Universal state-selective approach to multi-reference coupled-cluster theory

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In recent years one could witness an intensive development of theoretical formulations for dealing with quasi-degenerate electronic states. This effort incorporates formalisms driven by various design principles to account for the electron correlation effects including: multi-reference many-body perturbation theory (MRMBPT), density matrix renormalization group (DMRG) techniques, and (3) multi-reference coupled-cluster (MRCC) methodologies.   In this presentation, we will outline universal state-selective MRCC formalism for describing multi-reference systems.   In particular, we will analyze flexibility of the universal state-selective approach in adopting various sufficiency conditions underlying state-specific MRCC formulations. We will also discuss its size-extensivity, approximate invariance under rotations of active-orbitals, and efficiency in addressing intruder-state problem.