Chem 442: Homework for lecture L10

(only turn in **BOLD** assignment first lecture next week; do <u>all</u> assignments)

1. In lecture, we talked about how the vibrating molecule Hamiltonian (energy operator) is symmetrical in p and x because it depends on the square of both. We made use of this symmetry to find out that a Gaussian is the lowest energy state (ground state) of the harmonic oscillator, and its energy is $\hbar\omega/2$. We also to derived an expression for the Hamiltonian in terms of the raising operator $\hat{a}^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}(x - \frac{i\hat{p}}{m\omega})$ and lowering operator $\hat{a} = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}}(x + \frac{i\hat{p}}{m\omega})$: $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$

Now, work out $\hat{a}\hat{a}^\dagger$ to derive an equivalent representation for the Hamiltonian

$$\hat{H} = \hbar\omega\left(\hat{a}\hat{a}^\dagger - \frac{1}{2}\right).$$

That formula looks very similar to the one we derived in class, but the order of $\hat{a}^\dagger$ and $\hat{a}$ has switched.

Turn in 2. Remember, in quantum mechanics order matters: $x\hat{p} \neq \hat{p}x$ because momentum is a derivative. We showed $x\hat{p} - \hat{p}x$=$i\hbar$ several lectures ago.

a. What is $\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$ equal to? Is it zero, or does order matter? The 'leftover' difference is called a 'commutator' and is often abbreviated with square brackets as $[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}$. When you see [a,b] in quantum mechanics, think ab-ba!

BIG HINT: To make this really easy, use the two formulas for $\hat{H}$ from the previous problem!

b. Use your result above and the fact that $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$ to show that $\hat{H}\hat{a}^\dagger = \hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger$, the formula we used in lecture. **HINT:** $\hat{H}\hat{a}^\dagger = \hbar\omega\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hbar\omega\frac{1}{2}\hat{a}^\dagger$; now use the commutator from (a) to replace the $\hat{a}\hat{a}^\dagger$ in the first part by $\hat{a}^\dagger\hat{a}$ plus other stuff to get the answer.

c. What is $[\hat{a}^\dagger, \hat{a}^\dagger]$ equal to? **HINT: yes, this is easy!**

3. Prove that the Gaussian stationary state of the vibrating molecule that we derived in lecture L9 really is the lowest energy state, or ground state: the Heisenberg principle forbids the wavefunction from having a smaller Δx and 'squeezing down further' in energy.

To do this, recall from lecture that raising operator 'raises' an eigenstate to the next higher energy eigenstate, while the lowering operator 'lowers' an eigenstate to the next lower one. Simply show that for the Gaussian $\psi_0(x)$,

$$\hat{a}\psi_0 = 0.$$

This proves that there IS NO state lower in energy than the Gaussian, so the lowest eigenstate is the gaussian ψ_0 with energy $E_0 = \hbar\omega/2 = \hbar\omega(0 + \frac{1}{2})$. The next higher state, as we saw, is Ψ_1 with energy $E_1 = \hbar\omega(1 + \frac{1}{2})$, and so on up to $E_n = \hbar\omega(n + \frac{1}{2})$.