New Parameterizations of the Electronic Wave Function: From DMRG to Tensor Network States

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Over the last decade, we have witnessed the rise of the Density Matrix Renormalization Group (DMRG) algorithm in quantum chemistry [1] which had been successfully introduced in condensed matter physics. We showed that the DMRG algorithm is even applicable for non-linear, compact molecules like transition metal complexes and clusters [2] and proposed an extrapolation scheme that is able to control the error in the electronic energy during the iterations in order to provide an estimate for the converged energy and a criterion for terminating the iterations [3]. In the past few years, the DMRG algorithm has been discussed in terms of the parametrization of the wave function that is iteratively constructed. While we have decomposed the DMRG wave function in terms of a Slater determinant basis [4], which makes it comparable to a configuration-interaction (CI) wave function and thus analyzable, Rommer and Östlund showed already in 1995 that the DMRG wave function can be described as a matrix product state. Their work laid the foundations for a new family of states, the so-called tensor network states. The basic idea of tensor network states is to approximate the ground-state wave function of a strongly correlated system by constructing the complex high-dimensional CI coefficient tensor of a full-configuration-interaction wave function from a comparatively small set of coefficients relating the one-electron states. So far such states have been studied by several groups for simple spin Hamiltonians only. We have now analyzed electronic wave functions constructed in terms of such tensor network states for the full quantum chemical many-electron Hamiltonian [5].

Literature:

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