“QUANTUM ANALYSIS OF THE HYDROGEN ATOM: WAVE FUNCTIONS AND RADIAL PROBABILITY DISTRIBUTIONS OF 1S AND 2S STATES”

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Abstract: This article analyzes the wave functions corresponding to the 1s and 2s quantum states of the hydrogen atom. For the ground (1s) state, the wave function, probability density, and radial probability function are presented on a mathematical basis, and their physical meaning is explained in detail. Additionally, the most probable radius and the average distance of the electron are determined and compared with the results from the Bohr theory. For the 2s state, the wave function and the graph of the radial probability density are studied, demonstrating that the electron in this state is located, on average, much farther from the nucleus. The results show the intrinsic connection between quantum mechanics and the Bohr model.

Keywords: Hydrogen atom, wave function, probability density, radial probability function, Bohr radius, quantum states, 1s state, 2s state, quantum mechanics, electron cloud.

Because the potential energy of the hydrogen atom depends only on the radial distance r between nucleus and electron, some of the allowed states for this atom can be represented by wave functions that depend only on r. For these states, $f(\theta)$ and $g(\phi)$ are constants. The simplest wave function for hydrogen is the one that describes the $1s$ state and is designated $\psi_{1s}(r)$:

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \qquad (1)$$

where a_0 is the Bohr radius. Note that ψ_{1s} approaches zero as r approaches ∞ and is normalized as presented. Furthermore, because ψ_{1s} depends only on r, it is spherically symmetric. This symmetry exists for all s states.

Recall that the probability of finding a particle in any region is equal to an integral of the probability density $|\psi|^2$ for the particle over the region. The probability density for the $1s$ state is

$$|\psi_{1s}|^2 = \left(\frac{1}{\pi a_0^3}\right) e^{-2r/a_0} \qquad (2)$$

Because we imagine the nucleus to be fixed in space at $r = 0$, we can assign this probability density to the question of locating the electron. The probability of finding the electron in a volume element dV is $|\psi|^2 dV$. It is convenient to define the radial probability density function $P(r)$ as the probability per unit radial length of finding the electron in a spherical shell of radius r and thickness dr. Therefore, $P(r)dr$ is the probability of finding the electron in this shell. The volume dV of such an infinitesimally thin shell equals its surface area $4\pi r^2$ multiplied by the shell thickness dr (Fig. 1), so we can write this probability as

$$P(r)dr = |\psi|^2 dV = |\psi|^2 4\pi r^2 dr$$

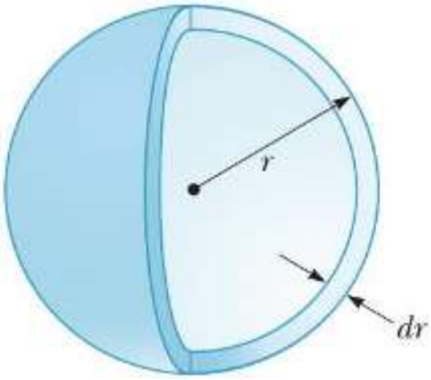


Figure 42.10 A spherical shell of radius r and infinitesimal thickness dr has a volume equal to $4\pi r^2 dr$.

Therefore, the radial probability density function for an s state is

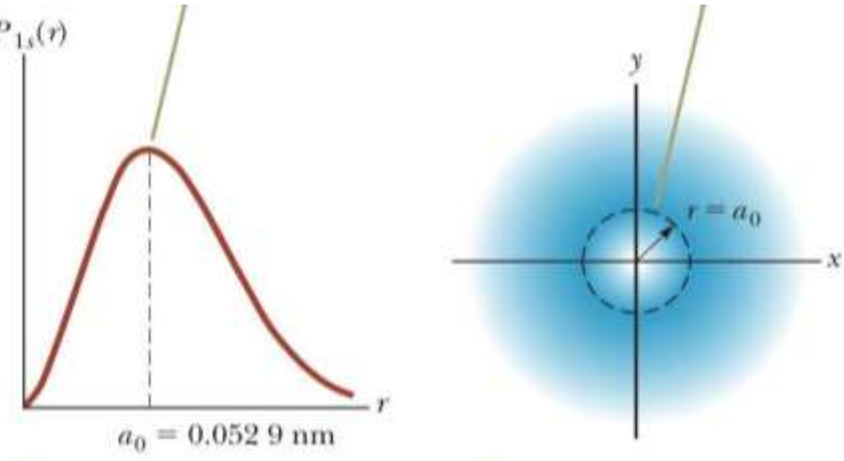
$$P(r) = 4\pi r^2 |\psi|^2 \quad (3)$$

Substituting Equation 2 into Equation 3 gives the radial probability density function for the hydrogen atom in its ground state:

$$P_{1s}(r) = \left(\frac{4r^2}{a_0^3}\right) e^{-2r/a_0} \quad (4)$$

A plot of the function $P_{1s}(r)$ versus r is presented in Figure 2a. The peak of the curve corresponds to the most probable value of r for this particular state. This peak occurs at the Bohr radius, the radial position of the electron when the hydrogen atom is in its ground state in the Bohr theory, another remarkable agreement between the Bohr theory and the quantum theory.

According to quantum mechanics, the atom has no sharply defined boundary as suggested by the Bohr theory. The probability distribution in Figure 2a suggests that the charge of the electron can be modeled as being extended throughout a region of space, commonly referred to as an electron cloud. Figure 2b shows the probability density of the electron in a hydrogen atom in the $1s$ state as a function of position in the xy plane. The darkness of the blue color corresponds to the value of the probability density. The darkest portion of the distribution appears at $r = a_0$, corresponding to the most probable value of r for the electron.



a) b)

Figure 2. (a) The probability of finding the electron as a function of distance from the nucleus for the hydrogen atom in the 1*s* (ground) state. (b) The cross section in the *xy* plane of the spherical electronic charge distribution for the hydrogen atom in its 1*s* state.

Example-1. Calculate the most probable value of r for an electron in the ground state of the hydrogen atom.

Solution. Do not imagine the electron in orbit around the proton as in the Bohr theory of the hydrogen atom. Instead, imagine the charge of the electron spread out in space around the proton in an electron cloud with spherical symmetry. Because the statement of the problem asks for the "most probable value of r," we categorize this example as a problem in which the quantum approach is used. (In the Bohr atom, the electron moves in an orbit with an exact value of r.)

The most probable value of r corresponds to the maximum in the plot of $P_{1s}(r)$ versus r. We can evaluate the most probable value of r by setting $dP_{1s}/dr = 0$ and solving for r.

Differentiate Equation 42.25 and set the result equal to zero:

$$\frac{dP_{1s}}{dr} = \frac{d}{dr}\left[\left(\frac{4r^2}{{a_0}^3}\right)e^{-2r/a_0}\right] = 0$$

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

$$2re^{-2r/a_0} + r^2(-2/a_0)e^{-2r/a_0} = 0$$

$$2r[1 - (r/a_0)]e^{-2r/a_0} = 0 \qquad (5)$$

$$1 - \frac{r}{a_0} = 0 \rightarrow r = a_0$$

Set the bracketed expression equal to zero and solve for r :

The most probable value of r is the Bohr radius! Equation (5) is also satisfied at $r=0$ and as $r \rightarrow \infty$. These points are locations of the minimum probability, which is equal to zero as seen in Figure 2a.

Examle-2. Calculate the probability that the electron in the ground state of hydrogen will be found outside the Bohr radius.

Solution. The probability is found by integrating the radial probability density function $P_{1s}(r)$ for this state from the Bohr radius a_0 to ∞. Set up this integral using Equation 4:

$$P=\int_{a_0}^{\infty} P_{1s}(r) dr=\frac{4}{a_0^3} \int_{a_0}^{\infty} r^2 e^{-2r/a_0} dr$$

$$P=\frac{4}{a_0^3} \int_2^{\infty}\left(\frac{z a_0}{2}\right)^2 e^{-z}\left(\frac{a_0}{2}\right) dz=\frac{1}{2} \int_2^{\infty} z^2 e^{-z} dz$$

Put the integral in dimensionless form by changing variables from r to $z=2r/a_0$, noting that $z=2$ when $r=a_0$ and that $dr=(a_0/2) dz$:

Evaluate the integral using partial integration;

$$P=-\frac{1}{2}(z^2+2z+2) e^{-z}\Big|_2^{\infty}$$

Evaluate between the limits:

$$P=0-\left[-\frac{1}{2}(4+4+2) e^{-2}\right]=5 e^{-2}=0.677 \text{ or } 67.7\%$$

Finalize This probability is larger than 50%. The reason for this value is the asymmetry in the radial probability density function (Fig. 2a), which has more area to the right of the peak than to the left.

If we were asked for the average value of r for the electron in the ground state rather than the most probable value?

Answer The average value of r is the same as the expectation value for r.

Use Equation 42.25 to evaluate the average value of r :

$$r_{\text{avg}}=\langle r\rangle=\int_0^{\infty} r P(r) dr=\int_0^{\infty} r\left(\frac{4 r^2}{a_0^3}\right) e^{-2r/a_0} dr$$

$$=\left(\frac{4}{a_0^3}\right) \int_0^{\infty} r^3 e^{-2r/a_0} dr$$

Evaluate the integral:

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

Again, the average value is larger than the most probable value because of the asymmetry in the wave function as seen in Figure 2a.

The next-simplest wave function for the hydrogen atom is the one corresponding to the $2s$ state ($n=2, \ell=0$). The normalized wave function for this state is

$$\psi_{2s}(r)=\frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0} \tag{6}$$

Wave function for hydrogen in the $2s$ state

Again notice that ψ_{2s} depends only on r and is spherically symmetric. The energy corresponding to this state is $E_2=-(13.606/4)\mathrm{eV}=-3.401\mathrm{eV}$. This energy level represents the first excited state of hydrogen. A plot of the radial probability density function for this state in comparison to the $1s$ state is shown in Figure 3. The plot for the $2s$ state has two peaks. In this case, the most probable value corresponds to that value of r that has the highest value of $P(\approx 5a_0)$. An electron in the $2s$ state would be much farther from the nucleus (on the average) than an electron in the $1s$ state.

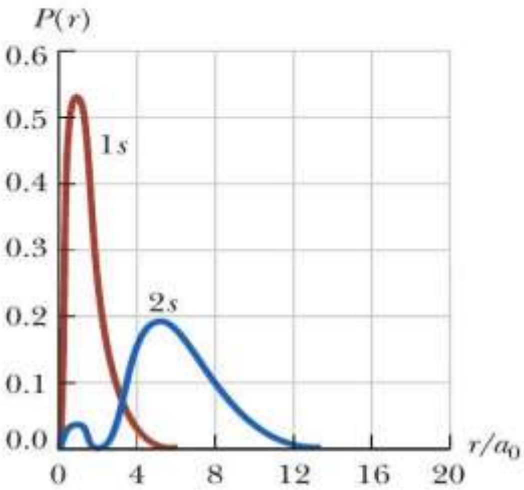


Figure 3. The radial probability density function versus r/a_0 for the $1s$ and $2s$ states of the hydrogen atom.

The research findings indicate that the spatial distribution of the electron in the 1s and 2s quantum states of the hydrogen atom can be clearly described through their wave functions. For the electron in the 1s state, the most probable radius is equal to the Bohr radius, which confirms the connection between quantum mechanics and the Bohr theory. The results obtained for the 2s state show that the radial probability density has two maxima and that the electron's average distance is significantly greater than that in the 1s state. This indicates a higher probability of the electron being located farther from the nucleus.

Thus, the wave functions obtained through quantum mechanics provide a deeper understanding of atomic structure beyond the framework of the traditional Bohr model. These analyses demonstrate that the mathematical and physical interpretations of quantum states can be effectively applied in the educational process, especially in atomic physics and quantum mechanics courses.

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