Solid State Physics 240A: Homework #7. Tight binding models.

Due Monday Nov. 2, 2015

1. Consider the single atom/cell, linear chain discussed in class. You are to compare two complementary choices using two parameters. In the first, you have 1st and 2nd neighbor hopping between orthogonal orbitals, with hopping amplitudes t_1, t_2 respectively. Set t_1=1 to fix the energy scale, so really only one parameter. In the second approach, only 1st neighbor hopping occurs but non-orthogonal basis functions are assumed, so you have an overlap parameter s_1, the only parameter for this case..

The objective is to compare using a 2nd neighbor hopping versus using an overlap parameter. Plot the band (what range is needed to see everything?) for $t_2 = \pm 0.25$, then plot the band for $s_1 = \pm 0.25$. What do the two approaches seem to do similarly, and what differently? It can be useful to make plots with more values of the parameters, all on the same plot. Don't let the parameters get too large, hence non-physical.

2. Diatomic chain. Consider a diatomic chain with atoms A and B, on-site energies $\varepsilon_A, \varepsilon_B$, 1st neighbor hopping $t_{AB} (\equiv t_{BA})$, and 2nd neighbor hoppings t_{AA}, t_{BB}.
(a) Construct the tight binding Hamiltonian matrix.
(b) Show that it reduces to the monatomic chain result in the appropriate limit, but with certain "complication(s)." Describe the complications.
(c) Expand the diatomic Hamiltonian, as is popular these days, in Pauli matrices and the unit matrix: $\sum_{j=0}^{3} h_j(k) \cdot \sigma$ to obtain the vector decomposition $\vec{h}(k)$. We will discuss this in class.

3. Construct the tight binding Hamiltonian matrix for "GaAs," which has the diamond structure except the two atoms in the primitive cell are different. However, let one atom (say, Ga) have two orbitals with different on-site energies, hence different hopping amplitudes t_a, t_b to the other atom. Account for all different on-site energies and nearest neighbor hopping only. This is practice in setting up a non-trivial but still straightforward TB Hamiltonian.