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Study of Structure Hydrogen Atom according to Schrödinger's Wave Equation

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ABSTRACT

The hydrogen atom, as the simplest atomic system, has played a fundamental role in the formation of quantum theories and helps us to achieve the research goal, which is the atomic structure. Based on the Schrödinger wave equation and using the time-independent Schrödinger equation and applying the Coulomb potential between the electron and the nucleus, the equation was decomposed into spherical coordinates and divided into radial and angular parts. Solving the angular part led to obtaining spherical harmonic functions and solving the radial part led to extracting Legendre polynomials. Finally, using Python computer programming, the data was obtained and the graphs of the spherical and radial parts were drawn to display the results. The results showed that the resulting wave function determines the probable density of electron presence in space and explains the concepts of orbitals. Ultimately, the findings show that the Schrödinger equation provides a solid theoretical foundation for understanding the structure of atoms and the quantum behavior of matter.

Keywords: Angular part, Electron probability density, Hydrogen atom, Radial part, Schrödinger equation.

1. INTRODUCTION

الْحَمْدُ لِلَّهِ رَبِّ الْعَالَمِينَ وَالصَّلَاةُ وَالسَّلَامُ عَلَى سَيِّدِ الْمُرْسَلِينَ وَعَلَى آلِهِ وَصَحْبِهِ أَجْمَعِينَ.

The investigation of the hydrogen atom, as the simplest atomic system, has played a fundamental role in the development of quantum mechanics. The first major step toward understanding atomic structure was made by Ernest Rutherford in 1911 with the experimental discovery of the atomic nucleus, leading to the planetary model of the atom. However, this classical model failed to explain the stability of atoms and the discrete nature of atomic spectra.

Subsequently, Niels Bohr (1913) introduced a quantized model of the hydrogen atom, proposing that electrons occupy discrete energy levels and emit or absorb radiation only during transitions between these levels. Although Bohr's model successfully explained the spectral lines of hydrogen, it remained semi-empirical and lacked a rigorous theoretical foundation.

A major conceptual breakthrough occurred with the hypothesis of matter waves proposed by Louis de Broglie in 1923, which suggested that particles exhibit wave-like properties. This idea paved the way for a wave-based description of atomic systems. Building on this concept, Erwin Schrödinger in 1926 formulated his wave equation, providing a comprehensive and fundamental framework for describing the behavior of electrons in atoms.

When applied to the hydrogen atom, the Schrödinger equation incorporates the Coulomb potential between the nucleus and the electron and is most effectively solved in spherical coordinates. The resulting equation separates into radial and angular components, yielding solutions that define the wavefunctions and discrete energy levels of the system. These solutions naturally introduce the quantum numbers (principal, azimuthal, and magnetic), which characterize the allowed states of the electron. Importantly, the theoretical predictions derived from this formulation are in excellent agreement with experimental observations of hydrogen spectra.

The physical interpretation of the wavefunction was later established by Max Born, who proposed that the square modulus of the wavefunction represents the probability density of finding the electron in a given region of space. This probabilistic interpretation replaced the classical notion of well-defined electron orbits with a statistical description of atomic structure.

In summary, the application of the Schrödinger wave equation to the hydrogen atom resolved the limitations of earlier atomic models and provided a rigorous theoretical basis for understanding atomic structure. It remains one of the most successful achievements of quantum mechanics and serves as a cornerstone for modern physics.

The main goal of this research is to analyze the structure of the hydrogen atom in the Schrödinger equation in order to extract the structure of the hydrogen atom based on this equation, which is urgently needed in the subject of atomic physics for third-case physics students.

The fundamental question is how can the structure of the hydrogen atom be accurately described and analyzed using the time-independent Schrödinger equation and generalized to other atoms?

The answers to these questions are presented as the findings of the research.

In this research, an analytical-theoretical and numerical computational method was used. First, the time-independent Schrödinger equation was written for the Coulomb potential. Then, using spherical symmetry, the equation was decomposed into angular and radial parts. The angular part was solved using spherical harmonic functions and the radial part with Legendre polynomials.

With the development of quantum mechanics, Erwin Schrödinger introduced an equation in 1926 that expressed the wave behavior of particles in the framework of a probabilistic description. In this model, the electron no longer moves as a particle in a specific orbit, but is described as a cloud of probabilities around the nucleus. Solving the Schrödinger equation for the hydrogen atom leads to the emergence of quantized wave functions (Ψ) and allowed energies, which are characterized by three principal quantum numbers. Based on this, examining the structure of the hydrogen atom in the Schrödinger model is considered the starting point for understanding the structure and behavior of atoms in quantum mechanics (Zettili, 2009).

2.MATERIALS AND METHODS

In this research, first, using existing equations and theories, the Schrödinger equation was formulated in three dimensions, then it was generalized to the hydrogen atom and radial and angular equations were obtained, and finally, data of these equations were extracted and plotted using the Python software.

According to the de Broglie hypothesis, each material particle corresponds to a wave whose wave function is:

$$\Psi(r, t) = Ae^{\frac{i}{\hbar}(\vec{p}\vec{r} - Et)} \quad (1)$$

Equation (1) is called the wave equation and represents the motion of a particle. This equation is a solution to the differential equation that Schrödinger first solved and named after himself (Sandrasekaran, et al, 2024).

To obtain the wave equation, first write the kinetic energy of the particle in terms of momentum and then in terms of the minus sign wave function. Finally, we generalize this particle to an electron that rotates around the nucleus of a hydrogen atom.

Suppose: A particle with mass m and velocity v moves, its kinetic energy is:

$$E_k = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} \\ \Rightarrow p_x^2 + p_y^2 + p_z^2 = 2mE_k \quad (2)$$

Now, according to equation (1), we write the particle wave equation:

$$\Psi(r, t) = Ae^{\frac{i}{\hbar}(\vec{p}\vec{r} - E_k t)} \quad (3)$$

We take the first derivative of equation (3) with respect to t (Agus & Anang2012).

$$\frac{\partial \Psi}{\partial t} = Ae^{\frac{i}{\hbar}(\vec{p}\vec{r} - E_k t)} \times \left(-\frac{i}{\hbar} E_k \right) \\ \frac{\partial \Psi}{\partial t} = \Psi \times \left(-\frac{i}{\hbar} E_k \right) \Rightarrow E_k = \frac{i\hbar}{\Psi} \times \frac{\partial \Psi}{\partial t} \quad (4)$$

Now we write the first and second derivatives of the particle's wave function (relation 3) with respect to its momentum in one dimension:

$$\begin{aligned}
\frac{\partial \Psi}{\partial x} &= \frac{i}{\hbar} p_x \Psi \\
\frac{\partial^2 \Psi}{\partial x^2} &= \frac{i}{\hbar} p_x \frac{\partial \Psi}{\partial x} = \frac{i}{\hbar} p_x \times \frac{i}{\hbar} p_x \Psi = \frac{i^2}{\hbar^2} p_x^2 \Psi \\
&= -\frac{1}{\hbar^2} p_x^2 \Psi
\end{aligned}$$

(Weideman 2025).

For the other two dimensions (y,z) we have

$$\begin{aligned}
\frac{\partial \Psi}{\partial y} &= \frac{i}{\hbar} p_y \Psi \\
\frac{\partial^2 \Psi}{\partial y^2} &= \frac{i}{\hbar} p_y \frac{\partial \Psi}{\partial y} = \frac{i}{\hbar} p_y \times \frac{i}{\hbar} p_y \Psi = \frac{i^2}{\hbar^2} p_y^2 \Psi \\
&= -\frac{1}{\hbar^2} p_y^2 \Psi
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \Psi}{\partial z} &= \frac{i}{\hbar} p_z \Psi \\
\frac{\partial^2 \Psi}{\partial z^2} &= \frac{i}{\hbar} p_z \frac{\partial \Psi}{\partial z} = \frac{i}{\hbar} p_z \times \frac{i}{\hbar} p_z \Psi = \frac{i^2}{\hbar^2} p_z^2 \Psi \\
&= -\frac{1}{\hbar^2} p_z^2 \Psi
\end{aligned}$$

Now we add the obtained second derivatives side by side.(Caruso et al.,2020)

$$\begin{aligned}
\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \Psi &= -\frac{1}{\hbar^2} (p_x^2 + p_y^2 + p_z^2) \Psi \\
\Delta \Psi &= -\frac{\Psi}{\hbar^2} (p_x^2 + p_y^2 + p_z^2) \\
p_x^2 + p_y^2 + p_z^2 &= -\frac{\hbar^2}{\Psi} \Delta \Psi \quad (5)
\end{aligned}$$

Now from relation (2) value $(p_x^2 + p_y^2 + p_z^2)$ We put in relation (5)

$$2mE_k = -\frac{\hbar^2}{\Psi} \Delta \Psi \quad (6)$$

$$\frac{\hbar^2}{2m} \Delta \Psi + \Psi E_k = 0 \quad (7)$$

This equation describes the motion of a free particle and is known as the Schrödinger equation. If the particle does not move with its potential (Young & Freedman, 2009), that is, it is not free and moves in the field of electrostatic force, such as the movement of an electron in the field of central force around the orbit of an atom, for example, a hydrogen atom (H), which expresses the purpose of the research, we write equation (7) using the laws of mechanical energy, which is the sum of kinetic and potential energy, as follows: (University of California, Davis, 2025).

$$E_k = E - u(r) \\ \frac{\hbar^2}{2m} \Delta \Psi + (E - u(r)) \Psi = 0 \quad (8)$$

This equation forms the basis of quantum mechanics, which actually describes the motion of an electron in the Coulomb field (Jeremy, 2022).

Now, if we apply the Schrödinger equation for the hydrogen atom in the system (c, g, s) we have that $u(r) = -\frac{e^2}{r}$

$$\frac{\hbar^2}{2m} \Delta \Psi + (E + \frac{e^2}{r}) \Psi = 0 \quad (9)$$

(LibreTexts,

2025).

Allowed energies E_1 For the wave Ψ_1 and E_2 For the wave $\Psi_2 \dots E_n$ For the wave Ψ_n is quantized in every waves. Its general solution is all pairs of (E, Ψ) and the specific solution is just one pair. (E_1, Ψ_1) It is possible. (Purwanto et al., 2012)

In some ways, $\left(\frac{e^2}{r} + E\right) \frac{2m}{\hbar^2} = K^2(r)$ and $k^2(r) \Psi + \Delta \Psi = 0$ are in

Cartesian coordinate form, but the electron's motion around the nucleus is spherical, so the Laplacian (Δ) must be spherical form, which is very

difficult and complicated to do manually using the chain differentiation rules. For this reason, we use the orthogonal curved coordinate system method, meaning that the Laplacian can be written using the Lamé coefficient h_i . According to Figure (1), we want to convert the Cartesian coordinates (x, y, z) to spherical coordinates (r, φ, θ) .

2. convert the Cartesian coordinates to spherical coordinates

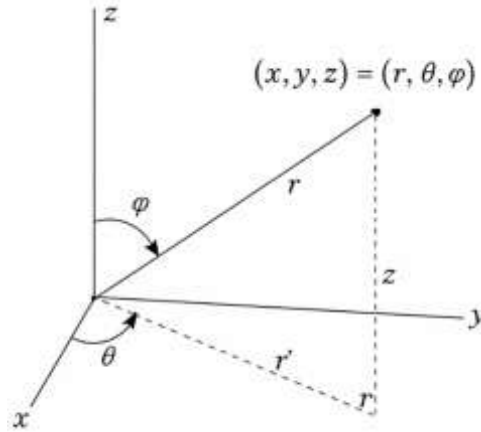


Figure (1): Shows a point in three-dimensional space where r is the distance of the point from the origin of the device, which is actually the radius of the atom.

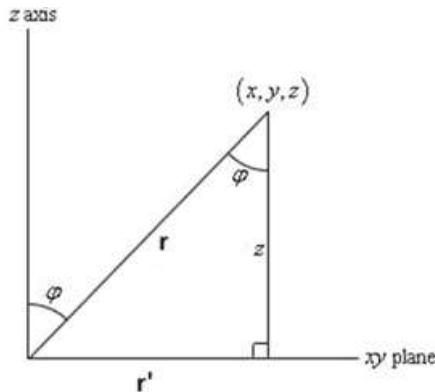


Figure (2): This is a continuation of Figure (1), in which the values of z and r are expressed in terms of φ .

$$y = r' \sin \theta$$

$$x = r' \cos \theta$$

$$z = r \cos \varphi$$

$$r' = r \sin \varphi$$

$$y = r \sin \theta \sin \varphi, \quad x = r \sin \varphi \cos \theta$$

$$\vec{r}(q_i, q_j, q_k) = \vec{r}(r, \theta, \varphi) \Rightarrow \vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$$

(Walet, 2024).

Now

$$\vec{r} = r \sin \varphi \cos \theta \vec{i} + r \sin \varphi \sin \theta \vec{j} + r \cos \varphi \vec{k}$$

$$\frac{\partial \vec{r}}{\partial r} = \sin \varphi \cos \theta \vec{i} + \sin \varphi \sin \theta \vec{j} + \cos \varphi \vec{k}$$

$$h_1 = \left| \frac{\partial \vec{r}}{\partial r} \right| = \sqrt{(\sin \varphi \cos \theta)^2 + (\sin \varphi \sin \theta)^2 + (\cos \varphi)^2}$$

$$= \sqrt{\sin^2 \varphi \cos^2 \theta + \sin^2 \varphi \sin^2 \theta + \cos^2 \varphi}$$

$$= \sqrt{\sin^2 \varphi (\cos^2 \theta + \sin^2 \theta) + \cos^2 \varphi} = 1$$

$$\text{in the same way } h_2 = \left| \frac{\partial \vec{r}}{\partial \theta} \right| = r, \quad h_3 = \left| \frac{\partial \vec{r}}{\partial \varphi} \right| = r \sin \varphi$$

Laplacian formula in spherical coordinates :

$$\Delta \Psi = \frac{1}{h_1 h_2 h_3} \sum_{i=1}^3 \frac{\partial}{\partial q_i} \left(\frac{h_2 h_3}{h_i} \frac{\partial \Psi}{\partial q_i} \right)$$

With substitutions $h_1 h_2 h_3$ and q_i , we have that

$$\Delta \Psi = \frac{1}{r^2 \sin \varphi} \left[\frac{\partial}{\partial r} \left(r^2 \sin \varphi \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial \Psi}{\partial \varphi} \right) + \frac{\partial}{\partial \theta} \left(\frac{1}{\sin \varphi} \frac{\partial \Psi}{\partial \theta} \right) \right]$$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2} \frac{1}{\sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial \Psi}{\partial \varphi} \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left(\frac{1}{\sin^2 \varphi} \frac{\partial \Psi}{\partial \theta} \right)$$

$$= \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{1}{\sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} \right) \right] + \frac{1}{r^2} \left(\frac{1}{\sin^2 \varphi} \frac{\partial^2}{\partial \theta^2} \right) \Psi$$

$$\Delta = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{1}{\sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} \right) + \frac{1}{r^2} \left(\frac{1}{\sin^2 \varphi} \frac{\partial^2}{\partial \theta^2} \right)$$

(Bayrak et al., 2025).

Therefore, the Laplacian (Δ) has been transformed into a spherical. Now we put this Laplacian value in equation (9)

$$\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{1}{\sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} \right) + \frac{1}{r^2} \left(\frac{1}{\sin^2 \varphi} \frac{\partial^2}{\partial \theta^2} \right) \right] \Psi + \left(\frac{e^2}{r} + E \right) \Psi = 0 \quad (10)$$

This is the Schrödinger equation in the spherical coordinate system, in which the Laplacian consists of two angular and radial parts, namely:

$$\Psi(r, \theta, \varphi) = R(r)Y(\theta, \varphi) \quad (\text{Stanizi \& Ahdyar, 2015}).$$

3. angular and radial parts in the spherical coordinate system

Now, considering that R is the radial function related to r and Y is the angular function related to (θ, φ) , we multiply both sides of equation (10) by RY.

$$\begin{aligned} & \frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{1}{\sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} \right) + \frac{1}{r^2} \left(\frac{1}{\sin^2 \varphi} \frac{\partial^2}{\partial \theta^2} \right) \right] RY \\ & + \left(\frac{e^2}{r} + E \right) RY = 0 \\ & \frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} RY + \frac{1}{r^2} \frac{1}{\sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} RY \right) + \frac{1}{r^2} \left(\frac{1}{\sin^2 \varphi} \frac{\partial^2}{\partial \theta^2} RY \right) \right] + \left(\frac{e^2}{r} + E \right) RY = 0 \quad (11) \end{aligned}$$

$$\partial_r (RY) = YR'(r)$$

$$\partial_\varphi (RY) = R \partial_\varphi Y$$

$$\partial_\theta (RY) = R \partial_\theta Y$$

so, expand the Laplacian terms

1- Radial pieces

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} RY \right) = \frac{Y}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right)$$

2 – Angular pieces

$$\frac{1}{r^2 \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} RY \right) = \frac{R}{r^2 \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} Y \right)$$

$$\frac{1}{r^2 \sin^2 \varphi} \frac{\partial^2 (RY)}{\partial \theta^2} = \frac{R}{r^2 \sin^2 \varphi} \frac{\partial^2 Y}{\partial \theta^2}$$

Now we substitute these values into equation (11) and then multiply

both sides by $\frac{r^2}{RY}$ that is:

$$\frac{\hbar^2}{2m} \left[\frac{Y}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{R}{r^2 \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} Y \right) + \frac{R}{r^2 \sin^2 \varphi} \frac{\partial^2 Y}{\partial \theta^2} \right] + \left(\frac{e^2}{r} + E \right) RY = 0$$

$$\frac{\hbar^2}{2m} \left[\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{1}{Y \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} Y \right) + \frac{1}{Y \sin^2 \varphi} \frac{\partial^2 Y}{\partial \theta^2} \right] + \left(\frac{e^2}{r} + E \right) r^2 = 0$$

$$\frac{\hbar^2}{2m} \frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left(\frac{e^2}{r} + E \right) r^2 = - \left[\frac{\hbar^2}{2m} \frac{1}{Y \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} Y \right) + \frac{\hbar^2}{2m} \frac{1}{Y \sin^2 \varphi} \frac{\partial^2 Y}{\partial \theta^2} \right]$$

multiply both sides by $\frac{2m}{\hbar^2}$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left(\frac{e^2}{r} + E \right) r^2 = - \left[\frac{1}{Y \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} Y \right) + \frac{1}{Y \sin^2 \varphi} \frac{\partial^2 Y}{\partial \theta^2} \right]$$

Left side depends only on r ; right side depends only on θ, φ . For this equality to hold for all r, θ, φ , both sides must be equal to the same constant. Conventionally choose that constant to be $l(l+1)$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left(\frac{e^2}{r} + E \right) r^2 = l(l+1)$$

$$\frac{1}{Y(\varphi, \theta)} \left[\frac{1}{Y \sin \varphi} \frac{\partial}{\partial \varphi} \left(\sin \varphi \frac{\partial}{\partial \varphi} Y \right) + \frac{1}{Y \sin^2 \varphi} \frac{\partial^2 Y}{\partial \theta^2} \right] = -l(l+1)$$

The solutions are the spherical harmonics:

$$Y_l^m(\varphi, \theta) = N_{lm} P_l^m(\cos \varphi) e^{im\theta}$$

with integer m satisfying $-l \leq m \leq l$ associated Legendre function p_l^m and the usual normalization constant. (Jackson, 1999).

$$N_{lm} = (-1)^m \sqrt{\frac{2l+1(l-m)!}{4\pi(l+m)!}}$$

Thus, the normalized spherical harmonics are

$$Y_l^m(\varphi, \theta) = (-1)^m \sqrt{\frac{2l+1(l-m)!}{4\pi(l+m)!}} P_l^m(\cos \varphi) e^{im\theta} \quad (12)$$

$$\text{They satisfy } \int_0^{2\pi} \int_0^\pi |Y_l^m|^2 \sin \varphi d\varphi d\theta = 1$$

(Makris et al., 2025).

3.RESULTS AND DISCUSSION

Quantum numbers: principal

$$n \geq 1$$

$$l = 0, 1, 2, \dots, n-1 (\text{orbital quantum number})$$

$$m = -l, \dots, l (\text{magnetic quantum number})$$

$P_l^m(x)$ is the associated Legendre polynomial.

$$\text{at the sample angles } \varphi \in \left\{0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \pi\right\} \text{ and } \theta \in \left\{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\right\}$$

Finally, for $l = 0, m = 0, \varphi = 0, \theta = 0$ we have:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \approx 0.28209$$

real and imaginary parts

$$e^{im\theta} = \cos(m\theta) + i \sin(m\theta) = 0.28209 + 0i$$

Tabal1- shows the defetnt valu of ϕ and θ for plot figur(3)

θ	ϕ	Re(Y)	Im(Y)	Y
0	0	0.2821	0	0.2821
0	$\pi/4$	0.2821	0	0.2821
0	$\pi/2$	0.2821	0	0.2821
0	$3\pi/4$	0.2821	0	0.2821
0	π	0.2821	0	0.2821
$\pi/2$	0	0.2821	0	0.2821
$\pi/2$	$\pi/4$	0.2821	0	0.2821
$\pi/2$	$\pi/2$	0.2821	0	0.2821
$\pi/2$	$3\pi/4$	0.2821	0	0.2821
$\pi/2$	π	0.2821	0	0.2821
π	0	0.2821	0	0.2821
π	$\pi/4$	0.2821	0	0.2821
π	$\pi/2$	0.2821	0	0.2821
π	$3\pi/4$	0.2821	0	0.2821
π	π	0.2821	0	0.2821

Note:

φ (**rad**) = Phi in radians (polar angle)

θ (**rad**) = Theta in radians (azimuthal angle)

$\text{Re}(\mathbf{Y})$ = Real part of the spherical harmonic $\mathbf{Y}$

$\text{Im}(\mathbf{Y})$ = Imaginary part of the spherical harmonic $\mathbf{Y}$

$|\mathbf{Y}|$ = Magnitude of the spherical harmonic $\mathbf{Y}$

Y_0^0 (s - state)

$Y_1^0, Y_1^{\pm 1}$ (p - state)

Y_2^m (d - state)

Now we just plot for Hydrogen Atom in Y_0^0 (s - state)

$|Y_0^0|$ on the sphere

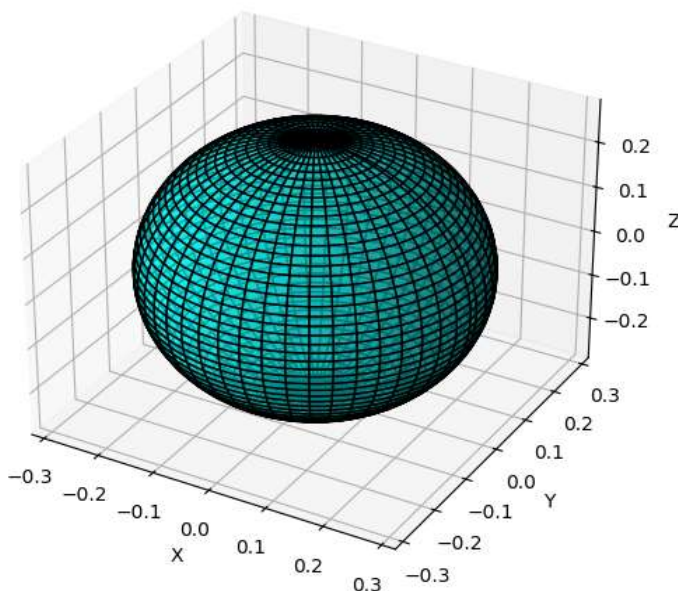


figure (3): The hydrogen atom in the ground state is completely isotropic. The probability of an electron changing only with r , not with direction.

Radial functions:

$$R_{nl}(r) = \frac{2}{n^2 a_0^{\frac{3}{2}}} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \left(\frac{2r}{na_0}\right)^l e^{\frac{-r}{na_0}} L_{n-l-1}^{(2l+1)}\left(\frac{2r}{na_0}\right) \quad (13)$$

we can check normalization by

$$\int_0^\infty |R_{nl}(r)|^2 r^2 dr = 1$$

and

$$\rho_{nl}(r) = r^2 |R_{nl}(r)|^2 \quad (14)$$

$$\begin{aligned} R_{10}(r) &= \frac{2}{1^2 \times 1^{\frac{3}{2}}} \sqrt{\frac{(1-0-1)!}{(1+0)!}} \left(\frac{2r}{1 \times 1}\right)^0 e^{\frac{-r}{1 \times 1}} L_{1-0-1}^{(2 \times 0 + 1)}\left(\frac{2r}{1 \times 1}\right) \\ &= 2\sqrt{1} \times (1) e^{-r} \times 1 = 2e^{-r} \end{aligned}$$

$$R_{10}(r) = 2e^{-r}$$

$$\Rightarrow \rho_{nl}(r) = r^2 |R_{nl}(r)|^2 = r^2 |2e^{-r}|^2 = 4r^2 e^{-2r}$$

for the hydrogen ground state ($n=1, l=0$) in atomic units (Bohr radius $a_0=1$)

the radial function is $R_{10}(r) = 2e^{-r}$ so $\rho_{10}(1) = 0.541341$

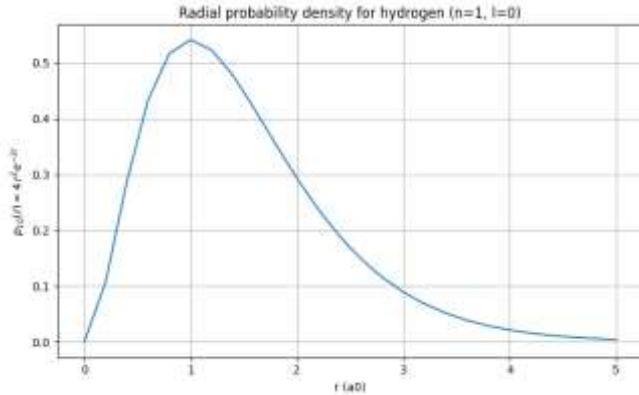


figure (4): shows the Hydrogen radial probability densities according to the relation (14)

Notes:

- The peak occurs at $r = 1a_0$ with $\rho_{10}(1) = 0.541341$

– Python programming was employed to obtain numerical data, and the corresponding graphs and the spherical structure of the hydrogen atom model were generated within a spherical coordinate system.

5.CONCLUSION

Based on the analysis using the Schrödinger wave equation, it is concluded that the hydrogen atom provides the simplest and most fundamental model for understanding quantum behavior in atomic systems. Within this framework, the electron is no longer considered a particle moving in a fixed, well-defined orbit, but rather is described by a wave function that represents a probability distribution of its presence around the nucleus. This marks a significant departure from classical atomic models.

The results show that the energy levels of the electron in the hydrogen atom are quantized, and each state is characterized by a set of quantum numbers n , l , and m . These quantum numbers determine not only the energy of the electron but also the shape and orientation of atomic orbitals. The use of a spherical coordinate system allows the Schrödinger equation to be separated into radial and angular parts, making the mathematical treatment more manageable and physically meaningful.

Furthermore, the analysis of the radial probability distribution reveals that the electron is most likely to be found at a specific distance from the nucleus. According to the results, this most probable radius is 0.541341 corresponding to the Bohr radius, where the probability distribution reaches its maximum. This demonstrates that although the exact position of the electron cannot be determined, regions of high probability can be clearly identified.

Finally, it is concluded that the hydrogen atom exhibits spherical symmetry, particularly in its ground state, where the probability distribution of the electron is uniform in all directions around the nucleus. Overall, the Schrödinger equation provides a highly successful and accurate description of atomic structure, effectively explaining the probabilistic nature of the electron and forming the foundation of modern quantum mechanics.

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