Solving Time-Independent Schrodinger Equation for a Double-Well Potential in Quantum Plasma Systems using Physics-Informed Neural Networks

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Abstract

The time-independent Schrödinger equation plays a fundamental role in describing quantum tunneling phenomena in systems governed by double-well potentials, which arise naturally as effective potentials in quantum plasma environments due to external fields and confinement effects. In this work, we employ Physics-Informed Neural Networks (PINNs) to solve one-dimensional Schrödinger equation for a symmetric double-well potential and obtain accurate ground and low-lying excited state solutions. The fully connected neural networks is used to obtain the wavefunctions, while the energy eigenvalues are treated as trainable parameters and determined through the minimization of a composite loss function enforcing the governing differential equation, boundary conditions, normalization, and orthogonality constraints. Even and odd-parity network architectures are used to directly capture symmetric and antisymmetric eigenstates. The PINNs results are validated against finite-difference matrix diagonalization technique, showing good agreement for the lowest energy levels and correctly reproducing the near-degeneracy caused by quantum tunneling between the wells. These results demonstrate that PINNs provide a flexible, accurate, and mesh-free alternative to conventional numerical techniques, making them well suited for modeling tunneling phenomena and effective quantum potentials in plasma-related systems.

1 Introduction

The time-independent Schrödinger equation plays a central role in quantum mechanics, governing the bound-state structure and tunneling dynamics of microscopic systems [1]. Among the class of exactly nontrivial quantum potentials, the symmetric double-well potential [2] occupies a distinguished

position due to its relevance in molecular inversion phenomena [3], quantum tunneling [4, 5], energy-level splitting [6] and plasma-modified quantum confinement [7]. In plasma environments, screening effects and collective interactions substantially modify the effective potential landscape, leading to rich quantum behavior that demands accurate and flexible computational approaches [8].

Traditionally, the Schrödinger equation for double-well systems has been solved using numerical techniques such as finite difference schemes, matrix mechanics [2], spectral methods [9], and shooting algorithms [10]. While these methods are well established and reliable, they often require dense spatial grids, careful treatment of boundary conditions, and repeated eigenvalue solvers to extract multiple states. Moreover, extending these approaches to plasma-modified or parameter-dependent potentials significantly increases computational cost and complexity [7].

In recent years, Physics-Informed Neural Networks (PINNs) have emerged as a powerful mesh-free framework for solving differential equations by embedding the governing physical laws directly into the training process of neural networks [11]. Unlike purely data-driven models, PINNs incorporate the Schrödinger equation as a soft constraint through automatic differentiation, enabling the simultaneous learning of wavefunctions and energy eigenvalues without discretizing the spatial domain [12]. This paradigm offers key advantages, including continuous representations of solutions, natural enforcement of physical constraints, and scalability to complex or parameterized potentials.

In this work, we employ the PINNs framework to solve the one-dimensional time-independent Schrödinger equation for a symmetric double-well potential relevant to quantum plasma systems. By explicitly incorporating parity symmetry, normalization, and orthogonality conditions into the loss function, the proposed approach accurately captures tunneling-induced near-degeneracy and reproduces low-lying energy eigenstates. The results demonstrate that PINNs provide an efficient and flexible alternative to traditional numerical solvers, particularly suited for plasma-modified quantum systems where adaptability and physical consistency are essential.

2 Methodology

The present study is based on the time-independent Schrödinger equation describing a quantum particle moving in an effective one-dimensional potential [13],

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \quad (1)$$

where $\psi(x)$ is the stationary wavefunction, E denotes the energy eigenvalue, and $V(x)$ represents the external potential [1]. In order to reduce the number of free physical parameters and improve numerical stability,

the equation is expressed in dimensionless form by adopting atomic units $\hbar = 1$ and $m = 1$. This leads to

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \quad (2)$$

Choice of Potential

To model tunneling and level splitting phenomena relevant to quantum plasma systems, we consider a symmetric double-well potential of the form [14]

$$V(x) = (ax^2 - b^2)^2 \quad (3)$$

where the parameters a and b control the curvature of the wells and the barrier height, respectively. This quartic form naturally produces two equivalent minima separated by a finite barrier and is widely used to study tunneling-induced near-degeneracy in bound states [15]. In the present work, the parameters are chosen as $a = 1$ and $b = 1.5$, ensuring well-separated minima and a finite tunneling probability for low-lying states.

Physics-Informed Neural Networks (PINNs) Framework

Within the Physics-Informed Neural Network (PINNs) framework [16], the wavefunction $\psi(x)$ is approximated by a fully connected neural network $\mathcal{N}(x;\theta)$ [17], where θ denotes the trainable parameters. Unlike conventional numerical solvers, the energy eigenvalues are treated as independent trainable parameters and learned simultaneously with the wavefunctions.

To explicitly enforce the parity symmetry of the double-well potential, separate neural architectures are employed for even and odd eigenstates [18], defined as

$$\begin{aligned} \psi_{\text{even}}(x) &= \mathcal{N}(x) + \mathcal{N}(-x), \\ \psi_{\text{odd}}(x) &= \mathcal{N}(x) - \mathcal{N}(-x). \end{aligned} \quad (4)$$

This construction ensures that the learned eigenfunctions possess the correct symmetry properties without additional constraints.

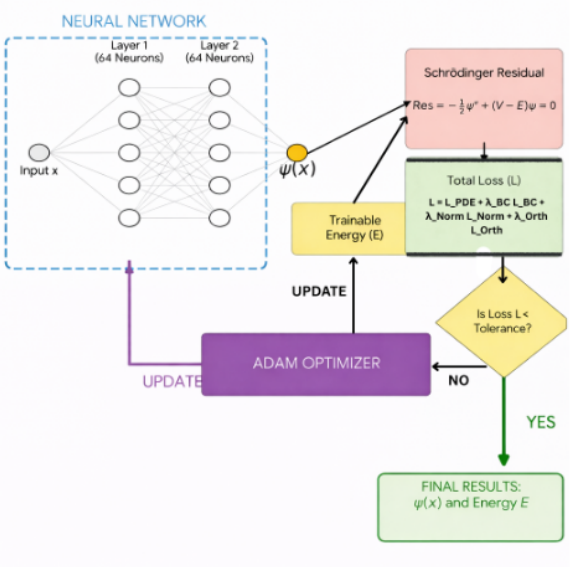

Figure 1: Workflow of the Physics-Informed Neural Network (PINNs) for solving the one-dimensional Schrödinger equation.The neural network approximates the wavefunction $\psi(x)$ while the energy E is treated as a trainable parameter, optimized using the ADAM optimizer by minimizing the total loss.

Loss Function and Training

The physics-informed neural network (PINNs) [19] is trained by minimizing a composite loss function that enforces the governing Schrödinger equation along with the physical constraints of the quantum system. The total loss is defined as

$$\mathcal{L} = \mathcal{L}_{\text{PDE}} + \lambda_{\text{BC}}\,\mathcal{L}_{\text{BC}} + \lambda_{\text{Norm}}\,\mathcal{L}_{\text{Norm}} + \lambda_{\text{Orth}}\,\mathcal{L}_{\text{Orth}}, \tag{5}$$

where the physics loss term enforces the time-independent Schrödinger equation and is given by

$$r_n(x) = -\frac{1}{2}\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_n(x) - E_n\psi_n(x) \tag{6}$$

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_c}\sum_{n=0}^{N_s-1}\sum_{i=1}^{N_c} |r_n(x_i)|^2 \tag{7}$$

The boundary condition loss ensures the wavefunctions vanish at the domain boundaries and is expressed as

$$\mathcal{L}_{\text{BC}} = \frac{1}{N_s}\sum_{n=0}^{N_s-1}\left(|\psi_n(-L)|^2 + |\psi_n(L)|^2\right). \tag{8}$$

To guarantee physical admissibility, the normalization loss enforces unit norm of each eigenstate,

$$\mathcal{L}_{\text{Norm}} = \frac{1}{N_s}\sum_{n=0}^{N_s-1}\left|\int_{-L}^{L}|\psi_n(x)|^2\,dx - 1\right|^2, \tag{9}$$

while the orthogonality loss ensures mutual orthogonality between distinct eigenfunctions,

$$\mathcal{L}_{\text{Orth}} = \frac{1}{N_s(N_s-1)}\sum_{\substack{m,n=0\\ m\neq n}}^{N_s-1}\left|\int_{-L}^{L}\psi_m(x)\psi_n(x)\,dx\right|^2. \tag{10}$$

The weighting parameters λ_{BC}, λ_{Norm}, and λ_{Orth} control the relative importance of each constraint during training. Equal weights $\lambda_{\text{BC}} = \lambda_{\text{Norm}} = \lambda_{\text{Orth}} = 10$ are used throughout the training.

The neural network consists of two hidden layers with 64 neurons each and hyperbolic tangent (*tanh*) activation functions. Training is performed using the Adam optimizer [20] with a learning rate of 10^{-3} over 10^4 epochs. Uniform collocation points are employed over the spatial domain, and automatic differentiation [21] is used to compute the second-order spatial derivatives.

3 Results and Discussion

The Physics-Informed Neural Network (PINNs) framework was applied to solve the time-independent Schrödinger equation for a symmetric double-well potential [22]. The model employed two hidden layers with 64 neurons each, using smooth activation functions to ensure differentiability of the wavefunction. Equal weights were assigned to the normalization, orthogonality, and boundary condition loss terms ($\lambda_{\text{Norm}} = \lambda_{\text{Orth}} = \lambda_{\text{BC}} = 10$), and the network was trained for 10^4 epochs for the three lowest eigenstates ($n = 0, 1, 2$).

The convergence behaviour of the energy

eigenvalues during training indicates stable and systematic learning. As training progresses, the total loss reduces by nearly three orders of magnitude, reflecting the simultaneous enforcement of the Schrödinger equation, boundary conditions, normalization, and orthogonality constraints. The final PINN-predicted energies are summarized below:

Table 1: Comparison of FD and PINN energy eigenvalues.

State	$E_{\mathrm{FD}}(hartree)$	$E_{\mathrm{PINN}}(hartree)$
$n = 0$	1.9705	1.9709
$n = 1$	2.0123	2.1500
$n = 2$	4.9079	4.9087

The ground state ($n = 0$) and second excited state ($n = 2$) energies obtained via PINNs are in excellent agreement with the finite difference (FD) results, with relative deviations below the percent level. The first excited state ($n = 1$) shows a comparatively larger deviation, which can be attributed to the increased sensitivity of higher-energy states to orthogonality enforcement and loss balancing during training. The Schrödinger equation is solved in dimensionless natural units by setting $\hbar = 1$ and $m = 1$, so the computed eigenvalues are energies in natural units that is the hartree (Ha).

The predicted wavefunctions using PINNs is compared with those obtained using the finite difference (FD) method as shown in figure 2. The excellent agreement in both amplitude and spatial structure demonstrates that the PINNs accurately captures

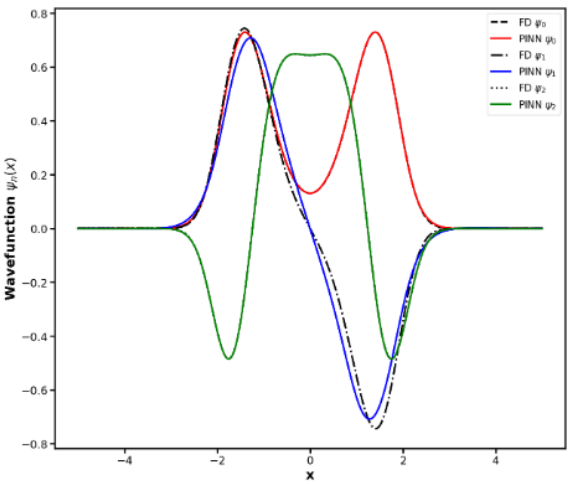

Figure 2: Comparison of eigenfunctions obtained using the Physics-Informed Neural Network (PINNs) and the Finite Difference (FD) method for the first three quantum states of the symmetric double-well potential. Solid colored curves represent PINNs solutions, while black dashed, dash-dotted, and dotted curves correspond to FD solutions for the ground, first excited, and second excited states respectively.

the nodal structure and tunnelling behaviour across the potential barrier. In particular, the smooth penetration of the wavefunctions into the classically forbidden region clearly illustrates quantum tunnelling, a hallmark feature of the double-well system.

The PINNs predicted low-lying eigenstates superimposed on the symmetric double-well potential is illustrated in figure 3. The wavefunctions are vertically shifted by their corresponding energy eigenvalues for clarity. The ground state ψ_0 exhibits even par-

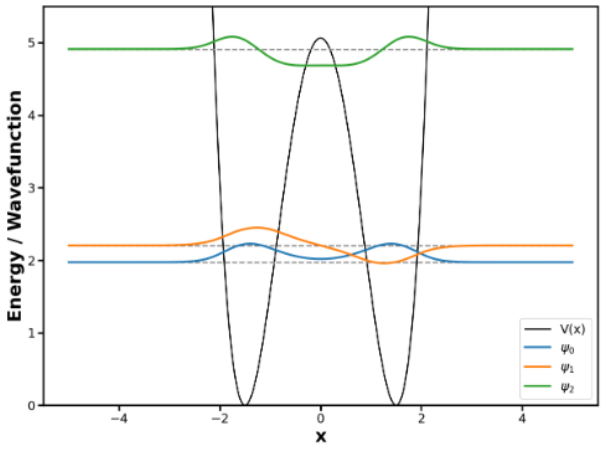

Figure 3: PINNs-computed eigenstates superposed on the symmetric double-well potential. The nonzero amplitude of the wavefunctions within the barrier region confirms quantum tunneling and results in a small energy splitting between the lowest two states.

ity with a finite amplitude at the center of the barrier, indicating strong tunnelling between the two wells [23]. The first excited state ψ_1 is antisymmetric, with a node at the center, as required by parity symmetry, while still displaying appreciable penetration into the classically forbidden region. The second excited state ψ_2 shows reduced tunnelling and increased localization within individual wells due to its higher energy.

The small energy separation between ψ_0 and ψ_1 reflects the lifting of degeneracy caused by quantum tunnelling through the finite potential barrier. This splitting would vanish in the limit of an infinitely high barrier, corresponding to fully localized states. The smooth and physically consistent behaviour of all eigenstates demonstrates the ability of the PINN framework to capture subtle quantum effects such as parity symmetry, tunnelling, and near-degeneracy without explicit basis construction or grid discretization.

An important physical feature of the symmetric double-well potential is the near-degeneracy of the ground and first excited states [22]. In the limit of an infinitely high barrier, these states would be exactly degenerate, corresponding to states localized in the left and right wells. However, due to finite barrier height, tunnelling lifts this degeneracy, resulting in a small energy splitting between the symmetric (even-parity) ground state and the antisymmetric (odd-parity) first excited state [24]. The PINN framework successfully captures this splitting, confirming its ability to resolve subtle quantum effects arising from wavefunction overlap across the barrier. This agreement also validates the parity-constrained network design used for the low-lying eigenstates.

Overall, these results demonstrate that PINNs provide a robust and flexible alternative to traditional numerical techniques [2, 10] such as finite difference and matrix mechanics methods. Unlike grid-based approaches, PINNs yield smooth, analytical representations of eigenfunctions, naturally incorporate physical constraints, and scale efficiently to higher-dimensional and more complex quantum systems.

4 Conclusion:

PINNs accurately solved the double-well Schrödinger problem using physics-based loss constraints and no spatial grid. The method reproduced eigenstates, tunneling behavior, and energy splitting in good agreement with finite-difference results, showing that PINNs are an efficient and flexible tool for quantum potential problems. However the present formulation assumes a one-dimensional, time-independent system and neglects explicit many-body and relativistic effects.

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