Homework 7: Bloch Electrons and Band Structure

(Note: To help students prepare for the upcoming Ph.D. screening exam).

1. The band structure of many semiconductors (particularly narrow-band-gap semiconductors) at the conduction band-edge is known to be somewhat non-parabolic. A good first approximation to the band structure about K = 0 is $\hbar^2 k^2 / 2m^* = U(1+\alpha U)$ where m* is the effective mass at k = 0, U is the energy, and α is the nonparabolicity parameter. Find an expression for the density-of-states in the conduction band.

2. Square lattice, free electron energies. (a) Show for a simple square lattice in 2-dim that the kinetic energy of a free electron at a corner of the 1^{st} Brillouin zone is higher than that of an electron at the midpoint of a side face by a factor of 2. (b) What is the corresponding factor for a simple cubic lattice in 3-dim ? (c) What bearing might the result of (b) have on the metallic or insulating nature of divalent elements having this band strucure ?

3. Kinematics of free electron energies in reduced zone for fcc lattice. (a) Plot in the [111] direction the energies of all bands up to six times the lowest band energy at the zone boundary **k** = (2π/a)(1/2,1/2,1/2). [Clue: an Excel spreadsheet works great for this problem]. Note that there should be crossing of the bands inside the 1^{st} BZ. Hence band-edges need not be located at the zone center or BZ boundary, since "turning on" the crystal potential energy will cause removal of the degeneracies at the crossings.

4. Square lattice with potential energy. Assume that the crystal potential energy is given by U(x,y) = -4Ucos(2πx/a)cos(2πy/a). Apply the central equation to find the energy gap at the corner point (x,y) = (π/a,π/a) of the 1^{st} BZ.

5. Silicon statistical mechanics
   (a) Show that the density of states associated with a single k-space ellipsoid in Si can be written $g_c(U) = \frac{\sqrt{2}}{\pi^2 \hbar^3} \left(m_d^*\right)^{3/2} \sqrt{U - U_c}$ where m_d^* is the density-of-states effective mass given by $m_d^* = \sqrt[3]{(m_t^*)^2 m_l^*}$
   (b) Evaluate the density-of-states mass, the effective density of states, and the intrinsic carrier concentration at 300 K and at 450 K (maximum safe operating temperature for Si power devices).