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Entanglement renormalization in interacting fermionic systems using single-particle transformations

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Abstract

One of the most powerful and popular quantum entanglement-based computation methods for the simulation of one-dimensional and quasi-two-dimensional strongly correlated materials is the Density Matrix Renormalization Group (DMRG) technique. A lower quantum entanglement between the system's degrees of freedom will result in a higher accuracy of the method. However, quantum entanglement between two complementary subsystems of a closed system depends on how the degrees of freedom have been distributed between them, and therefore, it is not in general invariant under arbitrary unitary transformations. Entanglement is invariant only under those unitary transformations which do not mix the degrees of freedom associated with the two subsystems. Consequently, a fundamental question is that if it is possible to construct, algorithmically, unitary transformations which minimize entanglement between degrees of freedom of the system and therefore maximize the DMRG technique. A general solution to this problem is highly nontrivial in general. In this paper, we study interacting fermionic models and by considering single-particle unitary transformations only. We define a novel and efficient method to find the optimal single-particle unitary transformations. In this framework, we show that using our algorithm, the accuracy of the DMRG method at a given bond dimension is increased and the ground-state energy is decreased and approaches to its exact value. Our method paves the way toward finding more general (many-particle) optimized unitary transformations and helps us to better understand the behavior of fermions in strongly correlated materials.

Keywords: entanglement, Density Matrix Renormalization Group (DMRG), entanglement renormalization, strongly correlated systems, Hubbard model, single-particle unitary transformations

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