Replica exchange molecular dynamics optimization of tensor network states for quantum many-body systems

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Variational quantum Monte Carlo (QMC) method with tensor network states(TNS) has been proved a powerful algorithm for simulating quantum many-body systems. However, because the ground state energy is a highly non-linear function of the tensors, it is easy to be trapped into local minima when optimizing the TNS of the simulated physical systems. To overcome this difficulty, we introduce a replica-exchange molecular dynamics optimization algorithm to obtained the TNS ground states, based on the variational QMC scheme, by mapping the TNS to a classical dynamical system. The method is expected to effectively avoid local minima. We make benchmark tests on a 1D Hubbard model based on matrix product states (MPS) and a Heisenberg J_1-J_2 model on square lattice based on string bond states (SBS). The results show that the optimization method is robust and efficient compared to the exist results.

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