PHYS 225 – Spring 2011 **Marie Lopez del Puerto**

HW #17

1. **(Kasap 4.1) Phase of an atomic orbital**

a. What is the functional form of a *1s* wavefunction $\psi(r)$? Sketch shematically the atomic wavefunction $\psi_{1s}(r)$ as a function of distance from the nucleus.
b. What is the total wavefunction $\psi_{1s}(r,t)$?
c. What is meant by two wavefunctions $\psi_{1s}(A)$ and $\psi_{1s}(B)$ that are out of phase?
d. Sketch schematically the two wavefunctions $\psi_{1s}(A)$ and $\psi_{1s}(B)$ at one instant.

2. **(Kasap 4.2) Molecular orbitals and atomic orbitals** Consider a linear chain of four identical atoms representing a hypothetical molecule. Suppose that each atomic wavefunction is a *1s* wavefunction. This system of identical atoms has a center of symmetry *O* with respect to the center of the molecule, and all molecular wavefunctions must be either symmetric or antisymmetric about *O*.

a. Using the LCAO principle, sketch the possible molecular orbitals.
b. Sketch the probability distributions $|\psi|^2$.
c. If more nodes in the wavefunctions lead to greater energies, order the energies of the molecular orbitals.