Physics 2403, Fall 2000

Problem Session Worksheet: Hydrogen Atom

The solutions to the three-dimensional Schroedinger Equation for the hydrogen atom (i.e., a central Coulomb potential) are composed of a function of *r*, the radius, alone multiplied by a function of ϕ, the azimuthal angle, alone multiplied by a function of θ, the polar angle, alone.

The solution wave functions are characterized by three quantum numbers n, l and m. In the absence of a magnetic field, the wave functions are degenerate in l and m, that is, the energies depend on n alone. All positive values of n are allowed, that is n > 0. However, for any particular value of n only certain values of l and m are allowed. For a particular n, $0 \le l \le n-1$ and $-l \le m \le +l$. Some examples of quantum numbers meeting these requirements are {n=1,l=0,m=0}, {2,0,0}, {2,1,0}, {2,1,±1}, {3,0,0}, {3,1,0}, {3,1,±1}, {3,2,0}, {3,2,±1}, {3,2,±2}.

The solution in ϕ, the azimuthal angle, is the simplest of the three separated functions.

$$\Phi(\phi) = \exp(\, im\phi)$$

The solution in θ, the polar angle, can be written as

$$\Theta(\theta) = (\sin\theta)^m P_{lm}(\cos\theta).$$

The functions $P_{lm}(\cos\theta)$ are known as the associated Legendre functions. While these functions depend on $\cos\theta$ alone, the form of the function depends on l and m. The associated Legendre functions can be calculated using the Rodrigues formula below in which $x = \cos\theta$.

$$P_l^m(x) = \frac{\left(1-x^2\right)^{m/2}}{2^l\, l!} \frac{d^{\,l+m}}{dx^{l+m}} \left(x^2-1\right)^l$$

The associated Legendre polynomials can also be calculated from recurrence relations (see the website http://mathworld.wolfram.com/LegendrePolynomial.html):

$$(l-m)P_l^m(x) = x(2l-1)P_{l-1}^m(x) - (l+m-1)P_{l-2}^m(x).$$

Exercise: Calculate the form of P_{00}, P_{10}, P_{11} and P_{20} using the formula above. Graph the functions $\Theta(\theta)$ based on these four P functions over the entire range of $-1 \le \cos\theta \le 1$. Remember that the probability of finding an electron at a particular value of $\cos\theta$ depends on the square of the wave function. What insights into the nature of the electron orbitals do you get from looking at your graphs?

The solutions in r, the radius, can be written as

$$R_{nl}(r) = \exp(-Zr/na_0)(Zr/a_0)^l\, G_{nl}(Zr/a_0).$$

Here a_0 is the Bohr radius and $G_{nl}(Zr/a_0)$ are a set of functions known as the associated Laguerre functions. The Rodrigues formula for these polynomials is given below. (k is the same as l, $x = Zr/a_0$).

$$\frac{e^x x^{-k}}{n!} \frac{d^n}{dx^n}\left(e^{-x} x^{n+k}\right)$$

Exercise: Calculate the form of G_{00}, G_{10} and G_{11}. Assume Z=1. Graph the functions R(r) based on these three G functions you have calculated for $0 \le r \le 10\ a_0$. What insights do you get from your graphs?

Problems for next week: Hand in your own copies of the 7 graphs described above along with your answers to the two questions about them.