PH575: Introduction to Solid State Physics SPRING 2017
Homework #3 DUE on **Wednesday**, 26 April 2017, in class

1. LCAO states

A chain of eight protons (periodic boundary conditions) supports eight LCAO states built from 1s orbitals. The x-axis passes through the eight protons.

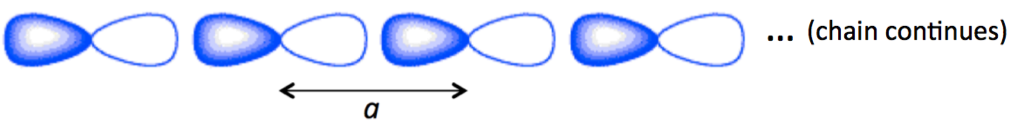
a) Consider the wavefuction with $k = \pi/4a$. Sketch the value of the wavefunction along the x-axis. Do separate plots for the real and imaginary components of the wavefunction.

b) Consider the wavefuction with $k = \pi/4a + 2\pi/a$. Show (mathematically) that this wavefunction is identical to $k = \pi/4a$.

c) Use vector notation in the atomic orbital basis to represent the state $k = \pi/4a$ and the state $k = \pi/2a$. Show that these two states are orthogonal.

2. LCAO states

Consider a 1d chain (periodic boundary conditions) of N identical atoms with spacing a along the x-axis. Each atom has only one p_x-orbital as shown below (dark represents negative, light represents positive). The molecular orbitals of this chain have the form $|\Psi\rangle = \sum c_n |n\rangle$, where $|n\rangle$ is the atomic orbital associated with the n^{th} atom.



a) What are the values of the first 4 coefficients, c_1, c_2, c_3, c_4, for the lowest energy LCAO wavefunction? What is k for this LCAO wavefunction?

b) What are the values of the first 4 coefficients, c_1, c_2, c_3, c_4, for the highest energy LCAO wavefunction? What is k for this LCAO wavefunction?

c) Sketch out the dispersion relationship, $E(k)$, for this system. Pay attention to the sign of the hopping integral, β. Assume that N is very large so that k is effectively a continuous variable.

3. Carbon nanotubes (CNTs) support 1-dimensional wave functions, similar to the LCAO states on a chain of protons. The changing phase of the wave function along the length of the carbon nanotube is described by k. Within the energy range of interest, the dispersion relation for the conduction band of a CNT is

$$E_c(k) = \alpha + \sqrt{\Delta^2 + (\hbar v_F k)^2},$$

and the dispersion relation for the valance band of a CNT is

$$E_c(k) = \alpha - \sqrt{\Delta^2 + (\hbar v_F k)^2}$$

(a) Find a piecewise expression for the 1-dimensional density of states (number of states per unit energy and unit length) for a CNT. The independent variable in your expression should be energy, not k.

(b) Sketch a graph of the answer you calculated in part a.