EOM-CCSD and EOM-MBPT(2) calculations with natural transition orbitals

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We present the excited state calculations based on the equation-of-motion coupled-cluster with single and double excitations (EOM-CCSD) and the second-order many-body perturbation theory (EOM-MBPT(2)). With the use of the natural transition orbital (NTO), the particular excitation, $I{\rightarrow}A$ is emphasized. We compare the single NTO excitations and discuss the reliabilities for different types of NTOs. Based on the simplified description of the NTO, we also propose the efficient scheme for the excited state. The reductions of single and double excitation vectors are discussed for the Rydberg and valence excitations.