Symposium 2
RDMFT for quantum chemistry: Computational and theoretical state-of-the-art and open challenges

Towards an in-principle-exact density matrix functional embedding theory

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Along the lines of a recent work on density-functional embedding theory for lattices [1], I would like to address in this (quite exploratory) presentation the one-electron reduced density-matrix functional exactification of *density matrix embedding theory* (DMET) [2], which is a promising approach for the description of strongly correlated electrons in both extended and molecular systems. After a brief review of DMET in the special case of non-interacting or mean-field electrons, where the approach is exact, I will discuss current implementations for interacting electrons and highlight the various approximations that are made [3,4]. In the latter case, mapping a correlated embedded fragment density matrix onto a (full-size) non-interacting system, which is a standard procedure inspired by *dynamical mean-field theory* (DMFT), raises serious representability issues. As an attempt to cure (or reduce) the ill-posed mapping problem of DMET, I would like to discuss the possibility of using an indirect mapping of the density matrix onto a (still non-interacting) non-hermitian system. We will also wonder how to retrieve such a system from a variational principle.

References

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[4] S. Sekaran, O. Bindech, and E. Fromager, *"Equivalence of the Singular Value Decomposition and the Block Householder Transformation in Density Matrix Embedding Theory"*, in preparation (2022).