General-Order Spin-Free Coupled-Cluster method

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A general-order coupled-cluster method is formulated using spatial orbitals, for both closed- and open-shell states. For open-shell states, we extended the partial-spin adaption scheme (Theor. Chem. Acc., 79, 1 (1991); J. Chem. Phys. 99, 5219 (1993)) to the full configuration-interaction limit by systematically improving the spin adaption. Additionally, double-coset techniques was used to simplify the canonicalization procedure (Comput. Phys. Commun. 157, 173 (2004)).