CHM 6480 – Problem Set 4
Due date: Sunday. November 22nd (by 11:59pm)
Do all of the following problems. Show your work.

1) The one dimensional harmonic oscillator is an exactly solvable problem in quantum mechanics. As such, it represents a good test case for variational theory, since variational calculations can be compared to the exact result for this system.

Consider the following function as a solution to the ground state of the harmonic oscillator

$$f(x) = \cos ax \qquad -\pi/2 < ax < \pi/2 \qquad (1.1)$$

$$f(x) = 0 \qquad ax \leq -\pi/2 \text{ or } ax \geq \pi/2 \qquad (1.2)$$

where a is our variable parameter.

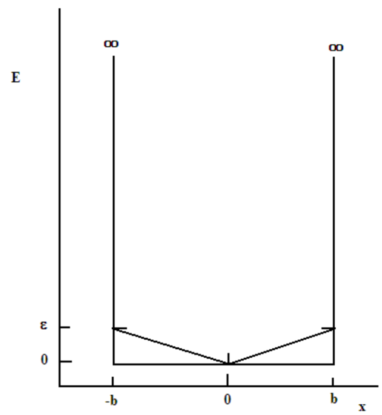
a) Find an expression for E_{trial}, given by the relationship

$$E_{trial} = \frac{< f \mid H \mid f >}{< f \mid f >} \qquad (1.3)$$

b) Find the value for a that minimizes the value for E_{trial}. Compare the minimum energy found to the ground state energy for the harmonic oscillator

$$E_1 = \frac{\hbar\,(k/m)^{1/2}}{2} \qquad (1.4)$$

2) Consider the following perturbed particle in an infinite box system.



Find the first order correction to the energy of this system for the n = 1 and n = 2 state.

3) As discussed in class, the energy of an atom is perturbed by spin-orbit coupling. Relative to the unperturbed energy, the perturbation energy due to spin orbit coupling is, to first order

$$E_{SO} = a\,[J(J+1) - L(L+1) - S(S+1)] \qquad (3.1)$$

Where L, S, and J are quantum numbers and a is a constant.

The ground electronic state for an oxygen atom is ^3P.

a) What are the possible values for J for the above state? What are the degeneracies for each of these states?

b) Using eq 3.1, find the value for E_{SO} for each of the J states of a ground state oxygen atom, relative to the energy in the absence of spin orbit coupling. Note that for the ^3P state of oxygen a = - 39. cm^{-1}.

c) The actual energies of the different J states of an oxygen atom (relative to the ground state energy) can be found at

https://physics.nist.gov/PhysRefData/ASD/levels_form.html

Enter “O I” in the box labeled “Spectrum” (this corresponds to the states for a neutral oxygen atom).

Compare your results in b to the experimental results, and comment on differences, if any.