CML 100: 2014-2015
Quantum Tutorial 2

(Submit answers to Q. 2,7,8 and 9 on 12th September 2014 during the lecture: Remember to write your group # along with the name and entry #)

1. Verify the recursion relation $H_{n+1}(z) - 2zH_n(z) + 2nH_{n-1}(z) = 0$ using the first few Hermite polynomials. Establish the condition when $\int \psi_f^* z\, \psi_i\, dz \neq 0$.
2. In the vibrational motion of HI, the iodine atom remains stationary because of its large mass. Assume that the hydrogen atom undergoes harmonic motion and that the force constant is $317\ \text{N m}^{-1}$, what is the vibrational frequency ν_0? What is the zero point energy if H is replaced by D? Assume that there is no change in the force constant.
3. Show that $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$ (Hint: Use the operator in Cartesian coordinates.
4. In the far infrared spectrum of $H^{79}Br$, there is a series of lines separated by $16.72\ \text{cm}^{-1}$. Calculate the values of the moment of inertia and the internuclear separation in $H^{79}Br$.
5. Show that $Y_1^{-1}(\theta,\phi)$is normalized and it is orthogonal to $Y_2^1(\theta,\phi)$.
6. Using the uncertainty principle argue that free electrons cannot exist in the nucleus. The diameter of a typical nucleus is 10^{-14} m.
7. For a hydrogen atom in the ground state find the classically forbidden region and calculate the probability of finding the electron in this region.
8. Where do the maxima in $r^2\psi_{2s}^2(r)$ occur?
9. What combinations of the d $(l = 2)$ atomic orbitals will produce the Cartesian function $d_{xz} = xzR_{nl}(r)$ and $d_{xy} = xyR_{nl}(r)$.
10. Consider the hygrogen wavefunction (very short answers)

$$\psi(r,\theta,\phi) = \left(\frac{3}{1944\pi}\right)^{1/2}\left(\frac{1}{a_0}\right)^{3/2}\left(4-\frac{2r}{3a_0}\right)\left(\frac{2r}{3a_0}\right)\cos\theta\ e^{-r/3a_0}$$

   a. Determine the values of the three quantum numbers.
   b. What is the ionization energy of the electron in this atom ?
   c. What is the degeneracy of this electronic level?
   d. Determine the position of the radial nodes.
   e. Sketch the radial part of the wavefunction.
   f. Plot the angular part as a function of x.
   g. Evaluate the probability of finding the electron in an infinitesimal volume around $x = 1, y = 2, z = 0$.
   h. To which of these states $(2s, 2p, 4d, 4f)$ would a transition occur?
   i. What is the most probable point in space at which the electron will be found?