Solving Hydrogen Atom using Physics- Informed Neural Network for ground state

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Submitted on 12-02-2026

Abstract

The hydrogen atom is a standard benchmark for testing and validating numerical techniques in quantum mechanics. Although high-precision studies in the literature include small quantum electrodynamic corrections such as the Lamb shift, the present work focuses on the numerical solution of the radial Schrödinger equation without incorporating these corrections.In this study, an unsupervised learning framework is employed to model radial wavefunctions at fixed energy values. A neural network is trained to learn physically acceptable solutions that satisfy boundary conditions and normalization behavior.
The obtained wavefunctions show strong agreement with expected theoretical profiles, reproducing correct nodal structures and asymptotic decay.The results demonstrate that unsupervised neural networks can serve as an effective numerical tool for approximating hydrogenic wavefunctions with good accuracy and precision. This approach provides a flexible foundation for future extensions toward more complex atomic systems and higher-order corrections.

1 Introduction

The hydrogen atom has long been a central model in quantum mechanics because it provides a clear and reliable framework for understanding atomic behavior. Since its exact analytical solution is known, it is often used to test the accuracy of numerical and computational methods.[1, 2] Studying the hydrogen atom also helps in analyzing subtle physical effects such as fine-structure corrections and the Lamb shift, which require highly precise calculations. For this reason, it remains an important system in modern computational physics.[3]

In earlier studies, researchers mainly relied on traditional numerical techniques to solve the radial Schrödinger equation. Methods such as finite-difference schemes and matrix approaches have been widely used[1] Among them, matrix methods with sine basis functions are popular because they provide stable eigenvalues and reason-

able wavefunctions. However, these methods depend on grid size and basis choice, which can sometimes reduce flexibility and accuracy, especially for excited states.[3]

More recently, Physics-Informed Neural Networks (PINNs) have emerged as a powerful approach for solving differential equations in quantum mechanics. By embedding physical laws and boundary conditions directly into the loss function, PINNs encourage solutions that remain smooth, stable, and physically consistent across the domain.[4, 5, 6] This physics-guided paradigm has gained considerable attention for integrating prior scientific knowledge into neural network training and for generating solutions that respect governing equations.[1, 7, 8]

Alongside these developments, an unupervised learning strategy is employed for the numerical simulation of the hydrogen atom.[9, 7] Rather than depending solely on physics-based constraints during optimization, the neural network is trained using Physics equations embedded in loss function.[10, 11, **?**] This data-guided formulation enables stable learning of radial solutions and captures the essential structure of hydrogenic states.[12, 13] The predicted wavefunctions agree well with theoretical expectations, exhibiting correct nodal patterns and physically meaningful asymptotic decay. [1]Such an unsupervised framework improves accuracy, maintains physical consistency, and reduces numerical errors.[14, 15] This makes it a useful and efficient method for studying quantum eigenvalue problems like the hydrogen atom.[**?**, 16, 7]

2 Modeling of the Physical System

In this section, we elaborate the four stages of the modeling theory as suggested by Hestenes,15 viz., Description, Formulation, Ramification, and Validation, to clearly delineate various aspects of the model.[3]

2.1 Description Stage

This stage comprises three components:

2.1.1 Object Description

1. **Object Type:** Hydrogen atom , the simplest constitutent of matter .
2. **Object Composition:** An electron and a proton.
3. **Object Variables:** The electron has a mass $m_e = 0.5109 \times 10^6\,\mathrm{eV}/c^2$. The proton mass is approximately 1837 times larger than the electron mass, with $m_p = 938.272 \times 10^6\,\mathrm{eV}/c^2$. Both particles carry electric charges of equal magnitude, one elementary charge, but with opposite signs.

2.1.2 Interaction Description

1. **Type of Interaction:** Electromagnetic interaction between the proton and electron [3, 10].

2. **Agents of Interaction:**

   (i) Proton as Coulomb (Attractive) source

   (ii) Range of interaction ; typically extends infinitely long [3]

   Interaction Variables: The behaviour of the hydrogen atom depends on a few fundamental quantities. The electron–proton distance r determines how the interaction varies in space. The Coulomb factor $e^2/(4\pi\epsilon_0)$ sets the strength of the electric attraction between the two particles.

2.1.3 Process Description

(a) **Reference System:**

The hydrogen atom can be rigorously reduced to an effective single- particle problem by introducing the reduced mass of the electron-proton system:

$$\mu = \frac{m_p m_e}{m_p + m_e} \approx m_e, \tag{1}$$

where the approximation arises from $m_p \gg m_e$. The electron can thus be treated as a particle moving relative to the center-of-mass of the system.

As the inter-particle interaction depends solely on the radial separation, the system possesses central symmetry. Consequently, **spherical polar coordinates (SPC)** constitute the most appropriate reference frame for its analysis.[9, 3]

(b) **State Variables:**

The wavefunction $\psi(r,t)$ completely specifies the quantum state of the system, with all physical observables derivable from it through appropriate operators.

2.2 Formulation Stage

At this stage, we first discuss the dynamical laws that govern the motion of the proton and then specify the interaction laws in their mathematical form. The initial and boundary conditions, if any, are then specified to complete the formulation of the mathematical model representing the physical system.

2.2.1 Interaction Laws

The hydrogen atom is governed primarily by the Coulomb attraction between the electron and the proton, which provides the central potential responsible for binding the system, expressed as $V(r) = -\dfrac{e^2}{4\pi\epsilon_0 r}$. Beyond this dominant interaction, additional effects arise from relativistic and quantum electrodynamical contributions. [17].

2.2.2 Dynamical Laws

The time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t) \tag{2}$$

is transformed into the time-independent Schrödinger equation (TISE) using the

method of separation of variables technique ,

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r})\, T(t)$$

, one obtains

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\,\psi(\mathbf{r}). \quad (3)$$

The non-relativistic radial Schrödinger equation is:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right] u_{nl}(r) = E_{nl}u_{nl}(r). \quad (4)$$

2.2.3 Boundary Conditions

For a physically acceptable solution of the hydrogen atom, the radial wavefunction must satisfy well-defined boundary conditions. The wavefunction and its derivative are required to exist and remain continuous for all values of r, ensuring a finite and physically meaningful solution. Dirichlet boundary conditions are imposed such that $u_{nl}(0) = 0$ and $u_{nl}(L) = 0$, which reflect the regular behaviour at the origin and the decay of the wavefunction at large distances. Additionally, the wavefunction must be normalisable so that the total probability of finding the electron in space remains finite.

2.3 Ramification Stage

An **unsupervised-learning-based Physics-Informed Neural Network (PINN)** is employed to numerically obtain hydrogenic radial wavefunctions at fixed energies while satisfying physical boundary conditions.

2.3.1 PINNs with Boundary, Normalization, and Orthogonality Constraints

A **Physics-Informed Neural Network** is employed to obtain the solution. The network takes the radial coordinate r as input and outputs the corresponding wavefunction $\psi(r)$.

The total loss function of the PINN is defined as:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{physics}} + \mathcal{L}_{\text{BC}} + \mathcal{L}_{\text{norm}} + \mathcal{L}_{\text{orth}}, \quad (5)$$

where:

(i) **Physics loss ($\mathcal{L}_{\text{physics}}$)**: Ensures the Schrödinger equation with is satisfied:

$$\mathcal{L}_{\text{physics}} = \frac{1}{N_r}\sum_{i=1}^{N_r}\left|\hat{H}\psi(r_i) - E\psi(r_i)\right|^2 \quad (6)$$

(ii) **Boundary condition loss ($\mathcal{L}_{\text{BC}}$)**: Enforces $\psi(0) = 0$ and $\psi(L) = 0$.

(iii) **Normalization loss ($\mathcal{L}_{\text{norm}}$)**: Ensures

$$\int_0^L |\psi(r)|^2\, dr = 1 \quad (7)$$

(iv) **Orthogonality loss ($\mathcal{L}_{\text{orth}}$)**: Ensures orthogonality of different eigenstates:

$$\int_0^L \psi_m(r)\,\psi_n(r)\, dr = 0 \quad (m \neq n) \quad (8)$$

2.3.2 Optimization Workflow

The overall workflow for the ramification stage is as follows:

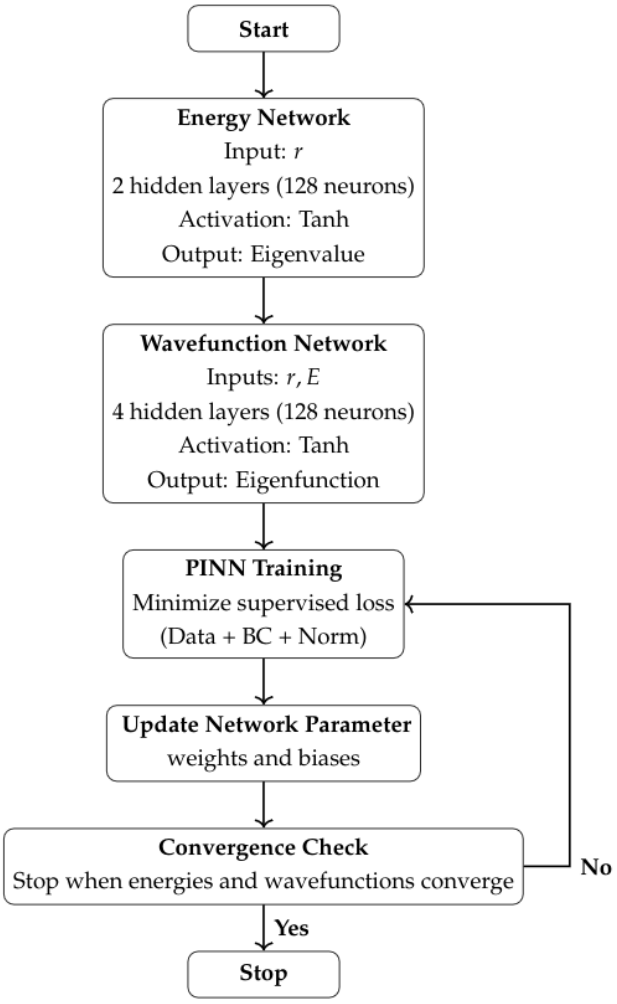

Figure 1: Optimization workflow.

2.4 Validation Stage

(i) Comparison can be made between theoretical and numerically Obtained energy eigenvalues and eigen functions from our simulation .

(ii) Finally, the energy level sequence that we obtain must also match with that expected from experimental considerations, so as to validate the deduced configurations.

3 Numerical Simulation

3.1 Choice of Units

All simulations are performed in atomic units ($\hbar = m_e = e = 1$), in which energies are measured in Hartree and lengths in Bohr radii. In this unit system, the electron–proton interaction reduces to the standard Coulomb form

$$V(r) = -\frac{1}{r},$$

and the exact nonrelativistic ground-state energy

$$E_{1s} = -0.5\,\text{Ha}$$

serves as a precise reference for evaluating numerical convergence.[3]

For higher orbital angular momentum, the effective potential is typically written as

$$V_{\text{eff}}(r) = -\frac{1}{r} + \frac{l(l+1)}{2r^2}, \tag{9}$$

highlighting its explicit l-dependence through the centrifugal term [3].

In the literature, Lamb-shift–related QED corrections are commonly treated by retaining the fine-structure constant α explicitly and extending the Hamiltonian with terms such as vacuum-polarization, Darwin, and self-energy contributions to enable stable evaluation of radiative level shifts.

3.2 Region of Interest

The radial coordinate is confined to a finite domain $r \in [0, R_{\max}]$, where $R_{\max}$ is chosen sufficiently large to ensure that bound-state wavefunctions decay to numerically negligible values at the boundary. For Physics-Informed Neural Network method , typical choices such as $R_{\max} = 20$–45 Bohr sufficient to produce hydrogenic energies upto atleast n=2 with accuracy . For principal quantum numbers $n \geq 3$, the radial cutoff is typically chosen in the range $R_{\max} = 80$–100 Bohr.[3]

3.3 Choice of Numerical technique

Accurate modelling of the hydrogen atom requires a method that remains stable near the Coulomb singularity and reliable for excited states. Conventional approaches such as finite-difference schemes and standalone basis expansions often demand fine discretization and careful boundary treatment. These requirements increase computational cost and can introduce numerical errors[18]. To address these issues, Physics-Informed Neural Networks (PINNs) using unsupervised learning was adopted. PINNs incorporate the governing equation and boundary conditions directly into the training process, reducing dependence on dense meshes[1]. This combination improves numerical stability and overall accuracy. It also produces smooth and physically consistent wavefunctions. This approach balances efficiency with precision. As a result, it serves as a practical alternative to traditional single-method techniques.

4 Results an Discussion

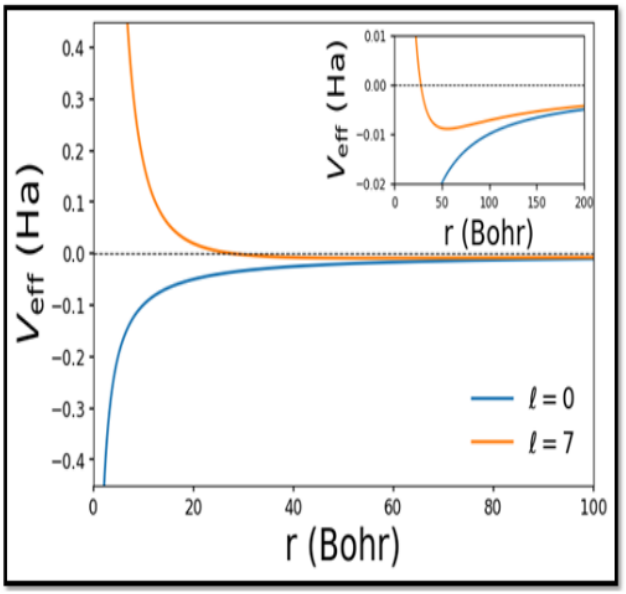

Figure 2: Effective Potential of Hydrogen atom for $l = 0$ and $l = 7$

Acknowledgments

A. Awasthi acknowledges the financial support provided by the DST, Govt. of India, through Grant No. DST-INSPIRE fellowship/2020/IF200538.

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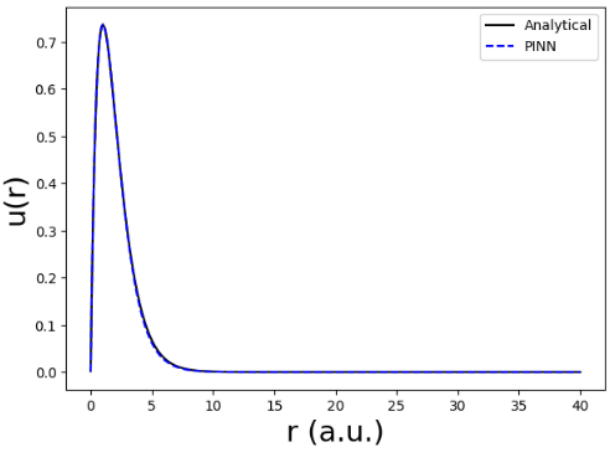

Figure 3: Comparison of analytical and PINN-predicted radial wavefunctions for the 1s state ($n = 1, l = 0$), achieving an accuracy of 2.576×10^{-4}.

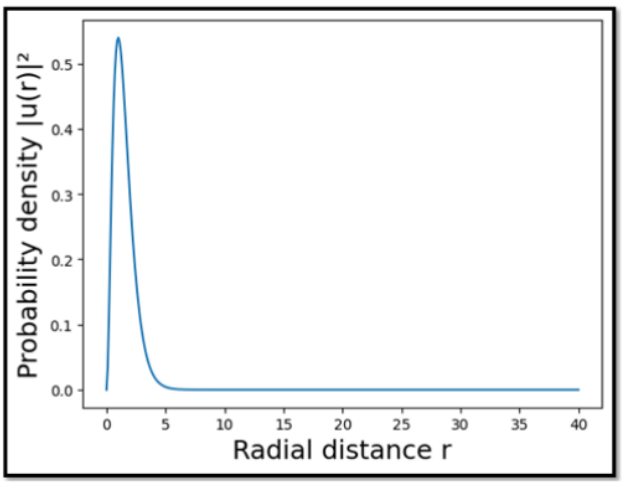

Figure 4: PINN-predicted Probability Density for the 1s state ($n = 1, l = 0$).

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