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

Abstract: We introduce a replica exchange molecular dynamics (MD) optimization algorithm to obtain the ground state in the representation of tensor network states (TNS), based on the Monte Carlo sampling techniques, by mapping the energy function of the TNS to that of a classical mechanical system. The method is expected to effectively avoid local minima of the energy functions. We make benchmark tests on a 1D Hubbard model based on matrix product states (MPS) and a 2D Heisenberg J1-J2 model on a square lattice based on string bond states (SBS). The results show that the optimization method is robust and efficient compared to the existing results.

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