Hydrogn Atom,Probability Functions

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I. Hydrogen Atom: Radial Distribution Functions

In this section we consider the question of the most probable distance from the nucleus at which the electron of a hydrogen-like atom is to be found. More precisely, *what is the probability of finding the electron at a particular value of r, regardless of the values of θ and ϕ*. That is, we are interested in finding the electron in a spherical shell of width dr at a radius r from the nucleus. This probablility is given, for a 1s orbital, by:

$$P(r)dr = \frac{1}{\pi a_o^3}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta r^2 e^{\frac{-2r}{a_o}} dr \quad (1)$$

$$= \frac{4}{a_o^3} r^2 e^{\frac{-2r}{a_o}} dr \quad (2)$$

For an s-type orbital, the integration over the spherical angles leads effectively to an averaging over these degrees of freedom. This is meaningful for spherically symmetric functions, such as the s-orbitals; however, since there is angular dependence on the radial probability density for orbitals for $l/gt0$, the *radial distribution function*, $P(r)dr$ is defined as:

$$P(r)dr = r^2 \left[R(r)\right]^2 dr \quad (3)$$

$$(4)$$

The form of this function arises from the full hydrogen atom wavefunction as seen by:

$$\psi^*\psi \; r^2 \; sin\theta \; dr \; d\theta \; d\phi = R(r)^* Y_l^{m*}(\theta,\phi) R(r) Y_l^m(\theta,\phi) \; r^2 \; sin \; \theta \; dr \; d\theta \; d\phi \quad (5)$$

$$= \left[r2R(r)^* R(r) dr\right] Y_l^{m*}(\theta,\phi) Y_l^m(\theta,\phi) sin\theta d\theta d\phi \quad (6)$$

Compare Figures 20.10 and 20.9 in Engel and Reid to see the differences in the forms of the above distribution functions. For the radial probability distribution

- Maxima move to larger r as principle quantum number increase.
- Electron is on average further from nucleus; less stronly bound as "n" increases.
- Nodes are present. Much like in the case of the particle in a box, since we are dealing with stationary states of the Schrodinger equation, nodes will be present in the standing wave solutions.
- Subsidiary maxima for hydrogenic orbitals demonstrate the wave nature of such particles. "interference" between waves.
- Number of nodes: For a certain principle quantum number, n, Nodes= $(n - l - 1)$ (excluding the one at ∞).
- Number of angular nodes: l