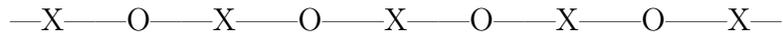


489 Spring 2004 Homework 8

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.



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 $\epsilon_s \gg \epsilon_p$, 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 $k=(1,0,0)(2\pi/a)$.
 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 E_n is the same for all bands n , i.e., $E_n = E$ 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; ...