Problem Set 4 CHEM 26100

## 4 Harmonic Oscillators II and the Hydrogen Atom

10/27: 1. The J=0 to J=1 transition for carbon monoxide ( $^{12}C^{16}O$ ) occurs at  $1.153 \times 10^5$  MHz.

- (a) Calculate the value of the bond length in carbon monoxide.
- (b) Predict the J=1 to J=2 transition for carbon monoxide.
- 2. The harmonic oscillator has a finite zero-point energy because of the uncertainty relation. In contrast, the lowest possible energy for the 2D rigid rotor is zero.
  - (a) For the ground state of the 2D rigid rotor, what is the expectation value of the angular momentum, and what is the uncertainty  $\Delta L_z$  in the expectation value? Recall that

$$(\Delta L_z)^2 = \langle \hat{L}_z^2 \rangle - \langle \hat{L}_z \rangle^2$$

- (b) In words, describe the uncertainty in position.
- (c) Using your answers to (a) and (b), explain briefly why the 2D rigid rotor can have a vanishing zero-point energy and yet still remain consistent with the uncertainty relation.
- 3. For the ground state of the hydrogen atom, compute
  - (a) The average distance from the nucleus for finding the electron.
  - (b) The most probable distance from the nucleus for finding the electron.
  - (c) Repeat the calculation for the second excited state (n = 3 and l = 0) and compare your results with the ground state.
- 4. Using non-relativistic quantum mechanics, compute the ratio of the ground-state energy of hydrogen to that of atomic tritium.
- 5. The Hamiltonian operator for a hydrogen atom in a magnetic field where the field is in the z-direction is given by

$$\hat{H} = \hat{H}_0 + \frac{\beta_B B_z}{\hbar} \hat{L}_z$$

where  $\hat{H}_0$  is the Hamiltonian operator in the absence of the magnetic field,  $B_z$  is the z-component of the magnetic field, and  $\beta_B$  is a constant called the Bohr magneton.

- (a) Show that the wave functions of the Schrödinger equation for a hydrogen atom in a magnetic field are the same as those for the hydrogen atom in the absence of the field.
- (b) Show that the energy associated with the wave function  $\psi_{n,l,m}$  is

$$E = E_n^{(0)} + \beta_B B_z m$$

where  $E_n^{(0)}$  is the energy in the absence of the field and m is the magnetic quantum number.