

The intermediate state EOM-CC approach for doubly excited dark states

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EOM-CCSD is a well-established method for obtaining excited states dominated by single excitations such as open-shell singlets. But excited states with significant double excitation contribution are not adequately treated by EOM-CCSD. Such states often required EOM-CCSDT and sometimes even EOM-CCSDTQ to be treated right. These methods are computationally demanding methods that scale as n^8 and n^{10} , respectively. Here we propose the intermediate state approach to obtain doubly excited states using EOM-CCSD, that scales as n^6 . Traditionally, EOM-CC is performed on a closed shell reference state for it has a well-described single-reference coupled-cluster (SRCC) wavefunction. This poster discusses our attempt on performing EOM-CCSD on a low spin open-shell reference state and its benefits. Considering spin contamination of such states with SRCC, various tools to obtain a better $M_s=0$ triplet state and open-shell singlet single reference CC wavefunction will be discussed. The accuracy of this approach is demonstrated with various examples.