Useful Parameters of DMRG for Everyday Quantum Chemistry Applications

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DMRG has been utilized to probe the character of acenes, to perform FCI calculations on diatomics, including Cr_2, and a wide array of large inorganic systems. Despite its successes to treat highly-correlated chemical systems, its usage has not expanded beyond the specialized research group. Principally, the wave-function ansatz needed requires both a particular set of orbitals, as well as a specific ordering to recover the appropriate correlations. In the present contribution, we provide a set of rules to enable the widespread use of DMRG for finite chemical systems. Specifically, we provide insight on the type and shape of orbitals that are useful in different situations, the degree of dimensionality that a system can be adequately described, and the effect of orbital ordering and noise and their effects of convergence. We will present these rules based on CASCI and CASSCF calculations using polyaromatic hydrocarbons and transition metal complexes. The latter includes systems that have complicated spin states that have been to-date difficult to elucidate using both single-reference methods and (small) active spaces.