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Physics-Informed Neural Networks based Solver for Time-Dependent Schrödinger Equation

We demonstrate the utility of Physics-Informed Neural Network based solvers for the solution of Time-Dependent Schrödinger Equation. We compare the computational efficiency and convergence behaviour of these solvers to traditional numerical techniques on simple quantum systems. The method developed here can be potentially extended as a surrogate model for the Time-Dependent Density Functional Theory workflow, enabling the simulation of large-scale calculations of electron dynamics in matter exposed to strong electromagnetic fields, high temperatures and pressures.

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