# Homework 7

Due 2/25/2010

1. [10 points + 5 extra credit] Consider a Kronig-Penney model with a delta function potential. In this model, we assume $U(r) = \sum_s U_0 a\delta(x - sa)$, where $a$ is the lattice constant of the 1D crystal under consideration. The eigenvalue equation for this potential is given by

$$\frac{P}{Ka}\sin Ka + \cos Ka = \cos ka \;\; \text{if}\, \epsilon_{k,n} > 0$$

$$\frac{P}{Ka}\sinh Ka + \cosh Ka = \cos ka \;\; \text{if}\, \epsilon_{k,n} < 0$$

where $P = \frac{mU_0a^2}{\hbar^2}$ [note: there is a factor of 2 mistake in Kittel for $P$] and $\epsilon_{k,n} = \frac{\hbar^2K^2}{2m}$ (the first equation) or $-\frac{\hbar^2K^2}{2m}$ (the second equation). Assume that $a = 2.76$ Å.

   a. Show that $U_G = U_0$ for any $G = \frac{2\pi n}{a}$.
   b. Numerically solve the above equation to plot the first three bands for $P = 0.3, 1, 3$ or $P = -0.3, -1, -3$. You will get extra credit if you choose to work with negative $P$ values, which will require you to check both positive and negative energy eigenvalues. In contrast, if you choose to work with positive $P$ values, then only the first equation above is necessary.
   c. Make a plot of the free electron dispersion shifted in energy by $U_0$ and compare, by over-plotting, it with the results of b. From your comparison, determine for which $P$ value the nearly free electron approximation works the best. Discuss the energy gap in view that approximation.
   d. Make a tight binding fit to the first band, i.e. the lowest-lying band, of b for each $P$ value as follows. As we learned in class, $\epsilon_{TB} = const - 2t\cos ka$. Take $const$ to be the mid-point in energy of the band, and $4|t|$ to be the energy width of the band. Compare this tight binding fit with the first Kronig-Penney band. What is the trend of the quality of the fit for the three values of $P$ in b? What would be your explanation for this trend?

2. [5 points] Kittel 7.2

3. [5 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 $|\lambda_{\vec{k}} - \lambda_{\vec{k}+\vec{G}}| \ll |U_{\vec{G}}|$). 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.

4. [10 points] Consider a 2 dimensional simple square crystal with two free electrons 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 (3(c) above), determine the geometry of Fermi surface(s). Explain why the Fermi surface can be thought of 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. [5 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 $\epsilon_k$ 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.