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 \( V=0 \), \( \psi_1 = \lambda \sin(k_1 x) \) and in region (2) where \( V=V_0 \), \( \psi_2 = B e^{-\varepsilon x} \) (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:

\[
\tan(k_1 L) + \frac{E}{\sqrt{V_0 - E}} = 0
\]

(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 $2.88 \times 10^{-25}$ kg, the difference in adjacent energy levels is $4.82 \times 10^{-21}$ 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.