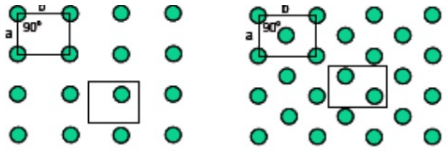
Physics 617 Problem Set 3 Due Weds., Feb. 15

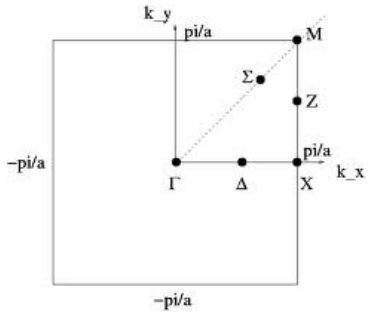
(1) Consider the 2D simple rectangular lattice (left in figure) and centered rectangular (right). Both are Bravais lattices and have can have rectangular *a*b* cells, but in the case of the centered lattice the rectangular cell is not primitive since there are 2 atoms/cell.



(a) Find a set of primitive vectors for the centered lattice, and the corresponding reciprocal lattice vectors.
(b) Show that the reciprocal lattice is also centered rectangular.
(c) Show that each reciprocal lattice position for the *a*b* centered lattice matches a reciprocal lattice position for the *a*b* simple lattice, however half of the simple-lattice reciprocal points are "missing" for the centered lattice. [Similar to the missing reflections for FCC and BCC in 3D that we discussed.]

(2) Degeneracies for Si and GaAs electron bands: For the diamond lattice (Si structure), show that the Fourier component of the lattice potential, $U_{\vec{K}}$, must be zero for the particular reciprocal lattice vector $\vec{K} = (2\pi/a)(2,0,0)$. (Hints: you could think of the lattice potential as superposition of atomic-like potentials located at the position of each atom, or a sleeker way to solve is to note that the potential *U* must be symmetric by translating along the vector corresponding to the Si near-neighbor spacing, and then inverting; consider the effect of this operation on the Fourier component of *U*.) Will this result also be true for the zincblende (GaAs) structure?

(3) Free-electron bands in a 3D simple cubic lattice, lattice constant *a*:
(a) Write down a general free-electron formula for $\varepsilon(k)$ along the (100) and the (111) directions, in terms of the magnitude of the wavevector, $|k|$. Do this in the reduced-zone scheme by adding/ subtracting wavevectors *K*, using *h, k,* and *l* to give the components of the *K* vectors used to fold the 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 *a* and fundamental constants? (Don't include the zero-energy point at Γ; look for the two next-lowest points where the bands "fold back" to the origin.) The figure shows a slice in the $k_x - k_y$ plane; by convention Γ is at $k = 0$ and X is the center of the square 1st BZ face at $k_x = \pi/a$.
(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? (In other words which reciprocal lattice vectors must be included in the energy calculation?)
(d) Sketch the three lowest energy bands in the Γ to X direction in the NFE model. (Don't solve for the energies, just give an approximate sketch.) What are the *degeneracies* of these bands

before the crystal potential splitting is applied? The degeneracies are equivalent to what is shown by the dots in figure 9.5 in the text for the FCC case.

(4) Consider a 2-dimensional honeycomb lattice, with distance a between atoms. As you recall, this is a lattice with a two-atom basis (such as graphene on the first HW).
(a) Find the dimensions of the real-space primitive cell, and the primitive cell in reciprocal space.
(b) Draw (carefully, use a ruler or computer) the reciprocal lattice for this structure, and construct enough bisector planes to map out the first 5 Brillouin zones.
(c) For the case of three electrons per atom in this structure (not per cell), find k_F assuming free electrons, and plot the Fermi surface (Fermi circle) on your drawing.
(d) Sketch the reduced-zone connected pieces of this Fermi surface, and show them as connected closed curves for each zone. Also indicate whether these form hole or electron pockets?