# Perturbative treatment of higher excitations in coupled-cluster theory

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Possibilities for the approximate treatment of higher excitations in coupled-cluster (CC) theory are discussed. Potential routes for the generalization of corresponding approximations to lower-level CC methods are analyzed for higher excitations. A general string-based algorithm is presented for the evaluation of the special contractions appearing in the equations specific to those approximate CC models. It is demonstrated that several iterative and non-iterative approximations to higher excitations can simply be implemented with the aid of our algorithm and that the coding effort is mostly reduced to the generation of the corresponding formulas. The performance of the proposed and implemented methods for total energies and thermochemical properties is assessed with special regard to quadruple and pentuple excitations. The applicability of our approach is illustrated by benchmark calculations for the butadiene and benzene molecules. Our results demonstrate that the proposed algorithm enables us to consider the effect of quadruple excitations for up to 10-12 atoms.