Physics 617 Problem Set 5 Due Monday, Mar. 20

1) Consider the 2D tight binding band from problem set 4. The band energy is,

$$\varepsilon(k) = \varepsilon_{\rm o} - 2 \left(t_2 \cos k_x a + t_1 \cos k_y b \right).$$

(a) Find a general expression for the semiclassical <u>real-space</u> trajectory of an electron, given a uniform electric field *E* pointing in an arbitrary direction, in terms of the components E_x and E_y . Assume that the electron starts at k = 0 at t = 0 and there is no scattering. Note, to do this you will need to find the semiclassical velocity vs. *k*, and convert to *t*-dependence using the time-dependence of *k*, and then integrate to find position.

(b) Find the Bloch oscillation trajectory in real space for the case of E which points along the (2, 1) direction, and sketch this trajectory.

2) For a 3D version of this band, consider a cubic case but with 3 different matrix elements, resulting in a band with energy,

$$\varepsilon(k) = \varepsilon_0 - 2 (t_1 \cos k_x a + t_2 \cos k_y a + t_3 \cos k_z a).$$

(a) Find the inverse effective mass tensor for a general vector k.

(b) For *k* close to zero, show that all principal values are all positive, and that the carrier pocket here will be an ellipsoidal electron pocket. For a Fermi energy just above the band minimum by a small energy difference δ , find the semi-major axes (e.g. the 3 radii) of the ellipsoidal pocket. (c) Show that just below the top of the band, the particles are holes with negative effective masses, and find the mass tensor.

(d) One of the saddle points will be position $(0,0,\pi/a)$. Find the inverse mass tensor at this point.

3) Ashcroft and Mermin problem #12.4.

4) 2D rectangular monatomic lattice, transverse vibrational modes: Assume a simple rectangular lattice with identical atoms separated by *a* in the x direction and *b* in the y direction, with nearest-neighbor interactions only. Assume displacements only in the z direction, and restoring forces (also in the z direction) $F_{(i,j),(i\pm 1,j)} = -K_1(u_{(i,j)} - u_{(i\pm 1,j)})$ for the "springs" along the x-direction, and $F_{(i,j),(i,j\pm 1)} = -K_2(u_{(i,j)} - u_{(i,j\pm 1)})$ for the y-direction "springs".

(a) Write an expression for the total elastic energy of the lattice, and then by taking appropriate derivatives obtain the equation of motion for the transverse modes. Substitute a solution of the form, $u_a \exp i[\vec{k} \cdot \vec{r} - \omega t]$, and show that the solutions have the form,

 $M\omega^{2} = 2K_{1}(1 - \cos k_{x}a) + 2K_{2}(1 - \cos k_{y}b).$

(b) Show that the allowed 2N solutions fill the first Brillouin zone, and determine the largest frequency among all the vibrational modes corresponding to this solution.

(c) Find the speed of sound in the *x* and *y* directions.