489 Spring 2004 Homework 8

Due Wednesday, April 14, 2004

1. Derive the electronic bands in the tight binding form for the following case, which is meant to be a one dimensional problem with bands similar to an ionic crystal like NaCl: a one dimensional crystal consists of two types of atoms equally spaced along a line.

   —X——O——X——O——X——O——X——O——X—

   One atom (X) has three p states oriented in the x, y, and z directions, with on-site matrix element of the Hamiltonian ϵ_{p_x}, ϵ_{p_y}, and ϵ_{p_z}. Although it is not required by symmetry, assume for simplicity that $\epsilon_{p_x} = \epsilon_{p_y} = \epsilon_{p_z} \equiv \epsilon_p$. The other atom (O) has one s state with energy $\epsilon_s > \epsilon_p$. There are interactions with nearest neighbors, but not to more distant neighbors.

   (a) Which nearest neighbor matrix elements are zero by symmetry?
   (b) In terms of the independent parameter(s) needed to describe the nearest neighbor interactions, give analytic expressions for the band energies $\epsilon_n(k)$.
   (c) Sketch the bands in the proper Brillouin Zone (You do not need to be accurate but show the important features.)
   (d) Show that there is a gap between the filled bands and empty bands in the case that $\epsilon_s >> \epsilon_p$, if there are just enough electrons per primitive cell to fill the p bands (as in real ionic materials like NaCl).

2. Consider the tight-binding s-band in a monatomic fcc lattice as described on p. 182 in A&M. Calculate the effective mass for electrons in terms of the tight-binding parameter γ (assume $\gamma > 0$) in the following cases: (a) at the bottom of the band. What is the k point where the minimum occurs?
   (b) at the top of the same band as in part (a). What is the k point where the maximum occurs? (c) The components of the anisotropic effective mass tensor at the X point k=(1,0,0)(2p/a).

3. A & M Problem 12-2(a). Note that the magnetic field is defined to be in the z direction.

4. A & M Problem 14-1.

5. A & M Problem 14-2.

Recommended other problems. Do not turn in:

A & M Problem 12-4. Note in part (a) that the electric field labelled En is the same for all bands n, i.e., En = E for all n. It is this fact that allows one to derive the desired result.

Show that the eigenvalues for a free electron in an H field in 2 d are indeed the same as for a harmonic oscillator of frequency ω_c. This is discussed in Landau & Lifshitz, Quant. Mech.; Peierls, Quant. Theory of Solids; Kittel; ...