

HYDROGEN ATOM - WAVE FUNCTION EXAMPLES

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.11.

A few more examples of working out the hydrogen atom wave functions. Using the formulas in the last example, we can get R_{20} . The recursion formula for $n = 2, l = 0$ is

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

The series has 2 terms, and we get $c_1 = -c_0$, so

$$R_{20}(r) = \frac{1}{r} u_{20}(r) \quad (2)$$

$$= \frac{1}{r} \rho e^{-\rho} v_{20}(\rho) \quad (3)$$

$$= \frac{1}{2a} e^{-r/2a} c_0 \left(1 - \frac{r}{2a}\right) \quad (4)$$

To find c_0 we normalize the radial function:

$$\int_0^\infty r^2 |R_{20}(r)|^2 dr = \int_0^\infty c_0^2 r^2 \left[\frac{1}{2a} \left(1 - \frac{r}{2a}\right) \right]^2 e^{-r/a} dr \quad (5)$$

$$= \frac{a}{2} c_0^2 \quad (6)$$

$$= 1 \quad (7)$$

So $c_0 = \sqrt{2/a}$ and $R_{20}(r)$ is

$$R_{20}(r) = \frac{1}{\sqrt{2}a^{3/2}} e^{-r/2a} \left(1 - \frac{r}{2a}\right) \quad (8)$$

The complete wave function is then

$$\psi_{200} = R_{20}(r) Y_{00}(\phi, \theta) \quad (9)$$

$$= \frac{1}{\sqrt{8\pi}} a^{-3/2} \left(1 - \frac{r}{2a}\right) e^{-r/2a} \quad (10)$$

For $R_{21}(r)$, we have

$$c_{j+1} = \frac{2(j+2) - 4}{(j+1)(j+4)} c_j \quad (11)$$

This time, there is only a single term in the series, so we have

$$R_{21}(r) = \frac{1}{r} u_{21}(r) \quad (12)$$

$$= \frac{1}{r} \rho^2 e^{-\rho} v_{21}(\rho) \quad (13)$$

$$= \frac{r}{(2a)^2} e^{-r/2a} c_0 \quad (14)$$

Doing the normalization integral for $R_{21}(r)$ gives $c_0 = \sqrt{2/3a}$ which gives the final result

$$R_{21}(r) = \frac{r}{2\sqrt{6}a^{5/2}} e^{-r/2a} \quad (15)$$

There are 3 wave functions corresponding to $n = 2$, $l = 1$, for which we need the spherical harmonics

$$Y_1^1 = -\left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{i\phi} \quad (16)$$

$$Y_1^{-1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{-i\phi} \quad (17)$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta \quad (18)$$

The three wave functions are thus

$$\psi_{211} = -\frac{1}{8\sqrt{\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \sin \theta e^{i\phi} \quad (19)$$

$$\psi_{21-1} = \frac{1}{8\sqrt{\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \sin \theta e^{-i\phi} \quad (20)$$

$$\psi_{210} = \frac{1}{4\sqrt{2\pi}} \frac{r}{a^{5/2}} e^{-r/2a} \cos \theta \quad (21)$$

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