Problem Set 5
More Separation of Variables, Postulates 0-3

1. A single particle of mass m free to move in one dimension (along the x axis) with potential energy given by $V=\frac{1}{2}m\omega^2x^2$ is in a state described by the following normalized function:

$$\Psi(x) = [2\omega m/h]^{1/4} \exp[-\pi\omega m x^2/h) \qquad \text{Eq. (1)}$$

Note that x goes from $-\infty$ to $+\infty$ in this case.

(a) Write the Schrödinger equation for this system.
(b) Determine if $\Psi(x)$ is an eigenfunction of the hamiltonian.
(c) What is the operator for linear momentum for this particle? Calculate the average value of linear momentum for the particle while in the state described by Eq. (1)
(d) Calculate the root mean square linear momentum when the particle is in state described by Eq. (1).
(e) What is the probability of finding the particle within an infinitesimal distance dx of the position $x = (h/\pi\omega m)^{1/2}$
(f) Calculate the average position of the particle while in the state described by Eq. (1).
(g) Calculate the root mean square position when the particle is in state described by Eq. (1).
(h) Calculate the product of the root mean square position and the root mean square linear momentum. [We will revisit this when we talk about the uncertainty principle.]
(i) For a diatomic molecule made up of atoms each having mass 2m, the "displacement of the internuclear distance R from the equilibrium distance R_{eq}" is $x = (R- R_{eq})$
and $\Psi(x)$ is given by the above function (Eq. (1)).
What is the mean displacement?
Calculate the mean square displacement.
When m is increased to M, what happens to the mean displacement and the mean square displacement? What does this tell you about the effect of isotopic substitution on amplitudes of vibrational motion?

2. Consider the physical system of a particle of mass m subject to a potential of the same type as in problem 1 above, but free to move in three dimensions x, y and z, that is, it has potential energy given by $V = \frac{1}{2}m\omega_x^2x^2 + \frac{1}{2}m\omega_y^2y^2 + \frac{1}{2}m\omega_z^2z^2$

(a) Write the Schrödinger equation for this system
(b) Show how you would find the eigenfunctions and eigenvalues of this physical system, <u>assuming that you already know the complete set of eigenfunctions and eigenvalues of the energy for the problem 1 above</u>. Note that you are not being asked to find the complete solutions to the Schrödinger equation for problem 1. The eigenvalues of energy for Prob. 1 are $E = (n+½)\, \hbar\omega$ where $n = 0, 1, 2, 3, 4, ...$

3. On separation of variables:
Imagine a universe with the following characteristics:

The gravitational attraction between two electrons a given distance apart is equal in magnitude to their electrostatic repulsion. All other gravitational interactions between elementary particles are the same as in our universe. The fundamental laws of physics have the same form in this universe as in our own.

(a) In this universe, what would be the Schrödinger equation for an atom with N electrons?

(b) Write the Schrödinger equation for the internal motion of the electrons in the presence of the He nucleus in this universe (that is, after separating out the translation of the whole atom in space).

(c) What are the eigenfunctions of this equation? what are the eigenvalues?

(d) Draw the energy level diagram for He atom in this imaginary universe. Express your answers in terms of $e^2/2a_0$, remembering that the energies of the one-electron in a hydrogen-like atom in our universe is $-(Z^2/n^2)\, e^2/2a_0$.

(e) What would be the ground state energy of the He atom in this imaginary universe? Compare it with the ground state energy of He atom in our universe: $-2.904\, e^2/2a_0$. Explain the difference.

(f) Discuss the structure and properties of atoms and molecules in the universe in question. Compare with the corresponding properties in our universe, giving explanations for any differences. ***Make the discussion as quantitative as you can*** and include as many as possible of the following points:

(1) Atomic energy level diagrams (for the free gaseous atoms).
(2) Electronic structure of the atoms - the nature of the periodic table.
(3) Ionization potentials.
(4) Atomic radii for the free atoms