Research Proposal

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

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Abstract: The Schrodinger equation describes how quantum systems evolve over time. Solving it for higher dimensional many-body systems can be computationally expensive using analytical methods. Physics-informed Neural Networks (PINNs) offer a promising alternative by using deep learning to find solutions while enforcing physical laws via loss functions. Through this research, I aim to develop a PINN framework to solve many-electron time-dependent Schrodinger equation (TDSE). The study will begin with a single-electron system in a one-dimensional harmonic potential then later scale the model to solve two-electron systems while considering electron-electron interaction. I will evaluate the model against know analytical solutions based on mean-squared error and probability density graph. Later on the study, I would also like to explore advanced training strategies like causal training and structure-preserving PINNs to improve performance. This research project is expected to provide a computationally efficient and scalable alternative for solving quantum wave functions.

Keywords: Neural Networks, Physics-informed Neural Networks, Schrodinger Equation, Quantum Physics, One-Dimensional harmonic oscillator, Many-Electron system.

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, are widely used but they will become computationally expensive when scaling to many electron high-dimensional systems. Physics-Informed Neural Networks (PINNs) offer a promising alternative by enabling efficient and flexible solutions to 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]. 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 modeling beyond 1D systems.

By combining the results 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.

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 in one-dimensional harmonic potential example. 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. We use separate uniform random points within the space and time domain to calculate each losses. For this example model, I am using 3140, 314 and 200 points to calculate the PDE loss, Initial condition loss and Boundary condition loss respectively.

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.

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 little to no labeled data for training.
- If we use structure-preserving training strategies [3], we can preserve the model stability for longer time domain.

3.2. Benefits to Research and Industry

- Quantum Computing & Materials Science: PINNs can efficiently model quantum dynamics for designing quantum circuits and semiconductors [5].
- Computational Efficiency: Unlike numerical solvers, PINNs are scalable and they can generalize to different system parameters without retraining [6].

4. Research Questions

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

1. Can PINNs accurately approximate the time evolution of a many-electron wavefunction?
2. How does the accuracy and computational efficiency of PINNs compare to numerical solvers?
3. What loss function modifications improve PINN training stability for long-time quantum wavefunction evolution?
4. How does the inclusion of electron-electron interactions affect PINN performance in many-electron systems?

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

5. Proposed Methodology

The proposed methodology involves defining the PINN architecture, training strategy and evaluation metrics. 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. Two inputs, x and t. Output will be the real and imaginary part of the corresponding wavefunction.
- Activation function: Here I am using *tanh* activation function. 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].
- Adam optimizer is used with $\beta_1 = 0.09$ and $\beta_2 = 0.999$
- Learning rate is initialized at $\alpha_0 = 0.001$ with exponential decay rate $\gamma = 0.9$ at decay steps $t_\gamma = 2000$ training steps with schedule $\alpha_t = \alpha_0 * \gamma^{t/t\gamma}$.

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 study, 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 everything 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,

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

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 the electron.

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

The initial condition loss can be found using the formula

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

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,

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

We can then calculate the total loss using the equation,

$$L=\lambda_{PDE}L_{PDE}+\lambda_{IC}L_{IC}+\lambda_{BC}L_{BC} \quad (10)$$

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

5.3. 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

In this study, I adheres to ethical guidelines by ensuring scientific integrity, transparency, and responsible use of resources.

- No human or sensitive data: This study does not involve human subjects, personal data, or confidential information.
- Research integrity and reproducibility: All methodologies, including dataset generation and model training, follow reproducible scientific practices. I used publicly available mathematical equations and standard machine learning frameworks, ensuring transparency.
- Responsible use of computational resources: The study is designed to minimize computational costs by optimizing training strategies and using efficient algorithms.
- Open science and Knowledge Sharing: I will document and share the finding of this project 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 one 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 wave functions.

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

- Introduce advanced training strategies 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 wavefunction evolution: The PINN model should achieve high accuracy, closely matching analytical solutions for single-electron and two-electron systems. The model should demonstrate stable long-time evolution of the wavefunction without numerical divergence.
- Computational Efficiency & Scalability: The PINN model should display good performance against numerical solvers in terms of computational cost and generalizability. Develop strategies for scaling the model to many-electron systems, incorporating electron-electron interactions.
- Contributions to Quantum Computing: The findings could impact quantum chemistry, condensed matter physics, and AI-driven PDE solvers, bridging the gap between machine learning and quantum mechanics.

Abbreviations

The following abbreviations are used in this manuscript:

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

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