Tensor decomposition in post-HF methods

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A new approximation for post-HF methods is currently being developed applying recent developments in tensor decomposition techniques [1-3]. In contrast to established approaches such as Cholesky decomposition, RI or density fitting [4-7] the tensor decomposition applied in this ansatz yields tensors of dimension *orbitals · rank* (*rank* being the expansion length of the tensor decomposition) as a representation for higher dimensional tensors like integrals, amplitudes and intermediates.

This approach has the potential to decrease the computational effort and the memory requirements of the algorithm drastically while allowing for rigorous truncation and error estimation. For methods from the Coupled-Cluster hierarchy for example, storage is reduced to $d \cdot rank \cdot orbitals$ (d being the dimensionality of the full tensor) and the computational effort is for all levels of approximation $rank^2 \cdot orbitals$. In this contribution first results for the the decomposition of the two electron integrals, the AO-MO transformation and the Coupled-Cluster amplitudes equations are presented. Furthermore, the scaling of the decomposition rank with system and basis set size is discussed for various quantities like integrals and amplitudes.

Literature:

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