

## HYDROGEN ATOM - MEAN RADIUS OF ELECTRON POSITION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.13.

We can work out the mean and mean square distances for an electron in a hydrogen atom using the standard method of interpreting the square modulus of the wave function as a probability density.

In the ground state, the quantum numbers are  $n = 1$ ,  $l = 0$ ,  $m = 0$  and the wave function can be worked out from the formulas we have used earlier.

$$\psi_{100} = R_{10}Y_0^0 \quad (1)$$

$$= c_0 \frac{1}{a} e^{-r/a} Y_0^0 \quad (2)$$

The constant  $c_0$  can be found from normalization as usual, and we have  $c_0 = 2/\sqrt{a}$  so, with the normalized spherical harmonic  $Y_0^0 = 1/\sqrt{4\pi}$  we have

$$\psi_{100} = \frac{1}{\sqrt{\pi}a^{3/2}} e^{-r/a} \quad (3)$$

Since the ground state does not depend on either angle, we have

$$\langle r \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty r |R_{10}|^2 r^2 |Y_0^0|^2 \sin\theta dr d\theta d\phi \quad (4)$$

$$\int_0^\infty r |R_{10}|^2 r^2 dr \quad (5)$$

$$= 4a^{-3} \int_0^\infty r^3 e^{-2r/a} dr \quad (6)$$

$$= \frac{3}{2}a \quad (7)$$

For the mean square:

$$\langle r^2 \rangle = \int_0^\infty r^2 |R_{10}|^2 r^2 dr \quad (8)$$

$$= 4a^{-3} \int_0^\infty r^4 e^{-2r/a} dr \quad (9)$$

$$= 3a^2 \quad (10)$$

Since the ground state is symmetric, we can work out the means for the rectangular coordinates separately without doing any more integrals:

$$\langle x \rangle = 0 \quad (11)$$

$$\langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle \quad (12)$$

$$= a^2 \quad (13)$$

The same results would be obtained for  $y$  and  $z$ .

For higher states, we don't have the spherical symmetry of the ground state. As an example, we'll look at the state  $n = 2, l = 1, m = 1$ . We need  $R_{21}(r) = \frac{1}{\sqrt{24}} a^{-3/2} (r/a) e^{-r/2a}$  from our previous example and the spherical harmonic  $Y_1^1(\theta, \phi) = -(\sqrt{3/8\pi}) \sin\theta e^{i\phi}$ . Using  $x = r \sin\theta \cos\phi$  we get

$$\langle x^2 \rangle = \int_0^{2\pi} \int_0^\pi \int_0^\infty (r \sin\theta \cos\phi)^2 \left( \frac{1}{\sqrt{24}} a^{-3/2} (r/a) e^{-r/2a} \right)^2 (\sqrt{3/8\pi} \sin\theta)^2 r^2 \sin\theta dr d\theta d\phi \quad (14)$$

$$= 12a^2 \quad (15)$$

using Maple to do the integrals.

We can use the same technique to find means for the other coordinates. Because  $\psi_{211}$  is independent of  $\phi$ ,  $\langle x \rangle = \langle y \rangle = 0$  and  $\langle y^2 \rangle = \langle x^2 \rangle = 12a^2$ . In the  $z$  direction, the wave function is even about the angle  $\theta = \pi/2$ , so we would expect  $\langle z \rangle = 0$ . We can work out  $\langle z^2 \rangle$  by doing the integral using  $z = r \cos\theta$  and we get  $\langle z^2 \rangle = 6a^2$ .

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