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# Are We There Yet? Implementation of All Triple Excitations in the Linearized Coupled Cluster Method

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## Abstract

The coupled-cluster (CC) method, originally developed for the needs of nuclear physics, is widely used in atomic physics and quantum chemistry as well. Its linearized version is used to perform high-precision calculations of different atomic properties. The CC method explores the state of an atomic system as a combination of excitations. It involves evaluation of all possible excitations - single (one excited electron), double (two electrons), etc. While the theory of the method is well developed, the implementation of the triple excitations is a computationally demanding task. Various approximate methods of including the triple excitations have been proposed. Some of them have become standard approaches routinely included in program packages. The most recent implementation includes the contribution of only valence triples. I will present my work on developing a code including and iterating the triple excitation amplitudes in the framework of the all-order method (linearized CC) used in our research group. The main computational issue comes from the storage requirements of the triple excitation amplitudes. Other implementations of the method usually avoid storing or even keeping those amplitudes in memory during the computation. For the sake of efficiency, a choice must be made based on the I/O time needed to access the pre-calculated array and the CPU time needed to evaluate the expressions involving the triple amplitudes. These expressions are complicated and the plan of action is not straightforward. In my presentation, I will explore the computational challenges and possible solutions involved in this research project.