Solving the Time-Dependent Schrödinger Equation for a Harmonic Oscillator and Extracting the Bohm Quantum Potential Using PINNs

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Submitted on 05-Feb-2026

Abstract

Physics-Informed Neural Networks (PINNs) offer an effective framework for solving partial differential equations by incorporating governing physical laws into the learning process. When applied to quantum mechanical differential equations such as the Schrödinger equation, this approach produces smooth wavefunctions suitable for computing both conventional observables and Bohmian quantities. In this work, a PINNs based framework is developed to solve the one-dimensional time-dependent Schrödinger equation for the Quantum Harmonic Oscillator, a fundamental model with broad relevance in quantum and plasma physics. A fully connected neural network is used to represent the real and imaginary parts of the wavefunction, with the Schrödinger equation enforced through the loss function together with appropriate initial and boundary conditions. Automatic differentiation is employed to compute the required derivatives and to extract physical quantities from the learned solution. The method accurately reproduces the ground-state wavefunction and yields a ground-state energy in agreement with the analytical result. The Bohm quantum potential obtained from the network also matches the corresponding analytical expression, demonstrating that the essential spatial structure of the quantum amplitude is well captured. These results demonstrate that PINNs constitute a reliable and conceptually transparent framework for solving the time-dependent Schrödinger equation. Within this differential equation based setting, PINNs also enable systematic exploration of Bohmian aspects of quantum systems, where Bohmian quantities such as the quantum potential provide physical insight into confinement effects and the emergence of effective potentials.

1 Introduction

The time-dependent Schrödinger equation (TDSE) plays a central role in quantum mechanics, governing the dynamical evolution of quantum systems [1]. It governs the evolution of quantum systems within the framework of non-relativistic quantum mechanics. Considering a particle of mass m in an external potential $V(x)$, its dynamics are governed by the one-dimensional time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t), \tag{1}$$

Here, $\psi(x,t)$ represents the system's complex wavefunction, and the probability of locating the particle at position x and time t is given by $|\psi(x,t)|^2$. Once the wavefunction is known, physical observables such as expectation values of position, momentum, and energy can be calculated [2]. The TDSE is required for describing a wide range of quantum phenomena, including wave-packet evolution, quantum tunneling, bound-state dynamics, and interactions with time-dependent external fields [3]. It provides a complete mathematical description of how quantum states change with time and is therefore essential in areas such as atomic and molecular physics, condensed matter physics, quantum optics, and plasma physics [4] . Accurate solutions of the TDSE are necessary for both theoretical investigations and practical applications involving quantum systems.

Only a limited number of idealized potentials admit analytical solutions of the TDSE, among them the free particle [5] , infinite well [6] , and harmonic oscillator [7]. Among these systems, the quantum harmonic oscillator (QHO) is of particular importance due to its wide applicability as an approximation for physical systems near equilibrium and its central role in quantum theory [8] . Analytical solutions of the harmonic oscillator provide closed-form expressions for energy eigenvalues and wavefunctions and serve as reliable reference results. Nevertheless, current research focuses not only on reproducing such solutions but also on developing methodologies that remain effective for systems lacking analytical solutions.

In this context, the QHO serves as an important benchmark problem. Its well-known exact solution allows direct validation of alternative computational approaches, enabling quantitative assessment of accuracy, stability, and physical consistency before extending these methods to more complex or analytically intractable systems.

To treat systems beyond analytical reach, several numerical methods have been developed for solving the TDSE, including finite-difference [9] , spectral and pseudo-spectral schemes [10] , split-operator techniques [11] , and implicit methods such as the Crank Nicolson approach [12] . Although traditional numerical methods have been successfully applied to many quantum

systems, they rely on explicit discretization of space and time using fixed grids. This dependence can increase computational cost, particularly for higher-dimensional problems, and may lead to numerical stability issues or the accumulation of errors during long-time evolution [13] . As a result, there is growing interest in alternative solution approaches that can provide smooth and accurate representations of quantum dynamics while reducing reliance on discretization.

To address these challenges, we employ Physics-Informed Neural Networks (PINNs) [14] , which allow us to approximate the wavefunction continuously over space and time without relying on fixed grids. PINNs incorporate the underlying physical laws, such as the Schrödinger equation, directly into the loss function, ensuring that the neural network solutions respect the governing quantum dynamics while enabling efficient and flexible computation [14] .

Until now, PINNs have been widely used to solve classical and quantum partial differential equations like the time-independent Schrödinger equation (TISE) and other evolution equations, where the neural network is trained to minimize the residuals of the governing equations across the computational domain [14] . By representing the solution as a neural network, we can evaluate it at any point in space and time, avoiding grid-based discretization and achieving a smooth and differentiable approximation. In this work, we extend the PINNs approach to solve the TDSE, enabling direct simulation of quantum dynamics and the evolution of wavefunctions in time, which is crucial for understanding dynamical processes in quantum systems.

Therefore, PINNs are employed in this work to solve the TDSE, using the QHO as a test system. The QHO is chosen not because its solution is unknown, but because it is a simple and well-understood system. Since its exact analytical solution is available, it provides a clear reference that allows new solution approaches to be tested and validated against known results before being extended to more complex quantum systems.

2 Methodology

To model the time evolution of quantum systems, we consider the TDSE. In this work, a one-dimensional QHO is selected as the physical system, where the external potential is well defined and analytically known. For an efficient neural-network-based treatment, the complex-valued wavefunction is decomposed into its real and imaginary parts, allowing the TDSE to be rewritten as a set of coupled real-valued partial differential equations. PINNs are then employed to approximate these components by embedding the governing equations together with the initial and boundary conditions directly into the learning framework.

The time evolution of the quantum system is described using the one-dimensional

TDSE .

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t), \tag{2}$$

where $\psi(x,t)$ is the complex-valued wavefunction and $V(x)$ denotes the external potential.

In this work, we consider the QHO potential,

$$V(x) = \frac{1}{2}m\omega^2x^2, \tag{3}$$

which serves as a simple and well-understood test system with an exact analytical solution.

For numerical convenience and improved training stability, the equation is expressed as dimensionless form by setting $\hbar = 1$ and $m = 1$. The TDSE then reduces to[15]

$$i\frac{\partial\psi(x,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}\omega^2x^2\psi(x,t). \tag{4}$$

Since neural networks operate on real-valued functions, the complex wavefunction is decomposed as

$$\psi(x,t) = u(x,t) + i\,v(x,t), \tag{5}$$

where $u(x,t)$ and $v(x,t)$ are the real and imaginary components, respectively. Substituting this form into the TDSE yields the following coupled system of real-valued equations [13]:

$$\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 v}{\partial x^2} - \frac{1}{2}\omega^2x^2v = 0, \tag{6}$$

$$\frac{\partial v}{\partial t} - \frac{1}{2}\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\omega^2x^2u = 0. \tag{7}$$

The problem is defined within a finite space–time region.

$$x \in [-L, L], \quad t \in [0, T], \tag{8}$$

where L and T are chosen sufficiently large to ensure that boundary effects do not influence the solution within the region of interest. This bounded domain is required for the effective implementation of PINNs, as it enables stable evaluation of the governing equation residuals and consistent enforcement of physical constraints throughout the computational region.

Initial condition is

$$\psi(x,0) = \psi_0(x), \tag{9}$$

which corresponds to

$$u(x,0) = \Re[\psi_0(x)], \quad v(x,0) = \Im[\psi_0(x)]. \tag{10}$$

Homogeneous boundary conditions are imposed as

$$\psi(-L,t) = \psi(L,t) = 0, \tag{11}$$

ensuring confinement and numerical stability.

The Physics-Informed Neural Network approximates the functions $u(x,t)$ and $v(x,t)$ by minimizing a composite loss function defined as

$$\mathcal{L} = \mathcal{L}_{\text{PDE}} + \lambda_{\text{IC}}\,\mathcal{L}_{\text{IC}} + \lambda_{\text{BC}}\,\mathcal{L}_{\text{BC}}, \tag{12}$$

where $\mathcal{L}_{\text{PDE}}$ enforces the TDSE residuals, while $\mathcal{L}_{\text{IC}}$ and $\mathcal{L}_{\text{BC}}$ impose the initial and

boundary conditions.The weighting parameters λ_{IC} and λ_{BC} regulate the relative importance of the initial and boundary condition constraints in the total loss function. Since different loss components may have different scales and convergence behaviors, these weights help balance the optimization process and prevent any single term from dominating the training [16] . Appropriate weighting improves numerical stability and convergence, and ensures that the learned solution simultaneously satisfies the governing differential equation and the prescribed physical conditions.
Within this bounded space-time domain, the solution of the governing equations is approximated using a Physics-Informed Neural Network. The PINNs framework enables the continuous representation of the wavefunction by embedding the TDSE and the associated constraints directly into the learning process.

To solve the governing equations within the defined space-time domain, we employ a framework which enables a mesh free solutions of partial differential equations by embedding physical constraints within the training process. Here, a PINNs is developed to model the real and imaginary parts of the quantum wavefunction over the full space–time domain.

The spatial and temporal coordinates (x, t) are used as inputs to the network, which outputs the real and imaginary components of the wavefunction, $u(x, t)$ and $v(x, t)$.Automatic differentiation is used to compute the required spatial and temporal derivatives, which are then substituted into the governing differential equations to evaluate the physics-based residuals. The total loss function is constructed by combining the differential equation loss with the losses corresponding to the initial and boundary conditions. By minimizing this total loss, the network parameters are optimized such that the predicted solution satisfies both the governing physical laws and the imposed constraints across the entire space-time domain.

2.1 Model Architecture and Training Setup

This section describes the network architecture and training configuration used in the PINNs framework. These choices determine the expressive capacity of the model, numerical stability, and convergence behavior during training.

The PINN employed in this work is implemented as a fully connected feedforward neural network designed to approximate the real and imaginary components of the quantum wavefunction.

- **Network architecture:** A fully connected feedforward neural network with three hidden layers, each containing 50 neurons.
- **Fully connected network:** A fully connected feedforward neural network is used, where each neuron is connected to all neurons in the next layer. This structure enables the learning of

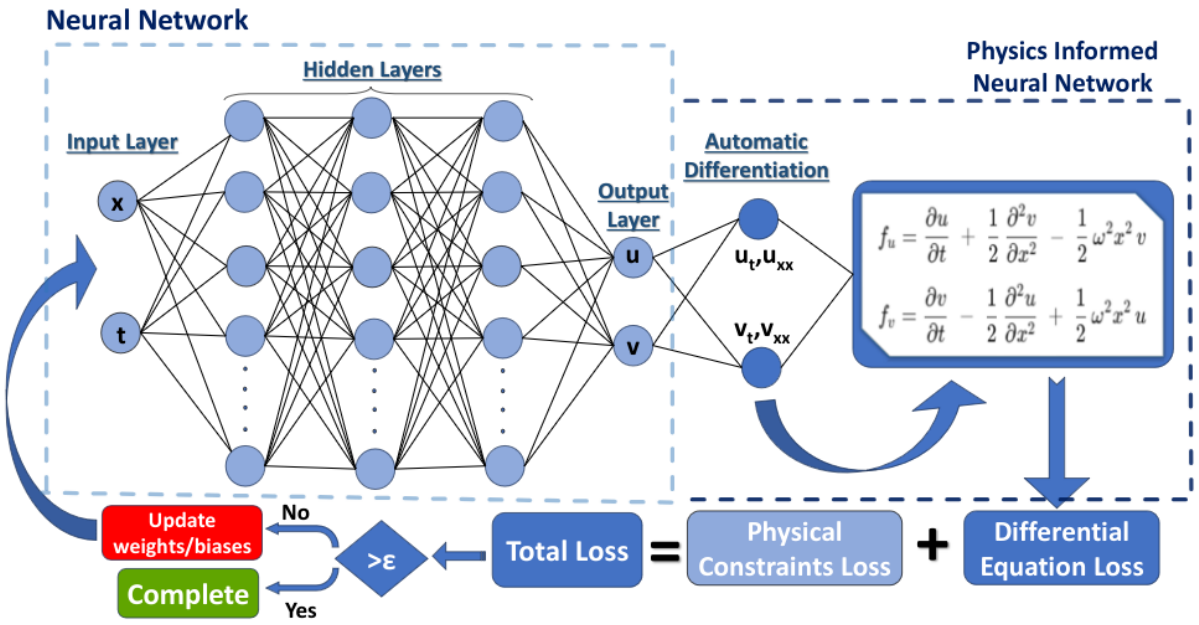


Figure 1: Architecture of a Physics-Informed Neural Network (PINNs). [17]

smooth, nonlinear mappings required for enforcing the governing physical equations within the PINNs framework [14].

- **Activation function:** The hyperbolic tangent (*tanh*) activation function is used in all hidden layers to ensure smooth approximations of the wavefunction and its derivatives.

- **Input variables:** Spatial and temporal coordinates (x, t).

- **Output variables:** The real and imaginary components of the wavefunction, denoted by $u(x,t)$ and $v(x,t)$, respectively.

- **Envelope function:** A Gaussian envelope $\exp(-x^2/2)$ is incorporated into the network output to enforce physical decay of the wavefunction at large spatial distances.

- **Training domain:** The bounded space time domain is defined as

$$x \in [-L, L], \quad L = 6, \qquad t \in [0, T], \quad T = 1,$$

.

- **Training points:** $N_f = 3000$ collocation points are randomly sampled within the interior of the domain to enforce the TDSE residual.
$N_{\text{IC}} = 900$ points are used to impose the initial condition at $t = 0$.

$N_{BC} = 900$ points are sampled at $x = \pm L$ to enforce boundary conditions.

- **Optimizer:** The Adam optimizer is used for training.
- **Learning rate:** A constant learning rate of 10^{-3} is employed.
- **Training epochs:** The network is trained for a total of 5000 epochs.
- **Automatic differentiation:** All spatial and temporal derivatives required for the loss function are computed using automatic differentiation.

2.2 Loss Function Formulation

The PINN is trained by minimizing a composite loss function constructed from physically motivated terms that enforce the governing time-dependent Schrödinger equation (TDSE), as well as the associated initial and boundary conditions. The total loss function is defined as

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{TDSE}} + \mathcal{L}_{\text{IC}} + \lambda_{\text{BC}}\,\mathcal{L}_{\text{BC}} + \lambda_{\text{phase}}\,\mathcal{L}_{\text{phase}}, \tag{13}$$

where λ_{BC} and λ_{phase} are weighting parameters that balance the relative contributions of the boundary and phase-consistency constraints.

- **TDSE residual loss:** Enforces the governing TDSE within the interior of the space–time domain [18]. It is defined as

$$\mathcal{L}_{\text{TDSE}} = \frac{1}{N_f}\sum_{j=1}^{N_f}\left[f_u(x_j,t_j)^2 + f_v(x_j,t_j)^2\right], \tag{14}$$

where f_u and f_v denote the residuals of the coupled real and imaginary TDSE equations [19].

- **Initial condition loss:** Enforces agreement between the network prediction and the prescribed initial wavefunction at $t = 0$.
- **Boundary condition loss:** Enforces physical decay of the wavefunction at the spatial boundaries by constraining both the wavefunction values and their spatial derivatives,

$$\mathcal{L}_{\text{BC}} = \left\langle u^2 + v^2 \right\rangle_{\pm L} + \left\langle (\partial_x u)^2 + (\partial_x v)^2 \right\rangle_{\pm L}. \tag{15}$$

- **Phase-consistency loss:** Preserves the correct eigenstate time evolution of the QHO,

$$\mathcal{L}_{\text{phase}} = \left\langle (u_t + E_0 v)^2 + (v_t - E_0 u)^2 \right\rangle, \tag{16}$$

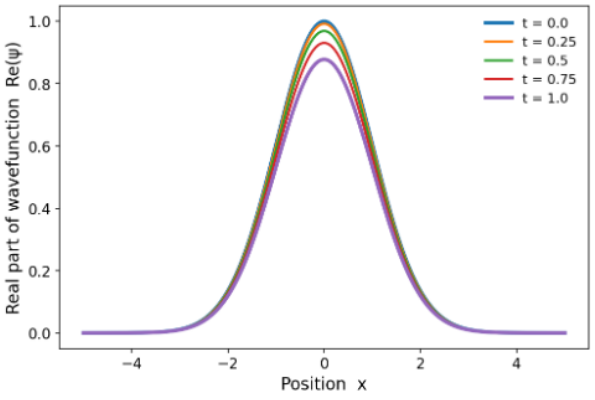
where $E_0 = \frac{1}{2}\omega$ is the ground-state energy.

These loss components collectively ensure accurate enforcement of the governing physics, numerical stability during training, and reliable approximation of the wavefunction over the entire space–time domain.

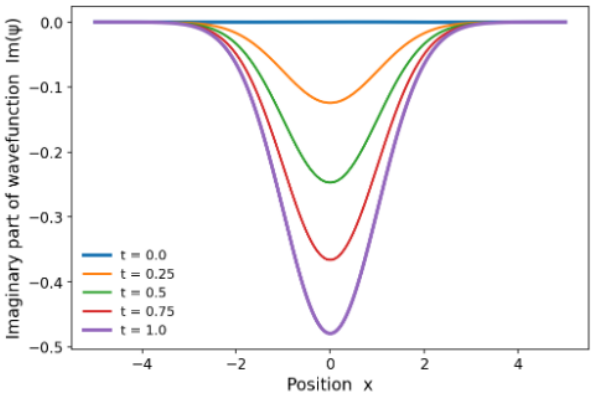
3 Result and Discussion

The Physics-Informed Neural Network (PINNs) accurately solves the TDSE for the one-dimensional QHO. The network is trained by enforcing the governing

equation, the ground-state initial condition, boundary constraints, and a phase-consistency condition to ensure correct temporal evolution.



(a)



(b)

Figure 2: Time evolution of the real (a) and imaginary (b) components of the wavefunction.

The real and imaginary components of the wavefunction in Fig. 2a and 2b demonstrate the correct time-dependent evolution. The wavefunction is purely real at the initial time, while the imaginary component develops smoothly as time progresses. The two components oscillate in time with a constant phase difference, demonstrating that the network preserves the correct quantum-mechanical phase structure. The use of a Gaussian envelope in the network architecture enforces proper spatial decay, while the imposed boundary constraints ensure numerical stability and prevent non-physical behavior near the domain boundaries. Overall, these results validate the effectiveness and physical consistency of the proposed PINNs framework for time-dependent quantum systems.

Using the learned wavefunction obtained from the PINNs solution, we further construct the Bohm quantum potential [20] , which provides an alternative description of quantum dynamics within the Bohmian formulation of quantum mechanics. In this approach, quantum effects are encoded through an additional potential term derived entirely from the wavefunction amplitude.

The complex wavefunction is written in polar form as

$$\psi(x,t) = R(x,t)\, e^{iS(x,t)},$$

where the amplitude $R(x,t)$ and phase $S(x,t)$ are real-valued functions. From the PINNs-predicted real and imaginary components,

$$\psi(x,t) = u(x,t) + i\, v(x,t),$$

the amplitude is computed as [21]

$$R(x,t) = \sqrt{u(x,t)^2 + v(x,t)^2}.$$

The Bohm quantum potential is defined as

$$V_{\text{Bohm}}(x,t) = -\frac{1}{2}\frac{\nabla^2 R(x,t)}{R(x,t)},$$

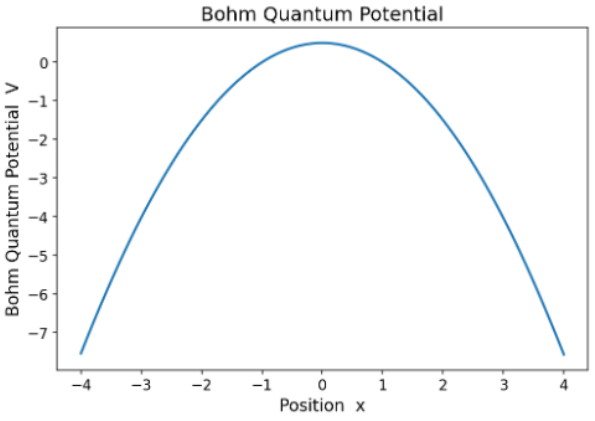
which, for the present one-dimensional system, reduces to

$$V_{\text{Bohm}}(x,t) = -\frac{1}{2}\frac{\partial^2 R(x,t)}{\partial x^2} \Big/ R(x,t).$$

All spatial derivatives required for the evaluation of the Bohm potential are computed using automatic differentiation [22], ensuring a smooth and accurate calculation without numerical discretization errors. The resulting Bohm potential in Fig. 3a exhibits a symmetric and well-behaved spatial profile, consistent with the expected structure QHO.

The Bohm quantum potential obtained in this work is direct relevance to quantum plasma physics, where it represents the leading-order quantum correction to classical fluid models [23] . In quantum hydrodynamic descriptions of plasmas, the Bohm potential accounts for wavefunction spreading and tunneling effects that arise from the quantum nature of charged particles [24].

The smooth and physically consistent Bohm potential constructed from the PINNs-predicted wavefunction demonstrates that the present work can accurately resolve quantum effects that are essential in dense or low-temperature plasmas. An important advantage of the PINNs-based approach is the accurate evaluation of the Bohm potential without numerical noise, since all spatial derivatives are computed using automatic differentiation. This feature



(a)

Figure 3: Bohm quantum potential corresponding to the ground-state wavefunction.

is particularly valuable for plasma applications, where small errors in the Bohm term can lead to unphysical instabilities in quantum hydrodynamic simulations.

These results indicate that the methodology developed here can be readily extended to quantum plasma models, providing a reliable tool for incorporating quantum effects into plasma simulations while avoiding the limitations of traditional grid-based numerical schemes.

4 Conclusion

In this study, the TDSE for a one-dimensional QHO was solved using a Physics-Informed Neural Network approach. The governing equation was embedded directly into the loss function along with suitable initial and boundary conditions, allowing the wavefunction to be learned without relying on traditional nu-

merical discretization methods. The QHO was chosen as a test system because its exact solutions are well known. The PINNs accurately capture the time evolution of both the real and imaginary components of the wavefunction. The extracted ground-state energy agrees closely with the expected analytical value, confirming the correctness of the model and training strategy.

An important outcome of this work is the construction of the Bohm quantum potential from the learned wavefunction. Using spatial derivatives obtained via automatic differentiation, the Bohm potential was calculated and found to match the expected behavior for the harmonic oscillator. This demonstrates that the PINNs solution is not only accurate at the wavefunction level but also reliable for computing derived physical quantities. Overall, the results show that PINNs provide a robust and a versatile framework for solving the time-dependent Schrödinger equation and analyzing quantum systems. The methodology presented here can be extended to more complicated potentials and boundary conditions, where analytical solutions are not available.

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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