Embedding Schemes Applied to Strongly Correlated Systems

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Two different embedding schemes are presented to study strongly correlated systems. In the first approach, an embedded FCI (full Configuration Interaction) is performed on top of the Distinguishable Cluster approximation (DCSD) [1]. In order to analyse the accuracy of this metod, a uniform dissociation of a 1D H-chain is studied. The latter still represents a difficult case for conventional methods [2]. In the second, a CEPA (Coupled-electron pair approximation) [3, 4] approach embedded in CISD (CI method with single and double excitations) is accomplished in order to investigate size-inconsistency issues in different open-shell transition metals. These systems are still an open question when based on the accuracy of a single-reference method.
Hydrogen systems For this we calculate two corrections: a basis set correction from explicitly correlated DCSD, and a correlation correction from an embedded FCI calculation on specific orbitals. These corrections, when applied on top of the DCSD calculations, give a good match with AFQMC+DMRG data by Motta et al. [2]. Further, uniform dissociation of 2 and 3 dimensional H-systems were also investigated. In all cases of dissociation the energy converges to the correct limit of separated Hydrogen atoms.
CEPA embedded in CISD The CEPA embedding in truncated CI method gives the possibility to study the effect of the excitation energies arising from the non-size-extensivity errors. The results of our calculations for three different compounds containing Cu^{2+} agree well with the conclusions from Giner et al. [5]. Embedding CISD in CEPA can be used to improve CEPA in bond-breaking situations.

References

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