Physics-Informed Neural Networks to Solve the Many Electron Time-Dependent Schrödinger Equation

Presented by,
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Introduction

- The **Schrödinger equation** is a fundamental equation in quantum mechanics that describes how the quantum state (wavefunction, Ψ) of a physical system evolves over time and space
- Traditionally, **Schrödinger equation** can be solved using analytical methods for simple systems or numerical techniques like finite difference or Crank–Nicolson methods for more complex systems
- In this project, I am trying to solve the **Schrödinger equation** using **Physics-Informed Neural Network (PINN)**, which are a type of neural network that learns to solve PDEs by embedding the relevant equations into its loss function
- The advantage of using **PINN** is that, since we are directly trying to satisfy the physical equation through loss function, we do not require large labelled datasets for training

Project Recap

- Successfully reproduced the baseline model of an electron in a 1D harmonic potential, based on the 2022 paper by Shah et al.
- Retrained the model using nanometer-picosecond (nm-ps) units instead of atomic units
- Experimented with various initial conditions
- Extended to a more complex problem: an electron in a moving quantum dot

Methods

- In this presentation, I will explain the two methods I have introduced to improve my **moving quantum dot PINN** model developed during the last trimester
- **Enforcing Causality**: In our context, causality means that the neural network should learn the wavefunction in a time-ordered manner, ensuring that what happens at later times depends on the learned behaviour at earlier times, just like in real quantum systems
- **Enforcing Normalization**: Normalizing the Schrödinger equation ensures that the wavefunction represent a valid probability distribution. Which means the probability of finding a particle anywhere in the spatial domain should be 1 at all times

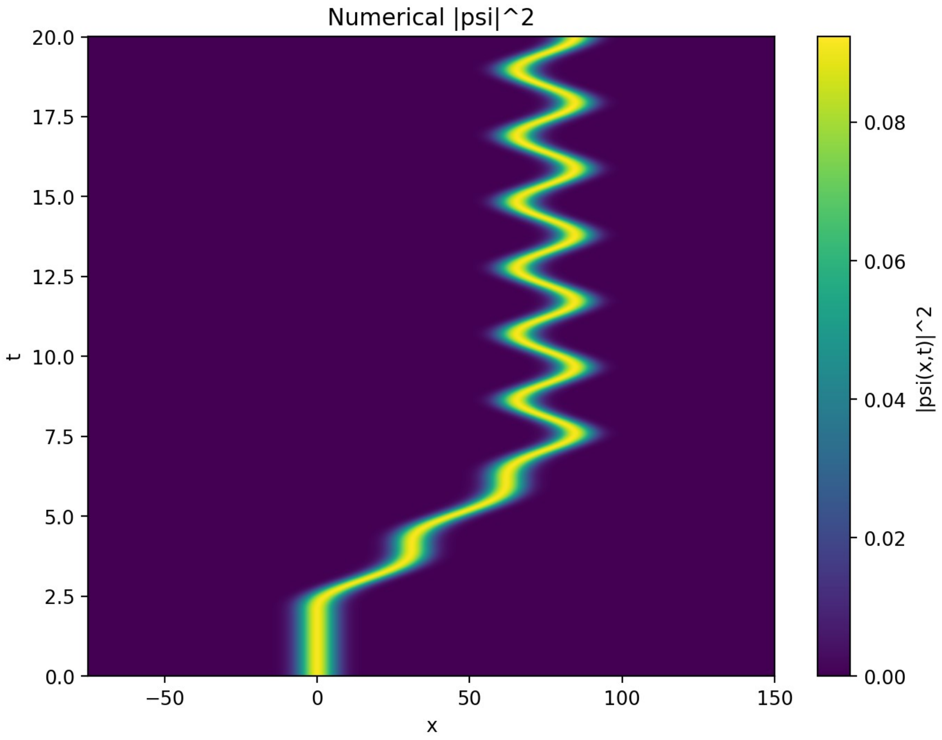
Causality

- To enforce causality during training, I divided the time domain into n equally spaced segments
- At each segment, the physics loss (PDE Loss, L_{PDE}) is computed as the sum of current segment’s loss and the cumulative losses from all previous segments
- This encourages the model to learn earlier segments accurately before learning later segments, satisfying causality

Causality

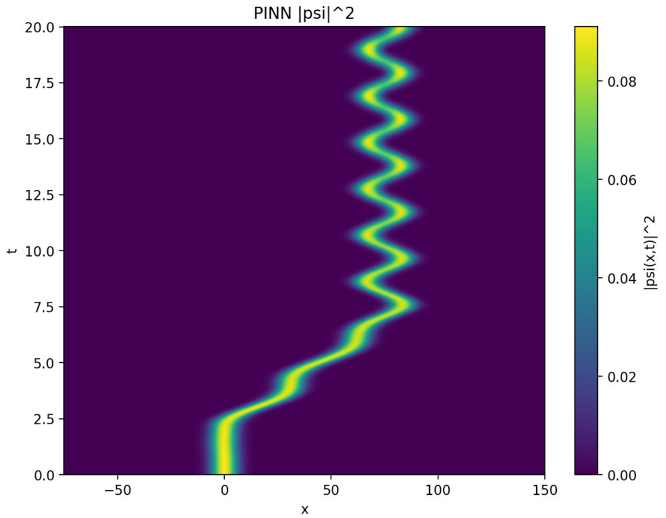
- Total PDE loss can be written as, $L_{PDE} = \frac{1}{N_{seg}} \sum_{i=1}^{N_{seg}} (\sum_{k=1}^{i-1} L_k) + L_i$
- Where,
  - N_{seg} = Number of segments
  - L_i, L_k = PDE Loss at segment i, k respectively
- The expression expands to,
  - $L_1 = L_1$
  - $L_2 = L_1 + L_2$
  - $L_3 = L_1 + L_2 + L_3$
  - $L_4 = L_1 + L_2 + L_3 + L_4$

Crank-Nicholson Solution

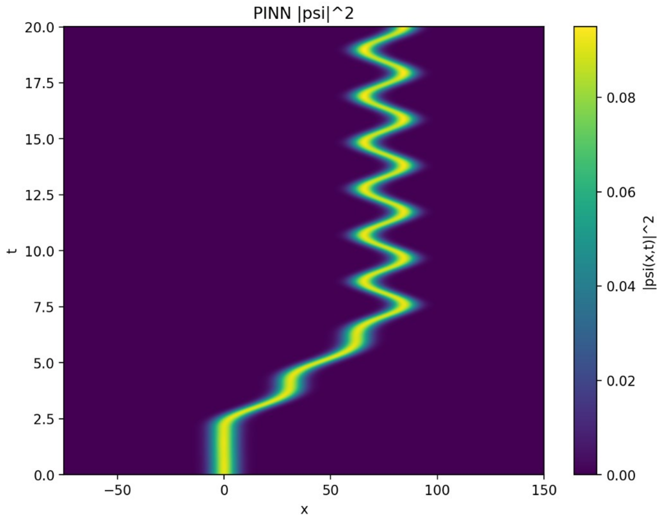


Results

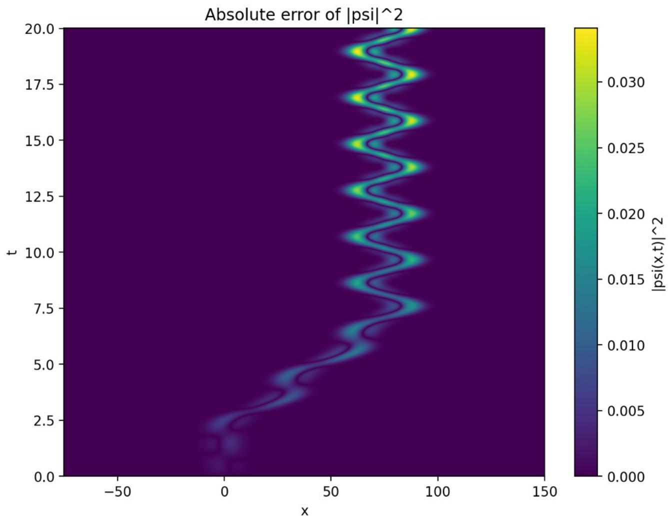
Base Model



Causal Model

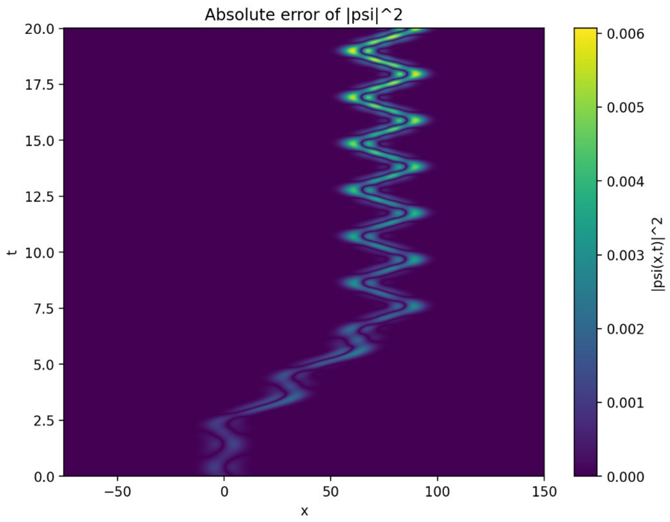


Base Model



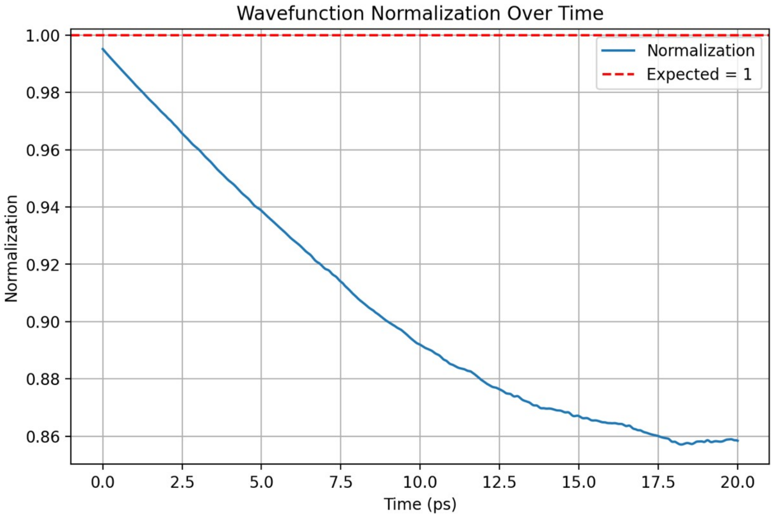
Mean	Standard Deviation	Min	Max
0.00073	0.00303	0.00000	0.03409

Causal Model



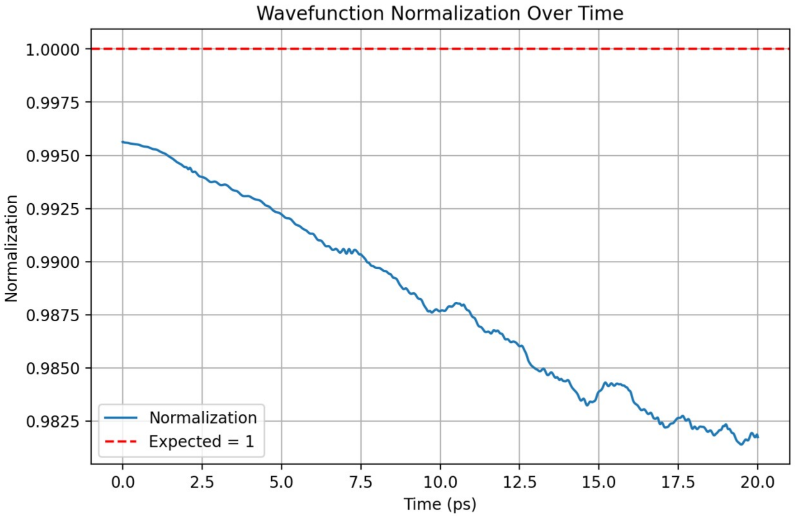
Mean	Standard Deviation	Min	Max
0.00012	0.00050	0.00000	0.00607

Base Model



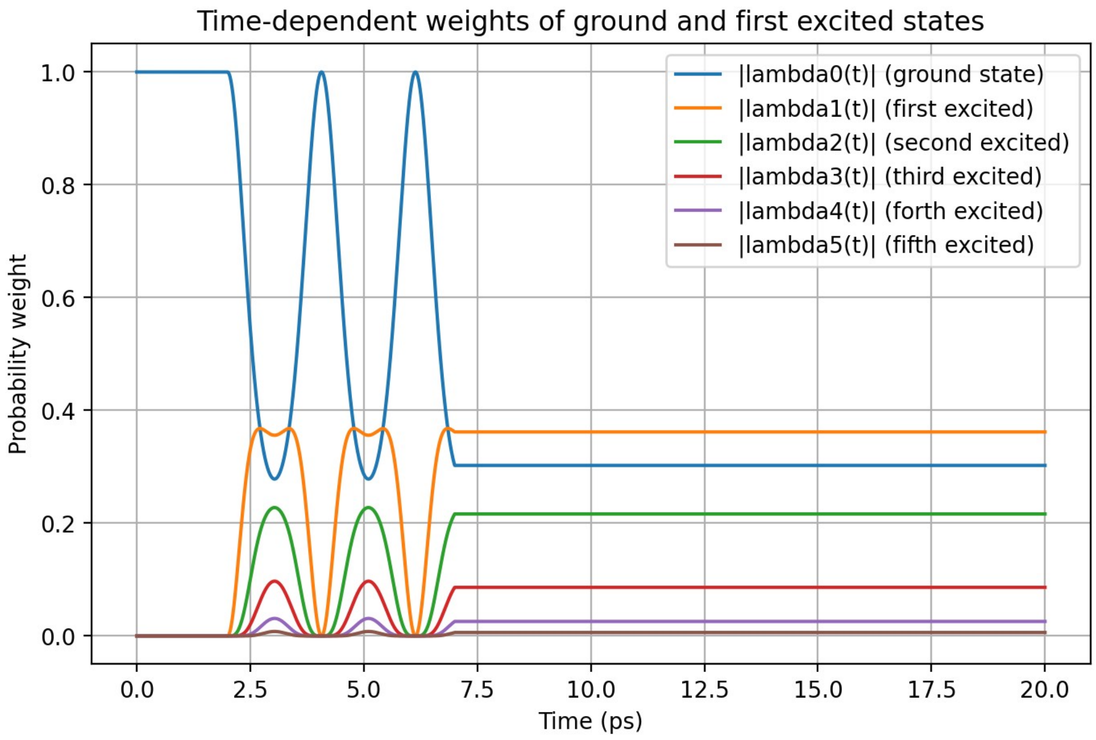
Mean	Standard Deviation	Min	Max
0.90468	0.04191	0.85709	0.99511

Causal Model

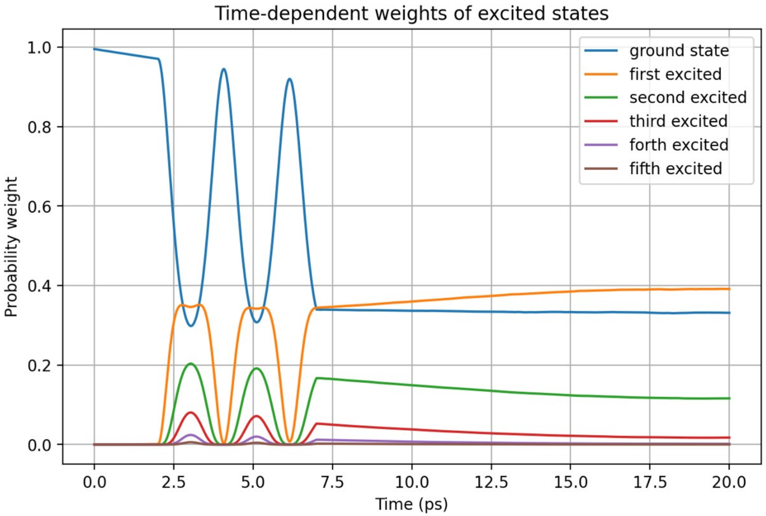


Mean	Standard Deviation	Min	Max
0.98813	0.00447	0.98139	0.99563

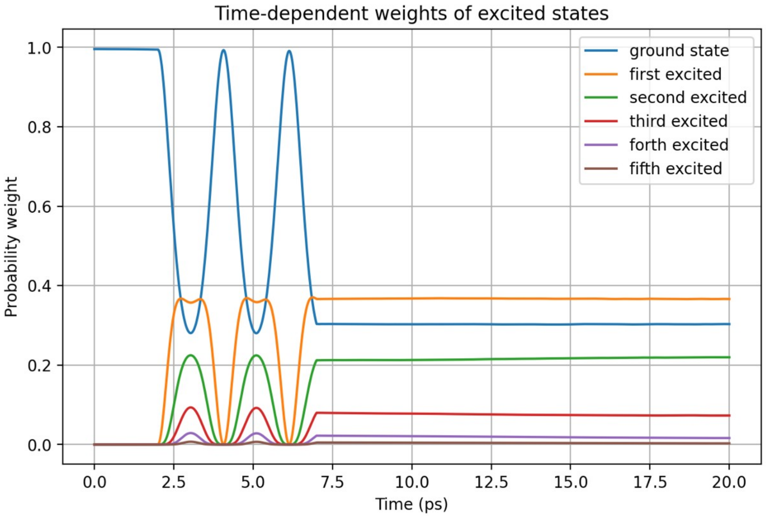
Crank-Nicholson Solution



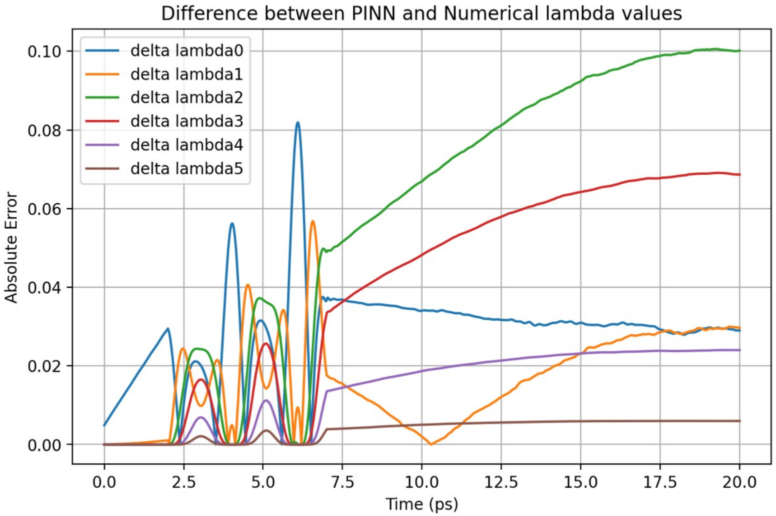
Base Model



Causal Model

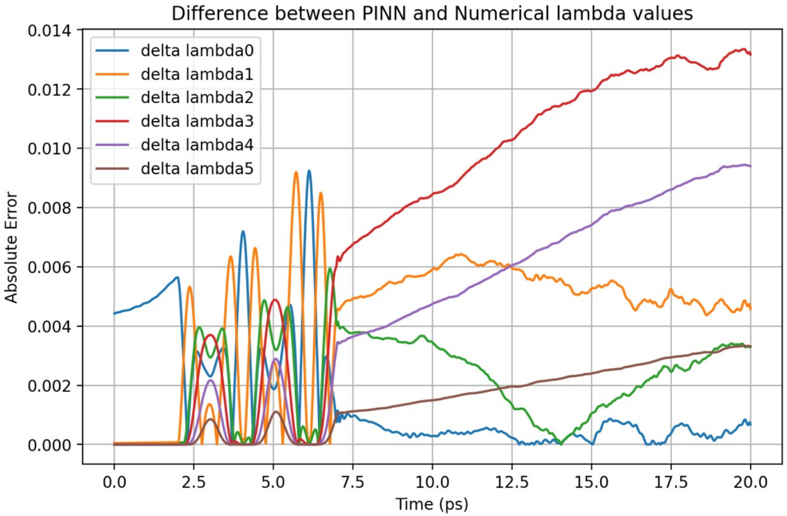


Base Model



Mean	Standard Deviation	Min	Max
0.05787	0.03653	0.00000	0.10055

Causal Model



Mean	Standard Deviation	Min	Max
0.00733	0.00489	0.00000	0.01335

Result Comparison

	$\Delta\Psi^2$ - max	norm - mean	norm - std	$\Delta\lambda_i$ - max
Base Model	0.03409	0.90468	0.04191	0.10055
Causal Model	0.00607	0.98813	0.00447	0.01335

$\Delta\Psi^2$ – max : Maximum deviation in the probability density $|\Psi|^2$ between the PINN and Crank–Nicolson solutions.

Norm – mean : Mean value of the wavefunction normalization over time, indicating how well probability conservation is maintained.

Norm – std : Standard deviation of the wavefunction normalization, reflecting fluctuations in total probability across time steps.

$\Delta\lambda_i$ – max : Maximum difference in the weight coefficients λ_i between PINN and Crank–Nicolson solutions.

Normalization

- When solving the Schrödinger equation, normalization ensures the wavefunction represents a valid probability distribution, which means the probability of finding a particle anywhere is exactly 1
- In the context of solving using PINNs, the wavefunction is not inherently normalized during training, we expect the model to naturally approximate normalization as it learns the correct solution
- However, by explicitly enforcing normalization as an additional term in the loss function, I observed improvement in the model performance

Normalization

- The probability of finding a particle in space is given by the integral of the probability density:

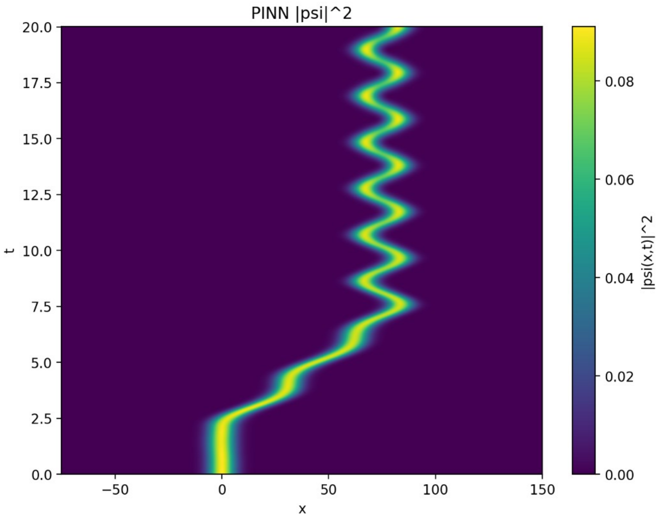
$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx$$

- We use Monte-Carlo approximation to find this integral during training:

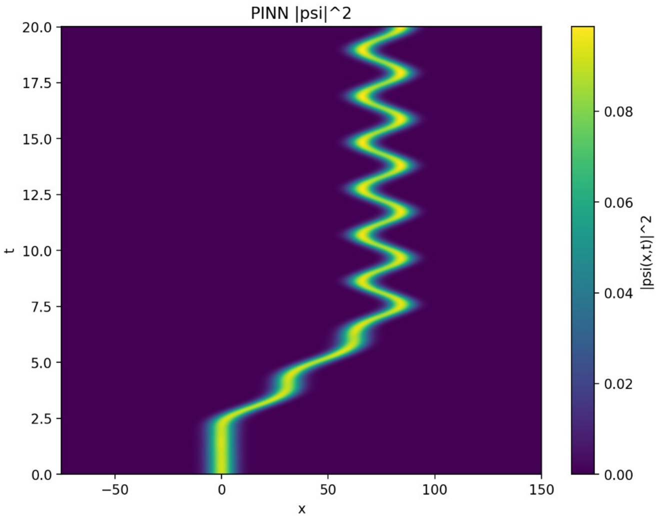
$$(x_{max} - x_{min}) \frac{\sum_{i=0}^{N} |\psi(x_i,t)|^2}{N}$$

Results

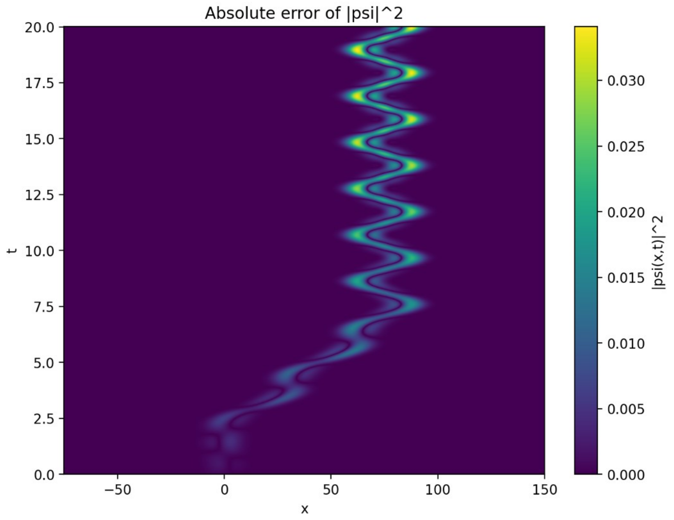
Base Model



Norm Model

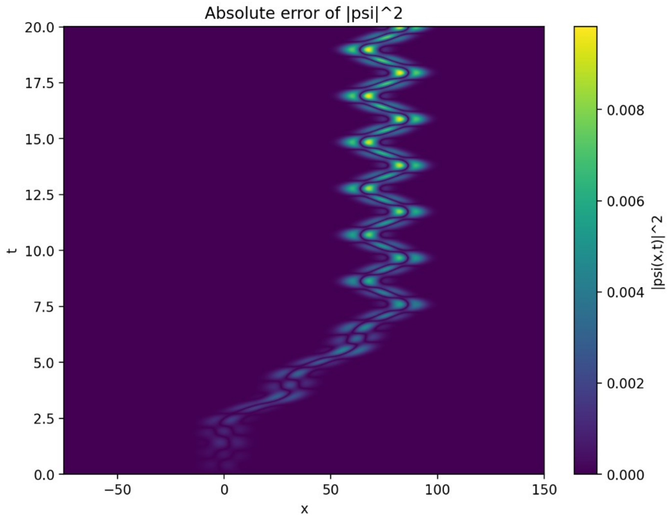


Base Model



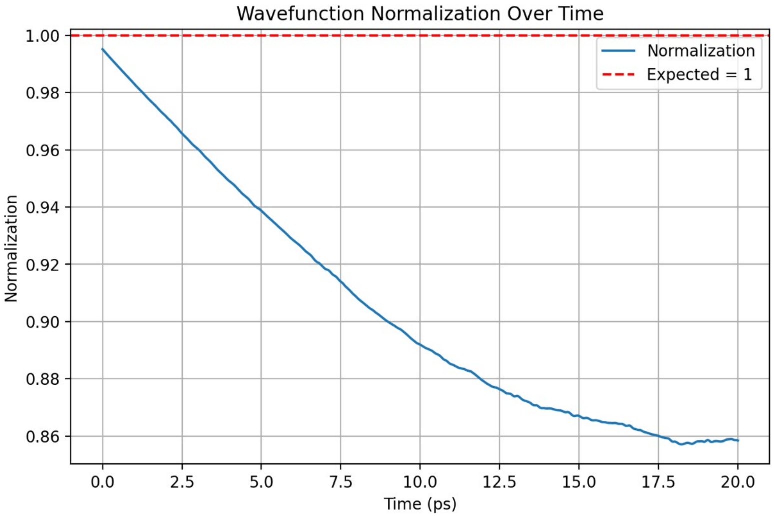
Mean	Standard Deviation	Min	Max
0.00073	0.00303	0.00000	0.03409

Norm Model



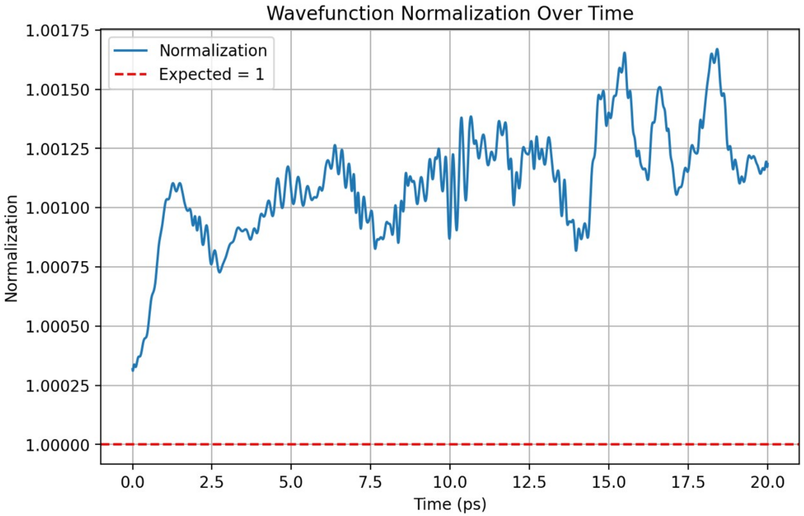
Mean	Standard Deviation	Min	Max
0.00019	0.00077	0.00000	0.00982

Base Model



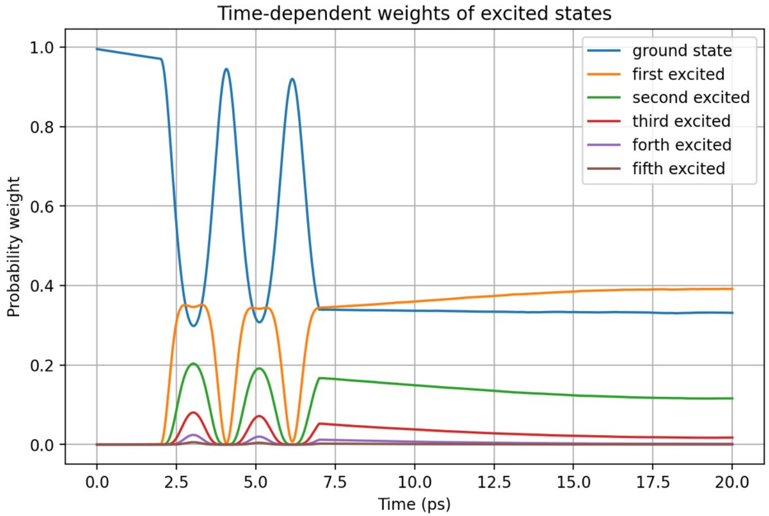
Mean	Standard Deviation	Min	Max
0.90468	0.04191	0.85709	0.99511

Norm Model

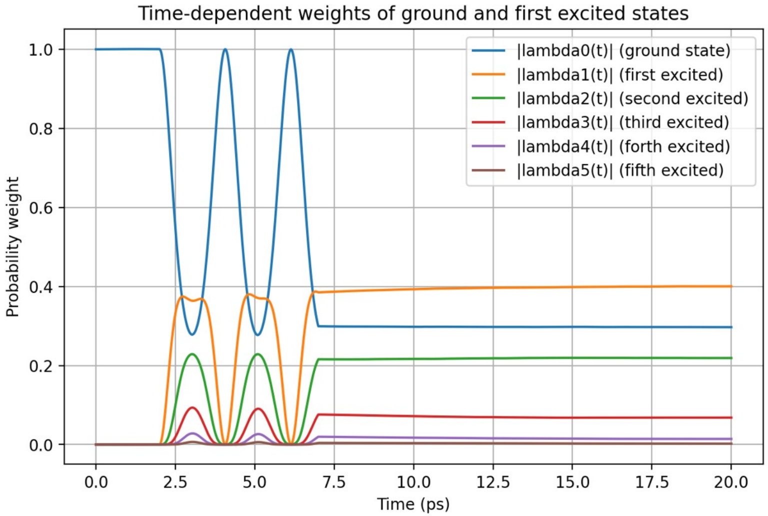


Mean	Standard Deviation	Min	Max
1.00111	0.00023	1.00031	1.00167

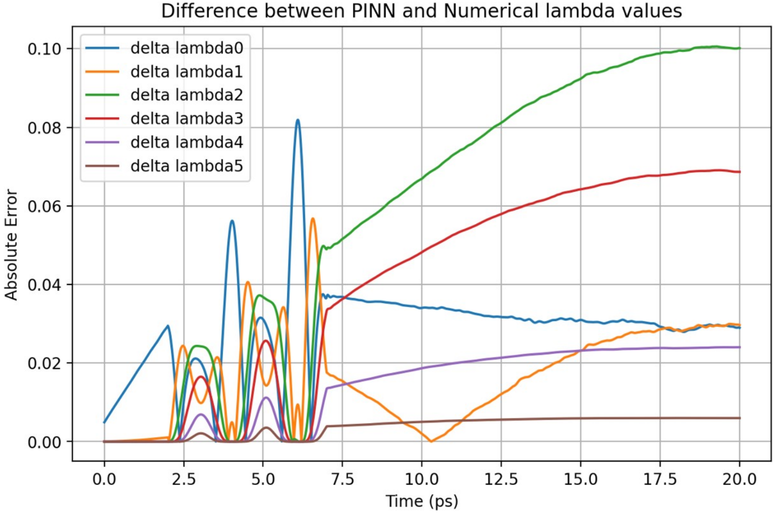
Base Model



Norm Model

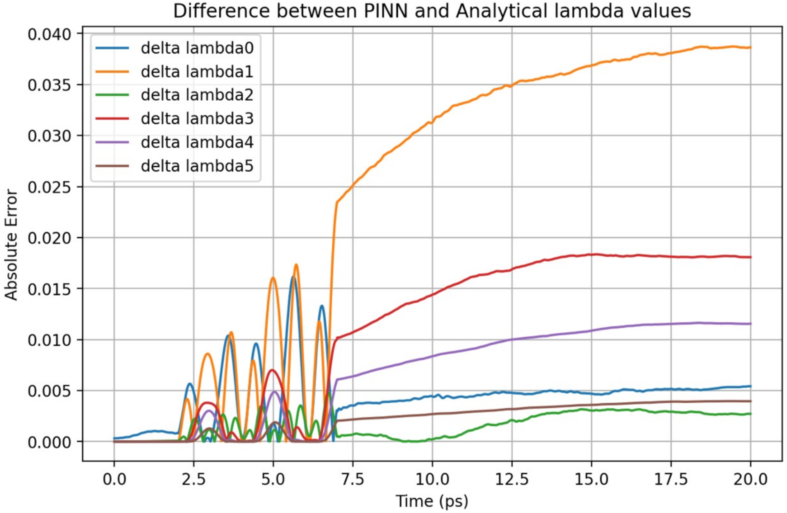


Base Model



Mean	Standard Deviation	Min	Max
0.05787	0.03653	0.00000	0.10055

Norm Model



Mean	Standard Deviation	Min	Max
0.02417	0.01470	0.00000	0.03872

Result Comparison

	$\Delta\Psi^2$ - max	norm - mean	norm - std	$\Delta\lambda_i$ - max
Base Model	0.03409	0.90468	0.04191	0.10055
Norm Model	0.00981	1.00111	0.00023	0.03872

$\Delta\Psi^2$ – max : Maximum deviation in the probability density $|\Psi|^2$ between the PINN and Crank–Nicolson solutions.

Norm – mean : Mean value of the wavefunction normalization over time, indicating how well probability conservation is maintained.

Norm – std : Standard deviation of the wavefunction normalization, reflecting fluctuations in total probability across time steps.

$\Delta\lambda_i$ – max : Maximum difference in the weight coefficients λ_i between PINN and Crank–Nicolson solutions.

Conclusion

- Introduced two key methods that improved the performance of the PINN model for a moving quantum dot
- Enforcing causality made sure that model training respected the time-ordered nature of quantum dynamics during training, leading to improvement in performance
- Normalization enforcement bought the total probability closer to one, stabilizing the wavefunction

Next Steps

- **Increase quantum dot speed**: Speed up the quantum dot movement and compare how the complexity of PINN and Crank-Nicholson is increasing
- **Extend to 2D systems**: Solve the TDSE for a electron in a two-dimensional quantum dot. Check if normalization and causality are improving the performance in higher dimensional models as well

Thank You