A Power Series Approximation in Symmetry Projected Coupled Cluster Theory

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Abstract

Projected Hartree-Fock theory provides an accurate description of many kinds of strong correlations but does not properly describe weakly-correlated systems. On the other hand, single-reference methods such as configuration interaction or coupled cluster theory can handle weakly-correlated problems but cannot properly account for strong correlations. Ideally, we would like to combine these approaches in a symmetry-projected coupled cluster approach, but this is far from straightforward. In this work, we provide an alternative formulation to identify the so-called disentangled cluster operators which arise when we combine these two methodological strands. Our formulation shows promising results for model systems and small molecules.