Physics 416 Problem Set 6 Due Monday, Oct. 24

(1) Start with the results of problem set 3, #1, for the Brillouin zones for 2-D triangular lattice, lattice constant a. You can use the dimensions given in the solutions, but you will need to do a bit of extra calculating for example to determine how far the 4th zone extends.

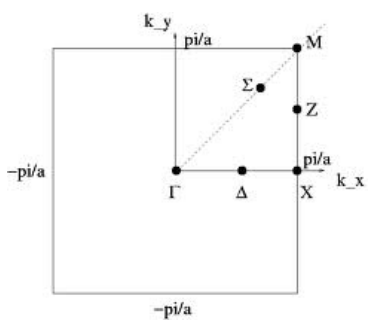
a) Consider a triangular lattice with one electron per primitive cell. Calculate the Fermi wavevector for a free Fermi gas, where the Fermi surface is circular. Don't forget to double up the state occupation for electron spin. Give the result in terms of a, and show that the Fermi surface fits entirely inside the first BZ.

b) Repeat this for the case that there are 4 free electrons per primitive unit cell: Find k_F and compare to the dimensions of the Brillouin zones. Which zone boundaries does the Fermi surface cross? Plot the Fermi surface on a simple sketch of the Brillouin zones in extended k-space.

c) Sketch the *connected* parts of the Fermi surface for the case of 4 electrons/cell. The results should be <u>connected closed curves</u> for each Brillouin zone, which you can get by folding into the first zone and in some cases also additional G-vector translations in reciprocal space. Defining an electron (hole) pocket as a closed surface containing occupied (unoccupied) states, identify your connected Fermi surface pieces as electron or hole pockets.

(2) Free-electron bands in a 3D simple cubic lattice:

(a) Write down a general <u>free-electron</u> ("empty lattice") formula for $\varepsilon(k)$ along the (100) and the (111) directions, for the case that the bands are all folded into the first zone. Do this in terms of $|k|$, and using h, k, and l to label the indices of the G vectors used to fold the band segments into the first zone.



(b) What are the energies of the lowest two band crossings at the Γ and X points, in terms of the lattice constant a and fundamental constants? The figure shows a slice at $k_z = 0$; by convention Γ is the origin, and X is the center of the square face, (100) direction.

(c) In the nearly-free electron model, which Fourier components of the crystal potential would be involved in determining band splittings at the lowest crossing at Γ?

(d) Sketch the three lowest energy bands in the Γ to X direction in the NFE model; what are the *degeneracies* of these bands?

(3) Kittel 7.4

(4) Kittel 7.6.