Nonrelativistic and Relativistic General Coupled Cluster Theory

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A novel method for performing coupled cluster calculations using an arbitrary excitation manifold from a single reference determinant is outlined. The new algorithm has the same operation count as traditional coupled cluster programs, where all interactions were explicitly coded. As examples of the possibilities of the new code, the dissociation of N_2 and the vibrational frequencies of O_3 are discussed. The generalization of the algorithm to relativistic two- and four- component methods are finally briefly discussed.