CH 107 Physical Chemistry QUIZ 1

17th October 2014 Total Marks = 20 Time 2 hours

All parts of a question MUST be answered together.
Fragmented answers will not be corrected

1. Justify or contradict the following:
   (a) Orbital approximation is given by $\Psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$ where $\Psi(r, \theta, \phi)$ is a one electron wavefunction.
   (b) The states given by $n_x = 2, n_y = 3$ and $n_x = 3, n_y = 2$ are always degenerate for a particlein a two dimensional box.
   (c) For any two wavefunctions Ψ_1 and Ψ_2, which are eigenfunctions of an operator **Â**, the linear combination $c_1\Psi_1 + c_2\Psi_2$ is always an eigenfunction of **Â**. **2 + 2 + 1**

2. (a) How many radial nodes and how many angular nodes does the following wavefunction possess? Where are these nodes situated?

$$\psi = (6 - r).r.e^{-r/3}.\sin\phi\sin\theta$$

   (b) Find the most probable distance of an electron from the nucleus, when it resides in

   i) 2s and ii) 2p orbital.

$\psi_{2s} = N_1(2 - \sigma)\, e^{-\sigma/2}$ and $\psi_{2p} = N_2\sigma\, e^{-\sigma/2}\cos\theta$ where $\sigma = r/a_0$ and N_1, N_2 are constants.

   Hence, sketch the radial distribution functions for the two orbitals. **2+3**

3. Suppose that the wavefunction for a system can be written as

$$\psi(x) = \frac{1}{2}\varphi_1(x) + \frac{1}{4}\varphi_2(x) + \frac{3 + \sqrt{2}\,i}{2}\varphi_3(x)$$

   where, $\varphi_1(x)$, $\varphi_2(x)$, $\varphi_3(x)$ are orthogonal to each other and are normalized eigenfunctions of the kinetic energy operator, with eigenvalues E_1, $3E_1$ and $7E_1$ respectively.

   (a) Is $\psi(x)$ normalized?
   (b) What are the possible values that you could obtain in measuring the kinetic energy on the system described by $\psi(x)$?
   (c) What is the average value of kinetic energythat will be obtained for a large number of measurements? **1+2+2**

4. (a) Writethe total Hamiltonian for a carbon atom.
   (b) What is a spin orbital?
   (c) Write the Slater determinant for the first singlet excited state of Li^+. **2+1+2**