Tensor Network Theory for Direct Simulations of Fermionic Ab Initio Hamiltonians on High Performance Computing Platforms

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Tensor network theory provides a well-developed mathematical framework for constructing efficient low-rank approximations of arbitrary tensors. As a numerical simulation technique, it has proven its power in condensed matter physics and quantum chemistry where it is used for constructing quantum many-body wavefunctions of the ground (and, sometimes, excited) states of the many-body Hamiltonians describing strongly interacting spins, bosons and fermions, in particular electrons. Although the many-body tensors constituting quantum-chemistry Hamiltonians expressed in second quantization are anti-symmetric with respect to the permutations of the electronic degrees of freedom, the standard tensor network machinery requires remapping of the particle Hamiltonians to the spin-site Hamiltonians by considering (spin-)orbital occupation numbers as effective 2- or 4-D spin spaces. As an alternative, here we are exploring a more direct technique where we keep the standard normal-ordered second-quantized Hamiltonian representation intact while slightly modifying the tensor network ansatz to enforce the fermionic symmetry. Although the resulting approach has a higher computational cost, the tensors entering the corresponding equations are larger and denser, making their processing more efficient on modern heterogeneous (GPU-accelerated) HPC architectures. The latter task is accomplished via the tensor network processing library ExaTN developed by us that can build and process arbitrarily complex tensor networks on any type of major computer hardware, from laptops to GPU-accelerated leadership HPC systems. We present the features and functionality of the ExaTN library and discuss its strengths in hope to facilitate the adoption of advanced tensor network representations in the electronic structure methods implemented in software packages widely used by quantum chemistry community.

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