Combining the Density Matrix Renormalization Group with Selected Configuration Interaction

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The density matrix renormalization group (DMRG) is a powerful method for solving quantum chemical systems with significant static correlation [1]. However, DMRG becomes too expensive for systems with very large active spaces (number of orbitals). Here, we propose to combine selected configuration interaction (SCI) techniques [2] with the DMRG. This is done by grouping orbitals located at the same atom into one site in the DMRG. The number of atoms then corresponds to the number of sites. Accordingly, the underlying representation of the DMRG describes selected many-body configurations instead of orbital occupations as is the case in conventional DMRG. The previously proposed active space decomposition (ASD) DMRG [3] is similar, but fundamentally differs by a restricted-active-space-based configuration selection and by using whole molecules as sites. Our SCI-based DMRG requires much smaller bond dimensions than conventional DMRG and is more general than ASD-DMRG. Preliminary results on hydrogen chains are presented.

References

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