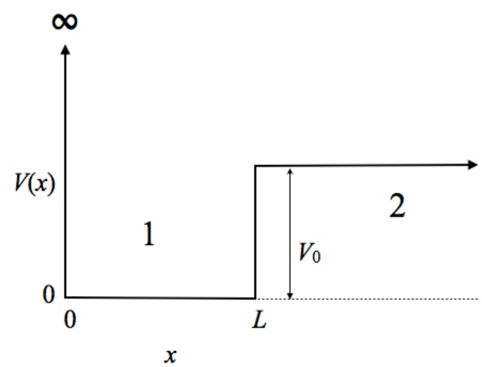
Chem 332: Problem Set #5

Due in class: Wednesday, Feb. 27th

(1) Consider the following 1-dimensional box that we discussed in class:



From lecture we know that in region (1) where V=0, $\psi_1 = A\sin(k_1 x)$ and in region (2) where V=V_0, $\psi_2 = Be^{-\varepsilon x}$ (for E<V_0), where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ and $\varepsilon = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$. Apply the boundary conditions at x=L, i.e., $\psi_1(L) = \psi_2(L)$ and $\psi_1'(L) = \psi_2'(L)$, and show this leads to the resulting quantization condition: $\tan(k_1 L) + \sqrt{\frac{E}{V_0 - E}} = 0$.

(2) Consider a simple harmonic oscillator with mass m and force constant k, and a particle with the same mass in a one-dimensional box of length L.

(a) What is the relationship between k and L such that the zero-point (ground state) energies of these two systems will be the same?

(b) If m is equal to the mass of a ^{1}H atom, what is the value of k (in N/m) corresponding to L=1.4 nm?

(3) For a certain harmonic oscillator of mass 2.88×10^{-25} kg, the difference in adjacent energy levels is 4.82×10^{-21} J. Calculate the force constant of the oscillator.

(4) For the ground state of the 1-dimensional harmonic oscillator, determine the expectation values of the kinetic energy (*T*) and the potential energy (*V*) and in doing so verify that $\langle T \rangle = \langle V \rangle$.

(5) If a H_2 molecule rotates in the plane of a crystalline surface (in a chemisorption situation), it can be approximated as a two-dimensional rigid rotor. Calculate (in kJ/mol) the lowest energy rotational transition for such a system. Take the mass of the rotor to be 1/2 the mass of a hydrogen atom with a value of *r* equal to the bond length of H_2, 0.7416 Å.