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Sliced Basis Density Matrix Renormalization Group

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The density matrix renormalization group (DMRG) and other tensor network algorithms have had tremendous success in simulating quantum lattice models. Formulated as a conventional wavefunction post-Hartree-Fock method, quantum chemistry DMRG (QCDMRG) now plays an important but limited role for the electronic structure of strongly correlated small to medium sized molecular systems. The key limitation of QCDMRG is non-optimal scaling of the computation time with the number of basis functions N.

Our recently introduced Sliced Basis DMRG (SBDMRG) uses conventional Gaussian basis functions only in two directions, while using a grid in the third direction, corresponding to the long direction of a chain or molecule. The complete locality in one direction reduces the number of Hamiltonian terms from N^4 to N^2. Using a compression method for these terms, we obtain a linear scaling algorithm. Sliced-basis DMRG produces near-exact correlated ground states within its basis. We have implemented SBDMRG for chains of hydrogen atoms, where we have been able to simulate up to 1000 atoms in a minimal basis.