Neural-network-based method for computing multiple excited states of the static Schrödinger equation

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Abstract

A neural-network-based method is proposed to solve the multiple excited-state energies and corresponding wave functions of the static Schrödinger equation. The neural network models are trained by minimizing a specific loss function, in which the main components are the energy and deflation terms. The loss function is trained to obtain the minimum value of the energy term which is the desired energy level. Moreover, the deflation term transforms the energies of all computed states to the appropriate shift, and enables us to compute the next consecutive state. The results show that the accuracy and efficiency of proposed method outperforms other neural-network-based solvers.