Homework 7

Due 3/9/2012 (extra office hours on Friday, March 2)

The total points = 120 points. However, 40 points will be extra credit.
If you earn extra credit points, then they will be applied to make up for any lost quiz scores, first. Any remaining extra credit points will be applied to the homework score. Please try all problems, extra credit or not!

1. [20 points] Consider the following matrix which is a generalization of the matrix that we considered in class. It is applicable to higher dimensions, and to the degenerate perturbation theory near the BZ boundary, not just at the BZ boundary (we assume $\left|\lambda_{\vec{k}} - \lambda_{\vec{k}+\vec{G}}\right| \ll \left|U_{\vec{G}}\right|$). This matrix is applicable near the BZ boundary that is the perpendicular bisector of $-\vec{G}$.

$$h = \begin{pmatrix} \lambda_{\vec{k}} + U_0 & U^*_{\vec{G}} \\ U_{\vec{G}} & \lambda_{\vec{k}+\vec{G}} + U_0 \end{pmatrix}$$

   a. Obtain eigenvalues of this matrix.
   b. Show that the group velocity satisfies: $\vec{v}_{\vec{k}} \cdot \vec{G} = 0$ if $\vec{k}$ is on the BZ boundary.
   c. Explain why (b) means that a constant energy surface (e.g. the Fermi surface) would cut the BZ boundary at the right angle.

2. [20 points] Extend the tight binding theory as we covered in class to 2D square lattice and 3D simple cubic lattice, and obtain the dispersion relation ϵ_k in each case. What is the band width in each case in terms of t? In this problem, assume that the 1s wave function at neighboring sites are orthogonal to each other.

3. [20 points] Kittel 7.2:

2. *Free electron energies in reduced zone.* Consider the free electron energy bands of an fcc crystal lattice in the approximation of an empty lattice, but in the reduced zone scheme in which all **k**' s are transformed to lie in the first Brillouin zone. Plot roughly in the [111] direction the energies of all bands up to six times the lowest band energy at the zone boundary at $\mathbf{k} = (2\pi/a)(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Let this be the unit of energy. This problem shows why band edges need not necessarily be at the zone center. Several of the degeneracies (band crossings) will be removed when account is taken of the crystal potential.

4. [20 points] Consider a 2 dimensional simple square crystal with two free electrons per unit cell.
   a. Within the free electron model, show that $k_F > 1.1\pi/a$ and $k_F < \frac{\sqrt{2}\pi}{a}$. Draw 9 adjacent BZs, consisting of 3 X 3 BZs. Sketch the Fermi surface (FS), paying close attention to which part of FS lies in which BZ. Do this in the repeated/periodic zone scheme, i.e., draw the FS around the origin of each BZ.
   b. Now focus on the BZ at the center. For the line $k_x = 0.9\pi/a$ within that zone, sketch free electron dispersions that are folded into that line, as a function of k_y. You should indicate where the Femi energy is. Does the dispersion have non-spin degeneracy? Answer the same questions for $k_x = \pi/a$.
   c. Suppose now we turn on a small potential $U_{2\pi} = \langle \vec{k} + \frac{2\pi}{a}\hat{x}|H|\vec{k}\rangle$. Assume that $U_{2\pi}$ is smaller than any finite energy difference at a fixed $\vec{k}$ for sketches made in (b). To leading order, write down what happens to those dispersion curves in (b). Make sketches.
   d. Using your results of (c) and the fact that Fermi surface is orthogonal to the BZ boundary (2(c) above), determine the geometry of Fermi surface(s). Explain why the Fermi surface can be thought of as a small "cigar" shaped [electron] pocket and a small "diamond" (or "circle") shaped [hole] pocket. From particle conservation, before and after turning on the potential, explain why there should be a definite relationship between the area of the "cigar" shape and the area of the "diamond" shape, and find that relationship.

5. [20 points] Crystal momentum conservation in photo-electric effect. In these experiments, light with energy of a few eV to a few hundred eV is directed to a crystal. As a result, electrons are ejected out, and they are called photo-electrons. For this process to occur, it seems clear (as a more sophisticated theory supports) that a scattering process

$$\nu + e \rightarrow e$$

must be occurring *inside* the crystal. This problem will demonstrate that for the full understanding of this scattering process it is essential to have the band theory, which Einstein did not have at his time.
   a. Assume a free electron model, with a non-relativistic energy dispersion relation $\frac{p^2}{2m}$, perfectly appropriate for this experiment. The scattering process can be most conveniently described in the rest frame of the

electron in the initial state. Solve the energy conservation equation $p_\nu c = \frac{p_e^2}{2m}$ and the momentum conservation equation $\vec{p}_\nu = \vec{p}_e$ simultaneously. Here, $\vec{p}_\nu$ is the momentum of the photon, and $\vec{p}_e$ the momentum of the electron in the final state. Can your result explain the experiment? For instance, is it possible to have the photoelectric effect with $h\nu = 10$ eV in this theory?

b. Now let us introduce the band theory. We consider a very nearly free electron model. In this extreme limit of $U_{\vec{G}} \to 0$, the dispersion relation is not modified at all from the free electron dispersion, except that it is now folded back into the first BZ, within the reduced zone scheme. This is a minimal model for our current purpose. To be concrete, consider a one dimensional crystal (a "quantum wire") with $a = 3$ Å, and choose $h\nu = 10$ eV. Choose the initial electron state to be a state in the first band, whose dispersion is $\frac{\hbar^2 k^2}{2m}$, and the final electron state to be a state in the 2nd band, whose dispersion is $\frac{\hbar^2\left(k' + \frac{2\pi}{a}\right)^2}{2m}$, with $|k|, |k'| \leq \frac{\pi}{a}$. [$\left(k' - \frac{2\pi}{a}\right)^2$ would work as well.] Assume that the momentum of the photon is parallel to the quantum wire. What is the final state of the electron? The crucial difference here is the use of the crystal momentum conservation.

6. [20 points] **Effective mass of semi-conductors**. Consider, again, the following matrix applicable near the BZ boundary that is the perpendicular bisector of $-\vec{G}$.

$$h = \begin{pmatrix} \lambda_{\vec{k}} + U_0 & U_{\vec{G}}^* \\ U_{\vec{G}} & \lambda_{\vec{k}+\vec{G}} + U_0 \end{pmatrix}$$

We shall consider a one dimensional crystal only.

a. Do the Taylor expansion of the resulting dispersion relations around the $k = -G/2$ to show that the dispersion is a parabolic function of $\tilde{k} = k + G/2$. From the parabolic form, obtain the effective masses of the electron and the hole in terms of m (bare mass of the electron), E_{Gap} (energy gap at the zone boundary $= 2\left|U_{\vec{G}}\right|$), and $\lambda \equiv \lambda_{k=-\frac{G}{2}}$.

b. To qualitatively estimate the effective mass, let us crudely map the case of GaAs, which has a direct band gap, to our 1D model above. The energy gap is 1.4 eV, the corresponding $\vec{G}$ value is $\frac{8\pi}{a}$ and $a = 6.56$ Å. Based on this information and the model of (a), estimate the effective mass. Compare it with the actual effective masses $m^*/m = 0.067$ (electron), $0.082, 0.45$ (hole), where m is the mass of the bare electron.

7. Submit (1) couple of paragraphs, describing your final project to be presented on March 19 and (2) your presentation file (pdf or ppt). These submitted materials and your presentation will be considered for your final grade. Your topic should be of relevance to the solid state physics, and your writing must include a key reference or two. I am open to discussions any time if you need help formulating your subject. Due March 19.