Chem 442: Homework for lecture L9

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

1. (Turn in) Use postulate (4) of quantum mechanics to prove very explicitly that the energy of a quantum particle with wavefunction $\Psi_n(x)\, e^{-\frac{i}{\hbar}E_n t}$ is simply E_n with 100% probability.

Remember what postulate (4) says IN GENERAL: if an observable A is measured, its value can't be just anything. It MUST BE one of the solutions of the equation $\hat{A}\varphi_n(x) = a_n\varphi_n(x)$. In this equation, a_n is called an "eigenvalue" of the operator $\hat{A}$ for the observable A, and $\varphi_n(x)$ is called an "eigenfunction." The probability of measuring that "n^{th}" eigenvalue as the actual value of A is $P(A=a_n) = |\int dx\varphi_n^*(x)\Psi(x,t)|^2$.

a. For the SPECIFIC case where A is the energy, write down the operator for A, the eigenvalue equation, and the probability $P(E=E_n)$; call the eigenvalues E_n and the eigenfunctions $\Psi_n(x)$ in this specific case.

b. Now assume that the wavefunction $\Psi(x,t)$ in your probability is not just any function, but the stationary state $\Psi(x,t) = \Psi_n(x)\, e^{-\frac{i}{\hbar}E_n t}$, and write down the probability formula.

c. Now remember that $e^{-\frac{i}{\hbar}E_n t}$ does not depend on x and can be pulled out of the integral, and that $e^{-a}e^{+a}=1$, and simplify the formula. Also remember that $\int dx|\Psi(x)|^2 = \int dx P(x) = 1$ to finally prove that $P(E=E_n) = 1$.

When the quantum particle has wavefunction $\Psi_n(x)\, e^{-\frac{i}{\hbar}E_n t}$, it is 100% guaranteed to have energy E_n!

2. a. Calculate the normalization integral of the Gaussian wavefunction $\Psi_0(x)=\exp(-ax^2)$ from $x = -\infty\ to\ \infty$. This integral is not equal to 1. Note $\Psi^*\Psi=\exp(-2a\,x^2)$

b. To normalize the Gaussian, it needs to be divided by the square root of the integral you got in part (a) Why the square root?

c. Write down the normalized Gaussian wavefunction.

d. Insert the function from (c) into the time-independent Schrödinger equation $\hat{H}\Psi_0(x) = E_0\Psi_0(x)$ for the vibrating molecule with mass m=1 and force constant k=1 we discussed in class and show that Ψ_0 is only a solution of the equation if $a=1/(2\hbar)$ and $E_0=\hbar/2$.

Note: this may seem pretty messy (the second derivative $\partial^2/\partial x^2$ of a Gaussian is already pretty ugly), but it is much easier than solving the differential equation from scratch if we had not proved in class that the solution must be a Gaussian!