Higher order contributions to LinearCCD

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The search for a better second-order perturbation theory for post Hartree-Fock correlation energy calculations is an important and fruitful avenue of current research. Over the past decade much progress has been made in various approximations to standard second order many-body perturbation theory using resolution-of-the-identity like methods or more straight forward ideas involving scaling the $\alpha\alpha$ and $\alpha\beta$ correlation contributions. Approaching the problem differently by looking for the optimal correlation energy while not requiring the best resulting scaling, second-order coupled cluster perturbation theory (CCPT(2), also notably recognized as linear CCD) is a promising infinite order method useful for the computation of molecular energies, gradients and Hessians. In this work we use a further perturbative expansion to derive consistent higher order contributions to the CCPT(2) energy. Using several prototypical systems we investigate the numerical effects of including these higher order terms.