Efficient implementation of an exponential multi-reference wavefunction ansatz

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An efficient implementation of an exponential multi-reference wavefunction ansatz [1] is presented. In accordance with the state universal coupled-cluster ansatz of Jeziorski and Monkhorst [2] the approach uses a reference specific cluster operator. In order to achieve state selectiveness the excitation and reference related amplitude indexing of the state universal ansatz is replaced by an indexing which is based on excited determinants. There is no reference determinant playing a particular role. The approach is size consistent, coincides with traditional single-reference coupled-cluster if applied to a single-reference and converges to full CI with an increasing cluster operator excitation level.

References

[1] M. Hanrath, J. Chem. Phys. **123** X (2005)

[2] B. Jeziorski, H. J. Monkhorst, Phys. Rev. A **24** 1668 (1981).