

Double excited states with EOM-CCSD

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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 dominated by double excitations are not accurately treated by EOM-CCSD. Even though double excitations are in the projection manifold of EOM-CCSD, triple excitations are required to provide a relaxation effect, which is an essential part of obtaining the correct answer. So, such states often required EOM-CCSDT and sometimes even EOM-CCSDTQ to be treated right. These are computationally demanding methods that scale as n^8 and n^{10} , respectively. Doubly excited closed-shell states are non-dipole allowed, making it spectroscopically dark. So, the availability of an appropriate theoretical method for such states can provide us with valuable information that cannot be gained from experiments. Here we explore the idea of using EOM-CCSD, which scales as n^6 , with an open shell determinant as a reference determinant to obtain doubly excited states.