Homework 6

Phys 155, Winter 2008, UCSC

Due Feb 25

1. [Group velocity; 5 points] We showed in class that at or near a zone boundary the following Hamilotonian is suitable for the first order perturbation theory, if there is a doubly degenerate free-electron state.

$$\begin{bmatrix} \varepsilon^0_{\vec{k}} + V_0 & V^*_{\vec{G}} \\ V_{\vec{G}} & \varepsilon^0_{\vec{k}+\vec{G}} + V_0 \end{bmatrix} \tag{1}$$

where

$$V_{\vec{G}} \equiv \langle \vec{k} + \vec{G} | H_1 | \vec{k} \rangle \tag{2}$$

and $\varepsilon^0_{\vec{k}}$ is the free electron energy. Below, let us ignore V_0 by re-defining the energy reference.

   (a) Is the zone boundary that we are considering a bisector plane of $\vec{G}$ or $-\vec{G}$?

   (b) Solve for the eigenvalues of the above matrix.

   (c) For each eigenvalue, say $\varepsilon_1 = \hbar\omega_1$, $\varepsilon_2 = \hbar\omega_2$, show that the group velocity $\vec{v} \equiv \partial\omega/\partial\vec{k}$ satisfies $\vec{v}\cdot\vec{G} = 0$ when $\vec{k}$ is <u>on</u> the zone boundary. [I think I wrote on blackboard $\vec{v}\cdot\vec{k} = 0$, which was incorrect. $\vec{v}\cdot\vec{G} = 0$ is correct.]

   (d) Discuss what (c) means for the movement of a wave packet formed around a point on the zone boundary. Consider the movement parallel to the zone boundary as well as perpendicular to it. Explain also that (c) means that any constant energy surface (e.g. a Fermi surface) should be perpendicular to the zone boundary plane.

2. [Divalent nearly free-electron metal in 2d; 10 points] Consider a 2 dimensional simple square crystal with two free electrons unit cell. The unit cell dimenion is $a \times a$.

   (a) Within the free electron model, show that $k_F > 1.1\frac{\pi}{a}$ and $k_F < \sqrt{2}\frac{\pi}{a}$. Draw 9 adjacent BZs, consisting of 3×3 BZs. Sketch the Fermi surface (FS), paying close attention to which part of FS lies in which BZ. Do this in the repeated zone scheme, i.e., draw the FS around the origin of each BZ.

   (b) Now look at 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 $V \equiv \langle \vec{k} + \frac{2\pi}{a}\hat{x} | H | \vec{k} \rangle$. Assume that V is smaller than any 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 (from 1(d)), 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 "circle" shape, and find what is the relationship.

3. [Tight-binding model in 2d – HTSC; 5 points] Consider a 2 dimensional simple square lattice with one valence electron per unit cell originating from a $1s$ orbital. The unit cell dimenion is $a \times a$. The tight-binding model is defined by

$$\begin{aligned} \langle ij|H|ij\rangle &= 0 \\ \langle i'j'|H|ij\rangle &= -t \,\text{if } (i'j') \text{ is a nearest neighbor of } (ij) \end{aligned}$$

Here ij (and $i'j'$) are integer indices for Bravais lattice points $ia\hat{x} + ja\hat{y}$.

(a) Derive the tight-binding electron energy $\varepsilon(\vec{k})$?

(b) Find and plot the Fermi surface, given that there is one valence electron per unit cell. [Hint: The Fermi energy is 0. Assume this and show that it is correct.]

(c) Explain why this model of a high temperature superconductor (i) is consistent with Wilson's rule, but (ii) is in trouble, given that experiments show insulating properties for one valence electron per unit cell.

(d) [optional – 8 bonus points] Consider more "hopping integrals" $\langle i''j''|H|ij\rangle = -t'$ for $i''j''$ that are next-nearest neighbors of ij, and answer the same questions (a,b). [The second part is actually quite difficult (bad problem!) and should be <u>numerically</u> done, as opposed to (b), which can be done analytically. It is not recommended to try to solve the second part casually. Will give 3 points for the first part. Will give 5 points to the second part, if the correct FS is obtained for $t = 0.15$ and $t' = -0.05$.]