[P7] New Alternative Embedding Method applied on Model Hamiltonian

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Because it often appears that the region of interest is only one part of a much larger system, and considering strong electron correlation as essentially local, embedding approaches are mainly used in practice[i] and provide a relatively accurate description of the system while remaining computationally affordable. In these approaches, the whole system is usually mapped onto an embedded quantum problem, e.g. a small system called impurity and the rest of the system called the bath[ii]. As an example among many others, one can cite the *dynamical mean-field theory*[iii], the so-called *self-energy embedding theory*[iv] and the *density-matrix embedding theory* (DMET)[v].

An alternative in-principle exact embedding approach applied on model Hamiltonians, so-called *site-occupation embedding theory* (SOET) [vi,vii,viii] has been formulated and tested recently on the Hubbard model. This theory is a Density-functional theory (DFT)-based method, but where the reference system is partially-interacting instead of noninteracting as in standard Kohn-Sham DFT.

In this poster, I will present a projected formulation of SOET (p-SOET) using the Schmidt decomposition, in analogy with DMET but in a density functional framework[ix]. This formulation has many advantages: (i) the convergence criteria on the density is physically motivated in SOET (ii) the correlation potential is analytical, and self-consistently determined through its dependence on the density (iii) the analytical correlation energy density functionals are involved in the exact recovering of the per-site energy, the double occupation, the discontinuity in the chemical potential, the charge susceptibility and so on. In principle, the only source of error of p-SOET applied to the Hubbard model is in the Schmidt decomposition based the KS wavefunction instead of the physical one, and it is shown to be very small. In practice however, the exact functionals are not known, and density-driven error as well as functional-driven error might appear. Hence, the self-consistently determined occupation on the impurity(ies) may deviate from the exact one, as well as other physical quantities.

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