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 orbitals 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 \(2 \times 2\) matrix equation, whose eigenvalues give 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 \(\Gamma\) and \(X\), and state the degeneracy for each.