

Adaptive mode transformations in fermionic tensor networks

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Non-local fermionic models are frequently encountered in physics, most prominently in quantum chemistry, but also when capturing quantum lattice systems. If strong correlations are present in the system, traditional numerical methods such as HF, CI or CC reach in some instances their limits. In these cases tensor-network methods provide a new way forward at the cost of being more expensive. The long-range nature of the interaction of such systems, however, renders their straightforward numerical simulation using tensor-network methods difficult. When using a DMRG-based method, a suitable reordering of the orbitals will already reduce the computational effort. Still, one has more freedom to preprocess the Hamiltonian by means of unitary transformations from one set of fermionic modes to another, aiming at minimising the entanglement present in the system. Here, we present an adaptive method that aims at combining advantages arising from suitable local mode transformations and matrix-product updates "on the fly" in an iterative fashion. Our results - both for lattice models and for systems in quantum chemistry - show that by including such local mode transformations and applying known reordering techniques, one finds good approximations of the ground state already for low bond dimensions and optimises the entanglement structure present in the ground. In addition, in cases where they can be identified in advance, we are able to approximately recover optimal global mode transformations from the local ones for medium sized systems.