

Tailored Coupled Cluster method for multi-determinantal problems

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Single reference coupled cluster methods are well established that it gives the most accurate results for most non-degenerate closed-shell ground states. However, it can be inadequate when the zeroth-order wavefunction is dominated by more than one Slater determinant. Here we tailor SR-CC theory to approximately treat multi-determinantal cases by keeping few amplitudes fixed to predetermined values from an external source. We report this scheme being applied to excited states, open-shell molecules, and bond-breaking cases. For excited states, we determine appropriate amplitudes from spin and spatial symmetry. And for bond breaking cases, we use GVB as an external source to determine the dominant amplitudes. This scheme is expected to accelerate the process of approaching the exact solution which is generally achieved by including higher cluster operators. We also analyze the dependence of reference orbital on the wavefunction obtained from tailored CC.