

Learning DFT and inverse mean field theories

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We first start with an introduction on how to extract a mean field single particle Hamiltonian from a many body wave function of a fermionic system [1]. While we primarily discuss lattice models we also look at neon in an augccpvdz basis set as an example. Our approach allows us to discuss the result of a many particle wave function in terms of a non-interacting description. In contrast to density functional theory approaches on the lattice this approach allows the extraction of appropriate kinetic terms. In result the extracted mean field theories are closer to the physics of the problem under investigation. Therefore, the extracted mean field Hamiltonians may provide an improved starting point for perturbative approaches. As an application we discuss a self consistent cluster embedding (SCCE), where we extract the inverse mean field Hamiltonian from a cluster in real space which we then use to describe a bath Hamiltonian coupled to the cluster. In addition, the technique can be used to decide whether a density matrix renormalization group calculation for interacting fermions has converged to the true ground state.

Second we discuss how one can apply machine learning techniques to construct density functional theory (DFT) functionals from those calculations and provide an example for disordered, interacting 1D fermions.

[1] Physical Chemistry Chemical Physics, 2018, 20, 27600-27610.