

## HYDROGEN ATOM - RADIAL FUNCTION EXAMPLES

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Post date: 31 July 2021.

In solving the radial equation for the hydrogen atom, we used the following notation:

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi) \quad (1)$$

$$u_{nl}(\rho) = \rho^{l+1} e^{-\rho} v_{nl}(\rho) \quad (2)$$

$$u_{nl}(r) \equiv r R_{nl}(r) \quad (3)$$

$$\rho = \kappa r \quad (4)$$

$$\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa} \quad (5)$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} \quad (6)$$

The solution was expressed as a series:

$$v_{nl}(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \quad (7)$$

with the coefficients  $c_j$  satisfying a recursion relation:

$$c_{j+1} = \frac{2(j+l+1) - \rho_0}{(j+1)(j+2(l+1))} c_j \quad (8)$$

The series must terminate by requiring  $\rho_0 = 2n$ , and the initial constant  $c_0$  is determined by normalization. This condition gives the quantization of energy, since from above

$$\kappa = \frac{me^2}{2\pi\epsilon_0\hbar^2\rho_0} \quad (9)$$

$$= \frac{me^2}{4\pi\epsilon_0\hbar^2 n} \quad (10)$$

Thus the original radial function is given by

$$R_{nl}(r) = \frac{1}{r} u_{nl}(r) \quad (11)$$

$$= \frac{1}{r} \rho^{l+1} e^{-\rho} v_{nl}(\rho) \quad (12)$$

As an example, for  $l = 0$ ,  $n = 3$  the recursion formula is

$$c_{j+1} = \frac{2(j-2)}{(j+1)(j+2)} c_j \quad (13)$$

so  $c_1 = -2c_0$ ,  $c_2 = 2c_0/3$  and all higher coefficients are zero.

The radial wave function is, from above:

$$R_{30}(r) = \frac{1}{r} \rho e^{-\rho} c_0 (1 - 2\rho + 2\rho^2/3) \quad (14)$$

$$= \frac{1}{3a} e^{-r/3a} c_0 \left( 1 - \frac{2r}{3a} + \frac{2r^2}{27a^2} \right) \quad (15)$$

where  $a$  is the Bohr radius:

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2} \quad (16)$$

$$\kappa = \frac{1}{an} \quad (17)$$

$$\rho = \frac{r}{an} \quad (18)$$

We can find  $c_0$  by normalizing the function. Since we are dealing with the radial function (the angular parts of the wave function are included in the spherical harmonic  $Y_l^m$ ), the normalization integral is

$$\int_0^\infty r^2 |R_{nl}(r)|^2 dr = 1 \quad (19)$$

Working out the integral (using software), we get

$$c_0 = \frac{2}{\sqrt{3a}} \quad (20)$$

For  $l = 1$ ,  $n = 3$  the recursion formula is

$$c_{j+1} = \frac{2(j-1)}{(j+1)(j+4)} c_j \quad (21)$$

so  $c_1 = -c_0/2$ , and all higher coefficients are zero.

The radial wave function is:

$$R_{31}(r) = \frac{1}{r} \rho^2 e^{-\rho} c_0 (1 - \rho/2) \quad (22)$$

$$= \frac{r}{9a^2} e^{-r/3a} c_0 \left(1 - \frac{r}{6a}\right) \quad (23)$$

Normalizing gives

$$c_0 = \frac{4}{3} \sqrt{\frac{2}{3a}} \quad (24)$$

For  $l = 2$ ,  $n = 3$  the recursion formula is

$$c_{j+1} = \frac{2j}{(j+1)(j+6)} c_j \quad (25)$$

so and all coefficients above  $c_0$  are zero.

The radial wave function is:

$$R_{32}(r) = \frac{1}{r} \rho^3 e^{-\rho} c_0 \quad (26)$$

$$= \frac{r^2}{27a^3} e^{-r/3a} c_0 \quad (27)$$

Normalizing gives

$$c_0 = \frac{2}{3} \sqrt{\frac{2}{15a}} \quad (28)$$

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