Extending the Domain of Connectivity for MRexpT: Analysis and Results

Michael Hanrath[1]

[1] Institute for Theoretical Chemistry, University of Cologne, Greinstrasse 4, 50939 Cologne, Germany

Michael.Hanrath@uni-koeln.de

Enhancements of the multi-reference exponential ansatz (MRexpT) [1] will be presented. Based on a perturbational analysis showing new insides to the origin of the connectivity problem of MRCC two new variants of the MRexpT ansatz will be derived:

1. a Fermi vacuum invariant with extended connectivity and
2. a non-Fermi vacuum invariant, fully connected one.

Using a new connectivity test (allowing a simpler application than e.g. [2]) approaches (a) and (b) are checked to fulfill the expected connectivity properties.

Both approaches show very significant numerical improvements with respect to the original MRexpT ansatz for various model systems. For instance the non-parallelity error for BeH_2 is reduced by more than a factor of two at SDT level and more than two orders of magnitude at the SDTQ level outperforming other MRCC methods with results available for this system. Further promising examples on P4 and 2P4 (a cubic geometrical arrangement) will be given.

Variant (b) restores size-consistency also for non-localized orbitals at the price of loosing full Fermi vacuum invariance. Nevertheless, the results remain more accurate than for the SRMRCC [3] approach while symmetry breaking remains are less severe.

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