Density-functional theory without density functionals: A quantum embedding perspective

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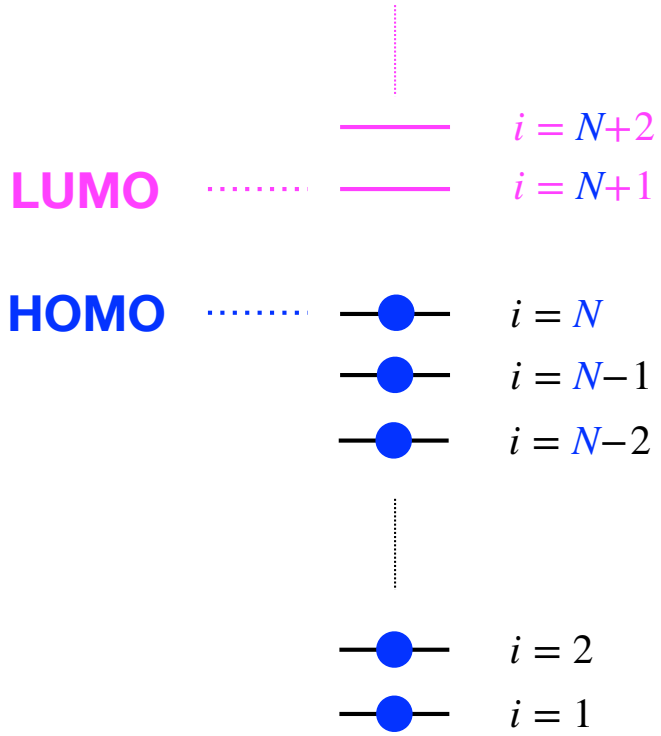
(Kohn-Sham) DFT for N-electron ground states

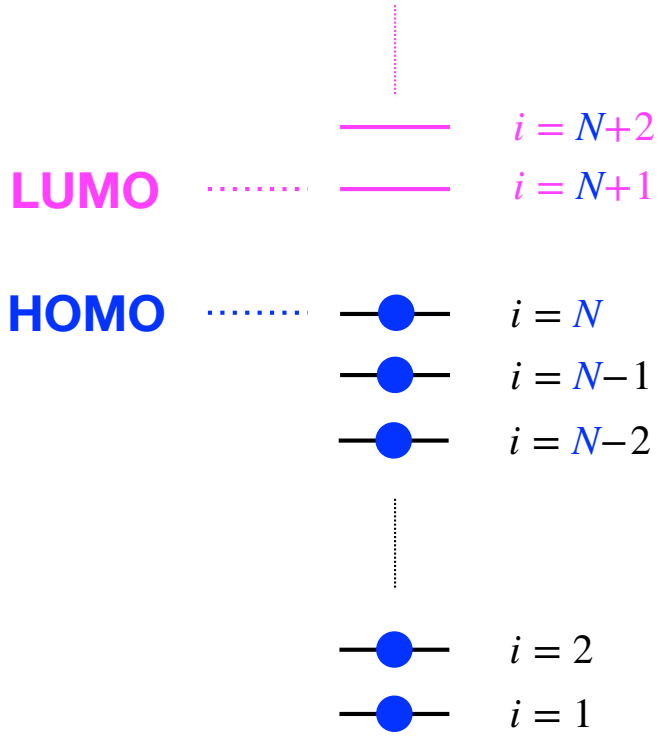
$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r})\right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$



(Kohn-Sham) DFT for N-electron ground states

One-electron picture

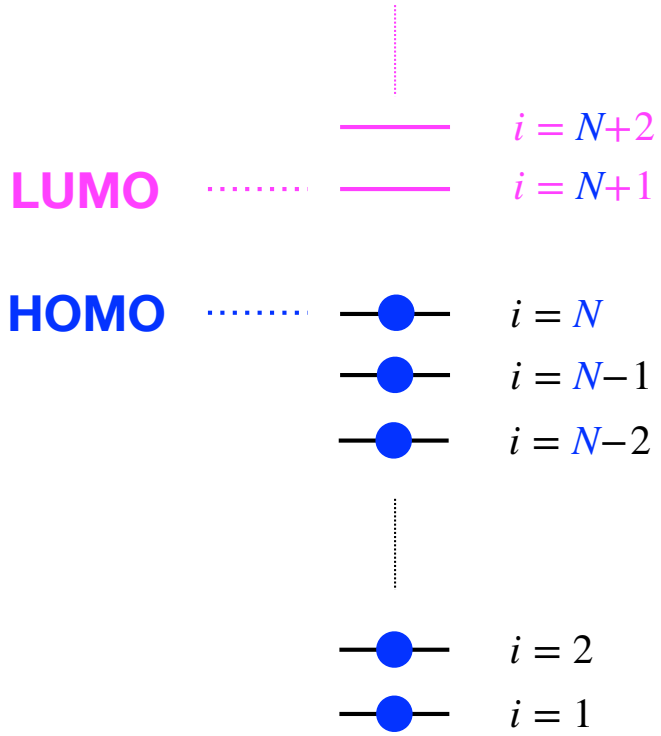
$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r})\right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$



DFT for N-electron ground states

$$\mathbf{r} \equiv (x, y, z)$$

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r}) \right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

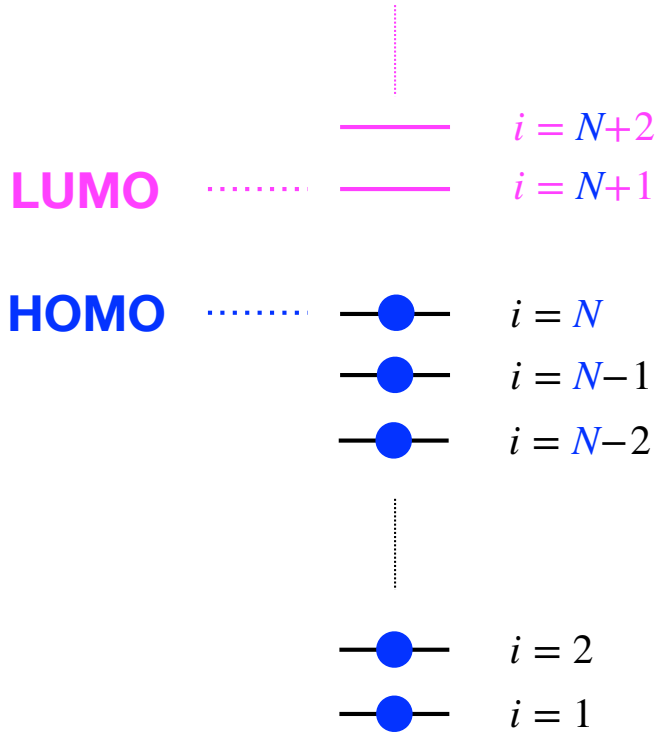


W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).

$$\nabla^2_{\mathbf{r}} \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

DFT for N-electron ground states

$$\left[-\frac{\nabla^2_{\mathbf{r}}}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r}) \right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

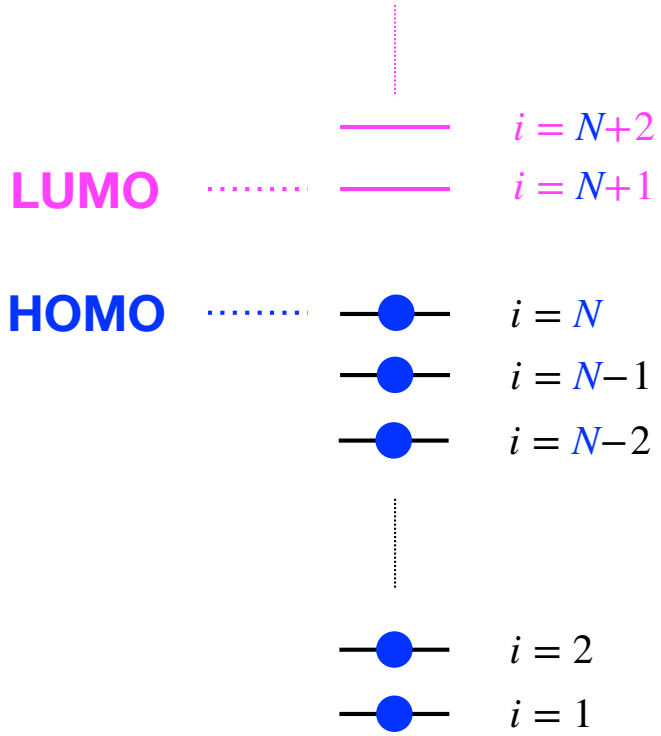


W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).

DFT for N-electron ground states

*"External" local and **multiplicative** potential*

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r})\right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$



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DFT for N-electron ground states

Nuclear potential *in quantum chemistry calculations*

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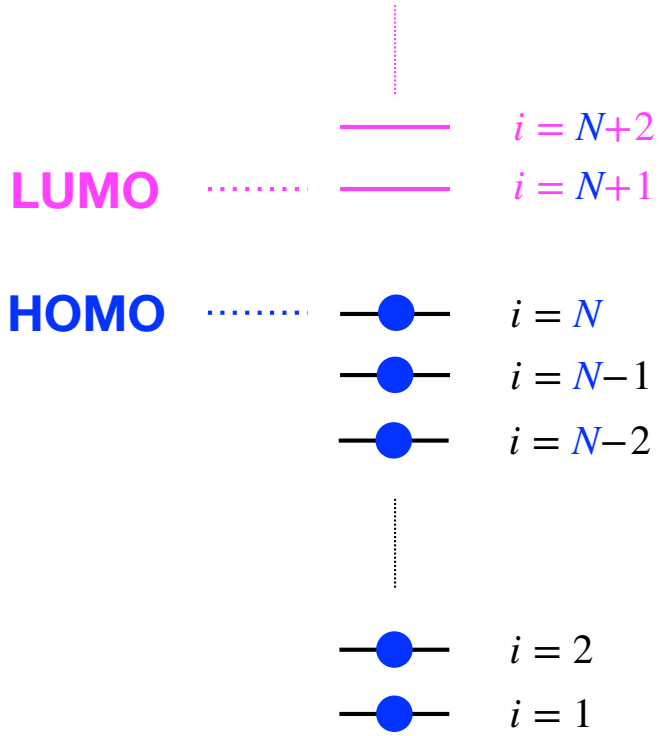
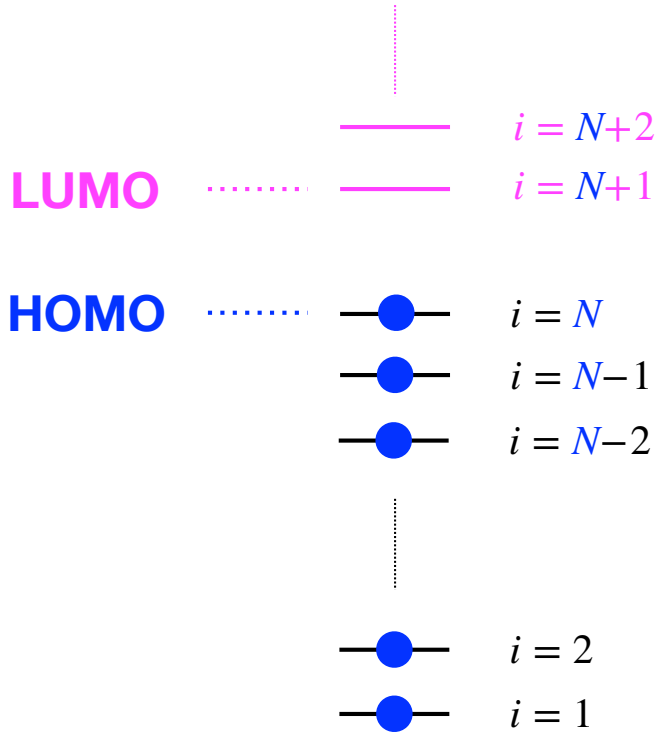


DFT for N-electron ground states

Hartree-exchange-correlation
local (multiplicative) ***potential***

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r})\right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$



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DFT for N-electron ground states

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r})\right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

$$n_0^N(\mathbf{r}) = \sum_{i=1}^{N} |\varphi_i(\mathbf{r})|^2$$

exact ground-state ***density***

W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).

DFT for N-electron ground states

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2} + v_{\text{ext}}(\mathbf{r}) + v_{\text{Hxc}}(\mathbf{r})\right] \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

Hartree-exchange-correlation ***potential***

$$v_{\text{Hxc}}(\mathbf{r}) = \left.\frac{\delta E_{\text{Hxc}}[n]}{\delta n(\mathbf{r})}\right|_{n=n_0^N}$$

W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).

DFT for N-electron ground states

$$\left[-\frac{\nabla_{\mathbf{r}}^2}{2}+v_{\mathrm{ext}}(\mathbf{r})+v_{\mathrm{Hxc}}(\mathbf{r})\right]\varphi_i(\mathbf{r})=\varepsilon_i\varphi_i(\mathbf{r})$$

*Hxc **energy** functional*

*Hartree-exchange-correlation **potential***

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Self-consistency!

W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).

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$$E_0 = -\frac{1}{2}\sum_{i=1}^{N} \int d\mathbf{r}\, \varphi_i(\mathbf{r})\, \nabla_{\mathbf{r}}^2 \varphi_i(\mathbf{r}) + \int d\mathbf{r}\, v_{\text{ext}}(\mathbf{r}) n_0^N(\mathbf{r}) + E_{\text{Hxc}}[n]\Big|_{n=n_0^N}$$

exact ground-state ***energy***

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DFT for N-electron ground states

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DFT for N-electron ground states

Once we have $E_{\mathrm{Hxc}}[n]$ we can run a DFT calculation for *any system*

DFT for N-electron ground states

Once we have $E_{\mathrm{Hxc}}[n]$ we can run a DFT calculation for *any system*

"Holy grail"

Local potential functional approach to DFT

Change of paradigm

$$n(\mathbf{r}) \longrightarrow v_{\text{ext}}(\mathbf{r})$$

Local potential functional approach to DFT

Change of paradigm

$$n(\mathbf{r}) \longrightarrow v_{\text{ext}}(\mathbf{r})$$

$$\left.\frac{\delta E_{\text{Hxc}}[n]}{\delta n(\mathbf{r})}\right|_{n=n_0^N} \equiv v_{\text{Hxc}}(\mathbf{r}) = v_{\text{Hxc}}[v_{\text{ext}}](\mathbf{r}) = ???$$

Local potential functional approach to DFT

Original N-electron Schrödinger equation

$$\hat{H}\Psi_0 = E_0\Psi_0$$

Local potential functional approach to DFT

Original N-electron Schrödinger equation

$$\hat{H}\Psi_0 = E_0\Psi_0$$

True physical Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{W}_{\text{ee}}$$

$$-\frac{1}{2}\sum_{i=1}^{N}\nabla_{\mathbf{r}_i}^2 \qquad \sum_{i=1}^{N} v_{\text{ext}}(\mathbf{r}_i) \qquad \sum_{1\le i<j}^{N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Local potential functional approach to DFT

Original N-electron Schrödinger equation

$$\hat{H}\Psi_0 = E_0\Psi_0$$

True physical Hamiltonian

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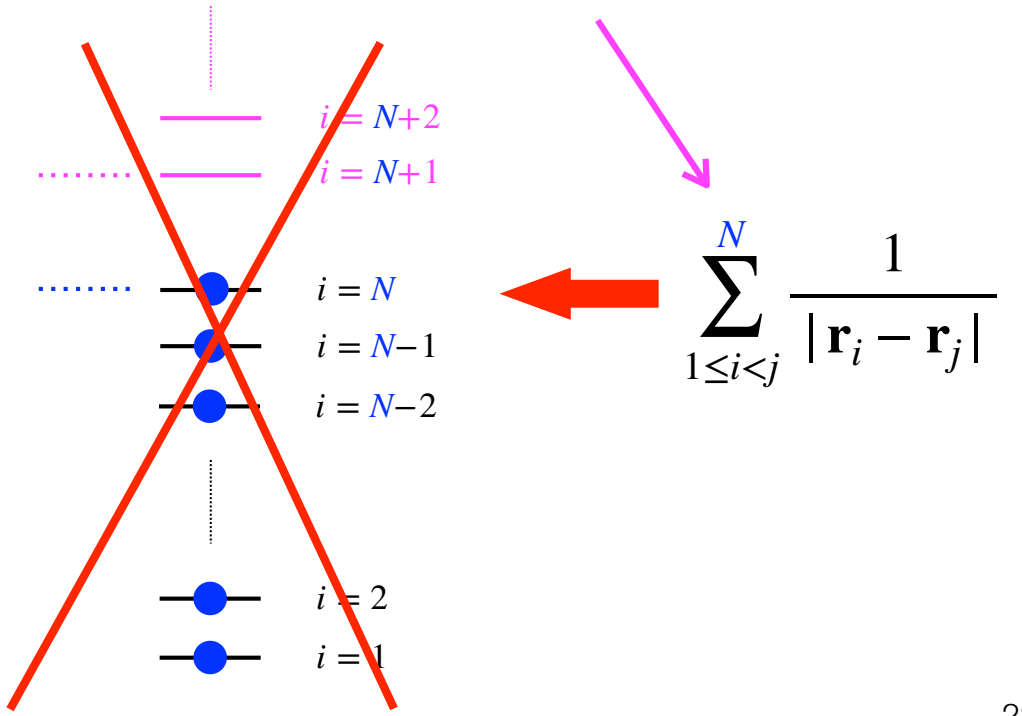

Local potential functional approach to DFT

Original N-electron Schrödinger equation $\hat{H}\Psi_0 = E_0\Psi_0$

True physical Hamiltonian $\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{W}_{\text{ee}}$ ***Known!***

Local potential functional approach to DFT

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*The Hxc potential is **completely unnecessary** here…*

Local potential functional approach to DFT

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The Hxc potential is completely unnecessary here…

…unless Ψ_0 ***is constructed (approximately) from the Kohn-Sham orbitals.***

Local potential functional approach to DFT

Original N-electron Schrödinger equation $\hat{H}\Psi_0 = E_0\Psi_0$

True physical Hamiltonian $\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{W}_{\text{ee}}$ ***Known!***

The Hxc potential is completely unnecessary here…

…unless Ψ_0 *is constructed (approximately) from the Kohn-Sham orbitals.*

The **approximate** one-electron **Kohn-Sham picture** and the **exact interacting picture** share the ***same density*** in this case

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

$$\sum_{i=1}^{N} v_{\text{Hxc}}(\mathbf{r}_i) \times$$

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

Ground (and excited)
KS pictures

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

Ground (and excited)
KS pictures

Slater determinants ← $\left\{ \Phi_I^{\text{KS}} \right\}_{I=0,1,2,\ldots}$

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

"perturbation"

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \underbrace{\left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)}$$

"perturbation"

$$E_0 = \langle \Phi_0^{\text{KS}} | \hat{H} | \Phi_0^{\text{KS}} \rangle + \sum_{I>0} \frac{\left| \langle \Phi_0^{\text{KS}} | \hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} | \Phi_I^{\text{KS}} \rangle \right|^2}{\mathscr{E}_0^{\text{KS}} - \mathscr{E}_I^{\text{KS}}} + \cdots$$

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \underbrace{\left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)}$$

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Görling-Levy perturbation theory

*A. Görling, M. Levy, Phys. Rev. A **50**(1), 196 (1994).*

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \overset{???}{\hat{V}_{\text{Hxc}}} + \underbrace{\left(\hat{W}_{\text{ee}} - \overset{???}{\hat{V}_{\text{Hxc}}} \right)}$$

"perturbation"

$$E_0 = \langle \Phi_0^{\text{KS}} | \overset{???}{\hat{H}} | \overset{???}{\Phi_0^{\text{KS}}} \rangle + \sum_{I>0} \frac{\left| \langle \overset{???}{\Phi_0^{\text{KS}}} | \overset{???}{\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}}} | \overset{???}{\Phi_I^{\text{KS}}} \rangle \right|^2}{??? \; \mathscr{E}_0^{\text{KS}} - \mathscr{E}_I^{\text{KS}} \; ???} + \cdots$$

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \overset{???}{\hat{V}_{\text{Hxc}}} + \underbrace{\left(\hat{W}_{\text{ee}} - \overset{???}{\hat{V}_{\text{Hxc}}} \right)}$$

"perturbation"

$$E_0 = \langle \Phi_0^{\text{KS}} | \overset{???}{\hat{H}} | \overset{???}{\Phi_0^{\text{KS}}} \rangle + \sum_{I>0} \frac{\left| \langle \overset{???}{\Phi_0^{\text{KS}}} | \hat{W}_{\text{ee}} - \overset{???}{\hat{V}_{\text{Hxc}}} | \overset{???}{\Phi_I^{\text{KS}}} \rangle \right|^2}{??? \; \mathscr{E}_0^{\text{KS}} - \mathscr{E}_I^{\text{KS}} \; ???} + \cdots$$

The evaluation of the energy **fully relies on** $\hat{V}_{\text{Hxc}}$

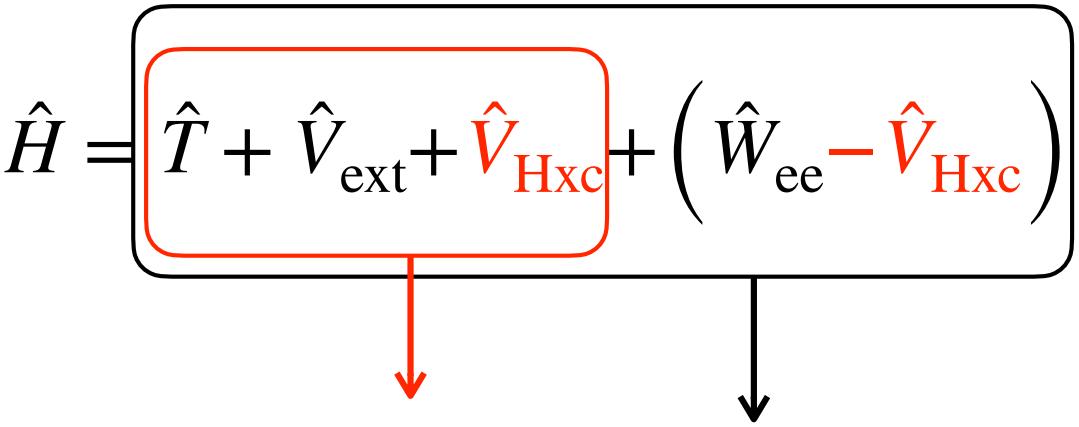
Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \overset{???}{\hat{V}_{\text{Hxc}}} + \underbrace{\left(\hat{W}_{\text{ee}} - \overset{???}{\hat{V}_{\text{Hxc}}} \right)}_{\text{“perturbation”}}$$

To-be-determined local potential
(hence the name of the approach)

The evaluation of the energy **fully relies on** $\hat{V}_{\text{Hxc}}$

Local potential functional approach to DFT



$$n_{\Phi_0^{\text{KS}}}(\mathbf{r}) = n_{\Psi_0}(\mathbf{r})$$

Exact density constraint

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

$$n_{\Phi_0^{\text{KS}}}(\mathbf{r}) = n_{\Psi_0}(\mathbf{r})$$

$$n_{\Phi_0^{\text{KS}}[v_{\text{Hxc}}]}(\mathbf{r}) = n_{\Psi_0[v_{\text{Hxc}}]}(\mathbf{r})$$

Self-consistent scheme
(when approximations are made)

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

$$n_{\Phi_0^{\text{KS}}[v_{\text{Hxc}}]}(\mathbf{r}) = n_{\Psi_0[v_{\text{Hxc}}]}(\mathbf{r})$$

Approaching the ground state Ψ_0 *of the full system is* ***computationally demanding***

R. J. Bartlett, I. Grabowski, S. Hirata, and S. Ivanov, J. Chem. Phys. 122, 034104 (2005).

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

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*The approach becomes interesting if a **reduced-in-size approximation** to* Ψ_0 *can be used*

Local potential functional approach to DFT

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{V}_{\text{Hxc}} + \left(\hat{W}_{\text{ee}} - \hat{V}_{\text{Hxc}} \right)$$

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The approach becomes interesting if a ***reduced-in-size approximation*** *to* Ψ_0 *can be used*

Quantum embedding!

Condensed Matter > Strongly Correlated Electrons

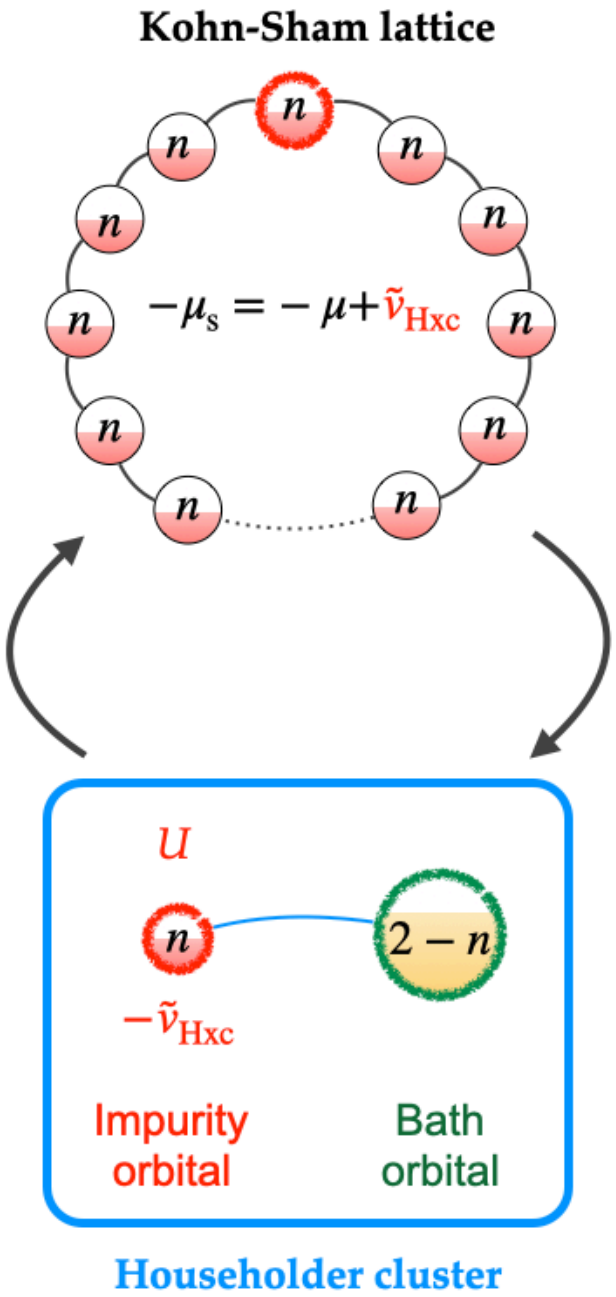
[Submitted on 16 Feb 2022]

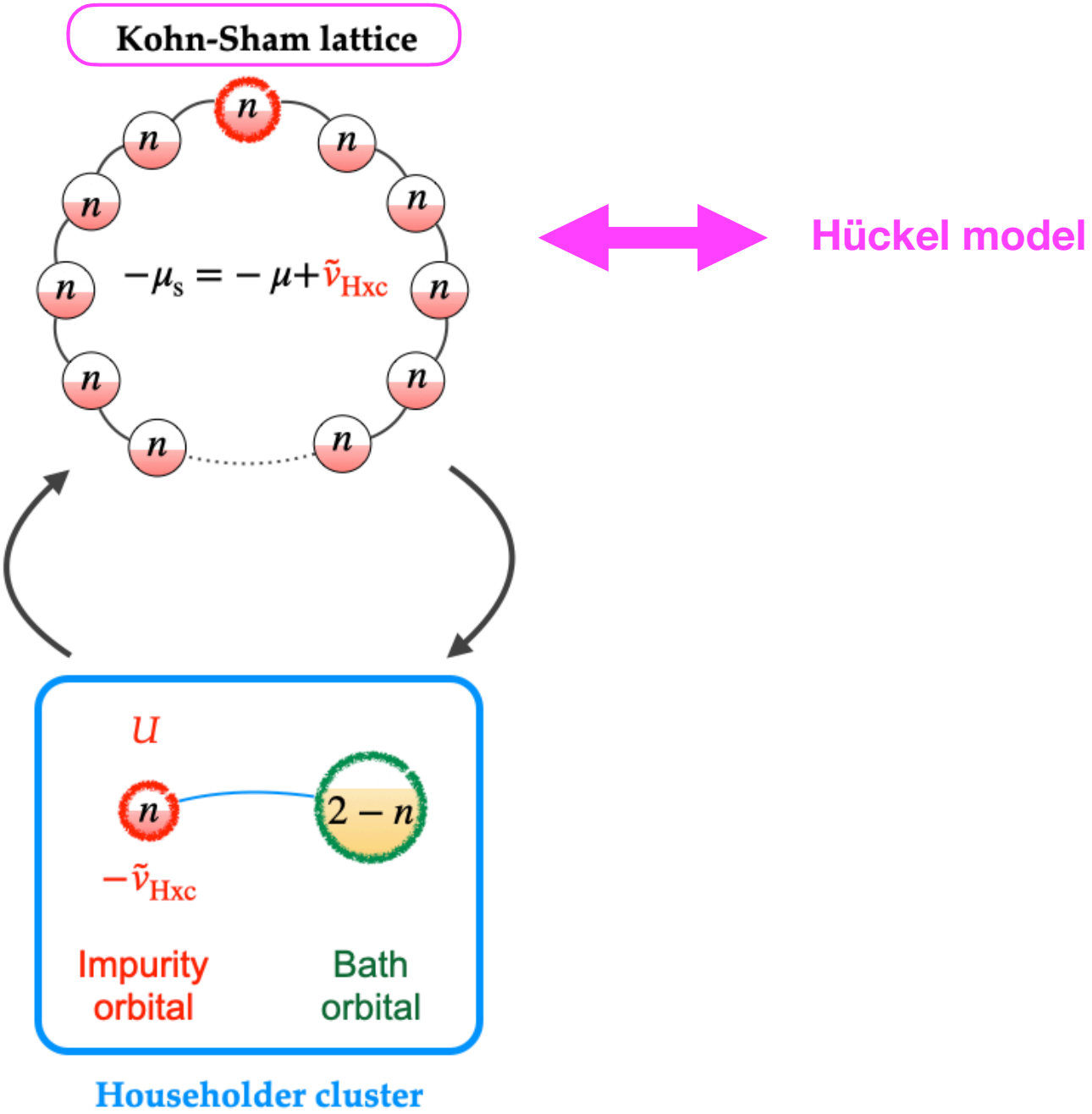
Local Potential Functional Embedding Theory: A Self-Consistent Flavor of Density Functional Theory for Lattices without Density Functionals

Sajanthan Sekaran, Matthieu Saubanère, Emmanuel Fromager

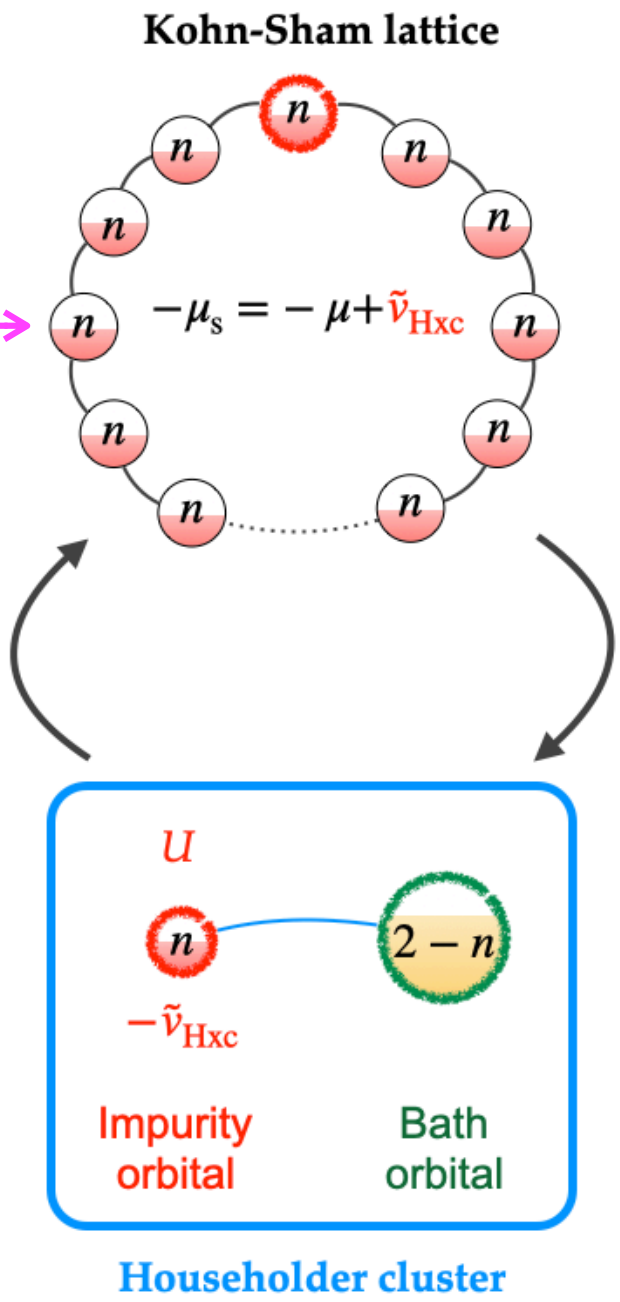
The recently proposed Householder transformed density-matrix functional embedding theory (Ht-DMFET) [Sekaran et al., Phys. Rev. B 104, 035121 (2021)], which is equivalent to (but formally simpler than) density matrix embedding theory (DMET) in the non-interacting case, is revisited from the perspective of density-functional theory (DFT). An in-principle-exact density-functional version of Ht-DMFET is derived for the one-dimensional Hubbard lattice with a single embedded impurity. On the basis of well-identified density-functional approximations, a local potential functional embedding theory (LPFET) is formulated and implemented. Even though LPFET performs better than Ht-DMFET in the low-density regime, in particular when electron correlation is strong, both methods are unable to describe the density-driven Mott-Hubbard transition, as expected. These results combined with our formally exact density-functional embedding theory reveal that a single statically embedded impurity can in principle describe the gap opening, provided that the complementary correlation potential (that describes the interaction of the embedding cluster with its environment, which is simply neglected in both Ht-DMFET and LPFET) exhibits a derivative discontinuity (DD) at half filling. The extension of LPFET to multiple impurities (which would enable to circumvent the modeling of DDs) and its generalization to quantum chemical Hamiltonians are left for future work.

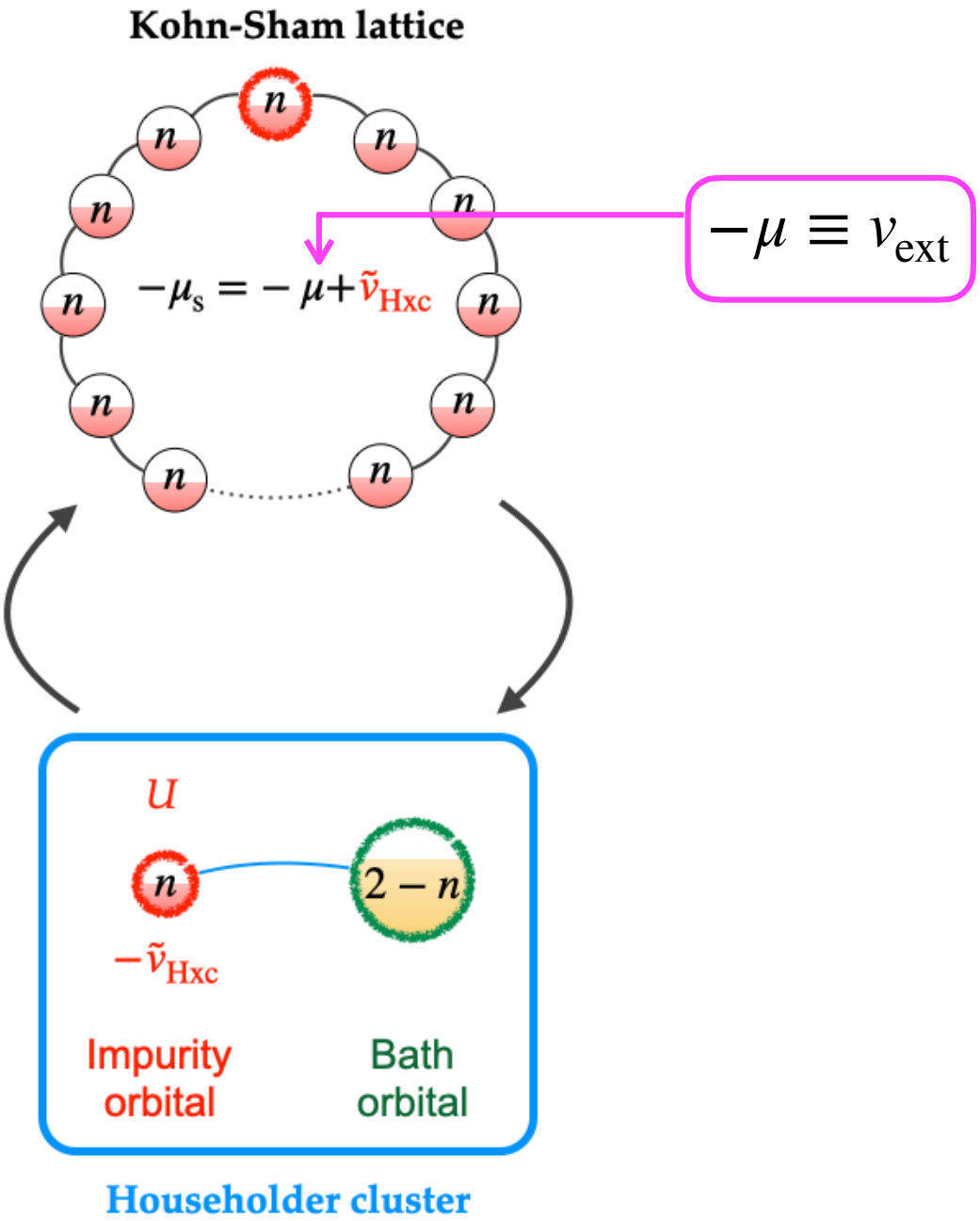
Application
to Hubbard lattices
(ring of hydrogen atoms)




Kohn-Sham lattice
$-\mu_s = -\mu + \tilde{v}_{Hxc}$
Hückel model
U
n
$2-n$
$-\tilde{v}_{Hxc}$
Impurity orbital
Bath orbital
Householder cluster

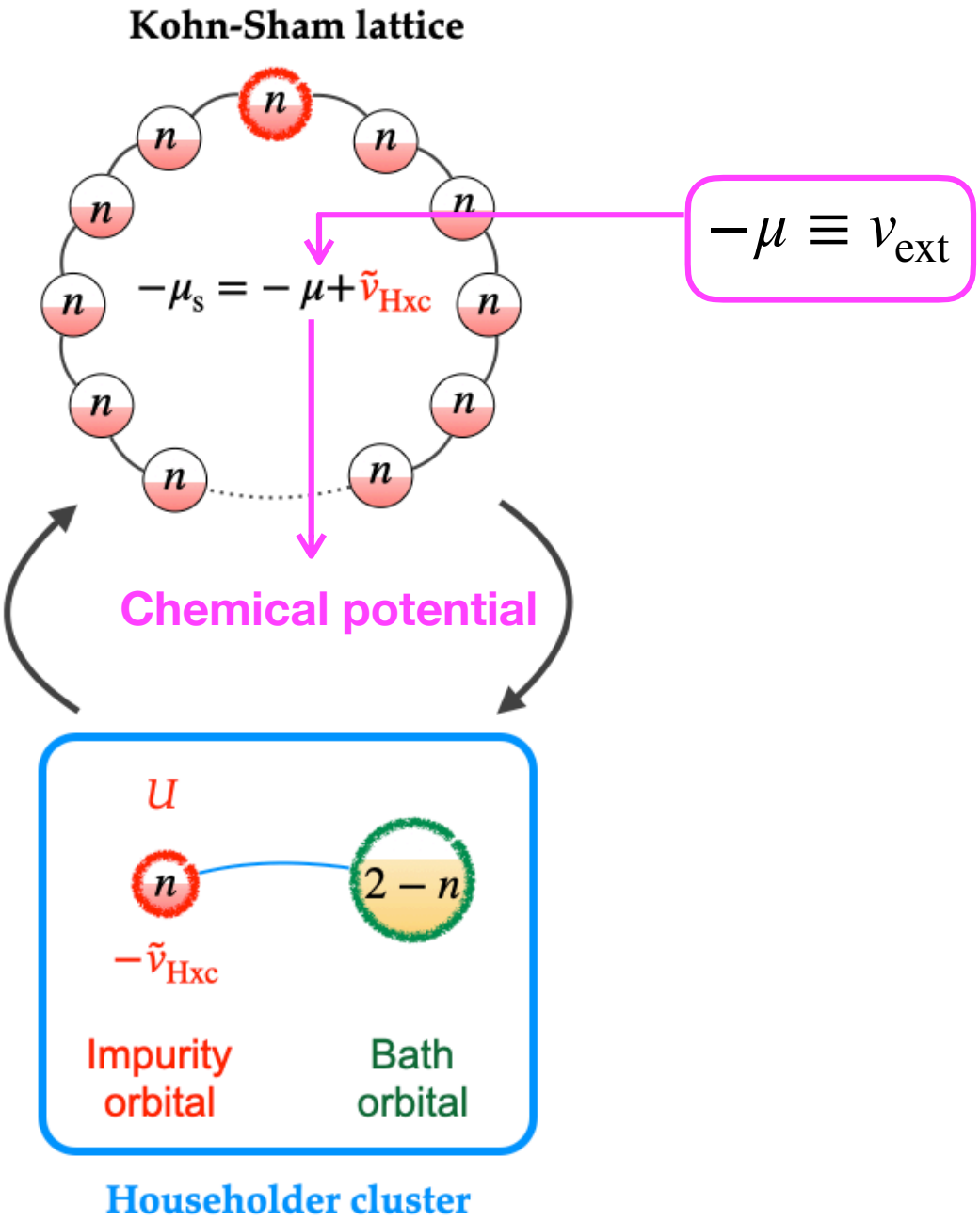
Uniform occupation n of the atomic orbitals

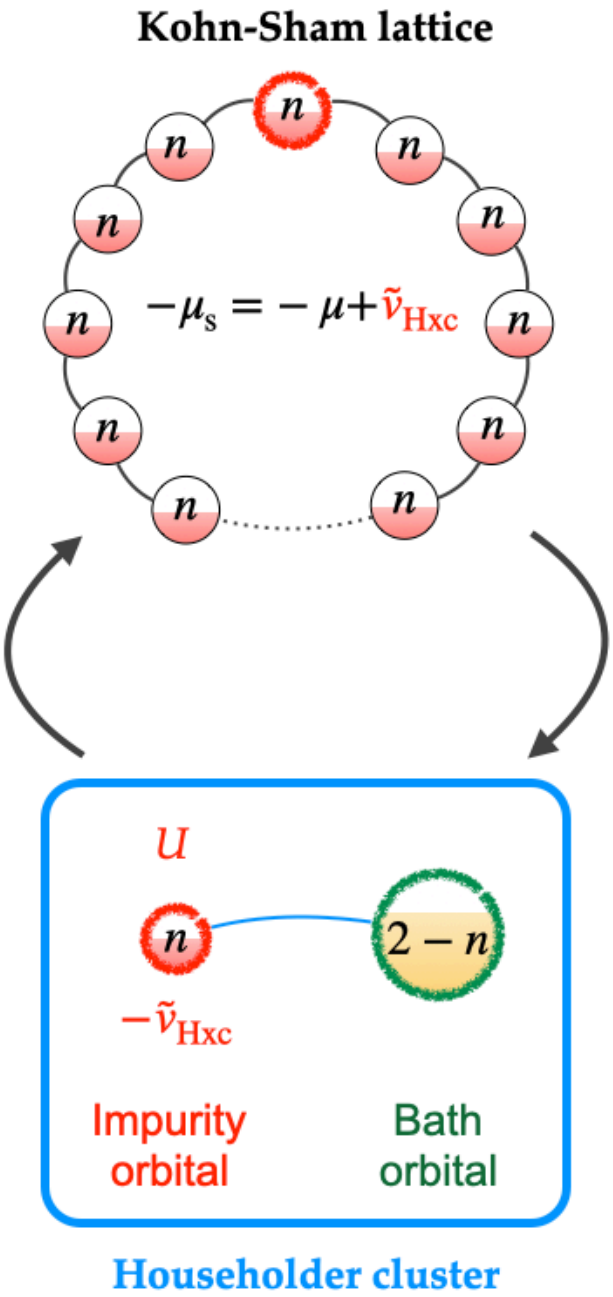



Kohn-Sham lattice
$-\mu_s = -\mu + \tilde{v}_{Hxc}$
$-\mu \equiv v_{ext}$
U
n
$2-n$
$-\tilde{v}_{Hxc}$
Impurity orbital
Bath orbital
Householder cluster

$$n = \frac{N}{L}$$

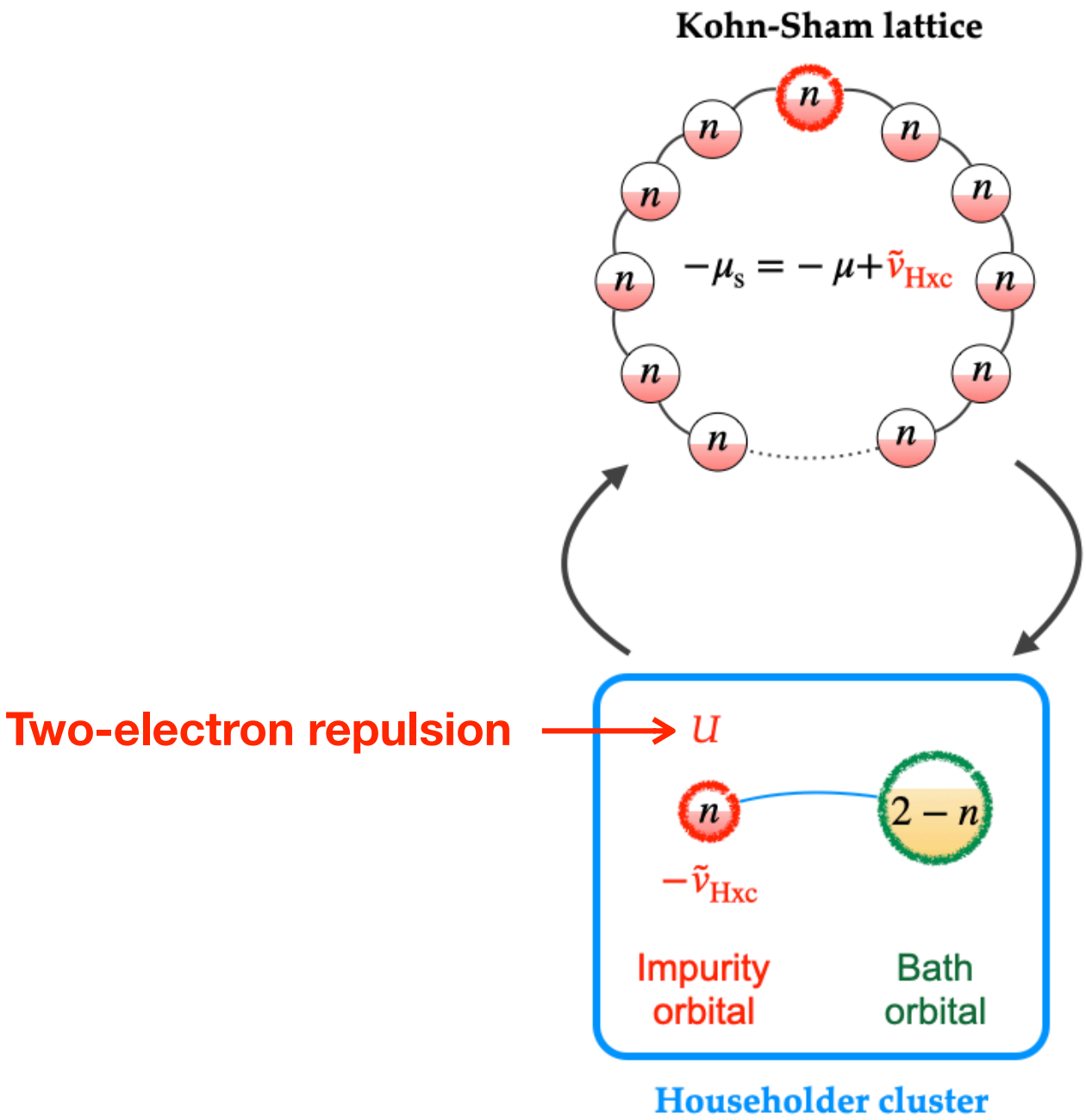
Fixed number of atomic orbitals

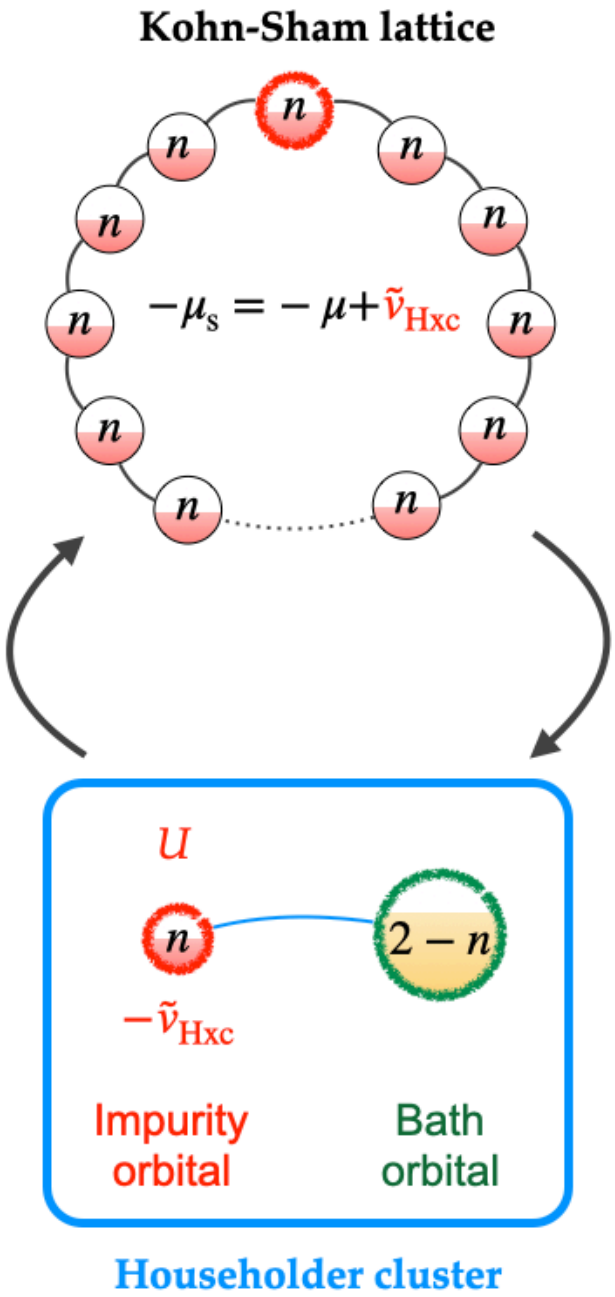




Embedding cluster

S. Sekaran, M. Saubanère, and E. Fromager (2022), Preprint: ***arXiv:2202.08071***
S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B ***104****, 035121 (2021).*

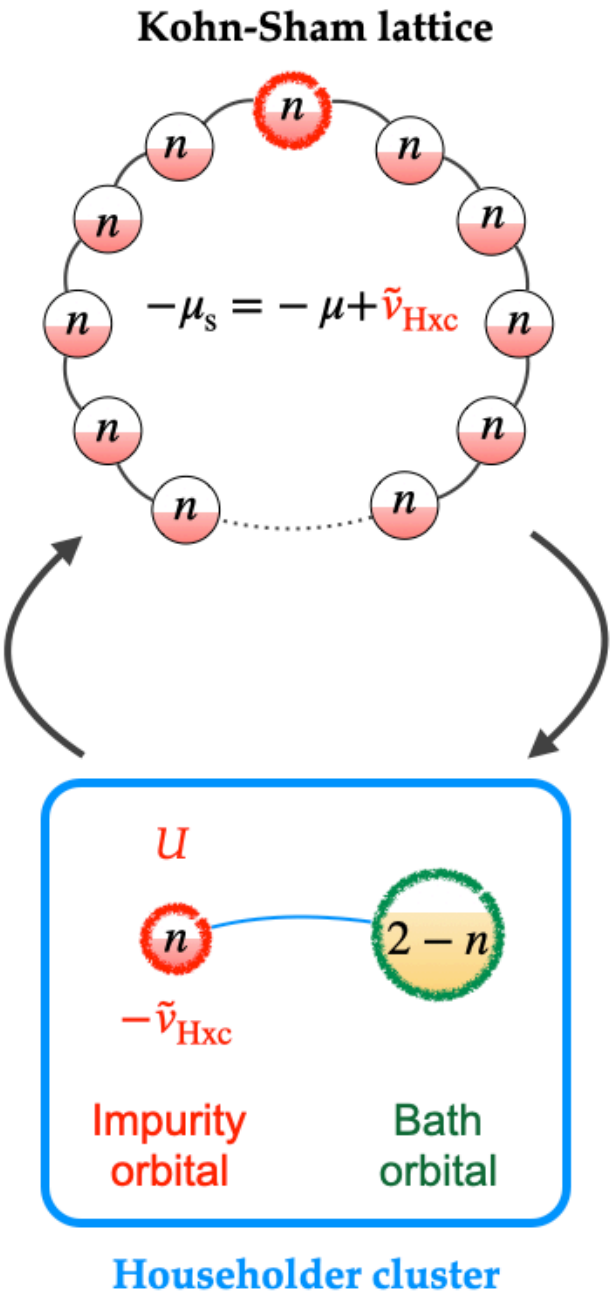

Kohn-Sham lattice
$-\mu_s = -\mu + \tilde{v}_{\mathrm{Hxc}}$
Two-electron repulsion
U
n
$2-n$
$-\tilde{v}_{\mathrm{Hxc}}$
Impurity orbital
Bath orbital
Householder cluster



Embedding cluster

Reduced-in-size version of the full **interacting** lattice

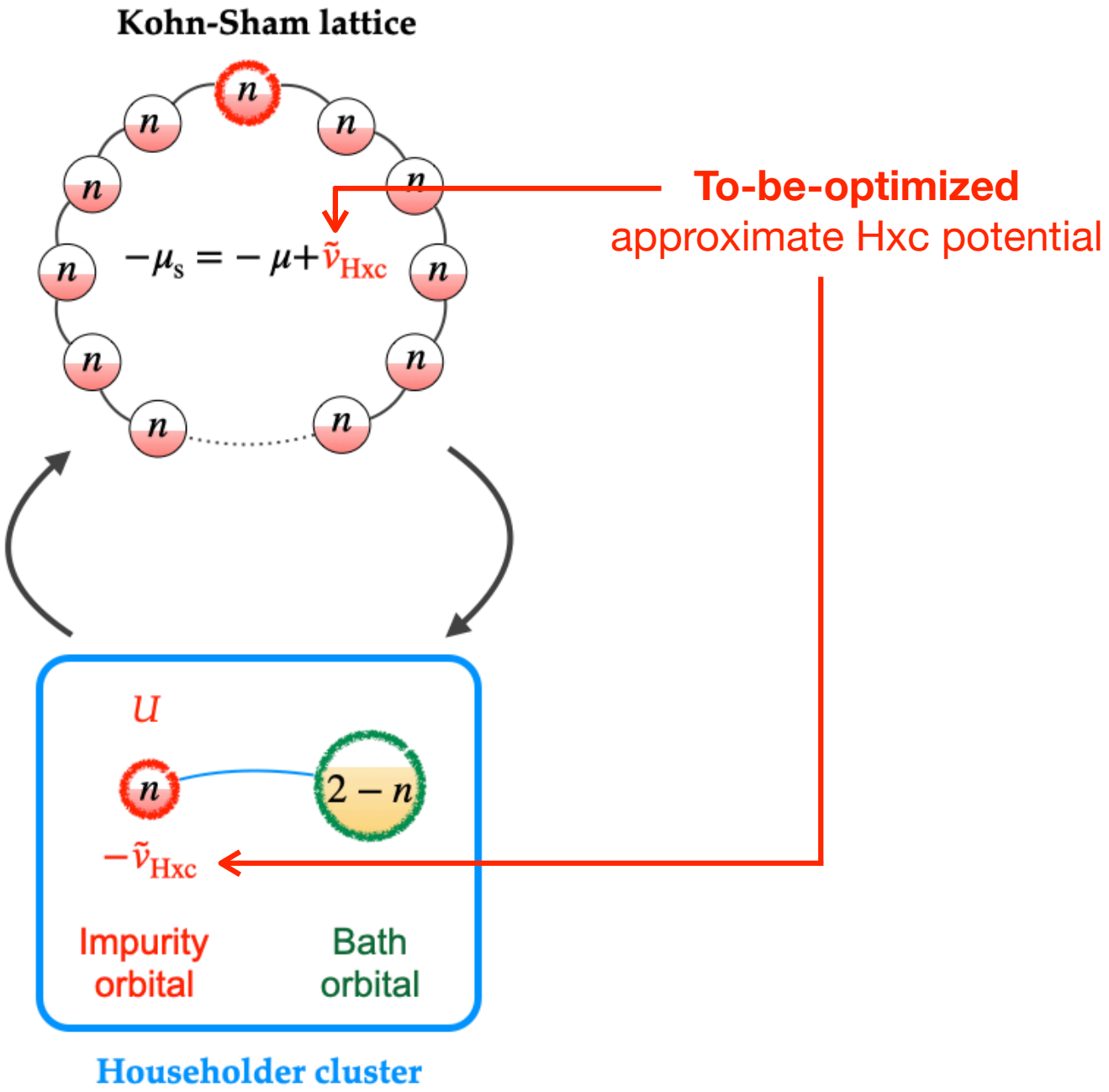
$$\Psi_0 \rightarrow \Psi_0^{cluster}$$

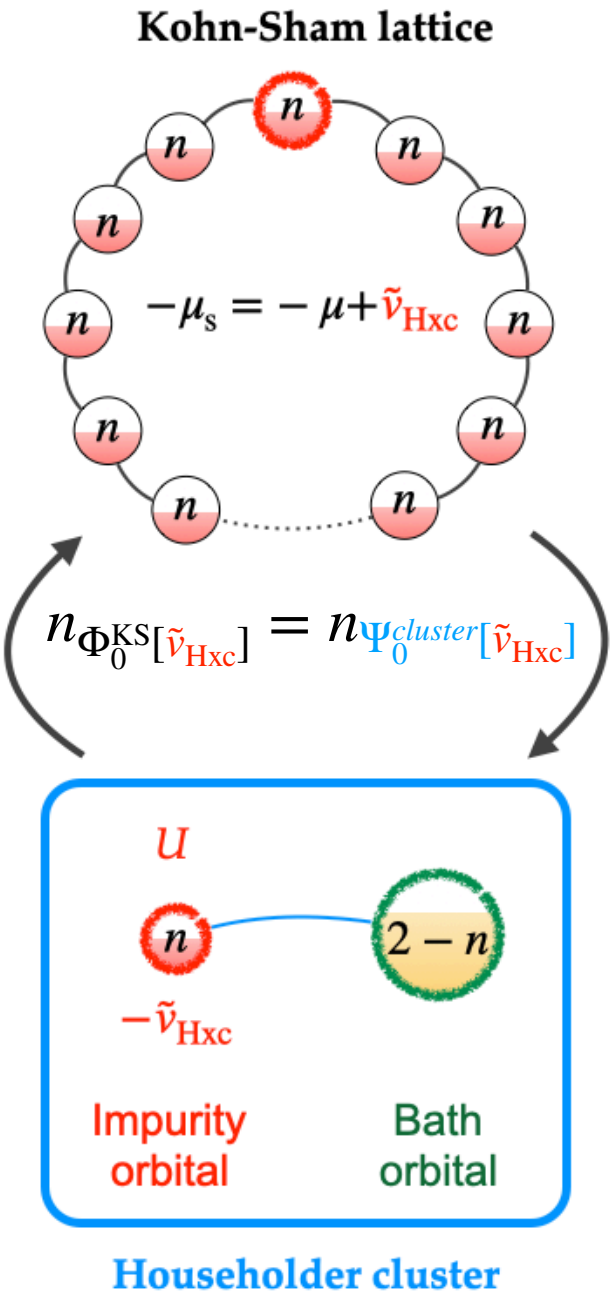


Embedding cluster

Can be solved exactly!

$\Phi_0^{\mathrm{KS}}[\tilde{v}_{\mathrm{Hxc}}]$





Self-consistency loop

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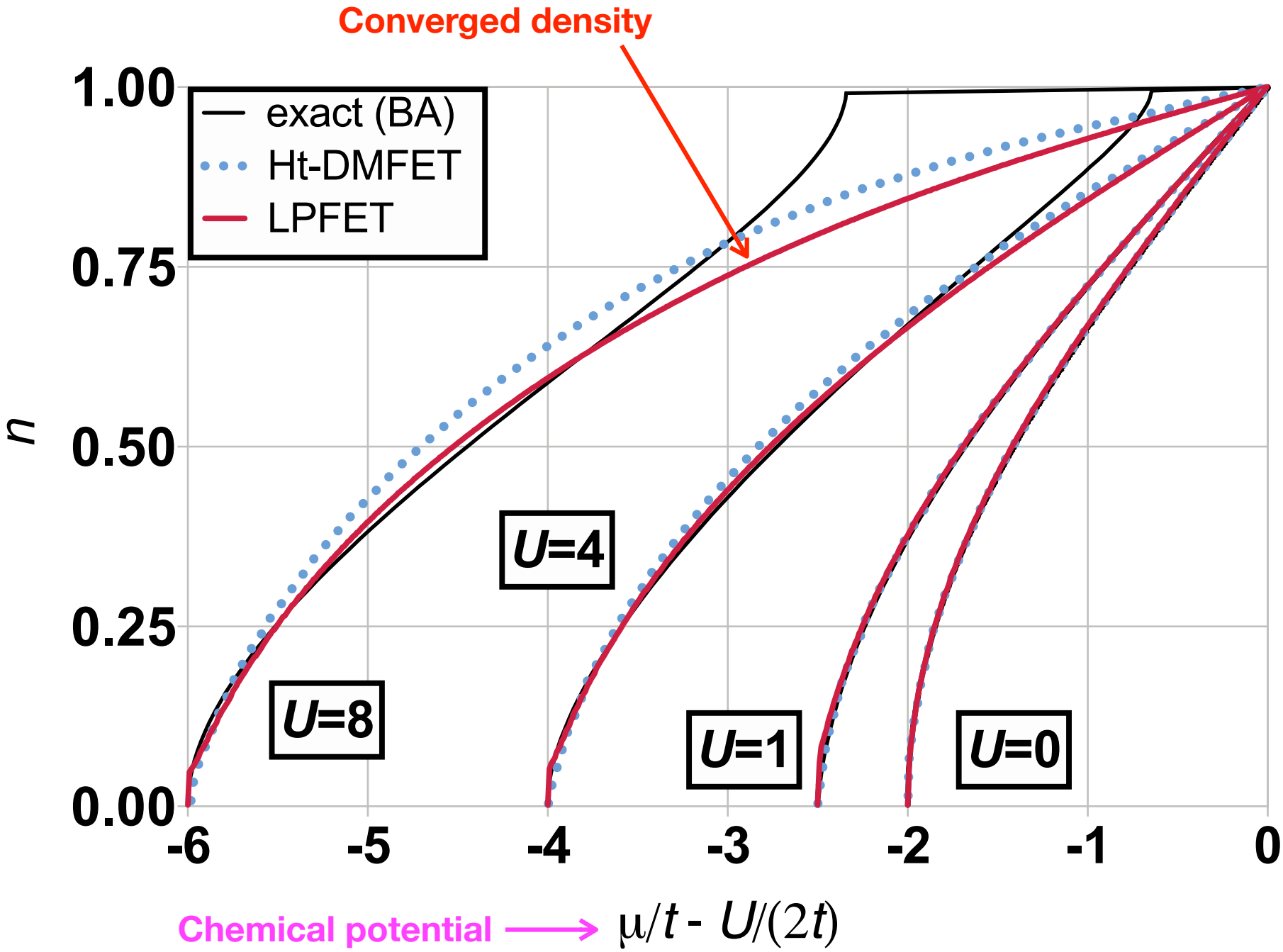
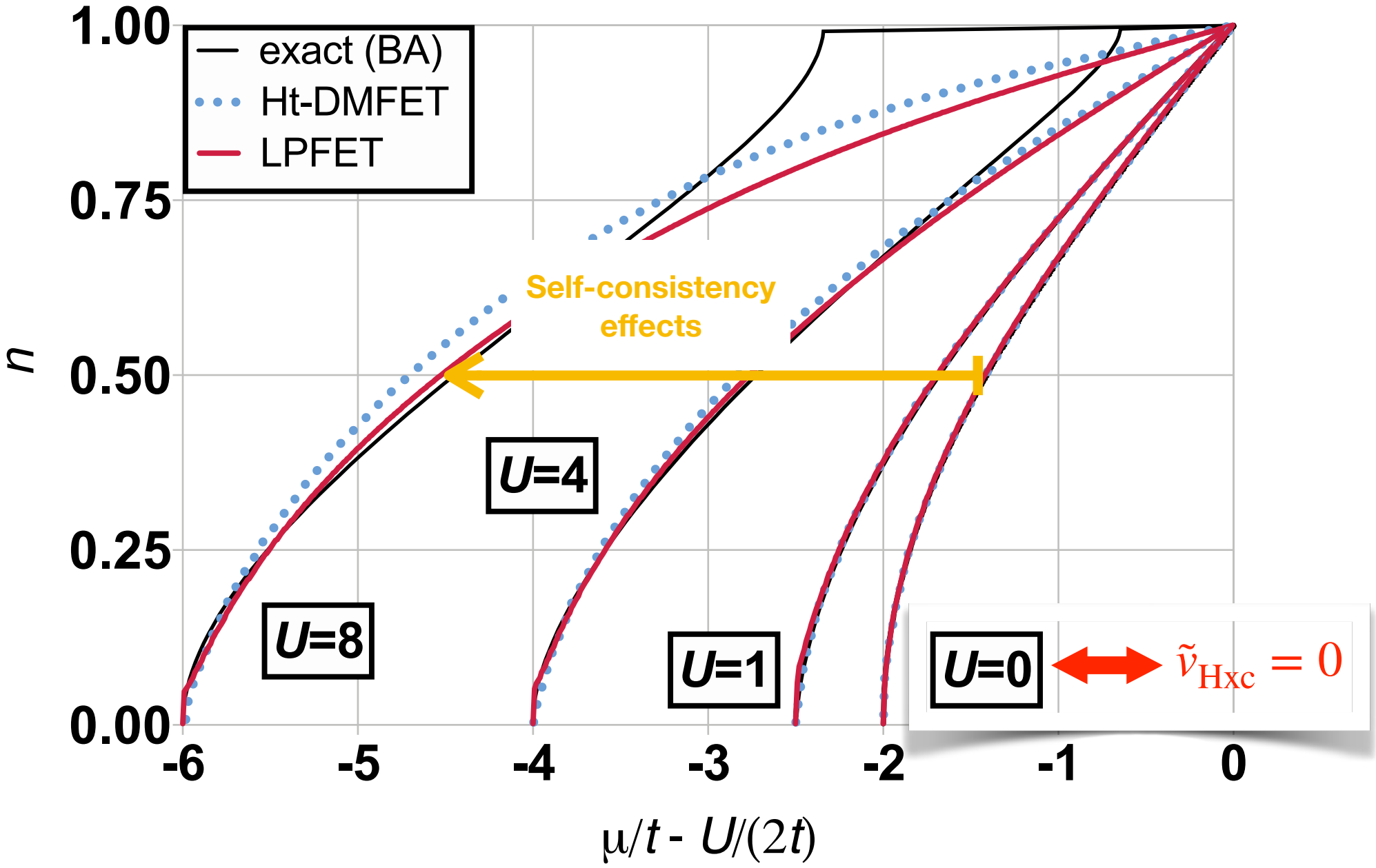
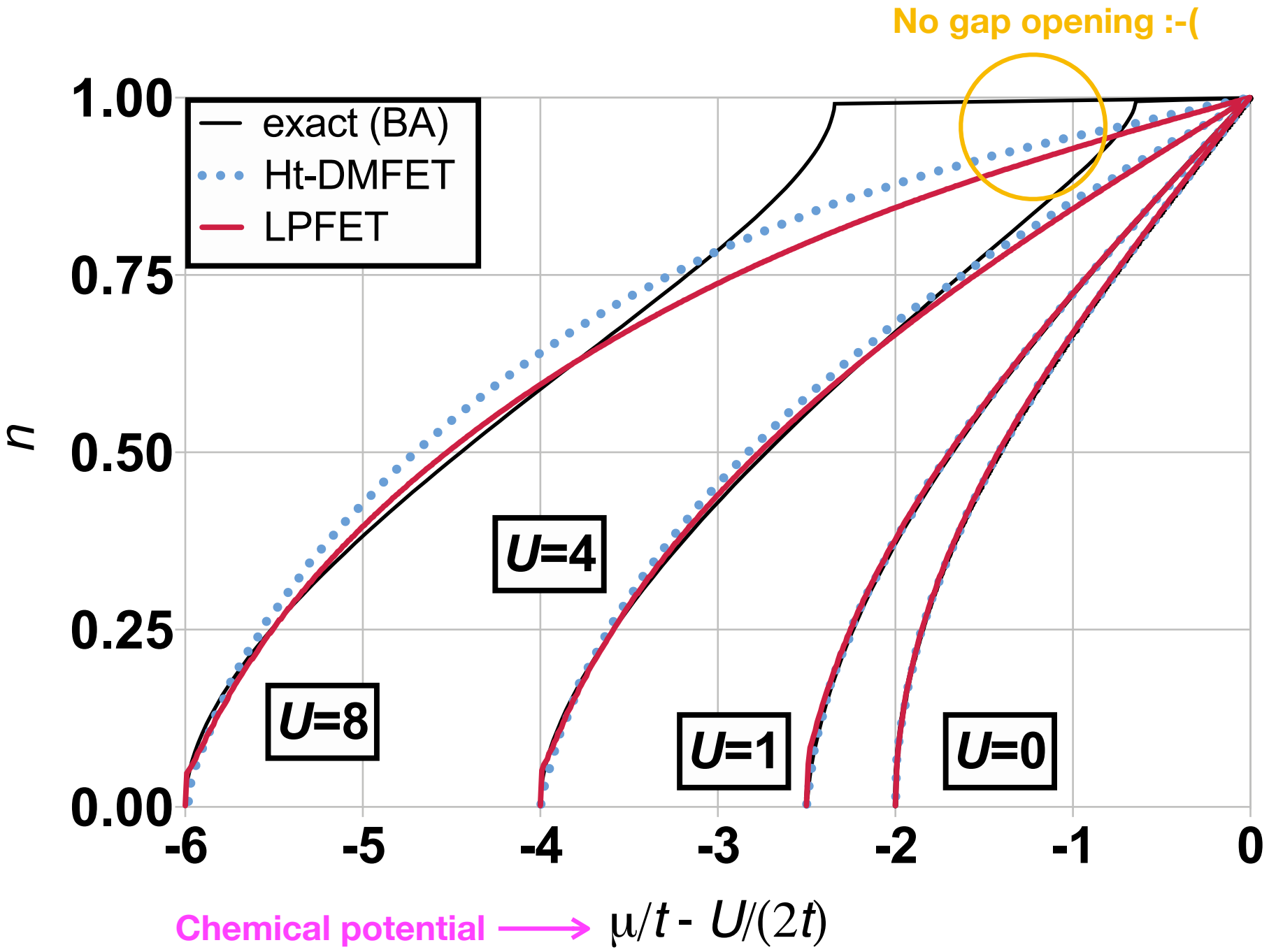
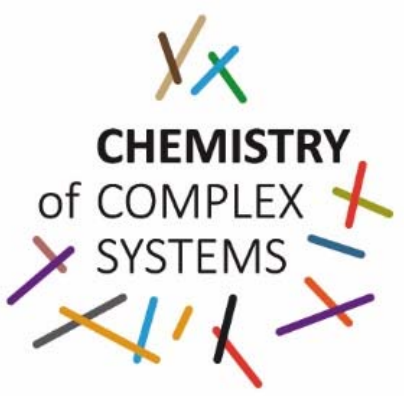

Converged density
exact (BA)
Ht-DMFET
LPFET
1.00
0.75
0.50
0.25
0.00
n
U=4
U=8
U=1
U=0
-6
-5
-4
-3
-2
-1
0
Chemical potential
μ/t - U/(2t)


1.00
0.75
0.50
0.25
0.00
n
-6
-5
-4
-3
-2
-1
0
μ/t - U/(2t)
exact (BA)
Ht-DMFET
LPFET
Self-consistency effects
U=4
U=8
U=1
U=0
$\tilde{v}_{\mathrm{Hxc}} = 0$


No gap opening :-(
exact (BA)
Ht-DMFET
LPFET
1.00
0.75
0.50
0.25
0.00
n
U=8
U=4
U=1
U=0
-6
-5
-4
-3
-2
-1
0
Chemical potential
μ/t - U/(2t)

Funding

“Lab of Excellence” project:
LabEx CSC (ANR-10-LABX-0026-CSC)



« Initiative d’Excellence » (IdEx) grant
University of Strasbourg

CoLab ANR project