

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

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

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

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

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

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

To find c_0 we normalize the radial function:

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

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

$$(7) \quad = 1$$

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

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

The complete wave function is then

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The three wave functions are thus

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

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

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

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