Exploring an Alternative Tensor Network Ansatz for Fermionic Systems

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We introduce and study an alternative tensor network ansatz for fermionic many-body systems. Specifically, we suggest a tensor factorization scheme that automatically takes care of the antisymmetry of fermionic many-body tensors via appending layers of the so-called ordering projectors to a chosen tensor network decomposition. In contrast to traditional tensor network theory, we do not use spin site mapping and the corresponding occupation number representation. Instead, we directly work with fermionic many-body tensors either in the particle or hole-particle representation. Thus, the size of our ansatz only depends on the number of correlated particles/holes, but not on the basis set size. Furthermore, our ansatz allows us to work directly with the original Hamiltonian tensors without the need to perform the Jordan-Wigner transformation or compute some factorized form. It also allows computing the 1- and 2-body low-rank reduced density matrices of fermionic many-body systems in a standard particle/hole representation. The evaluation of the reduced density matrices Hamiltonian expectation values as well as gradients with respect to the parameterizing tensor factors can be efficiently parallelized on multicore and multi-node computing platforms. However, the absolute computational cost of the full configuration interaction (FCI) method approximated by our ansatz is still higher than that of the traditional tensor network formalism due to our current inability to exploit the highly sparse nature of the ordering projectors. As such, the main goal of this presentation is to introduce an alternative fermionic tensor factorization scheme and describe its pros and cons.

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