CHEM 361B - Lecture 9 Activity

The Simple Harmonic Oscillator

1. The ground state wavefunction for the harmonic oscillator is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$$

   (a) Show that $\langle x \rangle = 0$.

   (b) Since $\langle x \rangle = 0$ for the simple harmonic oscillator, $\sigma_x = \sqrt{\langle x^2 \rangle}$. Given that the fundamental frequency of $^1H^{19}F$ is 4138.32 cm^{-1}, show that the root-mean-square displacement ($\sqrt{\langle x^2 \rangle}$) of the ground state ($\psi_0$) is 6.546×10^{-12} m. Use

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$$

   and the fact that $\omega = \sqrt{\frac{k}{\mu}} = \frac{2\pi c}{\lambda}$

   (c) Compare σ_x it to its equilibrium bond length of 91.68 pm. What does this result mean interms of experimentally measuring the equilibrium bond length?

2. In this question we will use the raising and lowering operators

   (a) Find ψ_1 by applying the raising operator to ψ_0:

$$\psi_1 = A_1 a_+ \psi_0$$

   to get

$$\psi_1 = A_1 \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}} x e^{-\frac{m\omega}{2\hbar}x^2}$$

   (b) Normalize your result from 2a) and show that $A_1 = 1$.

   (c) (Challenge) Apply $\hat{H}$ to ψ_1 and show that $E_1 = \frac{3}{2}\hbar\omega$.

   (d) What is the difference in energy between E_0 and E_1. Is this what you expected? In general, what is the difference in energy between all adjacent energy levels in the simple harmonic oscillator potential?