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.

$$\psi_{100} = R_{10}Y_0^0 \tag{1}$$

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

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

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

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

$$\langle r\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} r|R_{10}|^2 r^2\left|Y_0^0\right|^2\sin\theta\, dr\, d\theta\, d\phi \tag{4}$$

$$\int_0^{\infty} r|R_{10}|^2 r^2 dr \tag{5}$$

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

$$= \frac{3}{2}a \tag{7}$$

For the mean square:

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

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

$$= 3a^2 \tag{10}$$

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

$$\langle x\rangle = 0 \tag{11}$$

$$\langle x^2\rangle = \frac{1}{3}\langle r^2\rangle \tag{12}$$

$$= a^2 \tag{13}$$

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

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

$$= 12a^2 \tag{15}$$

using Maple to do the integrals.

We can use the same technique to find means for the other coordinates. Because ψ_{211} is independent of ϕ, $\langle x\rangle=\langle y\rangle=0$ and $\left\langle y^2\right\rangle=\left\langle x^2\right\rangle=12a^2$. 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 $\left\langle z^2\right\rangle$ by doing the integral using $z=r\cos\theta$ and we get $\left\langle z^2\right\rangle=6a^2$.

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