Multireference Driven Similarity Renormalization Group Truncated to One- and Two-Body Operators

Chenyang Li and Francesco A. Evangelista

Department of Chemistry and Cherry Emerson Center for Scientific Computation, Emory University, Atlanta, GA, 30322

We extend the driven similarity renormalization group (DSRG) theory[1,2] to a multi-configuration reference wavefunction based on the generalized normal ordering of Kutzelnigg and Mukherjee.[3] In the DSRG ansatz, the Hamiltonian is partially unitary-transformed to include dynamic correlation effects, and the cluster amplitudes are determined by a set of many-body conditions.[4] The DSRG thus helps build simple and robust multireference (MR) theories: (1) the partial transformation of the Hamiltonian ensures the avoidance of intruders, and (2) the many-body conditions solve the redundancy problem of the excitation manifold. Moreover, the complexity of MR-DSRG is independent with respect to the number of configurations in the reference wavefunction. In this work, we approximate the MR-DSRG equations by truncating the operator rank to at most two-body interactions, and apply a recursive linear commutator approximation of the Baker–Campbell–Hausdorff expansion. The resulting MR-LDSRG(2) theory requires only 39 diagrams and scales as $\mathcal{O}(H^2P^2N^2)$. Here H, P, and N stand for the number of hole (core + active), particle (active + virtual), and total orbitals, respectively. Finally, the MR-LDSRG(2) is compared to MR configuration interaction and MR coupled cluster theory with singles and doubles on the dissociation of N_2 ($X\,^1\Sigma_g^+$).

References

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