CHEM 361B - Lecture 12 Activity

The Hydrogen Atom

1. The solution to the Schrödinger equation for the Hydrogen atom is from multiplying three terms together: $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$. Solutions to the angular part are bundled in $Y(\theta,\phi)$.

   (a) Using the radial solution to the Schrödinger equation show that

   $$R_{21} = \frac{1}{2\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}$$

   (b) Using the angular solution to the rigid rotator show that

   $$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

   (c) Multiply R_{21} with Y_1^0 to get the $2p_z$ orbital

   $$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}\cos\theta$$

2. The typical shape of orbitals can be sketched out by looking at their dependence on θ and rotating it 360° around ϕ. Using the polar plot paper provided, sketch

   (a) The $2p_z$ orbital

   (b) the $3d_{z^2}$ orbital given that

   $$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}(3\cos^2\theta - 1) \tag{1}$$

3. Comparing the Schrödinger solution to the Bohr model of the Hydrogen atom

   (a) Compare the energy of the Hydrogen atom as predicted by the Schrödinger solution and the Bohr model of the Hydrogen atom. Are they the same?

   (b) The solution to the Schrödinger equation contradicts one of Bohr's postulates. Discuss how each model physically describes the hydrogen atom and identify which of Bohr's postulates the solution to the Schródinger equation contradicts?

4. Consider an electron in the $2p_z$ state.

   (a) Show that $\langle r\rangle = 5a_0$.

   (b) Knowing that $\psi^*_{2p_z}\psi_{2p_z}dV$ is the probability of finding the electron in some volume element in the $2p_z$ state

i. Show that the probability of finding the electron on the shell of a sphere of radius r is

$$P(shell) = \frac{r^4}{24a_0^5}e^{-r/a_0}$$

Aside: this is called the radial distribution function.

ii. Show that the radius of the most probable shell that the electron in the $2p_z$ orbital will inhabit is $r = 4a_0$.