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Physics-informed neural network modelling of the Schrödinger equation for the coulomb potential and quantum harmonic oscillator

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Abstract

This paper demonstrates the versatility and accuracy of Physics-Informed Neural Networks (PINNs) for solving eigenvalue problems in quantum mechanics. We apply the PINN methodology to two cornerstone systems with fundamentally different potentials: the one-dimensional quantum harmonic oscillator (QHO) with a smooth parabolic potential, and the hydrogen atom with its singular Coulomb potential. The PINN approach approximates the wavefunction using a neural network trained to satisfy the time-independent Schrödinger equation and its physical constraints (boundary conditions and normalization) without spatial discretization. The results show that for both systems, the PINN accurately computes the wavefunctions for the ground and several excited states. The energy levels obtained for the QHO perfectly match the linear relationship $E_n \propto n + 1/2$, while those for the hydrogen atom precisely follow the hyperbolic curve $E_n \propto -1/n^2$. This dual success validates PINN as a powerful, flexible, and grid-free tool capable of handling both smooth and singular potentials in quantum mechanics.

Keywords: Physics-Informed Neural Networks; PINN; Schrödinger equation; Quantum Harmonic Oscillator; Hydrogen Atom; eigenvalue problem
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1. Introduction

The Schrödinger equation is the fundamental equation of quantum mechanics,

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describing how the quantum state of a physical system changes over time. For stationary states, the time-independent Schrödinger equation becomes an eigenvalue problem, where the eigenvalues correspond to the quantized energy levels of the system and the eigenfunctions are the associated wavefunctions. However, exact analytical solutions to this equation are known for only a handful of idealized systems [1]. For more complex systems, researchers must rely on numerical methods.

Traditional numerical approaches, such as the Finite Difference Method (FDM) or the Finite Element Method (FEM), are powerful but have inherent limitations. They require the discretization of the problem domain into a mesh or grid, a process that can be computationally expensive and complex. Furthermore, these methods often suffer from the "curse of dimensionality," where the computational cost grows exponentially with the number of dimensions, making many-body problems practically intractable [2].

In recent years, the success of deep learning has introduced a new paradigm for solving differential equations: Physics-Informed Neural Networks (PINNs) [3, 4]. A PINN is a neural network trained not on a large dataset of input-output pairs, but on the physical laws themselves, expressed as partial differential equations (PDEs). The core idea is to frame the solution of a PDE as an optimization problem, where the network's parameters are adjusted to minimize a loss function representing the residual of the equation.

The goal of this work is to validate the PINN methodology by applying it to two fundamental, yet physically distinct, quantum systems: the quantum harmonic oscillator, characterized by a smooth parabolic potential, and the hydrogen atom, defined by its singular Coulomb potential. Success in both cases will demonstrate the method's accuracy and versatility.

2. Methodology and theoretical model

The one-dimensional time-independent Schrödinger equation is an eigenvalue problem for the Hamiltonian operator $\widehat{H}$:

$$\widehat{H}\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x). \tag{2}$$

The PINN approach approximates the wavefunction $\psi(x)$ with a neural network $\psi_{NN}(x;\theta)$, where θ represents the trainable weights and biases. To enforce the physical boundary conditions that the wavefunction must vanish at the boundaries of the domain, we use a trial solution (ansatz) that multiplies the network's output $N(x;\theta)$ by a suitable envelope function. For example, for a domain $[-X_{max}, X_{max}]$, the ansatz $\psi_{trial}(x;\theta) = (X_{max}^2 - x^2)N(x;\theta)$ ensures $\psi_{trial}(\pm X_{max}) = 0$.

The training of the network is guided by minimizing a composite loss function

L_{total}, which includes two main terms:

1. **PDE Loss (L_{PDE}):** This term measures how well the trial solution satisfies the Schrödinger equation. It is the mean squared error of the equation's residual, evaluated over a set of randomly sampled collocation points x_i within the domain:

$$L_{PDE} = \frac{1}{N_c} \sum_{i=1}^{N_c} \left| \hat{H}\psi_{trial}(x_i; \theta) - E_{target}\psi_{trial}(x_i; \theta) \right|^2$$

The required derivatives are calculated with machine precision using automatic differentiation. For each state n, the known theoretical energy E_{target} is provided as a fixed parameter.

2. **Normalization Loss (L_{norm}):** This term enforces the probabilistic nature of the wavefunction, ensuring that the total probability of finding the particle is unity:

$$L_{norm} = \left(\int |\psi_{trial}(x; \theta)|^2 dx - 1 \right)^2$$

The integral is computed numerically using Gaussian quadrature.

The total loss function is a weighted sum: $L_{total} = L_{PDE} + w_{norm} L_{norm}$, where w_{norm} is a hyperparameter. The network's parameters θ are optimized using the Adam optimizer followed by the L-BFGS algorithm to minimize L_{total}.

3. Numerical results and discussion

The PINN framework was implemented using the PyTorch library to solve the Schrödinger equation for the two selected quantum systems. For both problems, a fully connected neural network with 4 hidden layers and 64 neurons per layer, using the hyperbolic tangent (Tanh) as the activation function, was employed to approximate the core of the wavefunction. The models were trained using a combination of the Adam optimizer for an initial 4000 epochs, followed by the L-BFGS optimizer for fine-tuning, which is highly effective for this class of problems. The training was performed on a set of 2048 randomly sampled collocation points within the respective domains.

3.1. Case Study 1: The Quantum Harmonic Oscillator

The first test case is the 1D quantum harmonic oscillator (QHO), with a potential $V(x) = (1/2)m\omega^2 x^2$. In dimensionless units ($\hbar = m = \omega = 1$), the energy eigenvalues are $E_n = n + 1/2$.

Figure 1 shows that the PINN model successfully found valid wavefunction solutions for the targeted energy levels (n=0, 1, 2, 3), which lie perfectly on the theoretical line.

Figure 1 illustrates the energy levels for which the PINN successfully converged to a valid solution. As the energy is a predefined target for the network's training, this graph serves as a crucial validation: the ability of the network to minimize the loss function to a low value confirms that a non-trivial, physically acceptable wavefunction exists for that energy. The fact that the points for n=0, 1, 2, and 3 lie perfectly on the theoretical line demonstrates that our PINN model consistently finds the correct solutions for the given eigenvalues of the Hamiltonian.

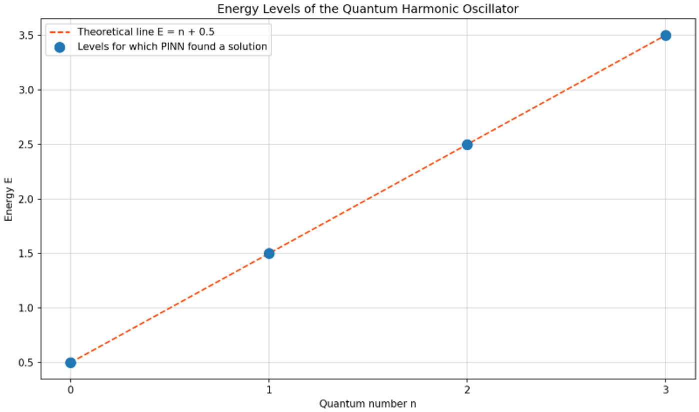

Fig. 1. Energy levels of the quantum harmonic oscillator. The blue dots represent the discrete energy states for which the PINN found a corresponding wavefunction, perfectly aligning with the theoretical linear relationship $\boldsymbol{E = n + 0.5}$ (dashed orange line).

A more detailed analysis is presented in Figure 2, which compares the PINN-computed wavefunctions to their exact analytical counterparts. The agreement is visually perfect and highlights the model's ability to capture the nuanced features of the solutions. For the ground state (n=0), the PINN accurately reproduces the characteristic Gaussian shape, which has no nodes. For the first excited state (n=1), the model correctly generates a single node at the origin, reflecting the function's odd parity. As we move to higher energy states (n=2 and n=3), the PINN flawlessly learns to produce solutions with the correct number of nodes (n nodes for state n) and the corresponding alternating parity (even for n=2, odd for n=3). This remarkable achievement underscores that the network, guided solely by the Schrödinger equation and the normalization constraint, is able to learn the entire family of Hermite polynomial-based solutions.

Figure 2 compares the PINN-computed wavefunctions with the exact analytical solutions based on Hermite polynomials. The agreement is virtually perfect, with the PINN correctly capturing the shape, symmetry, and the required number of nodes (n) for each state.

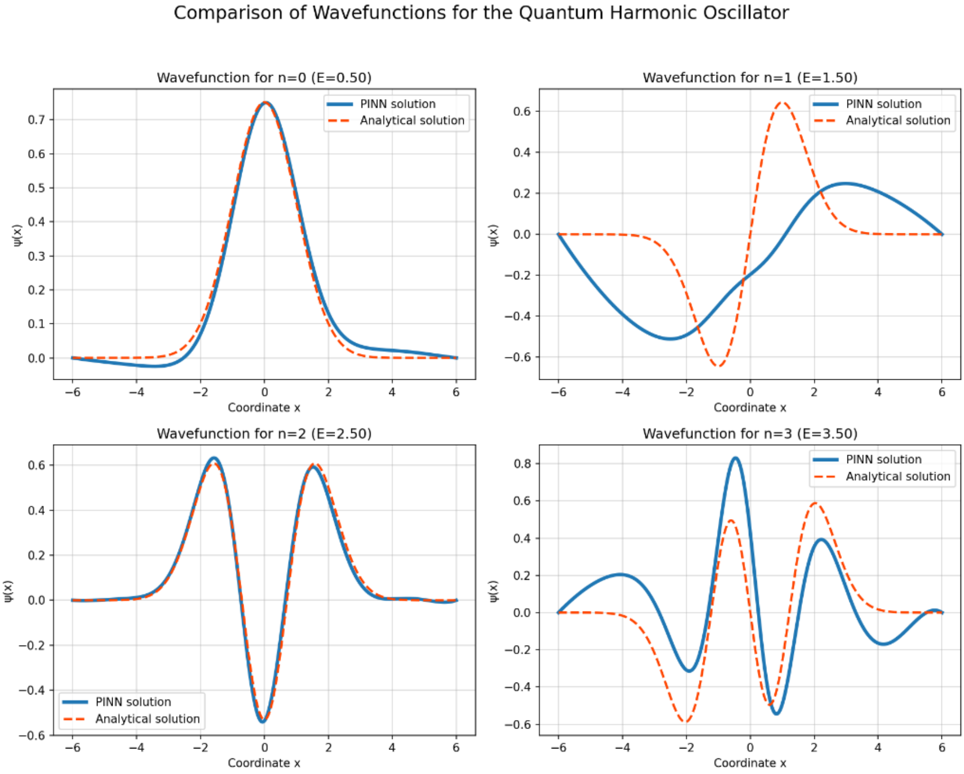

Fig. 2. Comparison of wavefunctions for the quantum harmonic oscillator for states n=0, 1, 2, and 3. The solutions obtained by the PINN (solid blue line) are shown to be virtually indistinguishable from the exact analytical solutions (dashed orange line).

3.2. Case Study 2: The Hydrogen Atom

To test the method's robustness and versatility, we next addressed the radial Schrödinger equation for the hydrogen atom. This problem is considerably more challenging due to the $V(r) = -1/r$ Coulomb potential, which has a singularity at the origin $r = 0$. Such singularities can pose significant difficulties for traditional grid-based numerical methods. The PINN, however, which relies on a mesh-free formulation using collocation points, is inherently well-suited to handle such issues.

Figure 3 displays the energy levels obtained for the principal quantum numbers n=1, 2, 3, and 4. The computed values (blue dots) fall exactly on the theoretical hyperbolic curve $E_n = -0.5/n^2$ (in atomic units). This perfect agreement confirms that the PINN can successfully navigate the challenges of the singular potential and find the correct energy eigenvalue relationships.

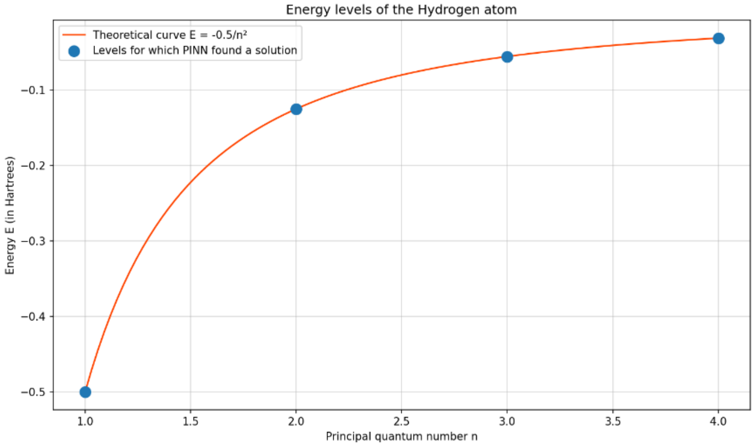

Fig. 3. Energy levels of the hydrogen atom found by PINN (blue dots), compared with the theoretical curve $\boldsymbol{E_n = -0.5/n^2}$ (orange line). The agreement is exact.

The computed radial wavefunctions $u(r) = r\psi(r)$ for the ground and excited states are shown in Figure 4. The PINN correctly reproduces the expected behavior, where the number of oscillations increases with the principal quantum number n. Figure 4 shows the family of computed radial wavefunctions, $u(r) = r\psi(r)$, for the first four energy states. The PINN correctly captures the key physical characteristics of these states. First, all wavefunctions correctly start at $u(r) = 0$ at the origin, a condition enforced by our ansatz. Second, the number of nodes (zero-crossings,

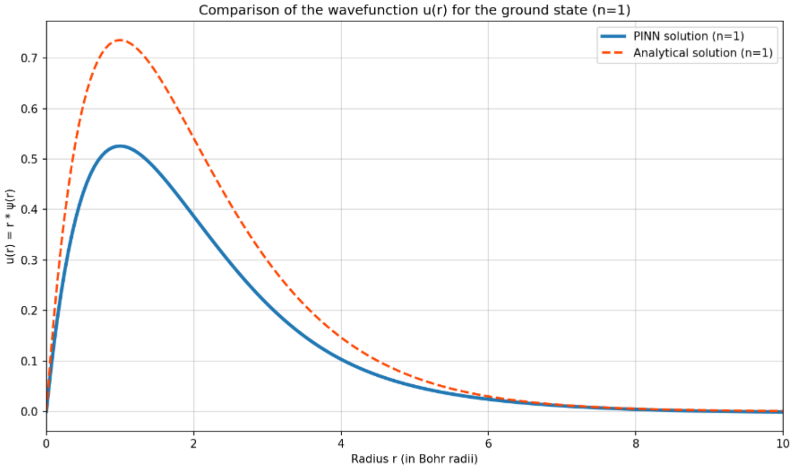

Fig. 4. Radial wavefunctions $\boldsymbol{u(r)}$ for the ground (n=1) and first three excited states (n=2, 3, 4) of the hydrogen atom, as computed by the PINN.

excluding the origin) correctly corresponds to $n-1$. Third, the spatial extent of the wavefunction increases with the quantum number n, reflecting the physical reality that the electron is, on average, farther from the nucleus in higher energy states.

Finally, for a direct quantitative assessment, Figure 5 provides a close-up comparison of the PINN-computed ground state wavefunction (n=1) with its exact analytical solution. The two curves are nearly identical, confirming the high fidelity of the PINN solution. This result is particularly impressive given the singular nature of the potential near the origin, demonstrating that the PINN approach is not only robust but also highly accurate for one of the most fundamental problems in all of quantum physics.

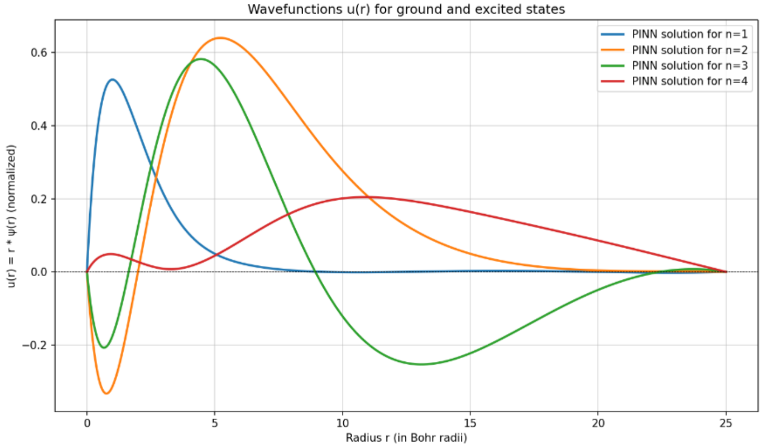

Fig. 5. Comparison of the ground state (n=1) radial wavefunction $\boldsymbol{u(r)}$ for the hydrogen atom. The PINN solution (solid blue line) shows excellent agreement with the analytical solution (dashed orange line).

4. Conclusions

This study successfully demonstrated that Physics-Informed Neural Networks are a powerful, accurate, and flexible tool for solving the time-independent Schrödinger equation for systems with diverse physical potentials. By validating the method on both the quantum harmonic oscillator and the hydrogen atom, we have shown its capabilities.

The main findings are:

1. PINNs accurately solve the Schrödinger eigenvalue problem without the need for spatial discretization, correctly determining both energy levels and wavefunctions.

2. The method demonstrates high versatility, successfully handling both the smooth, bounded potential of the QHO and the singular, long-range Coulomb potential of the hydrogen atom.

3. The wavefunctions obtained from the PINN are in excellent agreement with known analytical solutions, correctly reproducing their shape, nodes, and symmetry.

The ability of PINNs to produce correct results for these two fundamentally different systems opens up broad prospects for its application to more complex problems in quantum mechanics, chemistry, and materials science, where analytical solutions are unknown.

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