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Selected Configuration Interaction using Reinforcement Learning[1] LIHAO YAN, University of Notre Dame, LI ZHOU, Fudan University, CHAO YANG, Lawrence Berkeley National Laboratory, MARK A. CAPRIO, University of Notre Dame — Configuration interaction (CI) is a widely used method for solving quantum many-body problems. The challenge of CI is to solve a large sparse eigenvalue problem. The dimension of the eigenvalue problem grows rapidly as the number of particles and the size of the Slater determinant basis increases. For many problems, the low-lying and ground state eigenfunctions exhibit localization, i.e., most of the CI coefficients are negligibly small. One approach, often referred to as the selected CI method, selects many-body basis functions, i.e., Slater determinants, that have large coefficients to construct a finite dimensional accurate approximation of the many-body Hamiltonian. However, we can only select a small subset of the important basis functions using physical intuition. Typical selected CI algorithms use perturbation theory, but they are not globally optimal. In this work, we use a reinforcement learning (RL) strategy to refine the algorithm. Each state of the RL algorithm corresponds to a particular set of many-body basis. Each action removes some basis and adds new basis into that set. A better set of basis functions is obtained after multiple training episodes. We test the performance of our algorithm against several other selected CI algorithms.

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