Simulating Strongly Correlated Quantum Systems with Tree Tensor Networks

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We present a tree-tensor-network-based method to study strongly correlated systems with nonlocal interactions in higher dimensions. [1] Although the momentum-space and quantum-chemistry versions of the density matrix renormalization group (DMRG) method have long been applied to such systems, the spatial topology of DMRG-based methods allows efficient optimizations to be carried out with respect to one spatial dimension only. Extending the matrix-product-state picture, we formulate a more general approach by allowing the local sites to be coupled to more than two neighboring auxiliary subspaces. Following [2], we treat a tree-like network ansatz with arbitrary coordination number z, where the $z = 2$ case corresponds to the one-dimensional scheme. For this ansatz, the long-range correlation deviates from the mean-field value polynomially with distance, in contrast to the matrix-product ansatz, which deviates exponentially. The computational cost of the tree-tensor-network method is significantly smaller than that of previous DMRG-based attempts, which renormalize several blocks into a single block. In addition, we investigate the effect of unitary transformations on the local basis states and present a method for optimizing such transformations. For the 1-d interacting spinless fermion model, the optimized transformation interpolates smoothly between real space and momentum space. Calculations carried out on small quantum chemical systems support our approach.

References

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[2] Shi et. al., Phys. Rev. A, 74, 022320 (2006).