Physics 416 Problem Set 7 Due Wednesday, Nov. 2

(1) 2D rectangular lattice in tight binding: Consider a set of identical localized states $|m,n\rangle$ on a 2D simple rectangular lattice, where the integers m, n index the real-space positions of the states on the 2D lattice sites in x and y directions. Suppose that the Hamiltonian can be expressed as,

$$H = \sum_{m,n} \Big[\varepsilon_o |m,n\rangle\langle m,n| - t_1 \big(|m,n\rangle\langle m,n+1| + |m,n\rangle\langle m,n-1| \big) -$$

$$t_2 \big(|m,n\rangle\langle m+1,n| + |m,n\rangle\langle m-1,n| \big) \Big],$$

where ε_o, t_1, and t_2 are constants. This Hamiltonian couples nearest neighbors only along y (t_1 term) and x (t_2), thus these two constants have a role much like that of γ in our treatment of the cubic lattice in class. Assume lattice constants a (along x) and b (along y).

(a) Write down a Bloch wave function composed of the localized states $|m,n\rangle$. This should be very similar to the form shown in class, except there are two indices for the lattice positions showing explicitly the 2-D positioning; also I am using bra-ket notation instead of the function φ. In your answer express positions R explicitly in terms of a and b.

(b) Plug your wave-function into the Schrodinger equation, show that it is an eigenstate, and solve for the energy vs. k for the resulting band. Find the lowest and highest energies for the band, and identify the k-space coordinates of four saddle points in $\varepsilon(k)$. Sketch the first Brillouin zone and point out on your sketch the positions of the extrema and saddle points in the first Brillouin zone for this lattice.

(2) Kittel problem 8.1

(3) Kittel problem 8.2

(4) Consider a simple-cubic energy band, with energy vs. k the same as our result for an s-orbital tight-binding band, with γ as a parameter:

$$\varepsilon(k) = -2\gamma\left(\cos k_x a + \cos k_y a + \cos k_z a\right).$$

(a) Find the effective mass tensor (for a general $\vec{k}$).

(b) For $\vec{k}$ very close to the zone center, show that the effective mass is isotropic and positive, and find the value.

(c) Find the total bandwidth for this band (in eV) such that the small-k effective mass considered in the last part will be equal to 10 times the free-electron mass.

(d) For energies just below the top of the band show that, similar to part (b), the hole pocket effective mass is also isotropic, and find the value in terms of γ.

(e) Find a *saddle point* for the energy vs. k, and find the effective mass tensor at that point.

(f) What range of Fermi energies will exhibit open orbits for this band?