INTERNATIONAL CONFERENCE-CUM-ROUND TABLE ON TRANSLATIONAL RESEARCH AND INNOVATION IN BEAM TECHNOLOGIES (ICTRIBT-2026)

Contribution ID: **48** Type: **not specified**

Solving Time-Independent Schrodinger Equation for a Double-Well Potential in Quantum Plasma Systems using Physics-Informed Neural Networks (PINNs)

Background: The time-independent Schrödinger equation is central to the description of bound states and quantum tunneling in double-well potential systems. Such potentials are important in molecular inversion phenomena and can also arise as effective quantum potentials in plasma environments due to external fields, confinement effects, and plasma-surface interactions. Conventional numerical approaches, such as finite-difference matrix methods, rely on spatial discretization and can become computationally demanding for accurate solutions.
Purpose: The purpose of this study is to investigate the applicability of Physics-Informed Neural Networks (PINNs) for solving the one-dimensional time-independent Schrödinger equation with a symmetric double-well potential and to obtain accurate ground and low-lying excited state solutions relevant to quantum plasma systems.
Methods: A Physics-Informed Neural Network framework is employed in which the wavefunction is represented using fully connected feedforward neural networks, while the energy eigenvalues are treated as trainable parameters. The Schrödinger equation is enforced through a residual-based loss function, supplemented by boundary condition, normalization, and orthogonality constraints. Even- and odd-parity neural network architectures are used to directly capture symmetric and antisymmetric eigenstates. The PINN solutions are validated by comparison with reference results obtained from a finite-difference-based matrix diagonalization method.
Results: The PINN approach successfully reproduces the ground and low-lying excited states of the double-well potential. In atomic units ($\hbar = 1$, ⊠ = 1), the ground-state energy is obtained as ⊠0 ≈ 1.973, compared to the finite-difference value ⊠0 ≈ 1.971. The first excited-state energy is predicted as ⊠1 ≈ 2.220, while the corresponding finite-difference result is ⊠1 ≈ 2.012. The second excited-state energy is also well captured, with PINN and finite-difference values of ⊠2 ≈ 4.911and ⊠2 ≈ 4.908, respectively. The small energy separation between the lowest two states reflects the near-degeneracy characteristic of symmetric double-well potentials, arising from quantum tunneling between the wells.
Conclusions: This study demonstrates that Physics-Informed Neural Networks provide an accurate and flexible alternative to traditional numerical techniques for solving the Schrödinger equation with double-well potentials. The approach is suitable for modeling tunneling phenomena and effective quantum potentials in plasma-related systems.

Author: THAKUR, Tanisha (Central University of Himachal Pradesh)

Co-authors: Ms AWASTHI, Ayushi (Central University of Himachal Pradesh); Prof. SASTRI, O.S.K.S. (Central University of Himachal Pradesh)

Presenter: THAKUR, Tanisha (Central University of Himachal Pradesh)