What can Hartree-Fock theory tell us about the density matrix renormalization group?

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The density matrix renormalization group (DMRG) has an underlying variational ansatz, the matrix product state (MPS). The accuracy of this ansatz is controlled by its virtual dimension. In most applications for quantum chemistry this parameter is very large, and the high-accuracy or FCI regime is studied. With a good orbital choice and ordering, and by exploiting the symmetry group of the Hamiltonian, DMRG then allows to retrieve highly accurate results in active spaces beyond the reach of FCI [1,2].
However, DMRG can also be of use with smaller virtual dimensions. I will discuss how fundamental ideas from Hartree-Fock (HF) theory are transferable to DMRG. Both methods have a variational ansatz. The time-independent variational principle leads for HF and DMRG to a self-consistent mean-field theory in the particles and lattice sites, respectively. The time-dependent variational principle results in the random-phase approximation (RPA). RPA reveals the elementary excitations: particle and site excitations for HF and DMRG, respectively. Exponentiation of these excitations provides a nonredundant parameterization of the ansatz manifold, formulated by Thouless' theorem. A Taylor expansion in the nonredundant parameters leads to the configuration interaction expansion [3,4].

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