A New "Better Than CCSD" Method for EOM-CC Calculations

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A new theoretical method, CCSD(T)(a), is presented which includes a non-iterative "CCSD(T)-like" ground state correction to CCSD, as well as a natural extension to excited and ionized states using equation-of-motion theory (EOMEE and EOMIP, respectively). EOMIP-CCSD(T)(a) performs a full diagonalization in the 3h2p space using modified CC amplitudes for an overall cost which scales as N^7. For excited states, full EOMEE-CCSD(T)(a) scales as N^8, but can be reduced to N^7 by using the non-iterative EOMEE-CCSD* correction of Saeh and Stanton for the excited state (giving EOMEE-CCSD(T)(a)*). Results are presented for a variety of excited and ionized states, and the method is found to compare favorably to EOMEE- and EOMIP-CCSDT in many cases, particularly when properties of potential energy surfaces are compared.