Additional Problems

1) Consider the following diatomic molecules: H₂, He₂, B₂, N₂, O₂
   a) Make an energy diagram of the molecular orbitals formed by the LCAO method using the 1s, 2s, and 2p atomic orbitals.
   b) For each molecule assign the electrons to the molecular orbitals
   c) For each molecule calculate the bonding order
   d) Based on your answers in part c, which molecules are stable? Which are paramagnetic?

2) A quartic oscillator is defined by the Hamiltonian 
   \[ H = -\frac{\hbar^2}{8\pi^2m} \frac{d^2}{dx^2} + \frac{kx^4}{2} \]. Note this oscillator differs from the linear harmonic oscillator discussed earlier in that its potential energy goes like \( x^4 \).
   a) Using a trial wave function of the form 
   \[ \psi(x) = \left( \frac{\alpha^2}{\pi} \right)^{1/4} e^{-\alpha x^2/2} \], where \( \alpha \) is a constant, calculate the energy \( \langle E \rangle \) for the quartic oscillator and the ground state wave function.
   b) Determine the value of \( \alpha \) that minimizes the energy in part a.
   c) Using your result from part b, calculate the ground state energy of the quartic oscillator.

3) Suppose a hydrogen atom is initially in its ground state (i.e. the 1s orbital) defined by
   the wave function: 
   \[ \psi_{1,0,0}(x) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \].
   a) What frequency of radiation would be required to induce a transition from the 1s state to the n=2 state? To what region of the electromagnetic spectrum does this radiation belong?
   b) Calculate the transition moment for a transition from the 1s to the 2s orbital. That is, evaluate the integral
   \[ \int \psi^*_x \psi_{2,0,0} U^{1/2} d\tau \] where
   \[ U = -\mu V_0 |\cos \theta| d\tau = dx dy dz \], and
   \[ \psi_{2,0,0} = \frac{1}{\sqrt{32\pi a_0^3}} \left( 2 - \frac{r}{a_0} \right) e^{-r/2a_0} \]. You
perform this integral in spherical coordinates by setting

\[ d\tau = dx dy dz = r^2 \sin \theta dr d\theta d\phi, \]

and integrating \( r \) from 0 to infinity, \( \theta \) from 0 to \( \pi \), and \( \phi \) from 0 to \( 2\pi \). Is the transition moment non-zero? Will the transition be observed?

c) Will a transition occur from the 1s orbital to the 2p\(_x\) orbital? Prove you answer by evaluating the transition moment \( \int \int \int \psi_{2,1,0}^* U \psi_{1,0,0} d\tau \) where

\[ \psi_{2,1,0} = \frac{1}{\sqrt{32\pi a_0^3}} \left( \frac{r}{a_0} \right) \cos \theta e^{-r/2a_0} \]

\[ \psi_{2,1,\pm} = \frac{1}{\sqrt{64\pi a_0^3}} \left( \frac{r}{a_0} \right) \sin \theta e^{\pm i\phi} e^{-r/2a_0} \]

Explain.

d) Based on your answers in parts b and c, would you expect to observe transitions from the 1s state to the other 2p orbitals, described by the wave functions