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Object Oriented Structuring of Physics Informed Neural Network Solvers

In this work, we present an end-to-end system leveraging neural networks for objective function optimization in solving the Schrödinger and Dirac Differential Equations. We propose an object-oriented Python programming framework, enabling dynamic adaptation of user input for solving such equations via tunable hyper-parameters. This framework facilitates testing of various network architectures and minimization parameters through structured and extendable classes and methods that share essential attributes required for both equations.

This algorithm is initially applied to the 2-lepton system Muonium (Mu), characterized by a bound energy spectrum, but it can also be utilized for the description of other similar quantum systems. Through a series of ablation experiments, we have examined the effect of various correction terms (Breit, Darwin, etc.) of the Schrödinger Hamiltonian on the optimization in obtaining the corresponding wave functions and energies. Specifically, in solving the Dirac equation we explore several choices of network architecture (e.g., number of neurons, activation functions) for the low-lying energy levels. Our preliminary results indicate that only a few correction terms affect significantly the accuracy of the numerical solution compared to the analytical one.

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