CHEM442-001/002
College of Charleston
Spring 2000
Exam II

1(15). For atomic B

A) write the hamiltonian operator describing the internal atomic energy. Do not use summation notation, write out the complete set of terms.

B) write the determinant form for a trial wave function using atomic hydrogen orbitals. Do not expand the determinant.

C) write the ground state electron configuration. Is atomic B paramagnetic? _____

2(10). Classically, the one-dimensional kinetic energy of a particle is $(\frac{1}{2})k_B T$. Calculate the quantum number corresponding to this energy for a nitrogen molecule at 25 °C in a box that is 5.00 m wide.

3(20). A student was so thrilled at being able to do the homework assignment in which $\langle X \rangle$ and $\langle x^2 \rangle$ were determined for a particle in a three-dimensional box that he decided to derive the expression for $\langle x^3 \rangle$. Do likewise.
[Note that the integral that you will probably need is

$$\int x^n \sin^2 x \, dx = \frac{x^{n+1}}{2(n+1)} + \frac{n!}{4} \, abunchofnastytrigterms$$

however, time does not permit evaluating the "bunchofnastytrigterms", so omit them.]

4(20). The wave function for the SHO system is

$$\psi_v = \frac{1}{(2^v \, v!)^{1/2}} \left(\frac{a}{\pi} \right)^{1/4} e^{-ax^2/2} \, H_v(a^{1/2}x)$$

where

$$H_n(z) = (-1)^n \, e^{z^2} \, \frac{d^n}{dz^n} \, e^{-z^2}$$

Derive the wave function for $v = 5$ in terms of x and a.

5(20). Calculate the $\Delta\epsilon$ between the $J = 5$ and $J = 0$ rotational levels for HCl given $I = 2.679 \times 10^{-47}$ kg m^2.

Calculate $N_{J=5}/N_{J=0}$ at 100 K.

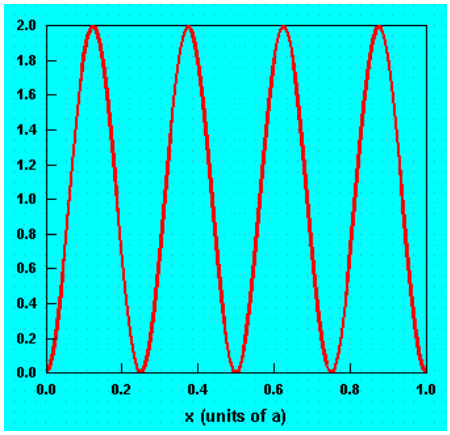
Calculate the $\Delta\epsilon$ between the v = 5 and v = 0 vibrational levels for HCl given ν_o = 8.65×10^{13} s^{-1}.

Calculate $N_{v=5}/N_{v=0}$ at 100 K.

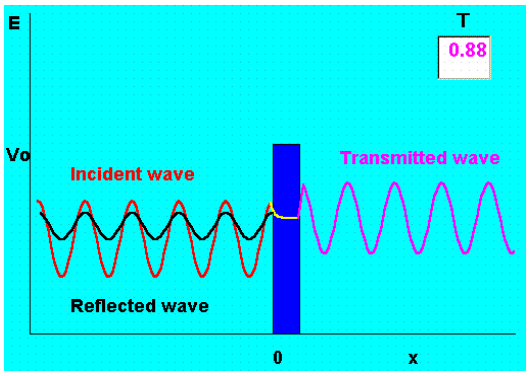
6(15). Answer the following questions for the screen captures from P-Chem:

A) For a particle in a one-dimensional box, is this $\psi^*\psi$ or ψ?

What is the value of the translational quantum number n?



B) This illustrates the phenomenon of _____



How will the diagram change if the barrier width increases?

C) Plot ψ for $v = 4$ on the appropriate energy line.