CHM 3411 – Problem Set 4

Due date: Wednesday, February 6st. (NOTE: The first hour exam is in class on Friday, February 8th. It will cover material from Chapters 7 and 8 of Atkins, including handouts.)

Do all of the following problems. Show your work.

1) Consider the following function as a possible solution to the particle on a ring TISE

$$f(\phi) = A \sin(2\phi) \qquad (1.1)$$

a) What value for A makes f(x) a normalized function?

b) Is f(x) an eigenfunction for the Hamiltonian operator for the particle on a ring? Recall that for this system

$$H = T + V = - (\hbar^2/2m)\, d^2/d\phi^2 \qquad (1.2)$$

If your answer is yes, what is the corresponding eigenvalue?

c) Is f(x) an eigenfunction for the operator L_z? Recall that

$$L_z = - i\hbar\, d/d\phi \qquad (1.3)$$

If your answer is yes, what is the corresponding eigenvalue?

2) What is the value for the following commutator

$$[\phi, L_z] \qquad (2.1)$$

where L_z is the z-component of the angular momentum vector (defined in the previous problem).

3) The solutions to the particle on a sphere TISE are the spherical harmonics $Y_{\ell,m_\ell}(\theta,\phi)$ (see Table 8.2 of Atkins), where the energy and possible values for the quantum numbers are

$$E_\ell = [\ \ell(\ell+1)\ ]\ \frac{\hbar^2}{2mr^2} = [\ \ell(\ell+1)\ ]\ E_0\ ,\ \text{ where } E_0 = \hbar^2/2mr^2 \qquad (3.1)$$

where $\ell = 0, 1, 2, \ldots$

$m_\ell = 0, \pm 1, \pm 2, \ldots \pm \ell$

Note that in the above expression the units for energy are J (Joule).

a) What is the energy and the degeneracy for the $\ell = 3$ states of the particle on a sphere? You may give your energy in terms of E_0 (defined above).

b) The wavefunction for the $\ell = 2$, $m_\ell = 2$ state of the particle on a sphere TISE is

$$Y_{2,2}(\theta,\phi) = (15/32\pi)^{1/2} \sin^2\theta \exp(2i\phi) \qquad (3.2)$$

Show by substitution into the eigenvalue equation that $Y_{2,2}(\theta,\phi)$ is an eigenfunction of the operator L_z (defined in problem 1), and find the corresponding eigenvalue.

4) The particle on a sphere is a good model for rotation of a diatomic molecule. Spectroscopic measurements can determine an experimental value for B, the rotational constant for the molecule. Since

$$B = \frac{h}{8\pi^2 c\mu r_e^2} \qquad (4.1)$$

where B is in wavenumbers, and μ, the reduced mass of a diatomic molecule AB, is defined as

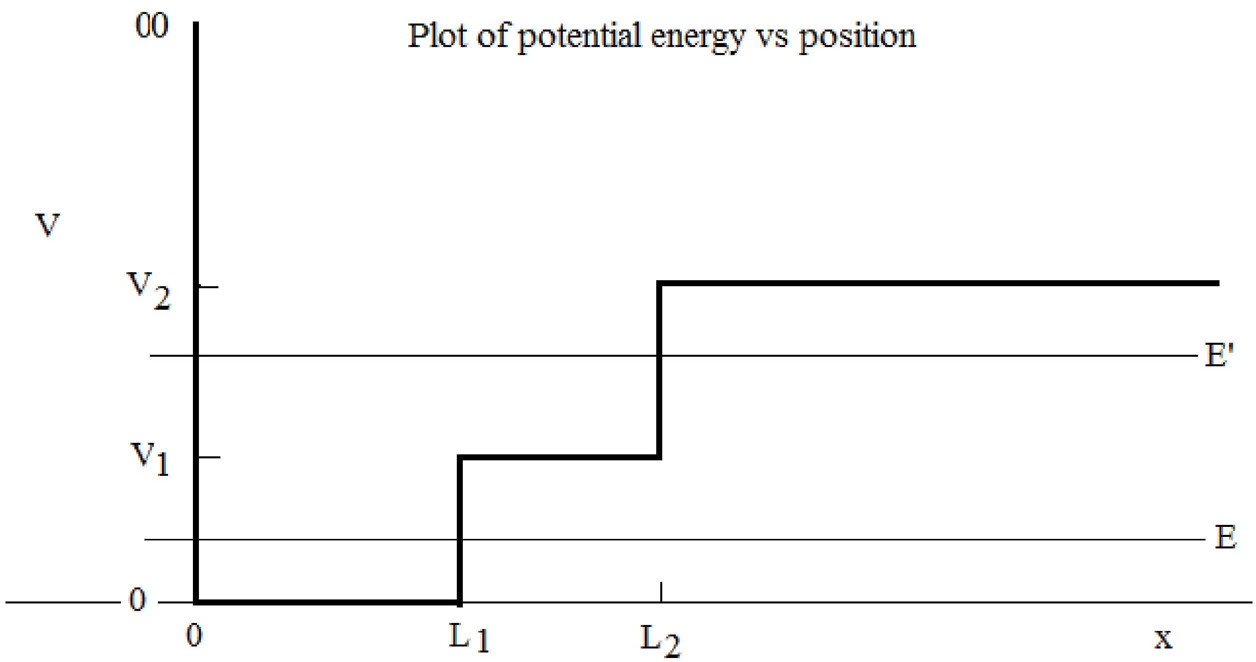
$$\mu = \frac{m_A m_B}{(m_A + m_B)} \qquad (4.2)$$

the value for B can then be used to find r_e, the equilibrium bond distance for the molecule.

Using the information below, find the value for r_e for the CN radical

$B(CN) = 1.900\ cm^{-1}$ $\qquad$ $m(^{12}C) = 12.0000$ amu $\qquad$ $m(^{14}N) = 14.0031$ amu

5) A plot of potential energy vs position is given below for a one dimensional system.



Sketch the following:

a) The wavefunction corresponding to an energy E, where E represents the ground state (lowest energy state) of the system.

b) The wavefunction for an excited state of the system that has two nodes and is at an energy E′.

Describe the "interesting" features of your two wavefunctions in the different potential regions.

Your sketches will be qualitative, but should be consistent with what we have discussed in class concerning wavefunctions for one dimensional systems.