Quantum chemical density matrix renormalization group, entanglement optimizations, and dynamical correlation extensions

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In this talk, the basic concepts of the quantum chemical density matrix renormalization group (QC-DMRG) method [1] will be overviewed. QC-DMRG, as the simplest from the family of tensor network state methods, has been developed extensively over the last decade and is now undoubtedly a well-established powerful multireference method capable of treating very large active spaces. The key ingredient of all the tensor network state methods is the entanglement (of the studied system) and its controlled manipulation is in fact essential for the efficiency of those methods. Recent developments of the local fermionic orbital optimization [2], which relies on the entanglement manipulation, will also be presented. Last, but not least, as the QC-DMRG active space in spite of being large cannot usually be the full Hilbert space, methods for computation of the missing dynamical correlation are necessary. The recently developed method combining the coupled cluster (CC) theory with QC-DMRG in the spirit of the tailored CC method [3, 4] will be discussed.

[1] S. Szalay *et al.*, *Int. J. Quant. Chem.* **115** (2015) 1342.

[2] C. Krumnow, L. Veis, Ö. Legeza, and J. Eisert, *arXiv:1504.00042*.

[3] T. Kinoshita, O. Hino, and R. J. Bartlett, *J. Chem. Phys.* **123** (2005) 074106.

[4] L. Veis, A. Antalik, Ö. Legeza, and J. Pittner, *to be submitted*.