Title: Open-Shell Tensor Hypercontraction

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Abstract

An extension of the least-squares tensor hypercontraction (LS-THC) approach to open shell MP2 and MP3 is presented. Complexity arising due to presence of Electron Repulsion Integrals (ERIs) is well known as a bottleneck in quantum chemical methods to steep scaling of the computational costs with the number of electrons. The LS-THC method is one of efficient approaches to approximate the ERI tensor, which has shown significant potential for practical application based on our previous work on closed shell MP3. In this method, the fourth order ERI tensor was expressed as a product of five second-order matrices, four of them are the orbitals evaluated at the grid points, the other one is core matrix evaluated at grid points matrices by fitting the wavefunction components, which paves the way to significant scaling through factorization. Continuing with previous work, the application of LS-THC to open shell MP2 and MP3 was performed using a mixed graphical-algebraic technique for deriving the working equations. Extension of THC-MP2 and -MP3 to open-shell systems will allow for the efficient calculation of molecular ions, radicals, and other reactive species. We will evaluate the energy errors and efficiency of our implementation for standard test systems as well as representative chemical reactions.