Density matrix renormalization group with dynamical correlation via adiabatic connection

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The quantum chemical version of the density matrix renormalization group (DMRG) method [1] has established itself as one of the methods of choice for calculations of strongly correlated molecular systems [2]. Despite its great ability to capture strong electronic correlation in large active spaces, it is not suitable for computations of dynamical electron correlation. In this conference contribution, we will present our recent work on electronic structure problem of strongly correlated molecules [3], in which DMRG is responsible for a proper description of the strong correlation, whereas dynamical correlation is computed via the adiabatic connection (AC) technique [4] which requires only up to two-body active space reduced density matrices. We will report benchmark results on different transition metal complexes.

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