

Local Potential Functional Embedding Theory based on the Householder Transformation

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INTRODUCTION

A new perspective of the Householder transformed density matrix functional embedding theory^[1] (Ht-DMFET) applied on the one-dimensional Hubbard model is presented. It follows the formalism of Kohn-Sham Density Functional Theory^[2] (KS-DFT) as the KS system tries to reproduce the density of a reduced-in-size interacting system. This formalism could be seen as a frequency-independent and local version of the two-site Dynamical Mean-Field Theory^[3] and offers an adequate strategy to treat Quantum Chemistry Hamiltonian.

BRIEF REVIEW OF HOUSEHOLDER TRANSFORMED DENSITY MATRIX FUNCTIONAL EMBEDDING THEORY

Replace the original full-size problem, by one or several simpler problems that preserve only a fragment of the original system. The fragment, which can be a single atomic site (often referred to as **impurity**) in a lattice, is embedded into a formal **bath** that is supposed to mimic the effects of the impurity's environment.

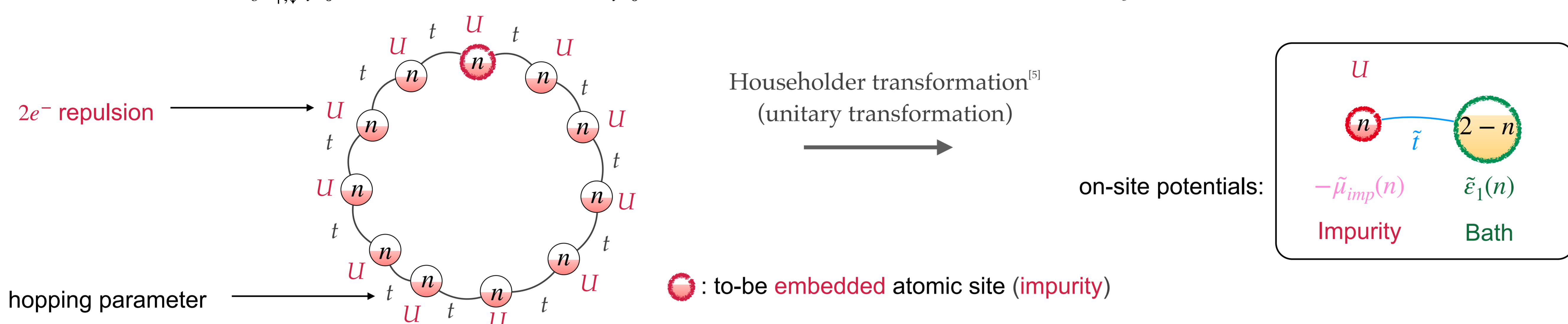
Divide and conquer^{[3],[4]}

400 sites uniform Hubbard model

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} \sum_{i=0}^{L-1} (\hat{c}_{i\sigma}^\dagger \hat{c}_{(i+1)\sigma} + H.c.) + U \sum_{i=0}^{L-1} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

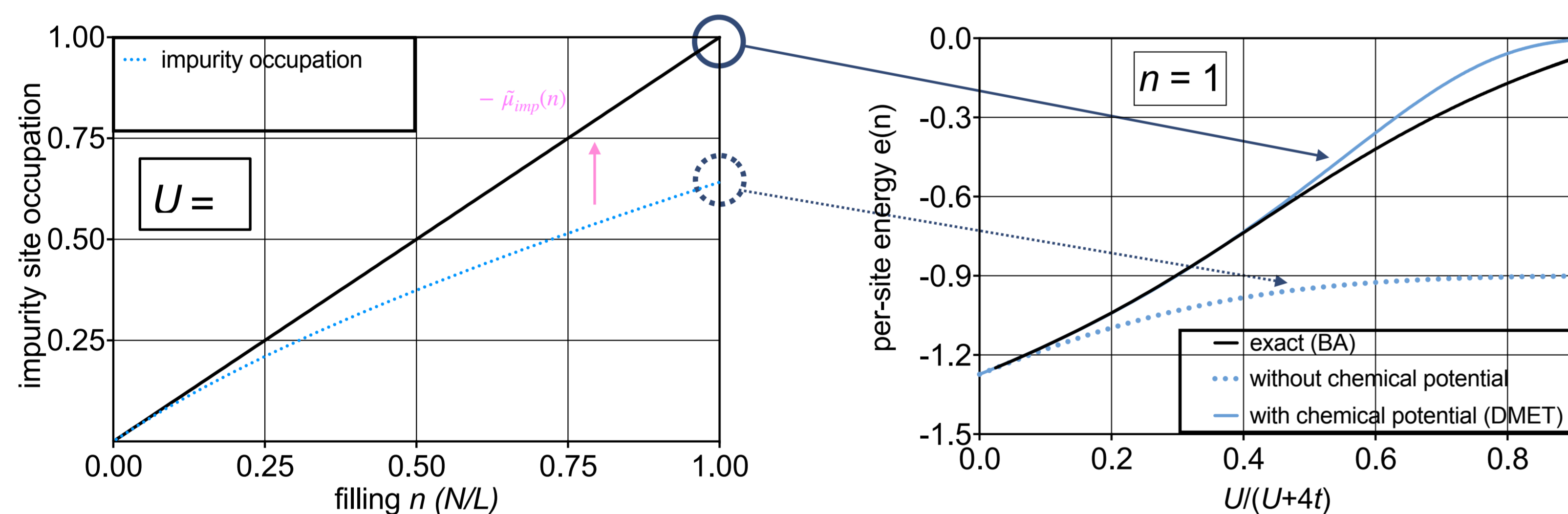
Embedded system: Householder cluster (dimer)^[1]

$$\hat{H}^{\mathcal{E}} = \sum_{\sigma} \left[-\tilde{t} (\hat{c}_{0\sigma}^\dagger \hat{d}_{1\sigma} + H.c.) - \tilde{\mu}_{imp} \hat{n}_{0\sigma} + \tilde{\epsilon}_1 \hat{d}_{1\sigma}^\dagger \hat{d}_{1\sigma} \right] + U \hat{n}_{0\uparrow} \hat{n}_{0\downarrow}$$



Density mapping

As in many embedding scheme (DMET^[4], DET^[6]), in the interacting case, the density profile obtained from the fixed number of electrons N in the lattice is **not** reproduced by the impurity site, thus leading in **substantial error** in the strongly-correlated regime of the per-site energies^[1]. A chemical potential $\tilde{\mu}_{imp}(n)$ is added on the impurity site to ensure the **density mapping**.



The motivation is to approximate **local properties** from the reduced-in-size system:

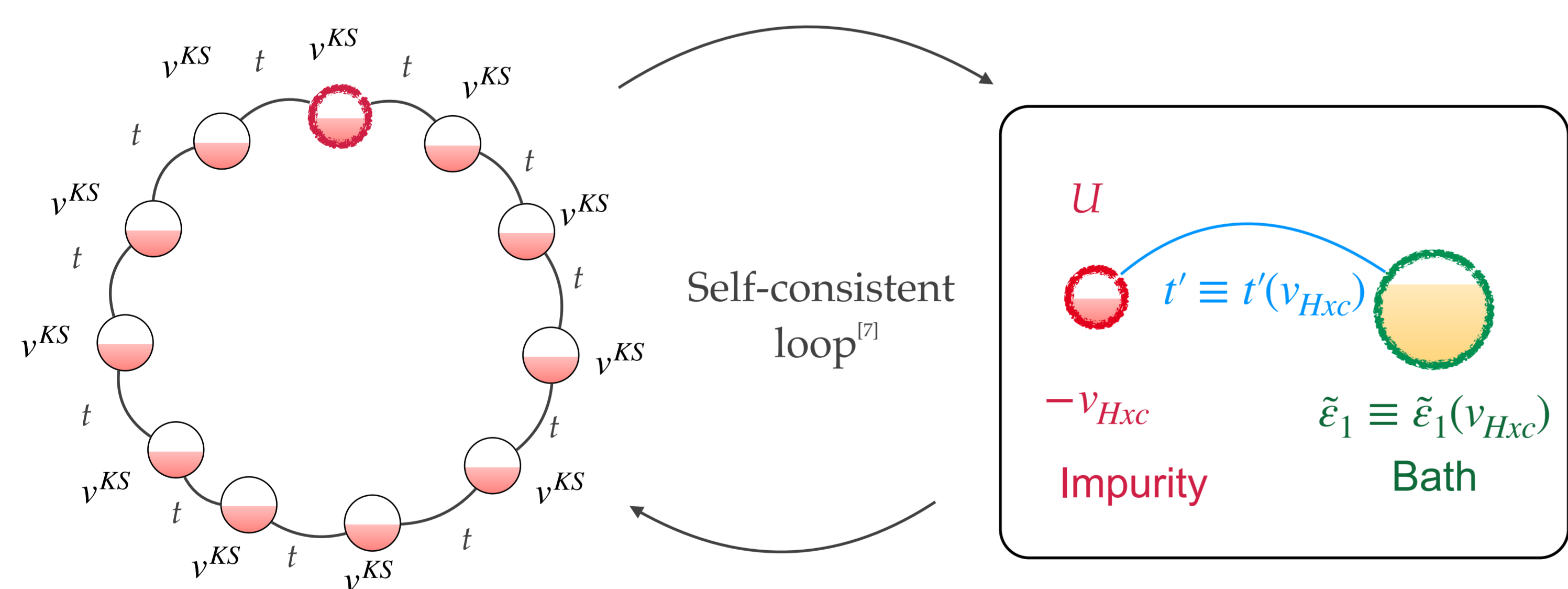
$$e(n) \approx -4t \langle \hat{c}_0^\dagger \hat{c}_1 \rangle_{\Psi^{\mathcal{E}}} + U \langle \hat{n}_{0\uparrow}^\dagger \hat{n}_{0\downarrow}^\dagger \rangle_{\Psi^{\mathcal{E}}}$$

$$\mu(n) = \frac{\partial e(n)}{\partial n}$$

In this special case, we construct the map $n \rightarrow \mu \equiv \mu(n)$.

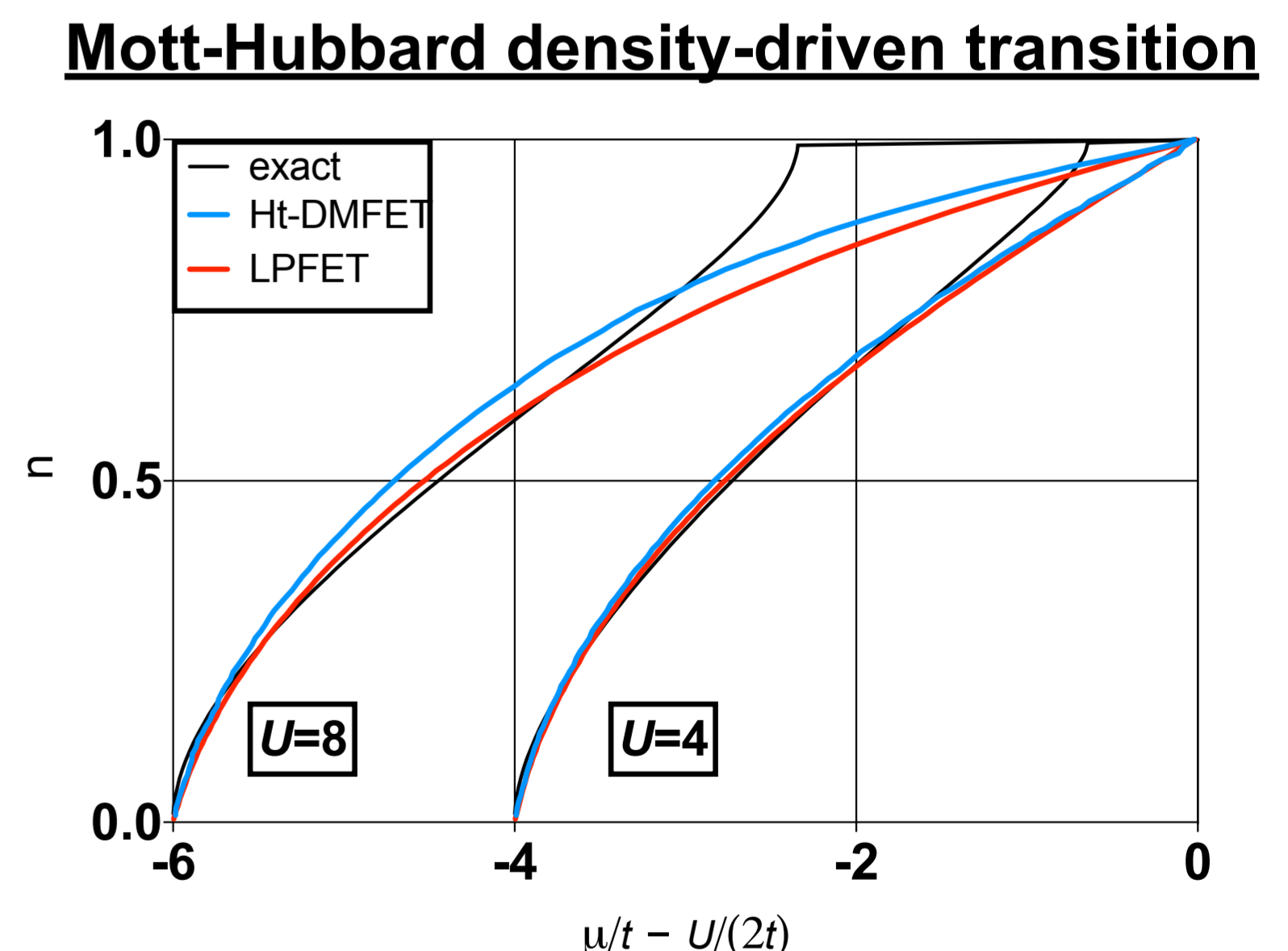
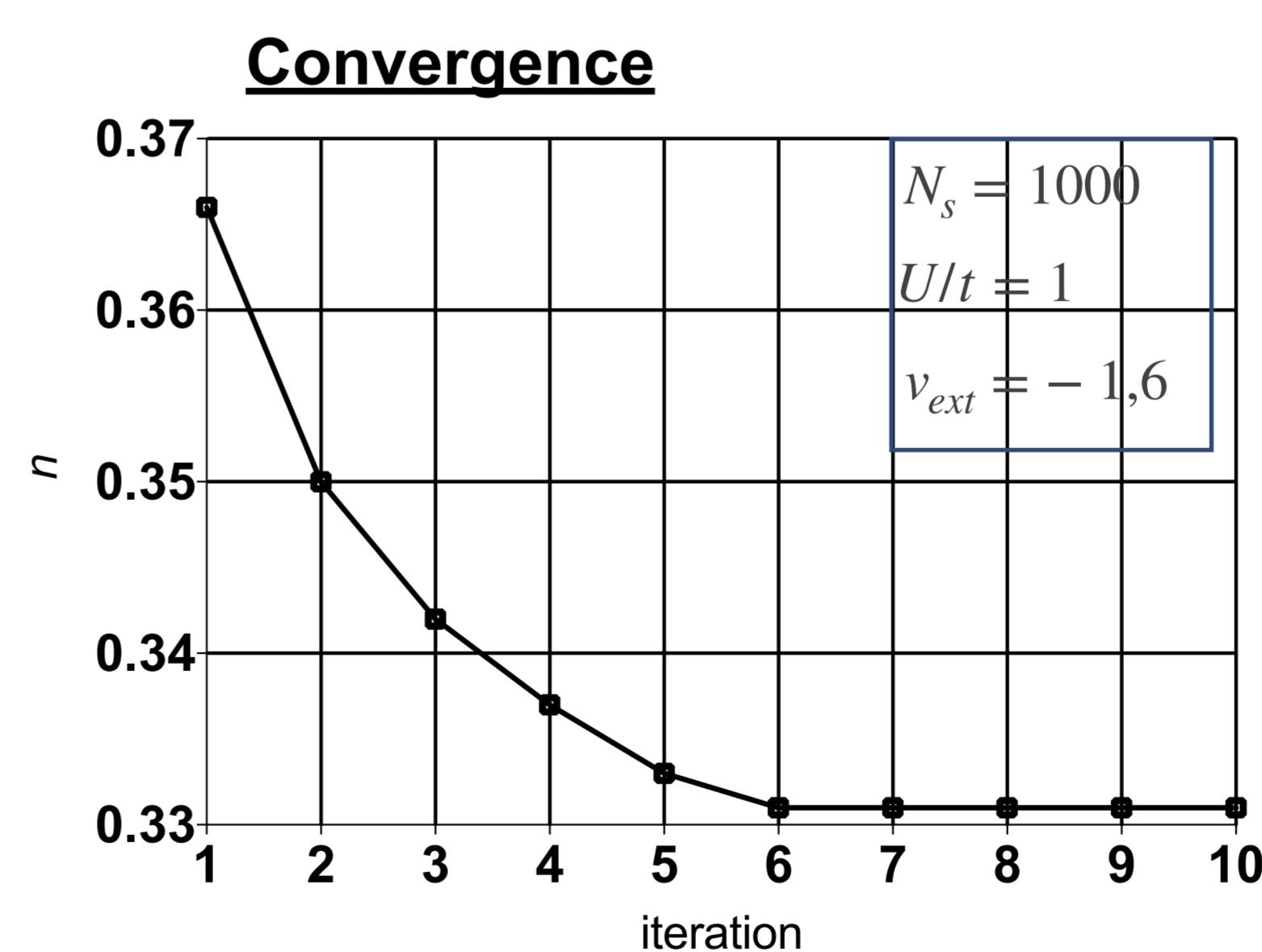
LOCAL POTENTIAL FUNCTIONAL EMBEDDING THEORY (LPFET)

In LPFET^[7], the Kohn-Sham density functional theory^[2] (KS-DFT) spirit is followed as we start the calculation with a **fixed** external potential v_{ext} and try to reproduce the density of the interacting system. The latter is replaced by a simpler reduced-in-size dimer, the Householder cluster. The density mapping constraint is at the origin of a **self-consistent loop**.



Density constraint $n_{KS \text{ lattice}}(-\mu + v_{Hxc}) \stackrel{!}{=} n^{\mathcal{E}}(v_{Hxc})$

With a fixed v_{ext} and a v_{Hxc} that need to be determined the following map is constructed: $v_{ext} = -\mu \rightarrow n(\mu)$.



CONCLUSION

- Establish clear connection with DFT
- LPFET can be seen as a frequency-independent and local version of two-site DMFT
- Strategy applicable to Quantum Chemistry

References

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