Approximations and exact properties of density functionals from the strong-interaction limit of DFT

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Abstract

The work presented in this thesis moves along a diverse path exploring both approximations and exact properties of density functionals.

It highlights the broad potential of model density functionals, based on interpolations along the adiabatic connection and containing the strong-interaction limit ingredient, for future applications on challenging compounds such as those containing noble metal clusters/complexes.

Furthermore, a novel approach towards an efficient resummation of the perturbation series expansion around the Hartree-Fock reference state is proposed which possesses many appealing properties at the theoretical level.

On a parallel track, several exact properties useful for density functional development, such as a sum-rule, a comparison between the two mostly used gauges in the definition of the exchange-correlation energy density, and an unexpected qualitative feature of the exact KS potential in the case of a stretched hetero-nuclear bond (among others), are reported for the first time.

Overall, this work shows that some distinctive features of the strong-interaction limit of DFT (and possibly also of HF theory) can be used as guidelines for developing density functional models that are accurate also for problematic cases such as strongly correlated systems or dissociation processes.