New Density Matrix Renormalization Group Approaches for Describing Quantum Many-body Systems under a Large Correlated Environment

Haibo Ma

Qingdao Institute of Frontier and Interdisciplinary Science, Shandong University, Qingdao 266237, China

Email: haibo.ma@sdu.edu.cn

Benefited by the efficient compression and localized representation of quantum states in its wave function's matrix product state (MPS) formulation, density matrix normalization group (DMRG) and its time-dependent variant (TD-DMRG) have been established as one of the most accurate methods in simulating the electronic structure and quantum dynamics of strongly correlated molecules with a large number of quantum degrees of freedoms (active orbitals or vibrational modes). However, the quantitative characterization of the quantum many-body behaviors of realistic strongly correlated systems requires a further consideration of the interaction between the embedded active subsystem and the remaining correlated environment (e.g. a huge number of external orbitals in quantum chemistry, or the infinite number of phonon modes in the condensed phase environment in quantum dynamics), which is intractable for DMRG and TD-DMRG. Here, we introduce our recent efforts on developing new DMRG and TD-DMRG approaches for accounting for these environmental effects: (1) Noticing that the DMRG wave function is highly redundant in the determinant space for chemical molecules, we introduced a stochastic approach to truncate and reconstruct the DMRG wave function. Further combined with the idea of external contraction (ec) and multi-reference configuration interaction (MRCI), we formulated a DMRG-ec-MRCI approach, which bypasses the bottleneck of computing high-order reduced density matrices (RDMs) and can hence handle much larger active spaces than other post-DMRG approaches. (2) We proposed a hierarchical mapping algorithm (HM) for TD-DMRG which uses quantum information theory (QIT) to identify a small number of effective environmental phonon modes couple to the system directly and performs block Lanczos transformations on the remaining indirect modes to transform the Hamiltonian matrix to a nearly block-tridiagonal form and eliminate the long-range interactions.

References:

1. Z. Luo, Y. Ma, X. Wang, H. Ma, *J. Chem. Theory Comput.* 14, 4747-4755 (2018).
2. Y. Xu, Z. Xie, X. Xie, U. Schollwöck, H. Ma, *JACS Au* 2, 335-340 (2022).
3. Y. Cheng, Z. Xie, H. Ma, *J. Phys. Chem. Lett.* 13, 904-915 (2022).
4. Y. Tian, Z. Luo, H. Ma, *J. Chem. Theory Comput.* doi: 10.1021/acs.jctc.2c00632 (2022).
5. H. Ma, U. Schollwöck, Z. Shuai, *Density Matrix Renormalization Group-based Approaches in Computational Chemistry*, Elsevier, Amsterdam (2022).