Generalized tensor methods and entanglement measurements for electronic structure calculations

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In the past decade, we have witnessed a breakthrough in electronic structure calculations due to the density matrix renormalization group (DMRG) method invented by S. R. White [1,2] which has become in recent years a rival to the conventional multiconfiguration wave function approaches [3-5]. Inclusion of the concepts of entanglement from quantum information theory (QIT) [6,7] has paved the road for identifying highly correlated molecular orbitals leading to an efficient construction of active spaces [6,8] and for characterizing the various types of correlation effects relevant for chemical bonding [9]. Quite recently, a reformulation of DMRG in terms of so-called matrix product states (MPS) has shown that it is only one special case in a much more general set of methods: the so-called tensor network states (TNS) [10], which is expected to even outperform DMRG/MPS in the near future [11,12].

In this tutorial contribution, we present an overview of the quantum chemistry version of the DMRG/MPS and tree-TNS algorithms and their applications to transition metal complexes [13]. Data sparse representation of the wavefunction in MPS and TNS is also investigated through advances in entanglement localization providing optimized tensor topologies. Entropy generation by the RG procedure, the mutual information leading to a multiply connected network of orbitals, reduction of entanglement by basis transformation and a configuration interaction based procedure which extends the active space dynamically (CI-DEAS) will be discussed.

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