Progressive Physics Journal
Volume 6, Nomor 2, Desember 2025
ISSN 2722-7707 (online)
http://jurnal.fmipa.unmul.ac.id/index.php/ppj

Application of Physics-Informed Neural Networks (PINNs) for the Numerical Solution of the Time-Independent Schrödinger Equation

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Article Info:
Received: 24-11-2025
Revised: 29-12-2025
Accepted: 29-12-2025

Keywords:
Physics-Informed Neural Networks, Schrödinger Equation, Quantum Harmonic Oscillator, Eigenvalue Approximation, Numerical Quantum Simulation.

Abstract

This work investigates the application of Physics-Informed Neural Networks (PINNs) as a proof-of-concept and qualitative approach for obtaining numerical solutions to the time-independent Schrödinger equation of the quantum harmonic oscillator in one, two, and three spatial dimensions. Fully connected neural network architectures are constructed to approximate wavefunctions over finite symmetric domains, while the corresponding energy eigenvalues are treated as trainable parameters. The training strategy employs randomly sampled interior points to enforce the Schrödinger operator residual and boundary points to impose vanishing wavefunction constraints. For the 1D quantum harmonic oscillator, the trained model yields a ground-state energy of E = 1.2939 after 12,000 training iterations. In the 2D case, convergence is achieved at E = 2.1352 within 14,000 iterations, while the 3D configuration attains E = 2.6377 after 12,000 iterations. While these results reproduce the expected qualitative trend of increasing ground-state energy with dimensionality, deviations from the exact analytical values remain significant, with relative errors of approximately 14% in 1D, 15% in 2D, and 25% in 3D. These discrepancies indicate that, in its current implementation, PINNs face optimization challenges and exhibit sensitivity to sampling density, boundary enforcement, and network architecture. Nevertheless, the trained models successfully capture the essential spatial symmetries and Gaussian-like profiles characteristic of harmonic oscillator ground states across all dimensions. Overall, this study should be regarded as a qualitative and pedagogical demonstration, highlighting the potential of PINNs for stationary quantum systems while emphasizing the need for further refinements – such as improved sampling strategies, loss-function balancing, and deeper network architectures – to achieve higher quantitative accuracy.

INTRODUCTION

The time-independent Schrödinger equation constitutes one of the fundamental pillars of quantum mechanics, as it governs stationary states and determines the energy spectrum of quantum systems subjected to a given potential [1]. For certain idealized potentials, such as the Quantum Harmonic Oscillator (QHO), exact analytical solutions for both eigenvalues and eigenfunctions can be derived through the eigenvalue–eigenfunction formulation [2][3]. Owing to its mathematical tractability and physical relevance, the QHO serves as a canonical benchmark model in quantum mechanics, with applications ranging from molecular vibrations and phonon dynamics to trapped particle systems.

In many realistic quantum systems, however, the potential landscape becomes spatially complex and analytically intractable. Under such conditions, numerical approaches are indispensable for solving the Schrödinger equation [4]. Conventional mesh-based numerical methods, including the finite difference method (FDM) and the finite element method (FEM), have been widely employed and have demonstrated high accuracy for a broad class of problems [5][6]. Nevertheless, these methods rely on explicit spatial discretization, which leads to rapidly increasing computational cost as the dimensionality of the system grows. This challenge is closely associated with the curse of dimensionality, which significantly limits the scalability of traditional numerical solvers for high-dimensional quantum systems [7][4].

Recent progress in machine learning and scientific computing has motivated the development of Physics-Informed Neural Networks (PINNs) as an alternative framework for solving partial differential equations [8][9]. PINNs incorporate physical laws directly into the training process by embedding the governing equations and boundary conditions into the loss function. Unlike mesh-based approaches, PINNs operate on randomly sampled collocation points and do not require explicit grid construction or large labeled datasets. This mesh-free characteristic provides conceptual flexibility and has enabled successful applications of PINNs in diverse areas, including fluid dynamics, nonlinear systems, and quantum mechanics [10][11][2].

Despite these advantages, the performance of PINNs is known to be sensitive to several factors, such as the stability of the optimization process, the distribution of collocation points, and the relative weighting of loss-function components [7][4][12]. Optimization difficulties, including gradient pathologies and the presence of multiple local minima, may hinder convergence toward accurate solutions, particularly for eigenvalue problems and higher-dimensional systems [13]. These limitations underscore the need for systematic studies that assess both the capabilities and constraints of PINNs when applied to fundamental quantum models.

In this study, PINNs are applied to solve the time-independent Schrödinger equation for the quantum harmonic oscillator in one, two, and three spatial dimensions using natural units ($\hbar = m = \omega = 1$) Under this formulation, the Hamiltonian takes the standard form

$$\boldsymbol{H} = -\frac{\mathbf{1}}{\mathbf{2}}\boldsymbol{\nabla^2} + \frac{\mathbf{1}}{\mathbf{2}}\boldsymbol{r^2},$$

for which the analytical ground-state energy is given by $E_0 = d/2$, where $d$denotes the spatial dimensionality. This well-established result provides a consistent reference for evaluating the performance of the PINNs-based approximation. The accuracy of the predicted eigenenergies and wave functions is assessed through direct comparison with the corresponding analytical solutions. Particular attention is given to the effect of increasing spatial dimensionality on training stability and solution accuracy. Rather than positioning PINNs as a replacement for established high-precision numerical solvers, this work aims to provide a qualitative and pedagogical evaluation of PINNs as a proof-of-concept framework for quantum eigenvalue problems. By clarifying both their strengths and limitations in a controlled benchmark setting, this study seeks to contribute to the broader understanding of machine-learning–based approaches for solving quantum systems with increasingly complex potential structures.

Mathematical Formulation

1. Time-Independent Schrödinger Equation

The fundamental equation employed in this study is the time-independent Schrödinger equation, which governs the stationary states of a quantum particle with mass moving in an external potential $V(\mathbf{r})$. This equation forms the basis of numerous quantum mechanical models and is widely adopted in Physics-Informed Neural Networks (PINNs) for solving eigenvalue problems [2][14][15].

The general eigenvalue formulation is expressed as :

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

where the Hamiltonian operator is given by :

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

Substituting the Hamiltonian into Eq. (1) yields the explicit form :

$$-\frac{\hbar^2}{2m}\nabla^2\,\psi\,(r) + V\,(r)\,\psi(r) = \mathrm{E}\,\psi\,(r) \tag{3}$$

For the quantum harmonic oscillator (QHO), the potential energy function is defined as:

$$\mathrm{V}(\mathrm{r}) = \frac{1}{2}\,m\omega^2\,|\,r\,|^2 \tag{4}$$

where ω denotes the angular frequency of the oscillator.

Here, the position vector is defined as $r = (x, y, z)$, and its Euclidean norm is given by :

$$|\,r\,|^2 = x^2 + y^2 + z^2$$

In lower-dimensional cases, this definition reduces accordingly. The quantum harmonic oscillator is frequently employed as an analytical benchmark in quantum mechanics because its eigenvalues and eigenfunctions are known exactly and exhibit well-defined symmetry properties [2][10].

1. **Natural Units**
   In this work, natural units are adopted by setting :

$$\hbar = 1,\ m = 1,\ \omega = 1, \tag{5}$$

which simplifies Equation (3) to the dimensionless form :

$$-\frac{1}{2}\nabla^2\,\psi\,(r) + \frac{1}{2}\,|\,r\,|^2\,\psi(r) = E\psi(r) \tag{6}$$

All subsequent one, two, and three dimensional formulations are derived consistently from Equation (6). The factor of 1/2 appearing in both the kinetic and potential energy terms is retained throughout, corresponding to the standard quantum harmonic oscillator Hamiltonian in natural units.

2. **One Dimensional Quantum Harmonic Oscillator (1D QHO)**
   For the one-dimensional case with spatial coordinate x, Eq. (6) reduces to :

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}x^2\psi(x) = E\psi(x) \tag{7}$$

3. **Two – Dimensional Quantum Harmonic Oscillator (2D QHO)**
   For the two-dimensional configuration with spatial coordinates (x, y) the Schrödinger equation becomes :

$$-\frac{1}{2}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}\right) + \frac{1}{2}(x^2 + y^2)\,\psi(\mathrm{x,y}) = E\psi(x, y) \tag{8}$$

4. **Three- Dimensional Quantum Harmonic Oscillator (3D QHO)**
   For the three-dimensional case with spatial coordinates (x, y, z) the governing equation is written as :

$$-\frac{1}{2}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + \frac{1}{2}(x^2 + y^2 + z^2)\psi(x, y, z) = E\psi(x, y, z) \tag{9}$$

Here, the Laplacian operator is defined consistently as :

$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right),$$

ensuring a correct formulation of the three-dimensional quantum harmonic oscillator.

Presentation of Tables and Figures

The main results of this study consist of the numerical approximation of ground-state eigenenergies and the qualitative visualization of wave-function profiles for the quantum harmonic oscillator (QHO) in one-, two-, and three-dimensional configurations using Physics-Informed Neural Networks (PINNs). A quantitative comparison between the eigenenergies predicted by PINNs and the corresponding analytical ground-state energies, defined as $E_0 = d/2$, is presented in Table 1. The spatial structure of the learned ground-state wave function for the one-dimensional case is illustrated in Figure 3. For the two- and three-dimensional configurations, the wave function profiles obtained using PINNs are shown in Figure 4, highlighting the symmetry and qualitative features of the ground states in higher dimensions.

Table 1. Comparison between ground-state energies obtained using PINNs (E_{PINN}) and analytical ground-state energies as ($E_0 = d/2$) for the quantum harmonic oscillator in one, two, and three spatial dimensions.

System	E_{PINN}	E_{analitik} ($E_0 = d/2$)
1D	1.2939	0.50
2D	2.1352	1.00
3D	2.6377	1.50

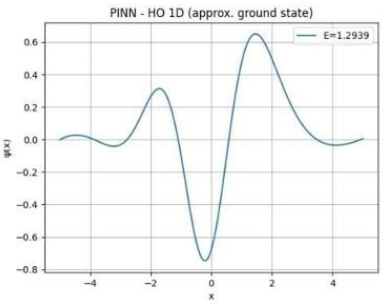
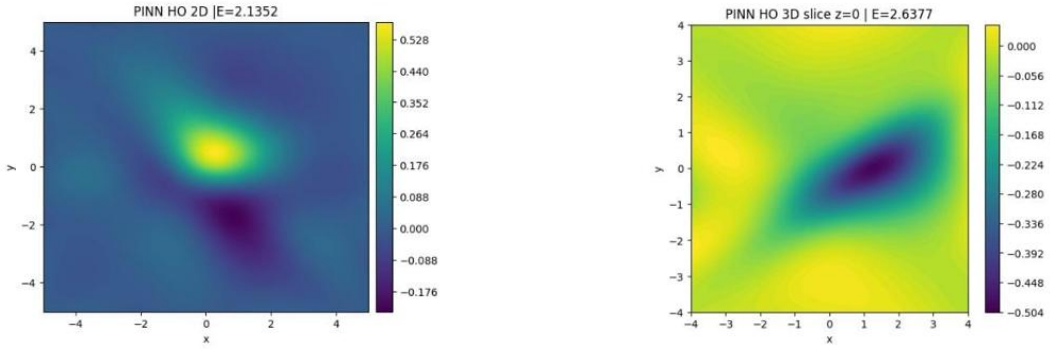


Figure 3. Visualization of the ground-state wave function of the one-dimensional quantum harmonic oscillator obtained using PINNs



(a) 2D (b) 3D

Figure 4. Visualization of the ground-state wave function of the quantum harmonic oscillator obtained using PINNs: (a) two-dimensional case and (b) three-dimensional case.

RESEARCH METHOD

This study employs a computational approach based on numerical simulation to solve the time-independent Schrödinger Equation using the Physics-Informed Neural Networks (PINNs) method. This approach is chosen because it integrates physical principles directly into the neural network training process through the minimization of differential equation residuals and the enforcement of boundary conditions, thereby eliminating the need for explicitly labeled datasets. [16]

1. **Physical Model**
   The system under investigation is the Quantum Harmonic Oscillator (QHO) in one-, two-, and three-dimensional configurations. The time-independent Schrödinger equation can be expressed as:

$$-\frac{1}{2}\nabla^2\psi(\boldsymbol{r}) + V(\boldsymbol{r})\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

   with $V(\mathbf{r}) = \frac{1}{2}|\mathbf{r}|^2$ as the harmonic potential. The QHO system is chosen because it has well-known analytical solutions, making it a suitable reference for evaluating the accuracy of PINNs predictions [17]

2. **PINNs Training**
   The neural network used in this study is a fully connected feed-forward neural network (FNN) with a hyperbolic tangent activation function. The model is trained to minimize a loss function consisting of:
   - the residual of the Schrödinger Equation,
   - boundary conditions, and
   - the normalization consistency of the wave function.

   The use of PINNs is motivated by their ability to approximate PDE solutions without requiring explicit discretization of the domain. Training parameters such as the number of collocation points, learning rate, and network size are adjusted to achieve stable convergence. Optimization is performed using the Adam algorithm and subsequently refined with the L-BFGS-B method. [18]

3. **Simulation Procedure**
   The simulation was conducted using the Python programming language. Libraries used include NumPy, SciPy, and Matplotlib for numerical computation, optimization, and visualization. The entire training and testing process was carried out in the Jupyter Notebook environment. The research procedure involves the following steps [19]:
   - Initialization of physical parameters (dimension, domain, and potential form).
   - Determination of collocation points within the domain using uniform random sampling.
   - Training of PINNs using a combined loss function.
   - Validation of the solution by comparing the eigenenergies with analytical solutions.
   - Visualization of the trained wave function.

4. **Evaluation Method**
   Evaluation is carried out by comparing the outputs of PINNs with the analytical solutions for the eigenenergy values and wave function profiles. In natural units ($\hbar = m = \omega = 1$), the theoretical ground-state energy is given by :

$$E_0 = \frac{d}{2}$$

where d denotes the dimensionality of the system. The error is calculated using the relative error, while the agreement of the wave function shape is visually evaluated through plots and contours.[20]

RESULT AND DISCUSSION

This section presents the research results and analysis of the application of Physics-Informed Neural Networks (PINNs) in solving the time-independent Schrödinger Equation for the Quantum Harmonic Oscillator (QHO) system in one-, two-, and three-dimensional configurations. The results are presented in the form of comparisons of eigenenergy values with analytical solutions, visualizations of wave functions, as well as evaluations of training convergence and sensitivity to collocation points.

1. Numerical Results of Eigenenergies

Based on the computational results, the PINNs model is able to estimate the ground-state eigenenergies for the 1D, 2D, and 3D QHO. The comparison is made with the analytical solution in natural units ($\hbar = m = \omega = 1$), so that the theoretical ground-state energy is given by:

$$E_0 = \frac{d}{2}$$

where d denotes the dimensionality of the system.

The results show that the predicted energies for the 1D and 2D cases are relatively close to the analytical solutions, while larger deviations are observed in the 3D configuration. In general, the relative error increases as the system dimensionality increases. This is consistent with the phenomenon of the curse of dimensionality, where higher dimensions expand the solution space, thereby increasing optimization complexity and reducing the stability of the PINNs approximation.

These findings are consistent with previous studies reporting that the performance of PINNs degrades in multidimensional systems. Several studies have shown that the prediction of the energy spectrum for multi-dimensional QHOs using PINNs tends to have larger errors compared to 1D systems [2][7][9]. Furthermore, [16] reported that energy errors can increase significantly as the potential structure becomes more complex, unless additional regularization strategies are applied to the loss function. Meanwhile, [11] demonstrated that the performance of PINNs in nonlinear Schrödinger systems is highly sensitive to optimization quality and training conditions.

Overall, these results indicate that increasing dimensionality is a factor that reduces the accuracy of energy predictions in PINNs, highlighting the need for advanced training strategies such as adaptive sampling or operator-based neural solvers to mitigate performance degradation.

1. Wave Function Visualiazation

The visualization of the wave function obtained from the trained PINNs model has been presented in the previous section. The wave function visualization from the PINNs training shows good agreement with the physical characteristics of the QHO.

For the 1D configuration, the wave function exhibits a Gaussian shape with a symmetric peak at the center of the potential ($x = 0$) and decays exponentially toward the edges of the domain. This profile is consistent with the analytical ground-state solution of the QHO, $\psi(x) \propto e^{-x^2/2}$, as derived in the standard formulation of quantum mechanics [21].

For the 2D configuration, the visualization results in the form of contours show the maximum probability density at the center $(x, y) = (0,0)$, then gradually decreasing radially outward, following the spherical symmetry dictated by the harmonic potential $V(x, y) = \frac{1}{2}(x^2 + y^2)$. This pattern demonstrates that PINNs can replicate the radial structure of the wave function without requiring a discrete mesh, supporting the findings of [22], which highlight the flexibility of PINNs in high-dimensional continuous domains.

Meanwhile, in the 3D configuration, a similar pattern is observed, with the highest probability concentration at the center and radial decay outward. However, the results exhibit larger numerical fluctuations compared to the 1D and 2D cases, potentially arising from optimization difficulties in high-dimensional systems and the sensitivity of collocation points to gradient errors [7][23]. This phenomenon indicates that, although the wave function shape remains physically acceptable, the numerical outputs in 3D tend to be less stable and require adaptive training strategies or additional regularization.

Overall, the visualization results indicate that PINNs have a strong capability in capturing the spatial characteristics of the wave function for the QHO, even when the eigenenergy accuracy is not optimal. These findings are consistent with [2], which reported that the representation of wave function shapes is generally more stable than the prediction of energy values. Additionally, [10] showed that in some 1D Schrödinger cases, the wave function distribution predicted by PINNs still aligns well with the exact solution, even when the exact energy exhibits a significant relative error.

These findings indicate that PINNs can provide a reliable representation of wave function shapes across various dimensions, even though increasing the complexity of the quantum system amplifies challenges related to stability and energy accuracy.

2. Training Convergence and Stability Analysis

Training convergence is observed through the reduction of the loss function during the optimization process. In the 1D system, the loss decreases steadily, indicating that PINNs can effectively learn the system dynamics. However, in the 2D system and especially in 3D, the loss reduction exhibits larger fluctuations, plateau tendencies, and slower convergence. Factors influencing performance degradation include :

- **Complexity of the optimization landscape**
  The presence of numerous local minima and saddle points in high-dimensional space complicates the training process [23][7].
- **Increase in the number of wave function parameters**
  Higher dimensions require networks with greater capacity to capture the structure of the wave function [2][14].
- **Gradient pathology**
  Extremely small or unstable gradients cause stagnation, resulting in the loss remaining nearly constant even as iterations continue [23].

These limitations are consistent with the literature, which states that PINNs are prone to training instability in high-dimensional domains [9]. Several approaches, such as adaptive sampling, curriculum training, and loss reweighting, are recommended to enhance stability and improve convergence.

3. Collocation Point Sensitivity Analysis

Sensitivity analysis based on variations in the number of collocation points shows that increasing the collocation point density significantly reduces energy errors in the

1D case. This indicates that sampling resolution has a strong impact on the accuracy of PINNs predictions. However, in the 2D and 3D configurations, a uniform increase in collocation points does not yield significant improvements in accuracy. This suggests that uniform random sampling is suboptimal for addressing the complexity of residual gradients and solution structures in multidimensional domains. Strategies such as adaptive collocation or importance sampling are considered more effective [4].

Several studies support this; for example, [24] demonstrated that the QR-DEIM method for adaptive point selection can enhance performance in multidimensional PDEs. Additionally, results from the PINNacle project [25] show that adaptive sampling and loss reweighting consistently outperform static sampling in high-dimensional PDEs. Thus, adaptive collocation point selection is a crucial step in improving the performance of PINNs in multidimensional quantum systems.

4. Limitation

Several limitations identified in this study include:

- **Errors increase significantlyin the 3D system**
  Influenced by the curse of dimensionality, which enlarges the solution space and makes optimization increasingly difficult [26].
- **Convergence difficulties and the emergence of stagnation (plateau)**
  The complex optimization landscape and the phenomenon of gradient pathology make it difficult for training to reach the optimal solution [7].
- **Random collocation point sampling is not yet optimal**
  Random points fail to capture regions with high residual gradients. An adaptive approach is required [27].
- **Treating energy as a trainable variable increases the nonlinearity of the system**
  When energy is included in the loss function, optimization becomes more difficult, as reported by [2].
- **Conventional MLP architectures are less efficient for high-dimensional radial systems**
  Feed-forward networks with tanh activation are less effective at capturing radial structures in 3D domains. Alternatives such as Fourier Neural Operator (FNO) or DeepONet have been reported to perform better in multidimensional systems [23].

CONCLUSION

This study has applied Physics-Informed Neural Networks (PINNs) to solve the time-independent Schrödinger Equation for the Quantum Harmonic Oscillator (QHO) system in one-, two-, and three-dimensional configurations. The results show that PINNs can approximate the eigenenergies and wave function shapes with varying quality, depending on the system's dimensionality. In the 1D and 2D configurations, the predicted eigenenergies are relatively close to the analytical solutions, whereas deviations increase significantly in the 3D system. This indicates that the performance of PINNs is strongly affected by the curse of dimensionality, which makes the optimization process more complex. Nevertheless, the wave function visualizations exhibit qualitative agreement with the physical characteristics of the QHO across all configurations, demonstrating that PINNs can still effectively represent spatial structures even when energy accuracy is not optimal.

Convergence and collocation point sensitivity analyses indicate that increasing the number of collocation points can reduce errors in low-dimensional systems, but is less effective in higher dimensions. Therefore, advanced training strategies, such as adaptive sampling, adaptive collocation, and alternative architectures like the Fourier Neural Operator or DeepONet, are recommended to improve training stability and prediction accuracy in multidimensional

systems. Overall, this study highlights the potential of PINNs as a physics-informed computational method for solving quantum problems, particularly in low-dimensional domains. On the other hand, computational challenges in multidimensional systems remain open for further exploration, especially in the context of architectural improvements and training strategies.

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