Chem 532: Problem Set #3

Due by 5pm: Friday, Sept. 30th

(1) We defined our simple harmonic oscillator ladder operators as:

$$\hat{a} = \frac{\hat{Q} + i\hat{P}}{\sqrt{2}} \quad , \quad \hat{a}^{\dagger} = \frac{\hat{Q} - i\hat{P}}{\sqrt{2}}$$

with $Q = \sqrt{\frac{m\omega}{\hbar}}\, x = \left(\frac{mk}{\hbar^2}\right)^{1/4} x$ and $P = -i\frac{d}{dQ}$

Show that the position and momentum can then be written as:

$$x = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^{\dagger}\right) \quad , \quad \hat{p}_x = i\sqrt{\frac{m\hbar w}{2}}\left(\hat{a}^{\dagger} - \hat{a}\right)$$

(2) Evaluate the following commutators

(a) $\left[\hat{a}^{\dagger}, \hat{a}\right]$

(b) $\left[\hat{H}, \hat{a}^{\dagger}\right]$, where H is the harmonic oscillator Hamiltonian

(3) Consider the <u>anharmonic</u> oscillator with $\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 + cx^3$.

Compared to the usual harmonic case, the first non-zero correction to the energy due to the anharmonic term cx^3 is given by weighted sums over the integrals $\langle \mathrm{v}' | x^3 | \mathrm{v} \rangle$, where $|\mathrm{v}\rangle$ are harmonic oscillator eigenfunctions with quantum number v (or v′). Evaluate this integral for a general $\langle \mathrm{v}'|$ and $|\mathrm{v}\rangle$ (*hint*: use the ladder operator representation of *x*)

(4) Single-walled carbon nanotubes can be approximated by a particle-on-a-cylindrical-surface model. Suppose the cylinder has length *L* and radius *a*, with the *z*-axis along the cylinder.

a) Write the kinetic energy operator of the electron in terms of the length z, the radius a, and the radial angle ϕ of the cylinder.

b) Combing ideas from the particle-in-a-box and particle-on-a-ring models, show that the wavefunction can be written as $\psi = Asin\left(\frac{n\pi}{L}z\right)e^{ik\phi}$. What are the allowed values of the quantum numbers n and k ?

c) Write the energy expression in terms of n, k, L, a, and fundamental constants. For a nanotube of radius 5.5 Å and length 120 Å, compute the energy spacing between the lowest energy levels.

(5) Convert the Laplacian operator from x,y cartesian coordinates to plane polar coordinates via the chain rule.