6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 5
Issued: 3-26-04   Due: 4-2-04 at the beginning of class.

Readings:
PSSA Chapter 7

Problem 5.1 1D monatomic chain

Consider a one dimensional monatomic lattice with each atom placed on the x-axis a distance a apart. Take two orbital for each atom, the $2s$-state and the $2p_z$-state. (See the drawing for problem 7.1 in PSSA but make the p-orbitals in the z-direction.

Write down the 2×2 matrix equation, whose eigen values gives you the bands (ignore the overlap matrix.)

(a) Under what conditions will the bands not overlap. Express your answer in terms of E_s, E_p, ($E_s < E_p$) and the appropriate V_{ijk}'s, and be careful of the signs. Hint: you should have found a diagonal matrix.

(b) Find an analytical expression for the density of states for each of the bands.

(c) Write down the tight binding wave function for the bottom band at $k = 0$, $k = \pi/4$ and $k = \pi/a$.

Problem 5.2 PSSA Problem 7.2

All the necessary .m files can be `ftp`-ed from the directory
`/afs/athena.mit.edu/user/o/r/orlando/Public`.

Problem 5.3 PSSA Problem 7.3

The programs are also in my Public Directory.

Problem 5.4 Free Electron Bands

Consider a 2D square lattice with lattice constant a.
(a) Plot (or draw, yes even by hand if you want) the first 6 energy bands along the k_y-direction in the reduced zone scheme.
(b) Also, determine the energy for each band at the symmetry points of Γ and X, and state the degeneracy for each.