HYDROGEN ATOM - RADIAL FUNCTION EXAMPLES

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.10.

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

$$\begin{aligned}
\psi_{nlm}(r,\theta,\phi) &= R_{nl}(r)Y_l^m(\theta,\phi) && (1)\\
u_{nl}(\rho) &= \rho^{l+1}e^{-\rho}v_{nl}(\rho) && (2)\\
u_{nl}(r) &\equiv rR_{nl}(r) && (3)\\
\rho &= \kappa r && (4)\\
\rho_0 &= \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa} && (5)\\
\kappa &= \frac{\sqrt{-2mE}}{\hbar} && (6)
\end{aligned}$$

The solution was expressed as a series:

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

with the coefficients c_j satisfying a recursion relation:

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

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

$$\begin{aligned}
\kappa &= \frac{me^2}{2\pi\epsilon_0\hbar^2\rho_0} && (9)\\
&= \frac{me^2}{4\pi\epsilon_0\hbar^2 n} && (10)
\end{aligned}$$

Thus the original radial function is given by

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

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

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

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

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

The radial wave function is, from above:

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

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

where a is the Bohr radius:

$$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \tag{16}$$

$$\kappa = \frac{1}{an} \tag{17}$$

$$\rho = \frac{r}{an} \tag{18}$$

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

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

Working out the integral (using software), we get

$$c_0 = \frac{2}{\sqrt{3a}} \tag{20}$$

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

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

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

The radial wave function is:

$$R_{31}(r) = \frac{1}{r}\rho^2 e^{-\rho} c_0 (1-\rho/2) \tag{22}$$
$$= \frac{r}{9a^2} e^{-r/3a} c_0 \left(1-\frac{r}{6a}\right) \tag{23}$$

Normalizing gives

$$c_0 = \frac{4}{3}\sqrt{\frac{2}{3a}} \tag{24}$$

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

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

so and all coefficients above c_0 are zero.

The radial wave function is:

$$R_{32}(r) = \frac{1}{r}\rho^3 e^{-\rho} c_0 \tag{26}$$
$$= \frac{r^2}{27a^3} e^{-r/3a} c_0 \tag{27}$$

Normalizing gives

$$c_0 = \frac{2}{3}\sqrt{\frac{2}{15a}} \tag{28}$$

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