academic work, and of the disciplinary guidelines and procedures applicable to breaches of such policy and regulations, as contained in the website http//www.cuhk.edu.hk/policy/academichonesty.

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