F 2013

Problem 4: Properties of the Hydrogen Atom

The wavefunctions for the ground state and first excited states of the hydrogen atom are given on the first page of this test.

(a) [2 pt] For the ground state of the hydrogen atom, determine the expectation value for the radial position of the electron, $\langle 1,0,0|r|1,0,0\rangle$.

(b) [3 pt] Define the radial probably density for the electron in a hydrogenic eigenstate: $P_{n,\ell,m}(r)dr$ as the probability of the electron being measured in the spherical shell between r and $r+dr$.

Write down expressions for $P_{1,0,0}(r)$ and $P_{2,1,1}(r)$, and sketch these as functions of r.

Hint: Remember that the integral of the probability density over r must be equal to one,

$$\int_0^\infty P_{n,\ell,m}(r)dr = 1 \tag{1}$$

(c) [3 pt] For the ground state of the hydrogen atom, determine the most probable radius for the electron. Compare your result to part (a) and explain the similarities and differences.

(d) [1 pt] What is the functional form for $P_{1,0,0}(r)$ in the limit as $r \to 0$? Explain your result considering that the ground state wavefunction is non-zero at $r=0$.

(e) [1 pt] What are the functional forms of $P_{1,0,0}(r)$, $P_{2,1,1}(r)$, and $P_{200}(r)$ as $r \to 0$? Explain the similarities and differences.

(a)

The ground state radial function is given by

$$|100\rangle_r = R_{10}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}$$

and the angular function is

$$|100\rangle_{\theta,\phi} = Y_{00}(\theta,\phi) = \frac{1}{\sqrt{4\pi}},$$

so our total ground state wavefunction is

$$|100\rangle = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}.$$

Then

$$\langle r\rangle_{100} = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \left(\frac{1}{\pi a_0^3}\right) e^{-r/a_0}\, r\, e^{-r/a_0}\, r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$= \frac{4\pi}{\pi a_0^3}\int_0^{\infty} r^3 e^{-2r/a_0}\, dr$$

$$= \frac{4}{a_0^3}\left(\frac{3!}{(2/a_0)^4}\right)$$

$$= \frac{24 a_0^4}{16 a_0^3}$$

$$\boxed{\langle r\rangle_{100} = \frac{3a_0}{2}}.$$

(b)

The radial probability density, in general, is

$$\frac{dP}{dr} = \rho = |\psi_r|^2 4\pi r^2.$$

So

$$\rho\, dr = |\psi_r|^2 4\pi r^2 dr,$$

and so $P_{n,\ell,m}(r)$ corresponds to ρ,

$$P_{n,\ell,m}(r) = |\psi_r|^2 4\pi r^2.$$

Then

$$P_{1,0,0}(r) = |R_{1,0}|^2 4\pi r^2$$

$$= \left(\frac{2}{a_0^{3/2}} e^{-r/a_0}\right)^2 4\pi r^2$$

$$\boxed{P_{1,0,0}(r) = \frac{16\pi}{a_0^3} r^2 e^{-2r/a_0}}$$

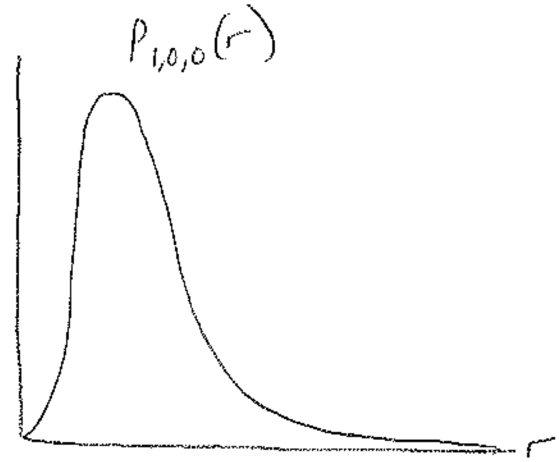
and

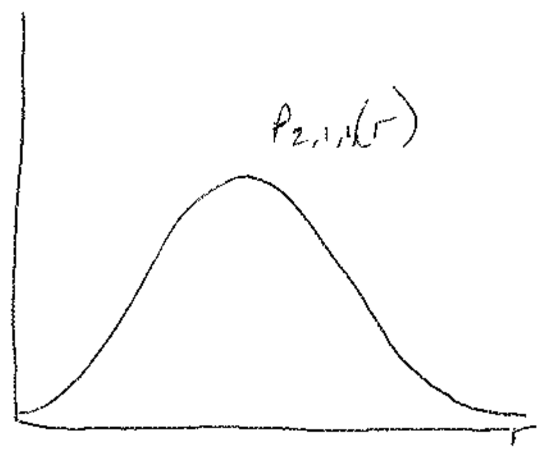
$$P_{2,1,1}(r) = |R_{2,1}|^2 4\pi r^2$$

$$= \left(\frac{1}{(2a_0)^{3/2}} \frac{r}{\sqrt{3}\, a_0} e^{-r/2a_0}\right)^2 4\pi r^2$$

$$\boxed{P_{2,1,1}(r) = \frac{\pi}{6a_0^5} r^4 e^{-r/a_0}}$$

(b), cont'd...





(c)

The most probable radius for the ground state is

$$\frac{dP_{1,0,0}}{dr} = 0$$

$$\frac{d}{dr}\left(\frac{16\pi}{a_0^3} r^2 e^{-2r/a_0}\right) = 0$$

$$\frac{d}{dr}\left(r^2 e^{-2r/a_0}\right) = 0$$

$$2r e^{-2r/a_0} - \frac{2}{a_0} r^2 e^{-2r/a_0} = 0$$

$$2r = \frac{2}{a_0} r^2$$

$$\boxed{r = a_0}$$

Both values in (a) and (c) depend on a_0, the bohr radius. The expectation value is the measurement result average after many measurements, whereas the most probable radius is what you would expect to measure if you took a single measurement.

(d)

We know

$$P_{1,0,0}(r) = \frac{16\pi}{a_0^3} r^2 e^{-2r/a_0},$$

so

$$\boxed{\lim_{r \to 0} P_{1,0,0}(r) = 0}.$$

This is a probability density result. The wavefunction may be non-zero at $r=0$, but the probability of finding the electron there is zero.

(e)

We know

$$P_{2,1,1}(r) = \frac{\pi}{6a_0^5} r^4 e^{-r/a_0}$$

and

$$P_{2,0,0}(r) = \frac{2\pi}{a_0^3} r^2 \left(1 - \frac{r}{2a_0}\right)^2 e^{-r/a_0}.$$

As $r \to 0$, we have

$$\boxed{P_{2,1,1} \to 0}$$

and

$$\boxed{P_{2,0,0} \to 0}.$$

Like $P_{1,0,0}$, we never expect to find the electron at the nucleus. The wavefunctions are non-zero there, as well.