Literature Review

Physics-Informed Neural Networks to solve the many-electrons time-dependent Schrödinger equation

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1. Introduction

The Schrödinger equation is a partial differential equation that governs the wave function of a non-relativistic quantum-mechanical system. The equation describes how quantum systems evolve over time. Solving the time-dependent Schrödinger equation (TDSE) will become challenging when dealing with many-electron systems, due to high dimensionality and electron-electron interactions. Numerical methods like Crank Nicholson work well for simple systems but their scalability and computational efficiency are limited for complex systems.

In recent years, Physics-Informed Neural Networks (PINNs) have been proposed as a new way to solve partial differential equations (PDEs) by embedding the driving physics equation into the loss function of the neural network [1]. This method removes the need for large scale labelled datasets and provides a noise free solution strategy. There are studies that have shown the potential of PINNs in solving one-dimensional TDSE problems [2] [3].

This literature review aim to explore how PINNs are currently used to solve TDSEs and whether they can be extended to practically solve the many-electron problem. This literature review will examine recent studies, identify existing challenges and highlight research gaps this project aims to fill.

2. Literature Search Process

To find relevant literatures for this review, I used multiple academic databases and platforms such as Google Scholar, ArXiv, ScienceDirect and the University of Adelaide library portal. The searching was mainly focused on recent works in Physics-Informed Neural Networks (PINNs) and their application to quantum physics, specifically related to solving the Schrödinger equation.

Keywords and phrases used includes: “Physics-Informed Neural Networks”, “PINN Schrödinger equation”, “Neural networks many body quantum systems”, “Neural PDE solvers” and “TDSE neural networks”. In addition to this, filters such as publication date from 2019 onwards, relevance and citation count were used to get better results. The inclusion criteria were:

- The paper must use deep learning frameworks such as PINN.
- The paper should focus on solving the TDSE or similar quantum PDEs.
- The paper must contribute to understanding PINN limitations, training or scalability.

Based on these processes, seven key papers were selected and reviewed in detail. The selected papers have a balance between understanding of PINN, quantum applications, numerical comparisons etc.

3. Academic Literature Review

This section reviews five papers that provide the theoretical foundation, technical approach and practical challenges related to solving the time-dependent Schrödinger equation using PINNs. These papers represent a combination of foundation, specific case studies, training strategies and evaluation metrics of PINNs in the context of quantum physics and PDEs.

1. Gardin et al. (2021): Non-Adiabatic Quantum Control of Valley States in Silicon [4]

This paper is included in this review to highlight the use of numerical methods in solving TDSE for real world quantum systems. The authors of this paper investigated the non-adiabatic evolution of an electron in a quantum dot within a silicon based heterostructure. They used Crank-Nicholson methods to simulate the TDSE and model valley state transitions in silicon qubits.

Their results showed how non-adiabatic control and electric field manipulation can be used to tune valley state populations. The study relies on accurate time domain modeling and boundary condition enforcement, two areas where PINNs can offer advantages. By comparing numerical methods with PINNs, future research can build hybrid models that combine the strengths of both. The work in this paper serves as a motivation for this project by demonstrating the difficulties of time-dependent quantum simulations.

2. Raissi et al. (2019): Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear PDEs [1]

This paper introduced the original Physics-Informed Neural Network (PINN) framework as a way to solve differential equations by embedding physical laws directly into the training process. In their work, a neural network is trained to minimize the residuals of the respective PDEs along with the initial and boundary conditions. This is done by designing a loss function composed of PDE residual loss, initial condition loss and boundary condition loss.

The key advantage of this method is that it removes the need for large scale labelled dataset, which is sometimes not available in physics problems. Instead, the model uses a small set of known boundary and initial condition and enforce the physical constrains throughout the problem domain. This approach is suitable for problems like the TDSE, where labelled data can be hard to find for complex situations.

This paper demonstrated their idea on PDEs such as the Burger's equation and the Navier-Stokes equation. They managed to get good results in both forward and inverse problem settings. They did not apply PINNs directly to the Schrödinger equation but their work can be considered as foundation for later studies. Their method shows potential for solving high-dimensional PDEs like the many-electron TDSE, but they also noted limitations such as difficulty in training over long time periods and capturing edge cases.

3. Shah et al. (2022): Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation [2]

In this paper, they applied PINNs directly to solve time-dependent Schrödinger for a one-dimensional quantum harmonic oscillator. They used Hartree atomic units to simplify the constants such as hbar, m_e and k_B to 1 and initialised their system with a superposition of the ground and first excited states. They employed a fully connected neural networks and trained it using a combination of PDE residual loss, initial condition loss and boundary condition loss.

A key challenge noted was that PINNs tend to focus too much on minimising the easier initial and boundary condition losses, often neglecting the PDE residual loss. To solve this, they experimented with adjusting the relative weights of each component of the loss

function and give more priority to the PDE loss. They managed to achieve a testing mean squared error (MSE) of 10-5 when tested in a 628×628 grid. This study provide valuable information regarding the training of PINNs for TDSE, particularly in handling long-time evolution and wavefunction complexity. While their work focuses on single electron systems, it lays the groundwork for extending PINNs to many-electron systems.

4. Hao et al. (2024): Structure-Preserving PINN for Solving Time-Dependent PDEs with Periodic Boundary Conditions [3]

This paper introduced a modification to the PINN framework called structure preserving PINN (SP-PINN), specifically designed for solving time-dependent PDEs with periodic boundary conditions. This paper does not solve the Schrödinger equation, but the proposed method can be considered relevant to quantum physics. The authors state that conventional PINNs fail to maintain the structural properties of the underlying PDE over longer time periods. For a TDSE, conservation of probability and long-time stability are crucial. SP-PINN address this by modifying the network architecture and loss function to preserve mathematical and physical structure of the problem.

They do this by introducing periodic basis functions into the neural network and by adding additional regularisation terms to the loss function that will punish structural violations. These changes help the model to maintain its periodicity and stability during time evolution. For quantum systems, such improvements can help scenarios involving periodic potentials, wave packets and systems with cyclic behaviours. The ideas presented in this paper can be adapted to improve training stability when solving TDSE using PINNs.

5. Grossmann et al. (2024): Can Physics-Informed Neural Networks Beat the Finite Element Method? [5]

In this paper, the authors conducted a comparison between PINNs and classical Finite Element Method (FEM) across various PDEs, including the Schrödinger equation. This study is important because it provides evidence of where PINNs excel and where they struggle compared to numerical solvers. According to their experiments, FEMs outperformed PINNs in terms of accuracy and convergence speed, while PINNs shows more flexibility and scalability for high-dimensional problems. For example, PINNs did not require structured grids to solve and they are easier to implement for complex boundary conditions.

For the Schrödinger equation, they states that PINNs could handle high-dimensional setups more naturally that FEMs, especially for irregular geometry and larger domain. However, PINNs sometimes trained for longer period of time to achieve higher accuracy. This comparisons help to justify the use of PINNs for many-electron TDSE problems, where FEM based solvers face challenges due to dimensionality and interaction complexity. At the same time, the paper also highlights the need for continued improvements in training strategies for PINNs.

These five papers provide a proper understanding of the current capabilities and limitations of PINNs in quantum applications. Gardin et al. presented a real world application of TDSE using numerical solvers, helping establish the importance and relevance of the problem. The paper by Raissi et al. laid the theoretical groundwork for PINN. Shah et al. extended this framework to the 1D TDSE and found some practical training challenges. Hao et al. proposed methods to enhance training stability and structural preservation. Finally, Grossman et al. conducted a performance comparison with FEM, highlighting the pros and cons of PINN over numerical methods.
Together, these works reveal that while PINNs are not outperforming classical solvers in all respects, they offer a reasonable method to solve high-dimensional quantum problems.

Considering the current limitations of PINN is important when doing many-electron TDSE. This literature report shows the direction of the current project and highlights where contributions can be made.

4. Existing Project Review

This section reviews two existing projects that aim to solve the many-electron Schrödinger equation using deep neural networks based approaches. These studies are not based on PINNs, but they provide valuable insights into alternative methods and architectures. Their findings support the direction and motivation of the current research project, which is to apply PINN to the many-electron time-dependent Schrödinger equation.

1. Han et al. (2019): Solving the Many-Electron Schrödinger Equation Using Deep Neural Networks [6]

In this paper, the authors introduced a method called DeepWF, which uses neural networks to represent many-electron wavefunctions. Instead of relying on orbital-based approaches, DeepWF learns the quantum wavefunction from scratch using the variational Monte Carlo (VMC) method to optimise the network. Their method respects the Pauli's exclusion principle by enforcing anti-symmetry in the network design. The wavefunction is modelled as a product of a symmetric function for spin-up electrons and two anti-symmetric functions for spin-down electrons.

The method was tested on several benchmark systems including H2, He, LiH, Be, B and a chain of 10 hydrogen atoms (H10). The method predicted ground-state energy values that closely matches the benchmark data. For example, the ground-state energy of the Be atom has a difference of only 0.03% from the reference values. Since this method does not rely on predefined atomic orbitals or basis sets, it it scalable.

DeepWF is not designed for time-dependent problems. But its success in solving the many-electron ground state problem supports the idea that neural networks can approximate any quantum wavefunctions. They also demonstrated that neural networks can capture electron correlation and spatial distribution without prior knowledge. These capabilities are essential for modelling many-electron systems and also justify further exploration into applying PINNs, which will consider physical laws to solve similar problems.

The authors also mentioned limitations of this model such as decreased accuracy for larger systems and challenges in training stability. To improve convergence, they suggest future improvements in both the anti-symmetric ansatz and sampling strategies. When applying PINN to similar problems, proper handling of symmetry and efficient training methods are important.

2. Nys et al. (2024): Ab Initio Variational Wave Functions for the Time-Dependent Many-Electron Schrödinger Equation [7]

In this paper, the authors proposed a different approach. They introduced a neural network based variational wavefunction to solve the time-dependent many-electron Schrödinger equation. This method combine quantum mechanics with deep learning by designing a flexible variational ansatz capable of learning complex time evolving quantum states.

Their model includes neural back flow transformations and time-dependent Jastrow factors. Both of these are optimised during training to follow the exact dynamics of the system. The study focuses on few-electron systems such as diatomic molecules and quantum dots, where electron-electron interactions make numerical methods computationally expensive.

One of the strength of this work is, it demonstrates the ability of neural networks to track time-dependent behaviour in systems governed by TDSE. This is highly relevant to the current research project, which aims to solve a many-electron TDSE problem using PINNs. While authors rely of variational principles and time evolution via optimisation, PINNs embed the TDSE directly into the loss function. Despite this difference, both methods aim for accuracy and scalability when solving the problem.

They also points out some challenges in this paper, including handling of high-dimensional Hilbert spaces and reaching numerical stability during long-time evolution. These are also key concerns in PINN-based modelling. Comparing the two methods will help identify what area of neural network architecture are most important.

Together, these two works show that neural networks can be powerful tools for solving the many-electron Schrödinger equation, both in a static ground state and dynamic time evolving forms. The paper by Han et al. show how deep neural networks can model ground states without orbitals, while Nys et al. show how neural variational model can follow time evolution in real systems.
However, both these approaches rely on sampling-based training and variational principles. But the current research project explores PINNs, which directly includes the TDSE into the training objective. This makes PINNs grid-free, data-efficient and more generalisable. The reviewed projects highlight the importance of handling symmetry, electron-electron interaction and long time stability.
In conclusion, while the reviewed methods use different training strategies, they validate the use of neural networks in quantum physics and support the relevance of applying PINNs to many-electron TDSE.

5. Conclusion

This literature review explored recent research on solving the many-electron time-dependent Schrödinger equation using PINNs and other deep learning techniques. The academic papers reviewed have shown the potential of PINNs to solve PDEs efficiently and identifying challenges like long-time stability and training imbalance. The review of existing projects demonstrated the success of deep neural networks in learning many-electron wavefunctions. These works also highlighted key issues such as scaling, physical accuracy and architecture design.

The combination of findings from both review categories shows that traditional deep learning models require extensive sampling, while PINN offer a promising, grid free and data-efficient alternative that can directly embed physical laws. However, PINN will still face challenges in training stability and performance for high-dimensional problems. This review support the direction of the current project, which focuses on extending PINNs to many-electron TDSEs. The project is positioned to contribute meaningful advancements to the intersection of machine learning and quantum physics.

Abbreviations

The following abbreviations are used in this manuscript:

PINN	Physics-informed Neural Networks
PDE	Partial Differential Equations
TDSE	Time-Dependent Schrodinger Equation
MSE	Mean squared error
SP-PINN	Structure-Preserving PINN
VMC	Variational Monte Carlo

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