Analytic gradients of EOM-CCSD*

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Understanding the process of molecule photoexcitation is crucial in various fields, including drug development, materials science, photovoltaics, and more. Two fundamental questions guide our exploration: What is the potential energy surface, and what are the molecular properties? Central to answering these inquiries is the evaluation of electronic energy derivatives. The introduction of the Z vector method has significantly enhanced the computational efficiency of analytic energy gradients. Owing to the favorable accessibility and predictable accuracy over a wide range of chemical problems, equation of motion coupled cluster singles and doubles (EOM-CCSD) has become the to-go method for predicting excited state properties. The great promise of the method has led to the implementation of analytic gradients of EOM-CCSD and numerous successful applications. However, challenges arise in specific cases where the inclusion of triple excitations becomes essential. Motivated by this need, EOM-CCSD* is developed to incorporate perturbative triple excitations. In what follows, we present a detailed formulation and implementation of analytic EOM-CCSD* energy gradients.