Physics-informed neural networks to solve the many-electrons time-dependent Schrödinger equation

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1. Introduction and Research Problem

The Schrödinger equation is a fundamental equation in quantum mechanics, governing the wave function of a non-relativistic quantum-mechanical system. Traditional numerical solvers, such as Crank-Nicholson and Runge-Kutta methods, are widely used but they will become highly complex when scaling to many electron systems. These methods require discretization, making them computationally expensive for high-dimensional quantum problems. Physics-Informed Neural Networks (PINNs) offer a promising alternative by integrating physical laws into neural networks, enabling efficient and flexible solutions to complex quantum equations [1]. PINNs are a type of universal function approximators that can embed the knowledge of any physical laws that govern a given data-set in the learning process, and can be described by partial differential equations (PDEs) [4].

My research project focuses on developing PINN-based solvers for the many-electrons time-dependent Schrödinger equation (TDSE). Prior studies, such as Shah et al. (2022), demonstrated the effectiveness of PINNs for single-electron 1D harmonic oscillator problems [2]. However, existing PINN models struggle with electron-electron interactions, long-time stability, and high-dimensional scalability. The recent work of Hao et al. (2024) on structure-preserving PINNs suggests a new techniques for improving stability in time-dependent PDEs, which could be adapted for quantum simulations [3].

This project aims to extend PINNs to many-electron systems, addressing:

- Electron-electron interactions using modified loss functions.
- Higher-dimensional modelling beyond 1D systems.
- Training stability improvements for long-time wavefunction evolution.

By leveraging insights from PINNs and scientific computing, this research project aims to develop a scalable and efficient Schrödinger equation solver, bridging the gap between machine learning and quantum mechanics. The findings could benefit quantum chemistry, condensed matter physics, and quantum computing, where solving many-body quantum systems remains a computational bottleneck [4].

2. Datasets

Since Physics-Informed Neural Networks (PINNs) do not require labeled data for training, we will generate random uniform collocation points within the spatial and temporal domain to enforce the Schrödinger equation along with initial and boundary conditions. I will demonstrate my method below using a single-electron one-dimensional example. Consider a single electron of mass m trapped in a one-dimensional time-independent harmonic potential. This example stand as a well understood benchmark for validating the PINN model before scaling to many-electron model [2].

For training, the spatial domain is set to $x \in [-50, 50]$ nanometers (nm), ensuring the wavefunction remains well-contained within a finite region. A time domain of $t \in [0, 50]$ picoseconds (ps) is chosen to analyze long-time evolution stability of the system.

For testing, initially we will define a 628×628 grid of evenly placed x and t points using the same domain we used for training. Later, based on the grid, an analytical solution will be generated using the equation:

$$\psi(x,t) = \psi(x,0)\, e^{-i\frac{E_0}{\hbar}t} \tag{1}$$

where,

$$\psi(x,0) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \tag{2}$$

and,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{3}$$

3. Task Selection and Benefit

The primary task for this research project is to develop a PINN framework that accurately models quantum wavefunction evolution, starting with a single-electron one dimensional harmonic potential before extending to many-electron systems [2].

3.1. Why PINNs for TDSE?

Traditional numerical methods suffer from computational inefficiency when scaling to high-dimensional many-body quantum systems. PINNs offer:

- Continuous solutions without explicit discretization.
- Integration of physics constraints, requiring minimal labeled data for training.
- Improved long-time stability, especially when using structure-preserving training strategies.

3.2. Benefits to Research & Industry

- Quantum Computing & Materials Science: PINNs can efficiently model quantum dynamics for designing quantum circuits and semiconductors [5].
- Computational Efficiency: Unlike traditional solvers, PINNs generalize to different system parameters without retraining, making them scalable [6].
- Physics-Informed AI: Advances in PINNs contribute to AI-driven scientific computing, bridging machine learning and theoretical physics [7].

By addressing the computational challenges of many-electron TDSE, this research project provides a newer and scalable approach for solving Schrödinger equation with higher accuracy and lower computational cost.

4. Research Questions

The following research questions ensure a clear focus on key computational and physical challenges:

- Can PINNs accurately approximate the time evolution of a many-electron wavefunction?
  - Evaluates the model's ability to capture quantum dynamics over extended time periods.
- How does the accuracy and computational efficiency of PINNs compare to traditional solvers?
  - Assesses whether PINNs offer advantages in scalability and long-time stability.
- What loss function modifications improve PINN training stability for long-time quantum wavefunction evolution?
  - Investigates strategies such as causal training and structure-preserving PINNs.
- How does the inclusion of electron-electron interactions affect PINN performance in many-electron systems?
  - Explores challenges in extending PINNs from single-electron to many-body quantum mechanics.

These questions guide the methodology, experimentation, and evaluation metrics, ensuring that the study addresses key limitations in PINN-based quantum solvers.

5. Proposed Methodology

For this research project, the proposed methodology involves defining the PINN architecture, training strategy, evaluation metrics and computational setup. Here I will use the same example of the one-dimensional single-electron model I mentioned in section 2.

5.1. PINN Architecture

- I used a fully connected feed forward neural network (FNN) with 6 hidden layers consisting of 512 neurons each.
  - Inputs: x, t
  - Outputs: Real and Imaginary part of the wavefunction
- Activation function: Tanh; The activation function has to $k + 1$ differentiable for a PDE of order k. So the activation function choices are limited to functions like *tanh* and *SiLU* [2].

5.2. Loss Function Components

Loss functions are crucial for every PINN because that is where we specify what the model should learn. A typical PINN model consists of mainly three loss functions:

1. PDE Loss (Physics Loss): This loss is created from the partial derivative equation (PDE) we are trying to solve. In the case of this project, it is the Schrodinger equation.
    - The first step is to create a residual using the PDE. The Schrodinger equation can be written as,

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

    - Then we will create the residual by bringing every at the RHS to LHS.

$$Residual, R=i\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-\frac{1}{2}m\omega^2x^2\psi(x,t) \tag{5}$$

    - During training, we will try to reduce this residual to zero. The PDE Loss can be found using the formula,

$$L_{PDE}=\frac{1}{N_{PDE}}\sum_{i=1}^{N_{PDE}}[R_{real}(x_i,t_i)^2+R_{imag}(x_i,t_i)^2] \tag{6}$$

2. Initial condition loss: Through this loss, we will enforce how the wavefunction should behave when t = 0. In our case, it is the ground state of electron.

$$\psi(x,0)=(\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}e^{-\frac{m\omega}{2\hbar}x^2} \tag{7}$$

    - The initial condition loss can be found using the formula

$$L_{IC}=\frac{1}{N_{IC}}\sum_{i=1}^{N_{IC}}[\psi_{NN}(x_i,0)-\psi_{IC}(x_i)]^2 \tag{8}$$

3. Boundary condition loss: Through this loss, we enforce how the model should behave at the spatial boundaries. We are using Dirichlet boundary conditions so the wavefunction will be zero at the boundaries. The boundary condition loss can be found using the formula,

$$L_{BC}=\frac{1}{N_{BC}}\sum_{i=1}^{N_{BC}}[\psi_{NN}(x_i,t_i)-0]^2 \tag{9}$$

We can then calculate the total loss using the equation,

$$L=\lambda_{PDE}L_{PDE}+\lambda_{IC}L_{IC}+\lambda_{BC}L_{BC} \tag{10}$$

where the λ variables are the respective regularization parameters for each losses.

5.3. Computational Setup

- I used Adam optimizers with Beta1 = 0.9 and Beta2 = 0.999
- The learning rate is initialized at a_0 = 0.001 with exponential decay rate = 0.9 at decay steps = 1000.

5.4. Evaluation Metrics

- Mean squared error between PINN prediction and analytical solution
- Probability density graph is compared between PINN prediction and analytical solution
- Probability conservation check: $\int|\psi(x,t)|^2dx=1$

6. Ethics Statement

This research adheres to ethical guidelines in computational physics and machine learning by ensuring scientific integrity, transparency, and responsible use of computational resources.

1) No human or sensitive data
    a) This study does not involve human subjects, personal data, or confidential information, eliminating privacy concerns.
2) Research integrity and reproducibility
    a) All methodologies, including dataset generation and model training, follow reproducible scientific practices.
    b) The study uses publicly available mathematical formulations and standard machine learning frameworks, ensuring transparency
3) Responsible use of computational resources
    a) The study is designed to minimize computational costs by optimizing training strategies and using efficient algorithms
    b) Ethical AI practices are followed to ensure fair and unbiased results
4) Open science and Knowledge Sharing
    a) Findings will be documented and shared for further research, contributing to open-access AI applications in quantum mechanics

7. Timeline

7.1. Phase 1: Literature Review and Model Setup (Weeks 1-4)

- Review relevant research papers on PINNs, TDSE and many-body quantum systems
- Define initial model architecture and loss functions based on previous paper
- Select benchmark problem: Single-Electron one-dimensional harmonic potential with a well defined analytical solution

7.2. Phase 2: Single-Electron PINN Implementation (Weeks 5-8)

- Implement PINN model for a single-electron TDSE in a one-dimensional harmonic potential
- Compare PINN solution to analytical wavefunctions

7.3. Phase 3: Stability and Model Refinements (Weeks 9-12)

- Introduce structured loss functions such as causal training and structure preserving PINNs
- Extend time domain and test long term stability

7.4. Phase 4: Many-Electron Model Extension (Weeks 13-16)

- Extend PINN model to two-electron systems in a double quantum dot
- Incorporate electron-electron iterations to the loss function

7.5. Phase 5: Final Testing and Research Report (Weeks 17-20)

- Conduct final model evaluation
- Summarize findings and prepare research project submission

8. Expected Outcome

The expected outcomes of this research project include:

- Accurate Quantum Wavefunction Evolution
    - The PINN model should achieve high accuracy, closely matching analytical solutions for single-electron systems.
    - Demonstrate stable long-time evolution of the wavefunction without numerical divergence.
- Computational Efficiency & Scalability
    - Compare PINN performance against traditional numerical solvers, assessing computational cost and generalizability.
    - Develop strategies for scaling to many-electron systems, incorporating electron-electron interactions.
- Contributions to Quantum Computing & AI-Driven Physics
    - The findings could impact quantum chemistry, condensed matter physics, and AI-driven PDE solvers, bridging machine learning and quantum mechanics.

These outcomes will validate PINNs for quantum simulations, providing a scalable, efficient alternative to traditional methods.

Abbreviations

The following abbreviations are used in this manuscript:

PINN	Physics-informed Neural Networks
PDE	Partial Differential Equations
TDSE	Time-Dependent Schrodinger Equation

References

1. M. Raissia, P. Perdikarisb, G.E. Karniadakisa, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, 2019
2. Karan Shah, Patrick Stiller, Nico Hoffmann, Attila Cangi, Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation, 2022
3. Baoli Haoa, Ulisses Braga-Netob, Chun Liua, Lifan Wangc, Ming Zhonga, Structure Preserving PINN for Solving Time Dependent PDEs with Periodic Boundary, 2024
4. Physics-Informed Neural Networks. Available online: https://en.wikipedia.org/wiki/Physics-informed_neural_networks (accessed on 10/03/2025)
5. Jannes Nys, Gabriel Pescia, Alessandro Sinibaldi, Giuseppe Carleo, Ab-initio variational wave functions for the time-dependent many-electron Schrödinger equation, 2024
6. Tamara G. Grossmann, Urzula Julia Komorowska, Can physics-informed neural networks beat the finite element method, 2024
7. Yaolong Zhang, Bin Jiang, and Hua Guo, SchrödingerNet: A universal Neural Network Solver for the Schrödinger Equation, 2025