Sparse and symmetry-preserving compression of tensor trains arising in quantum chemistry

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The quantum chemical density matrix renormalization group (QC-DMRG) is regarded as a powerful method for the resolution of the ground state energy of the many-body electronic Schrödinger equation. The construction of the quantum chemical Hamiltonian operator in matrix product or tensor train (TT) form is at the core of the QC-DMRG algorithm. Although the ranks of the exact TT representation grow quadratically with the system size d, $O(d^2)$, it can be reduced using the TT-SVD algorithm. However, this might destroy the sparsity as well as the symmetries of the original operator if it is not carefully done.

This study shows that the TT format of the Hamiltonians in QC-DMRG has an inherent structure that can be exploited to get a sparse and symmetry-preserving scheme. It is well known that the quantum chemical Hamiltonian has a variety of symmetries that can be exploited to design a more efficient TT representation. This not only results in reducing the computational cost but also preserves the properties of the original operator that are crucial for an accurate simulation. Therefore, we demonstrate that enforcing abelian symmetries such as the particle number results in a sparse block structured form in the TT cores of the TT representation of the Hamiltonian operator, leading to a symmetry-preserving, more structured, and organized representation, allowing for faster computation and manipulation.

In conclusion, this study highlights the potential for exploiting the new structure of the TT-cores of the TT representation of the Hamiltonian operator which can be used to reduce the cost of operations involved in the QC-DMRG algorithm.

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