Homework 4, Due Feb. 25

1. A crude model of an electron in a molecule treats it as a particle in a one-dimensional box whose length is on the order of the size of the molecule. a). For an electron in a box of length 4.0 Å, calculate the separation between the two lowest energy levels. b). Calculate the wavelength of a photon corresponding to a transition between these two levels. c). In what portion of the electromagnetic spectrum lies this wavelength?

2. Prove that the second and forth quantum states for particle in 1D box are orthogonal using the explicit wavefunctions.

3. The infrared absorption spectrum of $^{1}H^{35}Cl$ has its strongest band at 8.65×10^{13} Hz, which corresponds to the excitation from its ground vibrational state to the first excited vibrational state. a) Use the harmonic oscillator approximation to calculate the force constant of the bond in this molecule. b). Find the corresponding zero-point energy. c). predict the photon frequency of the strongest infrared band of $^{2}H^{35}Cl$. Use computer software to draw the wave functions of the first four eigenstates (using the harmonic oscillator approximation).

4. Verify that the ground state (n=0) wavefunction is an eigenstate of the harmonic oscillator Hamiltonian. Using the explicit wavefunction of the ground state to calculate the average potential energy $\left\langle 0\left|\hat{V}\right|0\right\rangle$ and average kinetic energy $\left\langle 0\left|\hat{T}\right|0\right\rangle$. (Hints: take advantage of the symmetry in integration and use the formula:

$\int_0^\infty x^{2n}e^{-ax^2}dx=\frac{1\times3\times5\times\cdots\times(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}$)