Risalah Fisika
Volume 6, Number 2, 2026 pp. 59-68
e-ISSN: 2548-9011
DOI: 10.35895/rf.v6i2.84

Computational Modeling and Visualization of Quantum Wavefunctions for the Particle-in-a-box and Hydrogen Atom

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ARTICLE INFO

Article history:
Received 23 February 2026
Revised 16 March 2026
Accepted 02 June 2026
Available online 15 July 2026

Keywords:
quantum mechanics; Schrödinger equation; hydrogen atom; particle in a box; computational modeling

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ABSTRACT

This study models and visualizes quantum wavefunctions in two fundamental systems-namely the one-dimensional particle-in-a-box and the hydrogen atom-using a computational Python-based approach. The Schrödinger equation is solved analytically to obtain the wavefunctions and probability distributions, which are subsequently visualized in both two and three dimensions. For the particle-in-a-box system, the results demonstrate clear energy quantization, increasing numbers of nodes, and waveform evolution that are aligns with theoretical predictions. In the hydrogen atom system, the modeling incorporates the radial and angular components of the wavefunction, producing realistic orbital representations such as 1s, 2p, 3p, and 3d according to the chosen quantum numbers n, l, and m. The resulting visualizations clearly illustrate the relationship between quantum numbers, nodal structure, and electron probability distributions. Overall, the study shows that computational modeling effectively bridges mathematical solutions and physical interpretation, providing a powerful tool for enhancing conceptual understanding in quantum mechanics education.

ABSTRAK

Penelitian ini memodelkan dan memvisualisasikan fungsi gelombang kuantum pada dua sistem fundamental, yaitu partikel dalam kotak satu dimensi dan atom hidrogen, menggunakan pendekatan komputasional berbasis Python. Persamaan Schrödinger diselesaikan secara analitik untuk memperoleh bentuk fungsi gelombang dan distribusi probabilitas, kemudian hasilnya divisualisasikan dalam bentuk dua dan tiga dimensi. Pada sistem partikel dalam kotak, hasil pemodelan menunjukkan pola kuantisasi energi, peningkatan jumlah node, serta evolusi bentuk gelombang yang konsisten dengan teori. Sementara itu, pemodelan atom hidrogen dilakukan dengan memanfaatkan kombinasi fungsi radial dan harmonik sferis, sehingga dihasilkan representasi orbital seperti 1s, 2p, 3p, dan 3d sesuai variasi bilangan kuantum n, l, dan m. Visualisasi yang dihasilkan secara jelas memperlihatkan hubungan antara bilangan kuantum, struktur nodal, dan distribusi probabilitas elektron. Studi ini menunjukkan bahwa pemodelan komputasional mampu menjembatani solusi matematis dan pemahaman fisik, serta menjadi media efektif dalam pembelajaran mekanika kuantum.

1. INTRODUCTION

Quantum mechanics has become a key pillar in describing particle behavior at the atomic and subatomic scales, where classical solutions are no longer able to describe wave-particle phenomena (Ling et al., 2021). The existence of electrons in atoms, for example, cannot be understood as points of mass orbiting the nucleus, as in the Bohr model, but rather as entities with a probabilistic distribution derived from the wave function ψ, which is a solution to the Schrödinger equation (Galler et al., 2021). The question of the shape of the wave function, how the probability of electron distribution changes with quantum numbers, and why atomic orbitals have certain shapes such as spherical, dumbbell, or other complex shapes are fundamental questions that encourage the use of computational modeling to obtain more intuitive visual representations (Azizi, 2021).

One simple system used as a basis for learning is the one-dimensional particle in a box. This model depicts a particle confined in a box with zero potential inside and infinity outside (Supriadi et al., 2020). Although simple, this model accurately describes how quantized energy naturally arises from mathematical solutions, and why

particles cannot exist at arbitrary energies. The second system discussed is the hydrogen atom, the only atom with a complete analytical solution to the three-dimensional Schrödinger equation (Al-Masaeed et al., 2024). By separating coordinates into radial and angular components, the hydrogen atom allows the visualization of orbitals such as 1s, 2p, 3d, and even orbitals with high quantum numbers. Computational modeling plays a crucial role in mapping these wave functions onto two-dimensional and three-dimensional graphs (Sathongpaen et al., 2024).

This study aims to systematically derive analytical solutions to the Schrödinger equation for both systems, implement them in the Python programming language, and display the wave functions and their probability distributions for various quantum numbers. Thus, this study not only provides theoretical insight but also provides a computational approach relevant to the study of modern physics.

2. SCHRÖDINGER'S EQUATION IS TIME INDEPENDENT

The time-independent Schrödinger equation for a particle of mass m with potential $V(r)$ is written as an eigenvalue operator:

$$\hat{H}\psi(r) = E\psi(r) \tag{1}$$

which $\hat{H}$ can be defined as (Singh, 2024):

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{2}$$

In one-dimensional coordinates (x) which will be used for the particle in the box case, the Laplacian operator becomes the second derivative with respect to x: $\nabla^2 \rightarrow d^2/dx^2$. An important physical interpretation is that the normalization solution of ψ must meet

$$\int |\psi|^2 \, dx = 1 \tag{3}$$

on all relevant domains.

3. Particles in a one-dimensional box

3.1. Differential equations and general form of solutions

Consider the potential of an infinite box:

$$V(x) = \begin{cases} 0, 0 < x < L, \\ \infty, otherwise \end{cases} \tag{4}$$

In the box ($0 < x < L$) the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{5}$$

We rearrange it into a standard form of differential equation

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \tag{6}$$

where

$$k^2 \equiv \frac{2mE}{\hbar^2}$$

The equation $\psi'' + k^2\psi = 0$ is a second-order homogeneous linear wave equation with a general solution

$$\psi(x) = A\sin(kx) + B\cos(kx) \tag{7}$$

where A and B are constants of integration (House, 2017).

3.2. Boundary conditions and quantization (k)

The physical condition comes from the infinite potential: the wave function must be zero at the walls of the box because the particle cannot be outside (the probability value is zero). So,

$$\psi(0) = 0 \quad \Rightarrow \quad A\sin(0) + B\cos(0) = B = 0.$$

For $B = 0$ the solution becomes (Griffiths & Schroeter, 2018):

$$\psi(x) = A\sin(kx) \tag{8}$$

The second boundary condition

$$\psi(L) = 0$$

gives

$$\psi(L) = A\sin(kL) = 0$$

For $A \neq 0$ (the trivial solution $\psi \equiv 0$ is unphysical, $sin\ (kL)$ must hold. The values of *k* that satisfy this are

$$kL = n\pi, \qquad n = 1,2,3,\ldots$$

so that

$$k_n = \frac{n\pi}{L} \tag{9}$$

3.3. Eigen energy

Since $k^2 = \frac{2mE}{\hbar^2}$, substitution equation (9) into it gives

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{10}$$

This shows discrete quantization of energy; where the energy scales with n^2 (Zettili, 2009).

3.4. Normalization and amplitude constant

The general wave function before normalization is $\psi_n(x) = A_n \sin(n\pi x / L)$ We determine A_n from the normalization condition.

$$\int_0^L |\psi_n(x)|^2\, dx = 1 \quad \Rightarrow \quad |A_n|^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \tag{11}$$

Using the trigonometric identity $\sin^2\alpha = \frac{1-\cos(2\alpha)}{2}$, produces

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \int_0^L \frac{1-\cos\left(\frac{2n\pi x}{L}\right)}{2} dx = \frac{1}{2}[x]_0^L - \frac{1}{2}\left[\frac{L}{2n\pi}\sin\left(\frac{2n\pi x}{L}\right)\right]_0^L. \tag{12}$$

The second term at the boundary becomes zero because $sin(2n\pi) = 0$. Then the integral becomes $\frac{L}{2}$ so that

$$|A_n|^2 \cdot \frac{L}{2} = 1 \quad \Rightarrow \quad |A_n|^2 = \frac{2}{L}$$

We take $A_n > 0$ to simplify the notation, so that the normalization constant (Dalal, 2018):

$$A_n = \sqrt{\frac{2}{L}} \tag{13}$$

Thus the normalized solution:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{14}$$

3.5. Probability density and node properties

The probability density of position is

$$P_n(x) = |\psi_n(x)|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right) \tag{15}$$

Nodes (where $\psi_n = 0$ inside $0 < x < L$) occur when $\sin(n\pi x / L) = 0$, that is, at ($x = \frac{jL}{n}$ for j = 0,1,…,n). The number of interior nodes (not counting the boundaries) is (n - 1). Physically, the number of nodes is directly proportional to the quantum number and explains the complexity of the waveform at higher energy levels (Griffiths, 1994).

4. Hydrogen atom

The hydrogen atom is a one-electron system in the Coulomb field of a charged nucleus (+e). The time-independent Schrödinger equation in three-dimensional coordinates is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r) \tag{16}$$

with the Coulomb potential (neglecting relativistic/spin corrections)

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}, \quad Z = 1 \text{ (hydrogen)} \tag{17}$$

Since the potential depends only on (r), we use spherical coordinates (r,θ,ϕ) and separate the variables (Griffiths & Schroeter, 2018). The Laplacian in spherical coordinates:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{18}$$

4.1. Separation of variables

Assume the solution $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$. Substituting into the Schrödinger equation and dividing by RY and multiplying by $2mr^2/\hbar^2$ yields

$$-\frac{r^2}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\big(E - V(r)\big) = \frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] \tag{19}$$

The left is just a function of r, the right is just the function of θ,ϕ. Both sides must be constants; define the separation constant $\ell(\ell+1)$ (convention). This yields two equations: the angular equation (which produces spherical harmonics) and the radial equation (Griffiths & Schroeter, 2018).

4.2. Angular equation: spherical harmonics

The angular equation becomes the eigenvalue for the angular operator (the angular momentum squared operator ($\hat{L}^2$):

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)Y \tag{20}$$

with the solution being the spherical harmonics $Y_\ell^m(\theta,\phi)$, where $\ell = 0,1,2,\ldots$ and $m = -\ell,\ldots,\ell$. The angular density $|Y_\ell^m|^2$ determines the angular distribution of the orbitals (Griffiths & Schroeter, 2018).

4.3. Radial equation

The radial equation obtained is

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[\frac{2m}{\hbar^2}\big(E - V(r)\big)r^2 - \ell(\ell+1)\right]R = 0 \tag{21}$$

For convenience, the substitution $u(r) = rR(r)$ is often used. With this substitution, we can write the equation (21) in one-dimensional form for $u(r)$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V(r)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u=Eu \tag{22}$$

This is the effective one-dimensional form of the Schrödinger equation with an efficient potential containing the centrifugal term $\frac{\ell(\ell+1)\hbar^2}{2mr^2}$ (Griffiths & Schroeter, 2018).

4.4. Radial solution for the Coulomb -transformation to the Laguerre equation

Substitute $V(r)=-\frac{Ze^2}{4\pi\varepsilon_0 r}$. To find a regular and normalized solution, follow the general steps (Zettili, 2009):

1) Introduce the Bohr constant $a_0=\frac{4\pi\varepsilon_0\hbar^2}{me^2}$ and the inert parameter $\rho\equiv\frac{2Zr}{na_0}$ ultimately $Z = 1$ for hydrogen. Here Z is kept for generality.
2) Using the substitution $R_{n\ell}(r)=\frac{u_{n\ell}(r)}{r}$ and the asymptotic form: for $r\to 0,\ u\propto r^{\ell+1}$ so that (R) is not singular), and for $r\to\infty$, u must decrease faster than the exponential for normalization, typically $e^{-\rho/2}$
3) By transformation of variables and substitution of the form $u(\rho)=\rho^{\ell+1}e^{-\rho/2}v(\rho)$, the radial equation transforms into an equation for $v(\rho)$ which is identical to the associated Laguerre polynomial equation. The discreteness of the energy arises from the requirement that $v(\rho)$ must be a polynomial so that it does not diverge when $\rho\to\infty$, thus yielding the quantization condition.

After working through the algebra (substituting into the equation and grouping the terms), we obtain the normalized radial solution (writing down the normalization constant $N_{n\ell}$:

$$R_{n\ell}(r)=N_{n\ell}\left(\frac{2Zr}{na_0}\right)^{\ell}e^{-Zr/(na_0)}L_{n-\ell-1}^{2\ell+1}\left(\frac{2Zr}{na_0}\right) \tag{23}$$

where $L_p^q(\rho)$ is the associated Laguerre polynomial and the index satisfies $p=n-\ell-1$ (nonnegative) such that $n\geq\ell+1$.

4.5. Eigen energy of hydrogen atom

The need for quantization produces eigenenergy

$$E_n=-\frac{me^4Z^2}{2(4\pi\varepsilon_0)^2\hbar^2}\cdot\frac{1}{n^2}\equiv-\frac{13.6057\cdot Z^2}{n^2}\text{eV} \tag{24}$$

For hydrogen (Z =1). This form comes from the requirement that $v(\rho)$ must be a polynomial of order $n-\ell-1$, which implies a relationship between energy and the principal quantum numbers $n=1,2,\ldots$

4.6. Normalization of radial constants

The normalization constant can be determined from the three-dimensional normalization conditions:

$$\int_0^{\infty}|R_{n\ell}(r)|^2\ r^2dr=1 \tag{25}$$

After substitution $\rho=\frac{2Zr}{na_0}$ and using the integral orthogonality of the Laguerre polynomials, the explicit constant is obtained

$$N_{n\ell}=\sqrt{\left(\frac{2Z}{na_0}\right)^3\frac{(n-\ell-1)!}{2n[(n+\ell)!]}} \tag{26}$$

The details of the proof utilize Laguerre's integral identity:

(27)

$$\int_0^\infty e^{-\rho}\rho^\alpha \left[L_k^\alpha(\rho)\right]^2 d\rho = \frac{(k+\alpha)!}{k!}$$

By substitution and factor arrangement, the above expression of $N_{n\ell}$ is obtained (Griffiths & Schroeter, 2018).

4.7. Complete wave function and probability

The complete stationary wave function for the pair n, ℓ, m is written

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r), Y_\ell^m(\theta,\phi) \tag{28}$$

The probability density of the three-dimensional space is

$$P_{n\ell m}(r,\theta,\phi) = |\psi_{n\ell m}(r,\theta,\phi)|^2 = |R_{n\ell}(r)|^2, |Y_\ell^m(\theta,\phi)|^2 \tag{29}$$

While the radial probability (probability of finding an electron in a radius surface from r *to* $r+dr$ is

$$P_{n\ell}(r), dr = |R_{n\ell}(r)|^2 \; r^2 dr \tag{30}$$

because of the volume factor of the sphere $4\pi r^2$ and the angular integration $\int |Y_\ell^m|^2 \, d\Omega = 1$ when the spherical harmonics are normalized (Zettili, 2009).

5. METHOD

This study uses a computational modeling approach to visualize the wave function and probability density of electrons in two quantum systems, namely a particle in a one-dimensional box and a hydrogen atom. In general, the method includes: determining simulation parameters, creating a numerical domain in the form of a spatial grid, applying the solution equations derived in the previous section, and graphical visualization in two and three dimensions using *Python*. The entire computational process is carried out using *NumPy*, *Matplotlib*, and *SciPy*, and is equipped with an interactive interface using ipywidgets to enable exploration of various quantum number values.

5.1. Particle-in-a-Box System Modeling Method

The modeling of a particle in a box is based on the analytical solution of the quantized wave function $\psi_n(x)$ expressed in Equation (14). The probability form of the particle's existence is calculated from the square of the wave function $|\psi_n(x)|$ as described in Equation (15). In the computational stage, a one-dimensional space domain is constructed using a grid from $x = 0$ to $x = L$ with 100 points generated using the *numpy.linspace()* function. The box length is set to $L = 1$, according to the parameters in the program code, so that all numerical calculations refer to the standardized domain. For visualization, the Python function psi(n, L, x) is used to calculate $\psi_n(x)$ directly from Equation (14), while psi_2(n, L, x) produces $|\psi_n(x)|^2$ based on Equation (15).

The program code then iterates over the first three quantum numbers n =1,2,3 to produce a graph of the wave function and its probability distribution. The first graph shows the shape of the sine wave of (x) for each value of n, while the second graph shows the square of the amplitude $|\psi_n(x)|^2$, which provides an idea of the most likely position where the particle is found. In addition to the static visualization. Thus, this modeling method combines Schrödinger's analytical solution with Python-based numerical visualization to enhance understanding of the relationship between energy quantization and wavefunction shape.

5.2. Hydrogen Atom System Modeling Method

The modeling of the hydrogen atom in this study is carried out based on the complete wave function $\psi_{n,l,m}$ (r,θ,ϕ), which has been derived in the Theoretical Basis and is expressed in Equation (28). The separation of the wave function into radial and angular components is carried out using the radial function $R_{n,l}(r)$ according to Equation (23) and the spherical harmonic function $Y_l^m(\theta,\phi)$ according to Equation (20). The probability of the electron's presence is calculated from $|\psi_{n,l,m}|^2$ as explained in Equation (29), while the radial distribution follows the definition of radial probability in Equation (30). In its implementation, this study visualizes two forms of probability representation: (1) two-dimensional visualization (electron density map in the xy plane), and (2) three-dimensional visualization (hydrogen atom orbital shape). For the 2D model, the program constructs a two-dimensional meshgrid from the Cartesian coordinates (x,y), then calculates the radius $R = \sqrt{x^2 + y^2}$.

The radial function is calculated based on Equation (23) using the Laguerre polynomial from the *numpy.polynomial.laguerre* library, while the total probability is obtained from $|R_{n,l}(r)|^2$, which represents the *xy*-plane projection of Equation (29). The calculation results are visualized using imshow with a viridis color palette to indicate the electron density. For 3D visualization, a spherical approximation is used through the (r,θ,ϕ) coordinates, which are calculated using the meshgrid. The radial function is calculated using the associated Laguerre polynomial *assoc_laguerre* from SciPy, according to Equation (23), while the angular component Ylm is calculated using the *sph_harm* function, according to Equation (20). Both components are combined to produce the complete wavefunction based on Equation (28). Its probability density is calculated as $|\psi|^2$ through Equation (29), then visualized as a 3D surface using plot_surface on the Cartesian coordinates resulting from the transformation of the *spherical_to_cartesian*(*r, \theta, \phi*) function. The entire hydrogen modeling provides an interactive interface so that the user can change the values of the three quantum numbers n, l and m, according to the quantum constraints described in the Theoretical Basis. By connecting Equations (23), (20), (28), and (29) in a single visualization flow, this method allows a direct mapping between quantum mechanical theory and the real shape of hydrogen atomic orbitals that appear in the simulation graph.

6. RESULT AND DISCUSSION

6.1. Particle-in-a-Box System Modeling

Figure 1 shows the shape changes of the wave function $\psi_n(x)$ and the probability distribution $|\psi_n(x)|^2$ for a particle in a one-dimensional box for three quantum number values, namely n = 1, 2, and 3. Fig. 1 (a) shows the wave function for the ground state n = 1, which is a single sine wave with no internal nodes, in accordance with Equation (14). This indicates that the electron has the highest probability at the center of the box and decreases towards the walls due to the boundary condition $\psi(0) = \psi(L) = 0$. As a counterpart, panel (b) shows the probability distribution $|\psi_1(x)|^2$ based on equation (15), which produces a single symmetric peak around x = 0.5L, reflecting the most stable and simplest ground state.

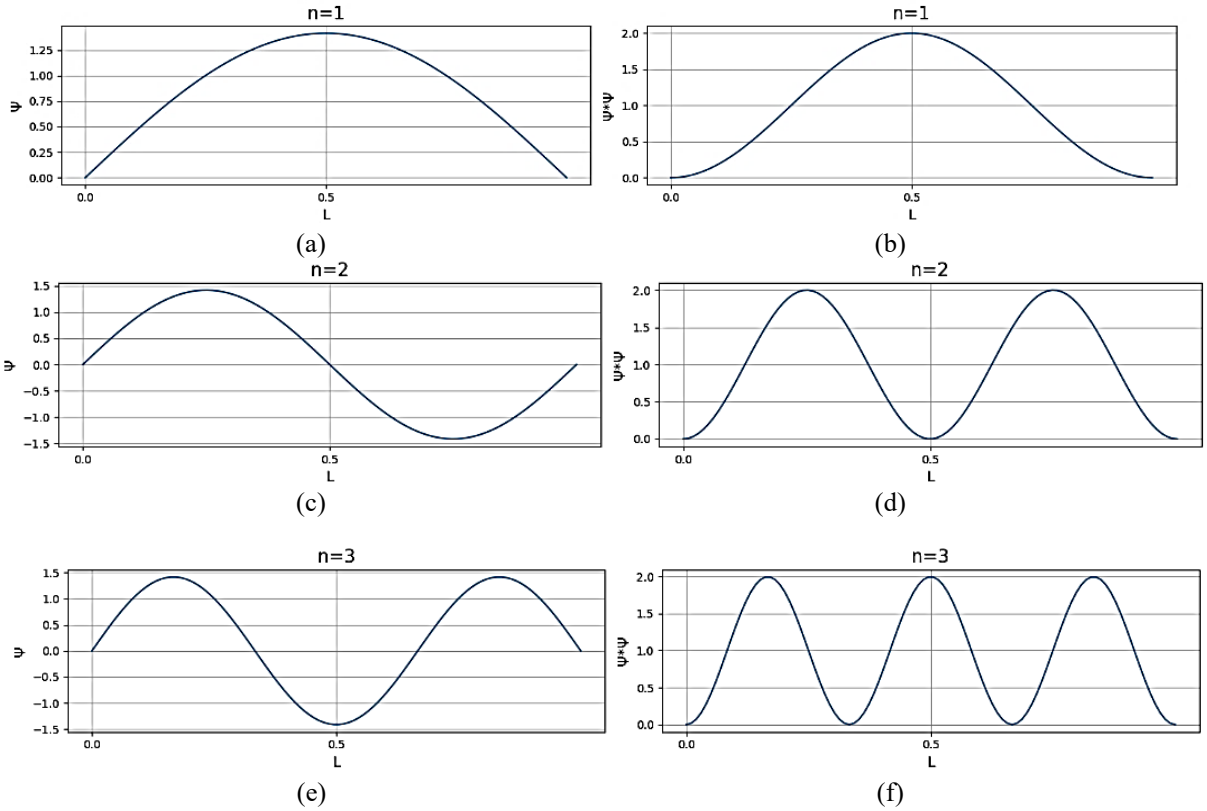


Figure 1. Visualization of the wave function $\psi_n(x)$ and the probability distribution $|\psi_n(x)|^2$ for a particle in a one-dimensional box at quantum numbers n = 1, 2, and 3: (a), (c), and (e) show the wave function $\psi_n(x)$; while (b), (d), and (f) show the probability distribution $|\psi_n(x)|^2$ respectively.

The changes begin to become apparent at n = 2. Panel (c) shows the wave function $\psi_2(x)$ with a single internal node in the center of the box, which is characteristic of excited states with more phase changes. This pattern is reflected in panel (d), the probability distribution $|\psi_2(x)|^2$, which now displays two peaks with zero probability

regions at these nodes. This phenomenon is consistent with the theory that increasing quantum numbers increases the energy of the system, resulting in a more complex wave structure that includes additional nodes.

The situation becomes clearer at $n = 3$. Panel (e) shows the wave function $\psi_3(x)$, which has two internal nodes and exhibits tighter oscillations than in the previous state. Panel (f), which visualizes $|\psi_3(x)|^2$, shows three relatively evenly spaced probability peaks while maintaining symmetry with respect to the box length. This pattern of increasing peaks aligns with the quantum mechanical principle that the number of significant probability regions increases proportionally with quantum number.

Overall, the visualization in Figure 1 illustrates a direct relationship between increasing quantum number and the number of nodes in the wave function and peaks in the probability distribution. The higher n, the more complex the spatial structure allowed for particles to exist, so that the probability distribution of the particle distribution becomes more divided but still bound by the sinusoidal structure according to the exact solution of equations (14) and (15). This visualization successfully shows the basic characteristics of the particle system in a box, namely energy quantization, the existence of nodes, and the evolution of the waveform at each energy level.

6.2. Hydrogen Atom System Modeling

The hydrogen atom modeling in this study was performed by combining radial and spherical harmonic functions to produce the complete wave function form $\psi_{n,l,m}(r,\theta,\phi)$. The visualization results shown in Figure 2 show two-dimensional and three-dimensional representations of the electron probability distribution for four different combinations of quantum numbers as summarize at Table 1. Each quantum number variation provides unique distribution characteristics, both in terms of the number of nodes, spatial symmetry, and lobe orientation, so the resulting graph provides a clear physical picture of the hydrogen orbital structure.

Tabel 1. Variation of quantum number of hydrogen atom

Variation	Quantum numbers		
	n	***l***	***M***
1	1	0	0
2	2	1	1
3	3	1	1
4	3	2	1

For the ground state ($n = 1$, $l = 0$, $m = 0$), Figure 2(a-b) shows that the electron distribution is spherically symmetric with a maximum intensity near the nucleus. The absence of radial or angular nodes is a characteristic feature of the 1s orbital. This shape arises because the spherical harmonic function for $l = 0$ is isotropic, so the electron distribution probability is identical in all directions. In the 3D visualization, this pattern appears as a single probability domain with no spatial splitting. These results are consistent with the analytical solution of the Schrödinger equation, which states that the ground state has no angular structure.

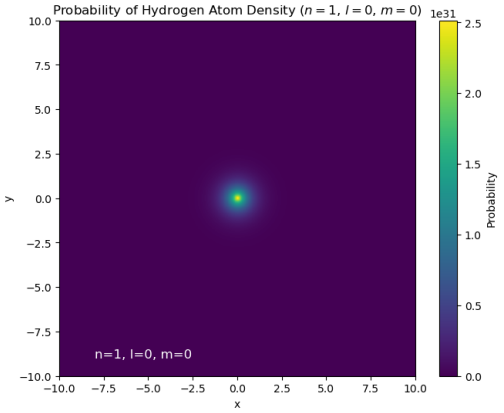
The change in the shape of the distribution begins to become apparent in the $n = 2$, $l = 1$, $m = 1$ states shown in Figure 2(c-d). The probability domain now forms two lobes, separated by a nodal plane passing through the nucleus. These angular nodes are a direct consequence of $l = 1$, which produces a spherical harmonic function with a single nodal plane. The $m = 1$ value causes the orbital orientation to be centered in a specific direction, resulting in a 2p orbital that is not axisymmetric but oriented according to the phase dependence $e^{\{im\,\phi\}}$. This shift in orientation demonstrates that the quantum number m does not change the basic shape of the orbital but rather determines the direction of the electron probability distribution.

In the higher-energy states, $n = 3$ and $l = 1$, shown in Figure 2(e–f), the probability distribution exhibits additional radial nodes. This is evident from the formation of rings or layers of probability regions that do not appear in the $n = 2$ state. Radial nodes arise because the value of n determines the number of nodes in the radial function, so orbitals at higher energies have a more complex spatial structure. In the three-dimensional visualization, the orbital lobes retain their p-characteristics (because $l = 1$), but the intensity pattern splits into two layers as a manifestation of these radial nodes.

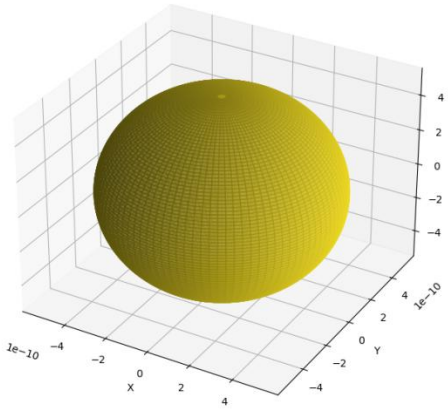
An even more complex situation is seen in Figure 2(g-h), for $n = 3$, $l = 2$, $m = 1$. In this configuration, the spherical harmonic function produces two angular nodes, so the probability distribution forms a d-orbital structure with several separate lobes. This geometric pattern depicts the five probability domains typical of d-orbitals, with their orientation determined by $m = 1$. The combination of radial and angular nodes in this state results in the three-dimensional visualization displaying a more complex multi-lobed shape than p-orbitals. This representation demonstrates increasing spatial complexity as the quantum number increases, in line with theoretical predictions regarding the wave behavior of electrons in the hydrogen atom.

Overall, Figure 2 shows that increasing quantum numbers not only increases the electron energy but also directly affects the probability geometry of the electron. Radial nodes appear as n increases, while angular nodes depend on the value of l, while m controls the spatial orientation of the orbitals. The resulting patterns indicate that

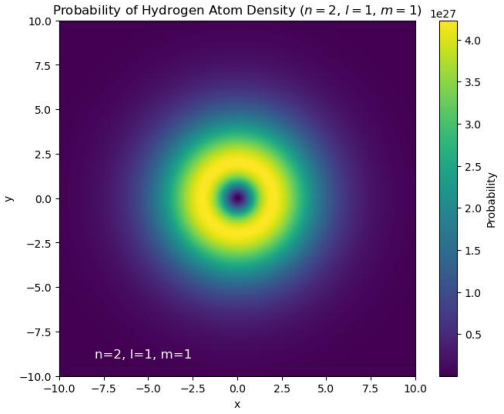
the shapes of the 1s, 2p, 3p, and 3d orbitals are not merely conceptual representations, but are direct mathematical solutions to the Schrödinger equation. Thus, this modeling provides an accurate computational visualization of the hydrogen orbital structure and clarifies the relationship between quantum numbers and the physical shape of the electron distribution.



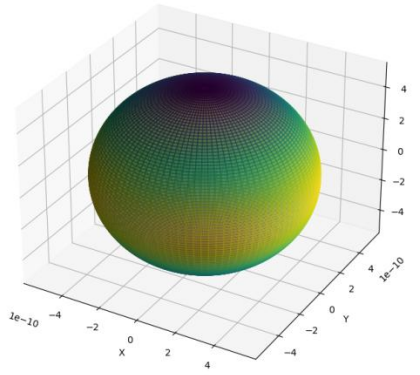
(a)



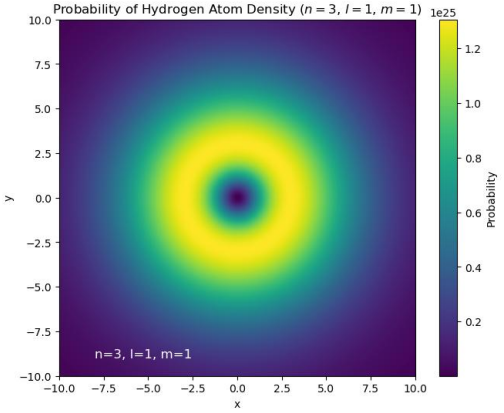
(b)



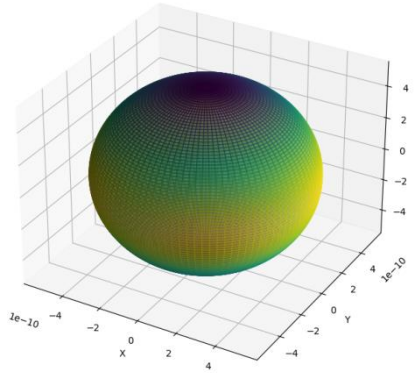
(c)



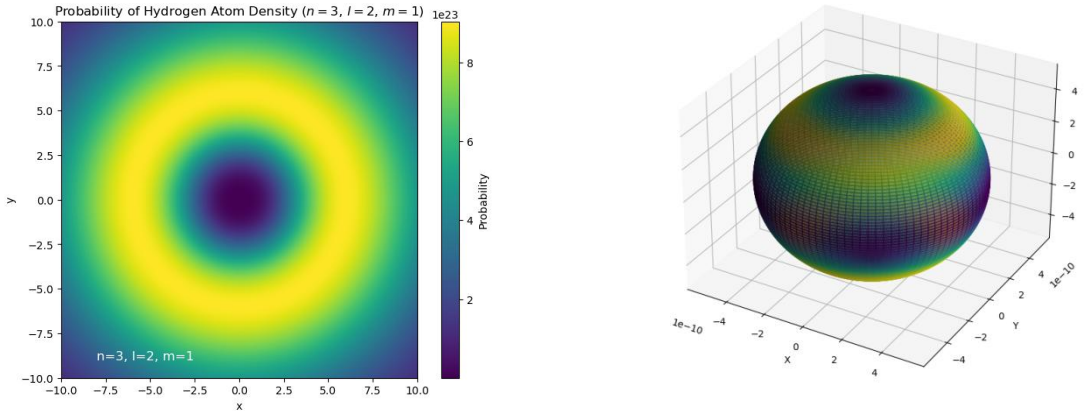
(d)



(e)



(f)



(g) (h)

Figure 2. Two- and three-dimensional visualization of the wave functions and electron probability distributions in the hydrogen atom for various quantum numbers (a-b) $n = 1$ $l = 0$ $m = 0$, (c-d) $n = 2$ $l = 1$ $m = 1$, (e-f) $n = 3$ $l = 1$ $m = 1$, (g-h) $n = 3$ $l = 2$ $m = 1$

7. CONCLUSION AND RECOMMENDATION

The results of quantum mechanical system modeling of particles in a one-dimensional box and hydrogen atom show that the computational approach is able to represent analytical solutions of the Schrödinger equation clearly. The visualization of waves and probability distributions in the particle-in-box system confirms the existence of energy quantization, the increasing number of nodes with increasing quantum numbers, and the periodic character of the wave function according to theory. Meanwhile, the hydrogen atom modeling successfully describes the three-dimensional orbital structure through a combination of radial and spherical harmonic functions, which show the change in complexity of the orbital shape due to variations in the quantum numbers n, l, and m. These results strengthen the understanding that quantum phenomena are both mathematical and physical, and that orbital structures are not just concepts, but rather forms of probability distributions that arise directly from the solutions of the Schrödinger equation. Thus, this study shows that Python-based computation is an effective tool for connecting quantum theory with visual representations, thereby improving conceptual understanding in modern physics learning.

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