Linear and Quadratic Internally Contracted Multireference Coupled-Cluster Approximations

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The reliable description of molecular phenomena, such as excitation energies and magnetic properties, often requires an accurate electronic wavefunction that goes beyond the scope of single-reference coupled-cluster techniques. Internally contracted multireference coupled-cluster (icMRCC) can be used to provide these accurate benchmark results and, when combined with embedding schemes, investigate large molecular complexes.
However, the standard icMRCC equations can become computationally expensive to solve, particularly if the embedding region in a molecule needs to be increased to capture the relevant chemistry. This is primarily due to the large number of terms that arise in the energy and amplitude equations which can far exceed the number of corresponding terms in single-reference coupled-cluster.
In response to this to this problem, linear and quadratic approximations have been developed which aim to decrease the computational expense and increase the scope and usage of icMRCC. These have been inspired by older methods, like the well known CEPA(0) approximation, based upon the unlinked coupled-cluster formalism. The approximations are benchmarked against full configuration interaction, to investigate the accuracy and shed light on interesting features of these methods. The quintet-triplet splitting energy of an $FeC_{72}N_2H_{100}$ complex is also investigated, suggesting a future use of these approximations.