Homework 8

Due 3/8/2011

1. [10 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.

2. [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.

3. [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

$$\nu + e \to e$$

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.

4. [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 $= 2|U_{\vec{G}}|$), 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.