Introduction to density matrix embedding theory

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Local and non-local one-electron bases

(One-electron reduced)
density matrix

$$\gamma(\mathbf{x},\mathbf{x}') = \langle \hat{\Psi}^{\dagger}(\mathbf{x})\hat{\Psi}(\mathbf{x}')\rangle = \sum_{kk'} \varphi_k^*(\mathbf{x})\varphi_{k'}(\mathbf{x}') \underbrace{\langle \hat{a}_k^{\dagger}\hat{a}_{k'}\rangle}_{\gamma_{kk'}}$$

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single determinant

$$= \sum_{k}^{occ.} \varphi_k^*(\mathbf{x})\varphi_k(\mathbf{x}')$$

$$\{\gamma_{kk'}\} \equiv \begin{bmatrix} 1 & & & & 0 \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \\ 0 & & & & 0 \\ & & & & & \ddots \\ & & & & & & 0 \end{bmatrix}$$

Local and non-local one-electron bases

(One-electron reduced)
density matrix

"Molecular orbital"
representation:
Non-local basis

$$\gamma(\mathbf{x},\mathbf{x}') = \langle \hat{\Psi}^{\dagger}(\mathbf{x})\hat{\Psi}(\mathbf{x}')\rangle = \sum_{kk'} \varphi_k^*(\mathbf{x})\varphi_{k'}(\mathbf{x}') \underbrace{\langle \hat{a}_k^{\dagger}\hat{a}_{k'}\rangle}_{\gamma_{kk'}}$$

Representation
in real space:
Local basis

$$\overset{single\ determinant}{=} \sum_{k}^{occ.} \varphi_k^*(\mathbf{x})\varphi_k(\mathbf{x}')$$

Local and non-local one-electron bases

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single determinant

$$= \sum_{k}^{occ.} \varphi_k^*(\mathbf{x})\varphi_k(\mathbf{x}')$$

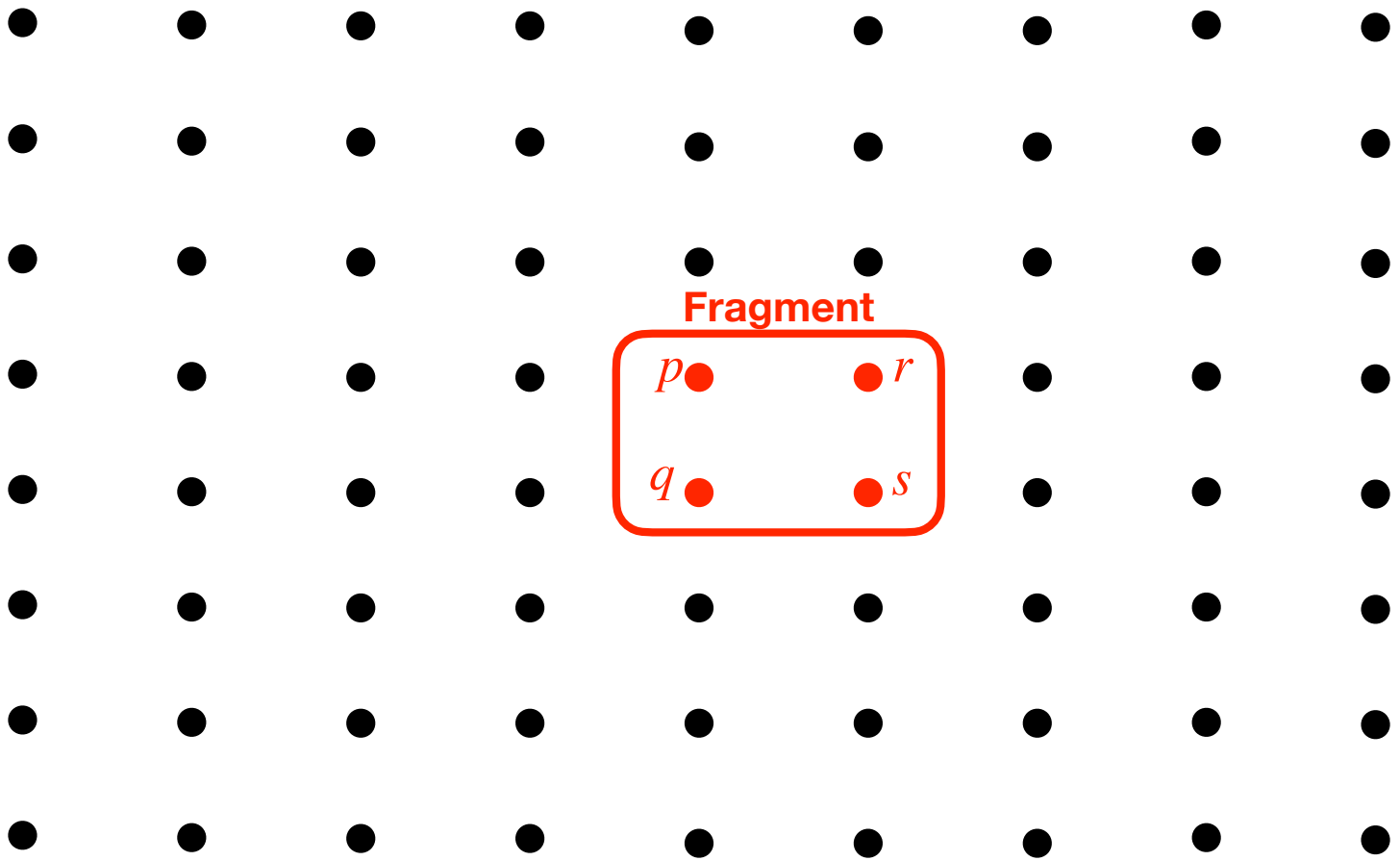
$$\{\gamma_{kk'}\} \equiv \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} = \{\gamma_{kk'}\}^2$$

Idempotency!

Local evaluation of the energy (in a localised spin-orbital basis)

So-called "lattice representation"

$$\langle \hat{H} \rangle = \sum_{pq} h_{pq} \underbrace{\langle \hat{c}_p^\dagger \hat{c}_q \rangle}_{\text{One-electron density matrix}} + \frac{1}{2} \sum_{pqrs} \langle pq \,|\, rs \rangle \underbrace{\langle \hat{c}_p^\dagger \hat{c}_q^\dagger \hat{c}_s \hat{c}_r \rangle}_{\text{Two-electron density matrix}}$$



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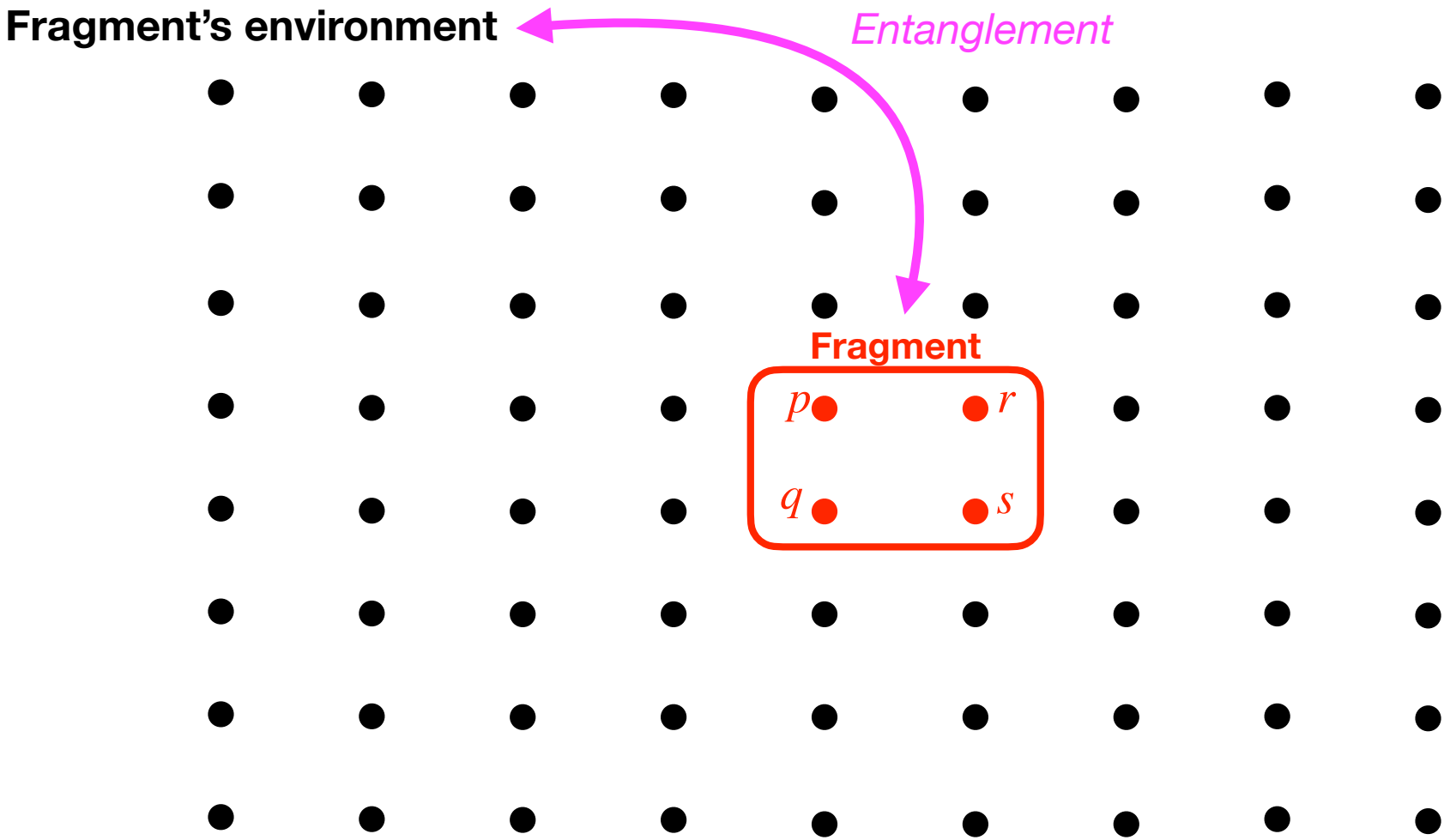
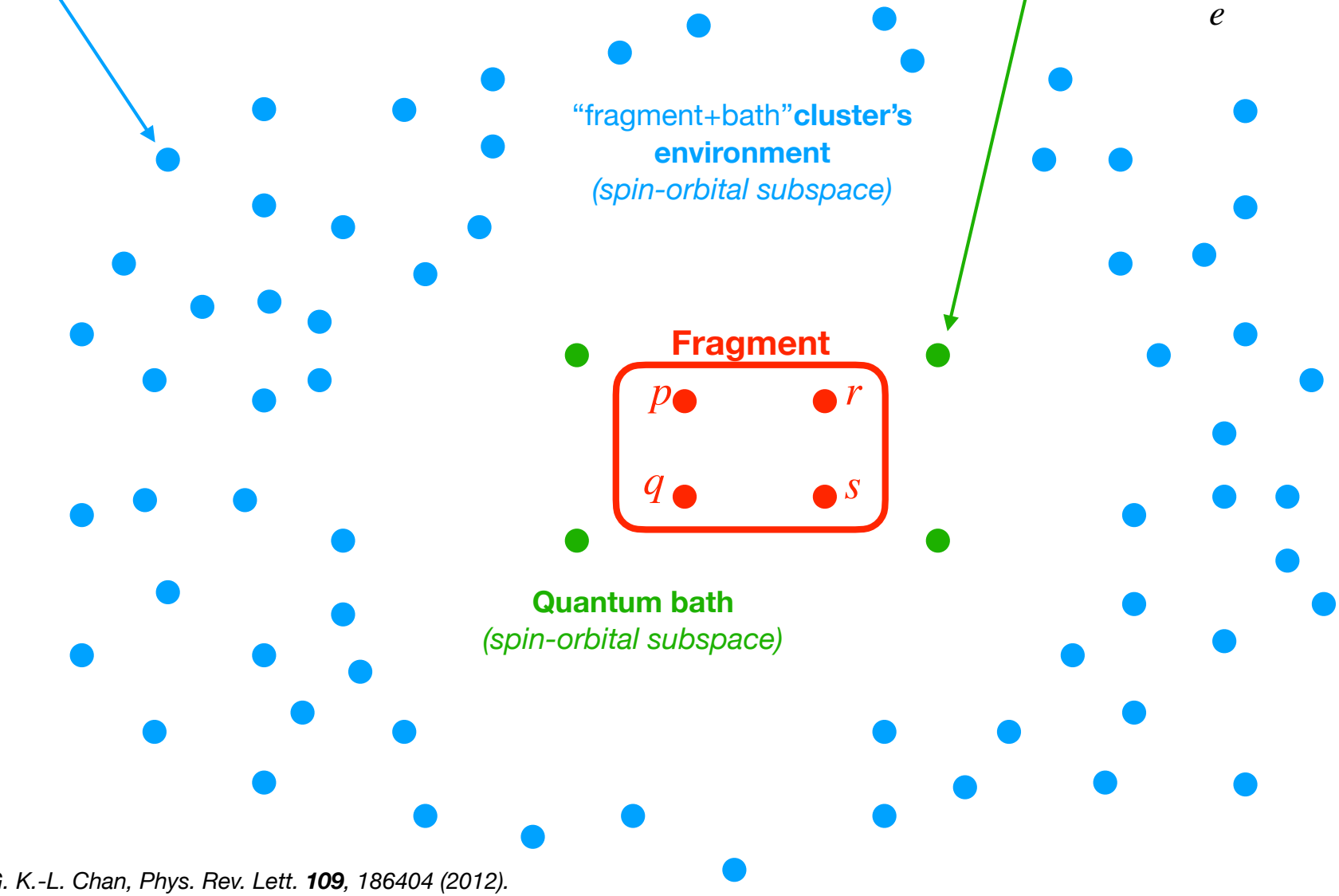


Clusterization through a unitary one-electron transformation

$$\hat{d}_{\mathscr{E}} = \sum_{e}^{environment} \mathcal{U}_{e\mathscr{E}}\,\hat{c}_e$$

$$\hat{d}_{b} = \sum_{e}^{environment} \mathcal{U}_{eb}\,\hat{c}_e$$



G. Knizia and G. K.-L. Chan, Phys. Rev. Lett. ***109****, 186404 (2012).*
S. Wouters, C. A. Jiménez-Hoyos, Q. Sun, and G. K.-L. Chan, J. Chem. Theory Comput. 12, 2706 (2016).

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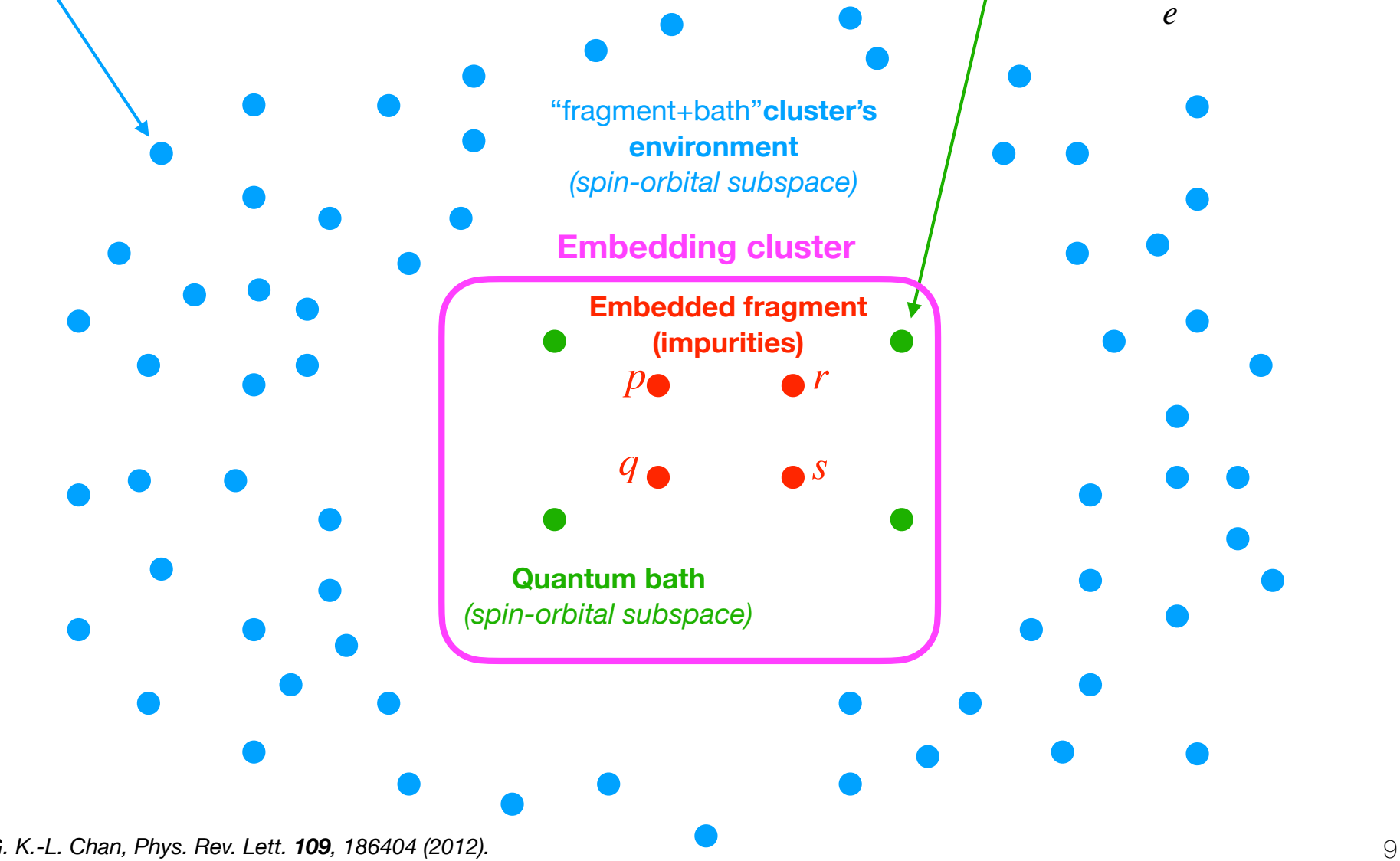

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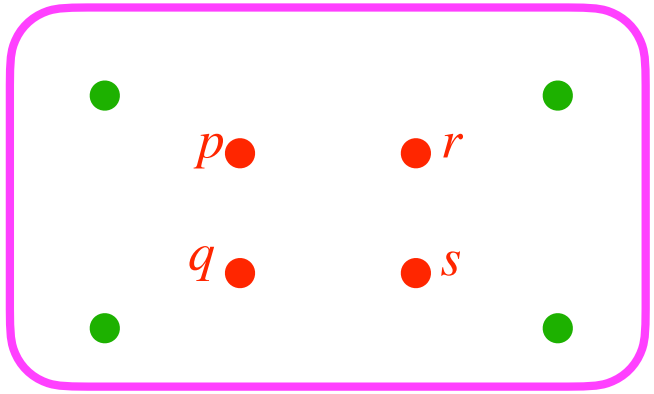
Density matrix embedding theory (DMET)

$$\langle \hat{H} \rangle = \sum_{pq} h_{pq} \langle \hat{c}_p^\dagger \hat{c}_q \rangle + \frac{1}{2} \sum_{pqrs} \langle pq \,|\, rs \rangle \langle \hat{c}_p^\dagger \hat{c}_q^\dagger \hat{c}_s \hat{c}_r \rangle$$

Original lattice representation

Quantum bath
≡ electronic reservoir

Closed embedding cluster



$\Psi^{\mathscr{C}}$ *(exact diagonalisation)*

$$\langle \hat{c}_p^\dagger \hat{c}_q \rangle \approx \langle \hat{c}_p^\dagger \hat{c}_q \rangle_{\Psi^{\mathscr{C}}}$$

$$\langle \hat{c}_p^\dagger \hat{c}_q^\dagger \hat{c}_s \hat{c}_r \rangle \approx \langle \hat{c}_p^\dagger \hat{c}_q^\dagger \hat{c}_s \hat{c}_r \rangle_{\Psi^{\mathscr{C}}}$$

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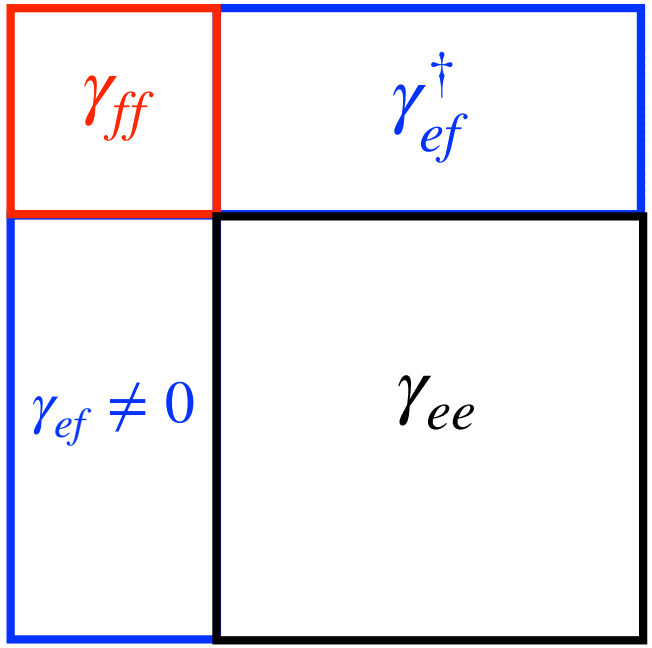
Clusterization through a unitary one-electron transformation

$$\gamma \equiv \left\{ \gamma_{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle \right\} \equiv$$



Change of spin-orbital basis

$$\hat{d}_j = \sum_l^{lattice} \mathcal{U}_{lj}[\gamma_{ef}]\, \hat{c}_l$$

Unitary transformation *of the density matrix*

$$\tilde{\gamma}_{ij} = \left\{ \langle \hat{d}_i^\dagger \hat{d}_j \rangle \right\} \equiv \mathcal{U}^\dagger[\gamma_{ef}]\, \gamma\, \mathcal{U}[\gamma_{ef}]$$

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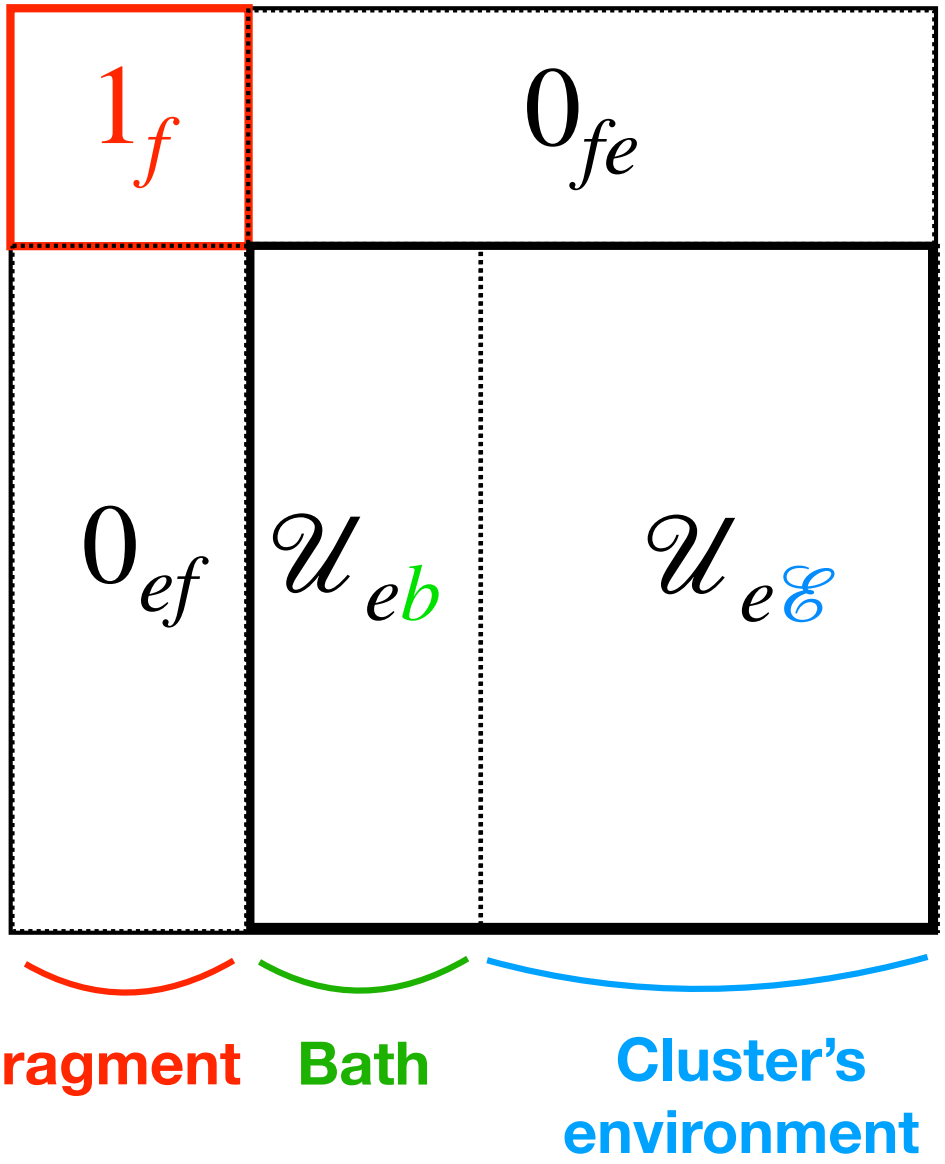
Clusterization through a unitary one-electron transformation

$$\mathcal{U} \equiv \mathcal{U}[\gamma_{ef}] =$$



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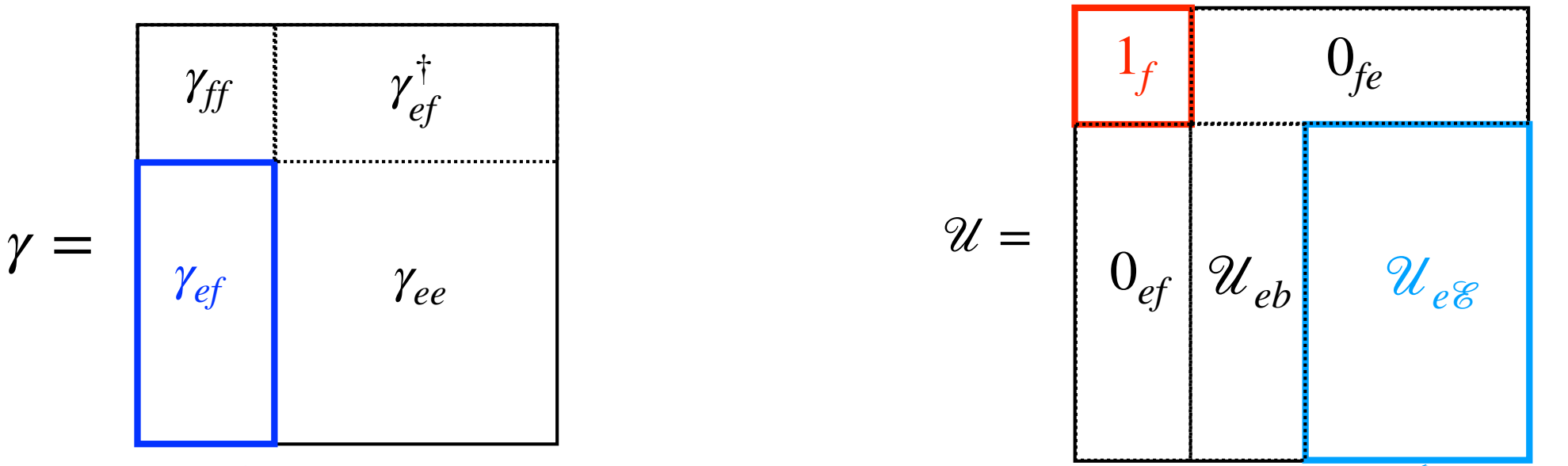
Clusterization through a unitary one-electron transformation



Environment of the embedding cluster
(usually neglected)

$$\gamma_{ef}^{\dagger}\,\mathcal{U}_{e\mathscr{E}} \equiv 0$$

Orthogonality constraint

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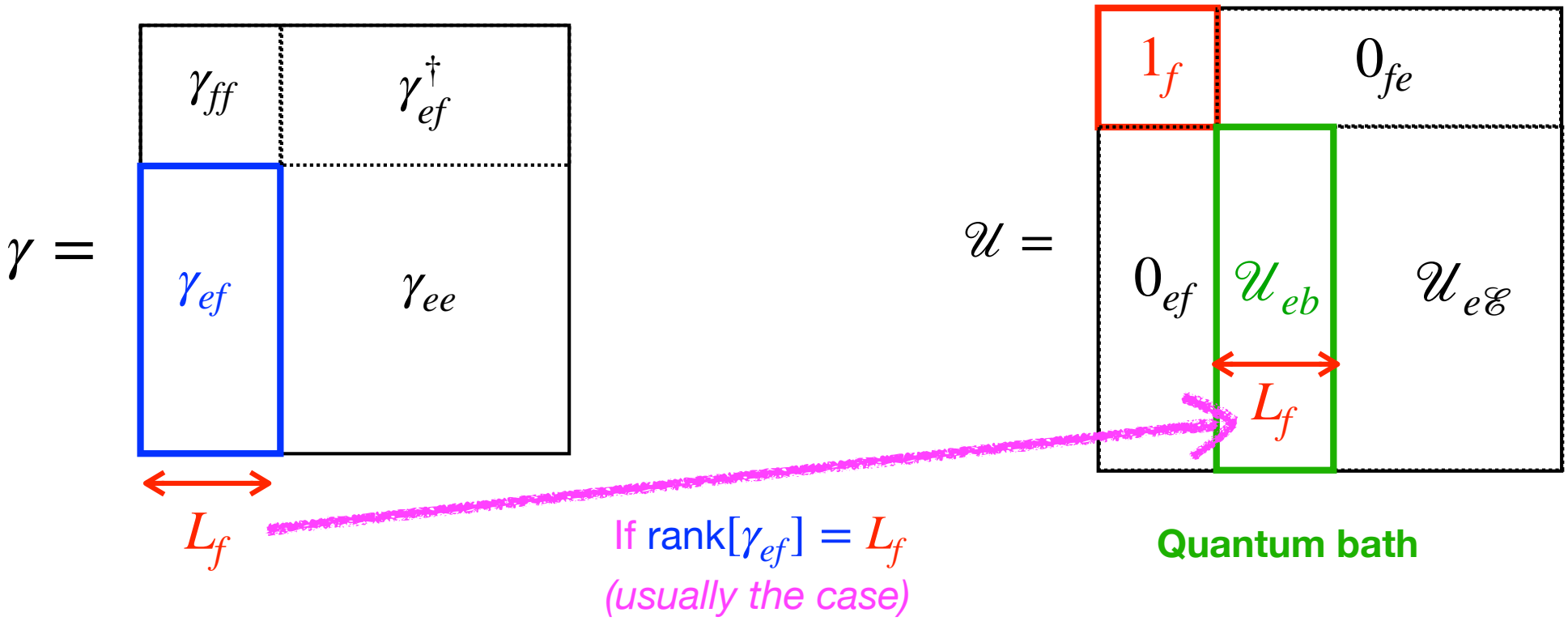
Clusterization through a unitary one-electron transformation



Bath spin-orbitals are generated from the *columns of* γ_{ef}

S. Sekaran, O. Bindech, and E. Fromager, to be submitted *(2022).*

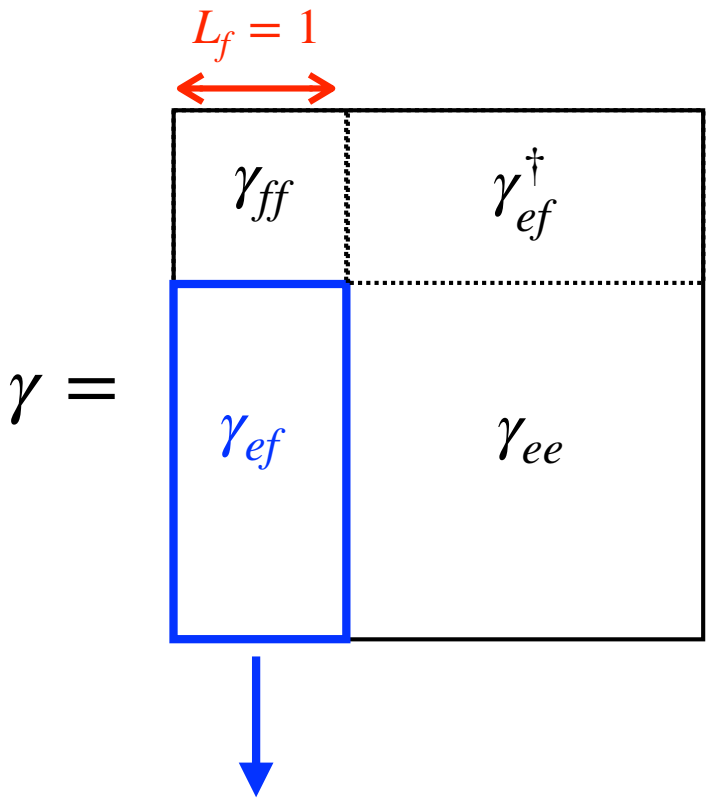
[1]*B.-X. Zheng, PhD thesis,* **arXiv:1803.10259** (2018).

[2]*F. Rotella and I. Zambettakis, Appl. Math. Lett.* ***12****, 29 (1999).*

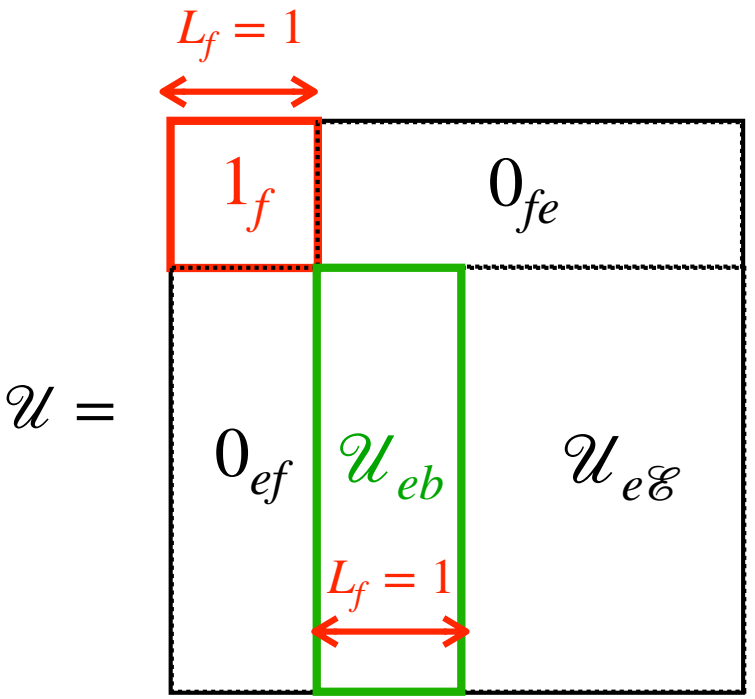
[3]*S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B* ***104****, 035121 (2021).*

[4]*S. Sekaran, M. Saubanère, and S. Yalouz,* to be submitted (2022).

Single-impurity case



Column vector



Quantum bath

$$\mathcal{U}_{eb} = \frac{\gamma_{ef}}{\sqrt{\gamma_{ef}^\dagger \gamma_{ef}}}$$

Column vector

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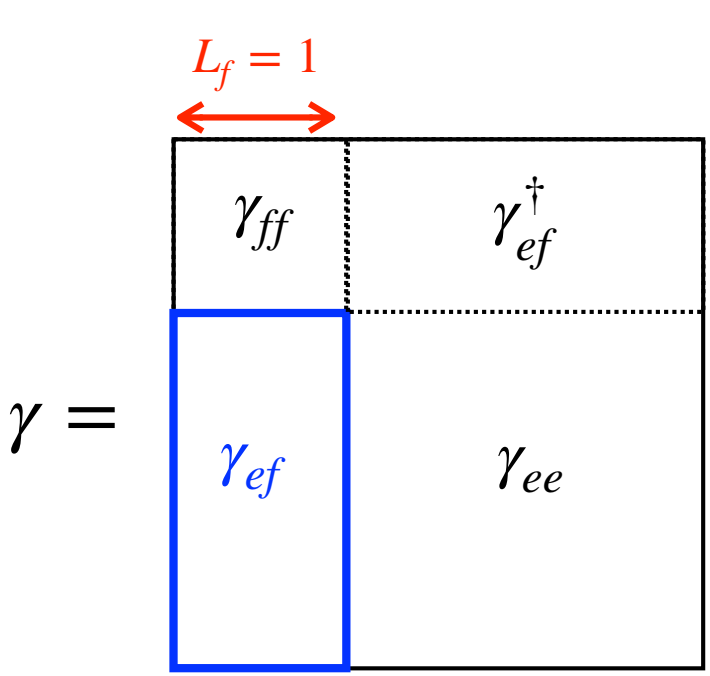
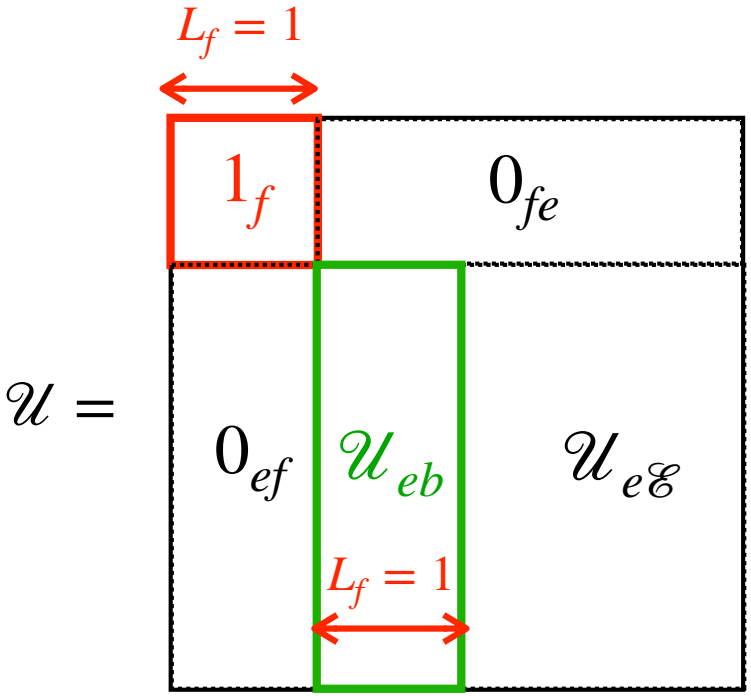
Single-impurity case





$$\hat{d}_{bath} = \frac{\sum_{e}^{environment} \gamma_{ef}\, \hat{c}_e}{\sqrt{\sum_{e}^{environment} |\gamma_{ef}|^2}}$$

$$\mathcal{U}_{eb} = \frac{\gamma_{ef}}{\sqrt{\gamma_{ef}^{\dagger}\gamma_{ef}}}$$

Column vector

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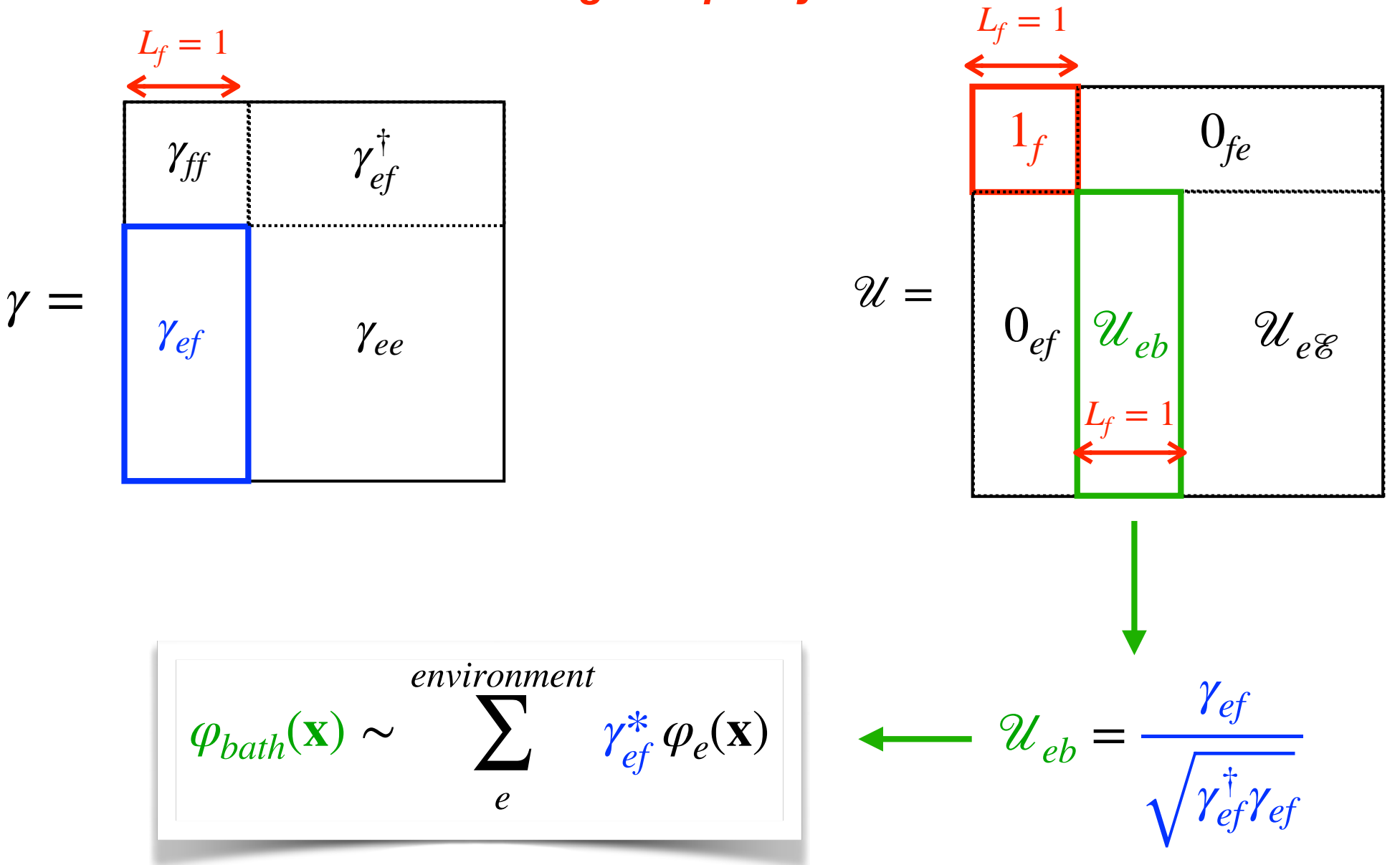
Single-impurity case



$$\varphi_{bath}(\mathbf{x}) \sim \sum_{e}^{environment} \gamma_{ef}^{*}\, \varphi_{e}(\mathbf{x})$$

$$\mathcal{U}_{eb} = \frac{\gamma_{ef}}{\sqrt{\gamma_{ef}^{\dagger}\gamma_{ef}}}$$

Column vector

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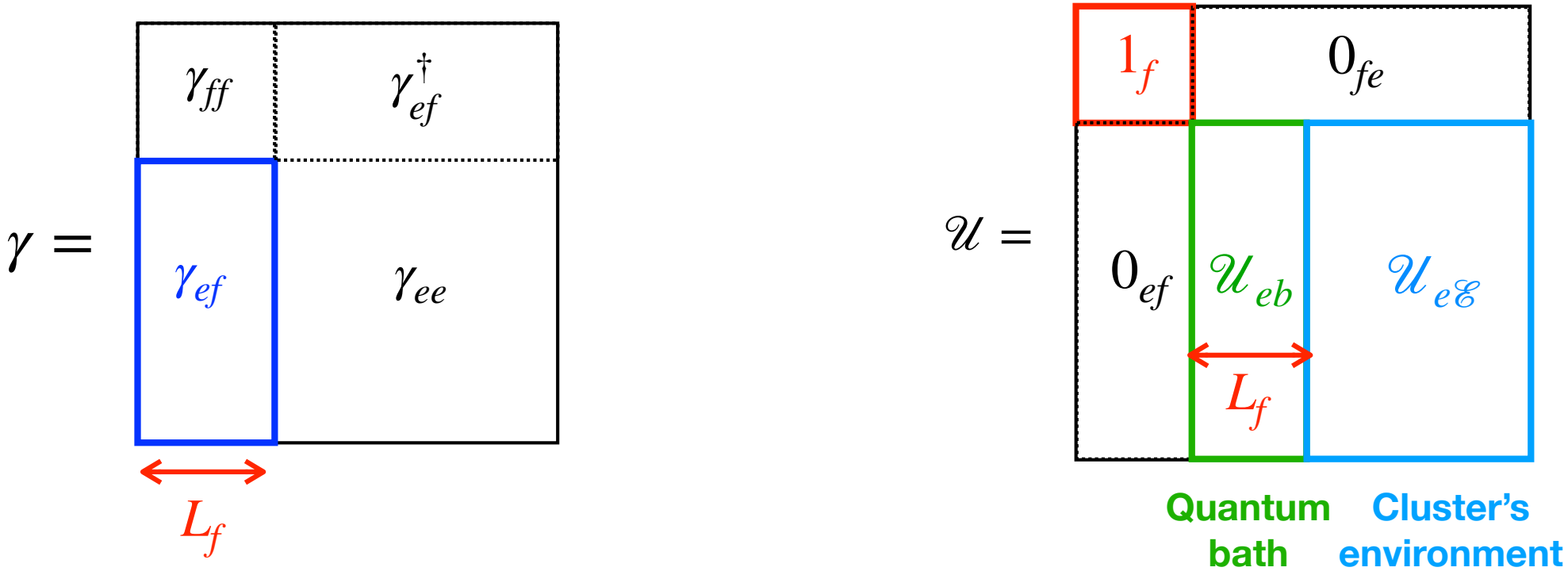
General multiple-impurity case



How to generate an ***orthonormal basis*** for the bath and the cluster's environment?

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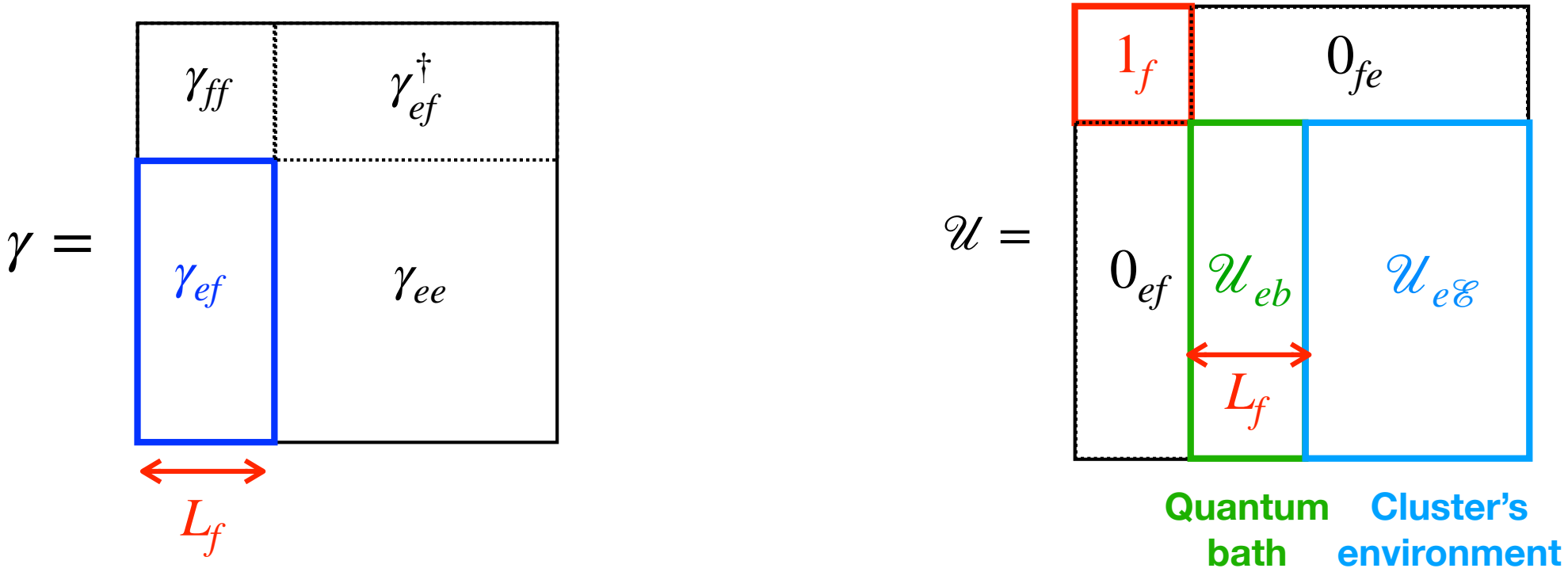
General multiple-impurity case



Diagonalise $\gamma_{ef}\gamma_{ef}^{\dagger}$ *!!!*

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[3]*S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B* ***104****, 035121 (2021).*

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General multiple-impurity case

$$\gamma = \begin{pmatrix} \gamma_{ff} & \gamma_{ef}^{\dagger} \\ \gamma_{ef} & \gamma_{ee} \end{pmatrix}$$

L_f

$$\mathcal{U} = \begin{pmatrix} 1_f & 0_{fe} \\ 0_{ef} & \mathcal{U}_{eb} \quad \mathcal{U}_{e\mathscr{E}} \end{pmatrix}$$

L_f

Quantum bath **Cluster's environment**

$$\gamma_{ef}\gamma_{ef}^{\dagger}\mathcal{U}_{e\mathscr{E}} = \mathcal{U}_{e\mathscr{E}}0_{\mathscr{E}\mathscr{E}}$$

Zero eigenvalues

General multiple-impurity case

$$\gamma = \begin{pmatrix} \gamma_{ff} & \gamma_{ef}^{\dagger} \\ \gamma_{ef} & \gamma_{ee} \end{pmatrix}$$

L_f

$$\mathcal{U} = \begin{pmatrix} 1_f & 0_{fe} \\ 0_{ef} & \mathcal{U}_{eb} \quad \mathcal{U}_{e\mathscr{E}} \end{pmatrix}$$

L_f

Quantum bath **Cluster's environment**

Bath spin-orbitals are generated from the *columns of* γ_{ef}

General multiple-impurity case

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L_f

Quantum bath **Cluster's environment**

Bath spin-orbitals are generated from the *columns of* γ_{ef}

$$\left(\gamma_{ef}\gamma_{ef}^{\dagger}\right)\gamma_{ef} = \gamma_{ef}\left(\gamma_{ef}^{\dagger}\gamma_{ef}\right)$$

Step-by-step construction of the bath

$$\left(\gamma_{ef}\gamma_{ef}^{\dagger}\right)\gamma_{ef} = \gamma_{ef}\left(\gamma_{ef}^{\dagger}\gamma_{ef}\right) \qquad \gamma_{ef}^{\dagger}\gamma_{ef} = \mathscr{W}\mathscr{D}\mathscr{W}^{\dagger}$$

$\sigma_i > 0$

Singular values of γ_{ef}

$$\begin{bmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \\ & & & \sigma_{L_f}^2 \end{bmatrix} = \mathscr{D}$$

Step-by-step construction of the bath

$$\left(\gamma_{ef}\gamma_{ef}^{\dagger}\right)\gamma_{ef} = \gamma_{ef}\left(\gamma_{ef}^{\dagger}\gamma_{ef}\right) \longleftarrow \gamma_{ef}^{\dagger}\gamma_{ef} = \mathscr{W}\mathscr{D}\mathscr{W}^{\dagger}$$

$\sigma_i > 0$

Singular values of γ_{ef}

$$\begin{bmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \\ & & & \sigma_{L_f}^2 \end{bmatrix} = \mathscr{D}$$

$$\left(\gamma_{ef}\gamma_{ef}^{\dagger}\right)\underbrace{\gamma_{ef}\mathscr{W}\mathscr{D}^{-1/2}}_{\mathscr{U}_{eb}} = \underbrace{\gamma_{ef}\mathscr{W}\mathscr{D}^{-1/2}}_{\mathscr{U}_{eb}}\mathscr{D}$$

Step-by-step construction of the bath

$$\left(\gamma_{ef}\gamma_{ef}^{\dagger}\right)\gamma_{ef} = \gamma_{ef}\left(\gamma_{ef}^{\dagger}\gamma_{ef}\right)$$

$$\gamma_{ef}^{\dagger}\gamma_{ef} = \mathscr{W}\mathscr{D}\mathscr{W}^{\dagger}$$

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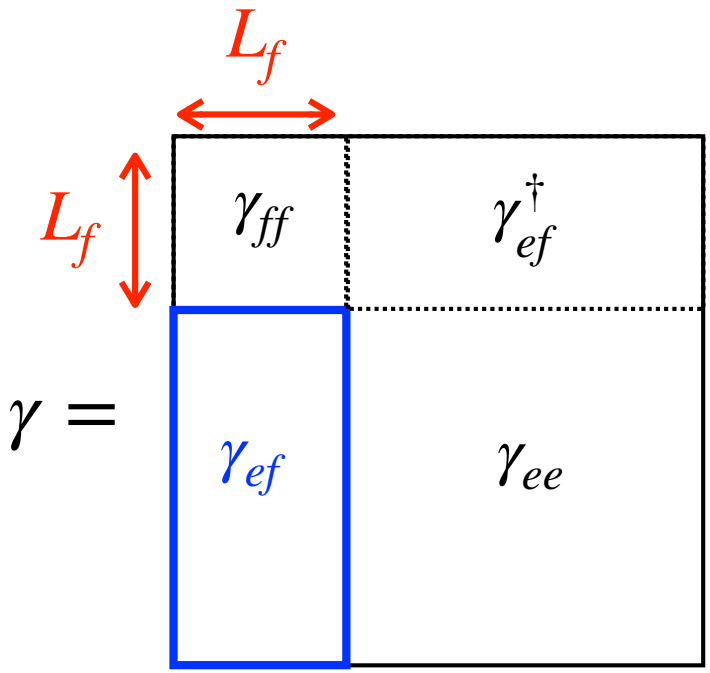
Singular values of γ_{ef}

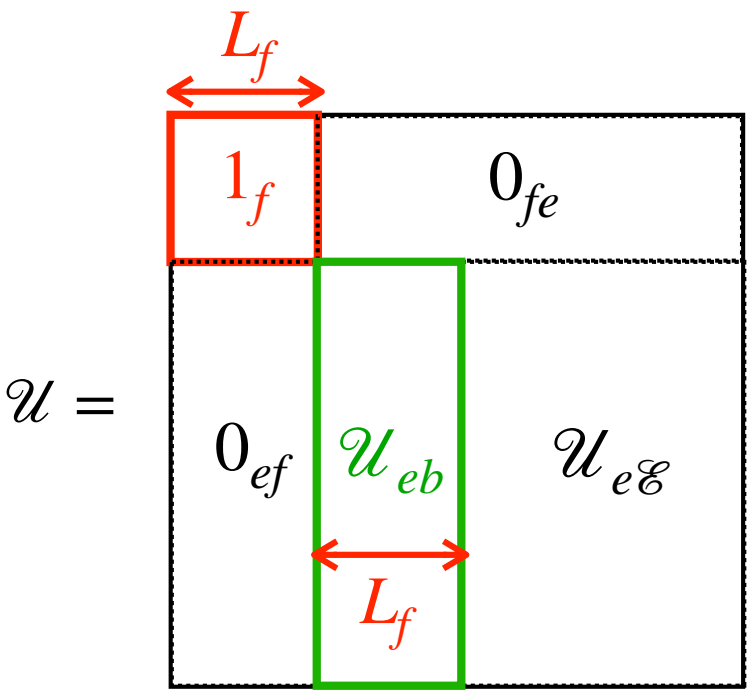
$$\begin{bmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & & \ddots \\ & & & \sigma_{L_f}^2 \end{bmatrix} = \mathscr{D}$$

$$\left(\gamma_{ef}\gamma_{ef}^{\dagger}\right)\underbrace{\gamma_{ef}\mathscr{W}\mathscr{D}^{-1/2}}_{\mathscr{U}_{eb}} = \underbrace{\gamma_{ef}\mathscr{W}\mathscr{D}^{-1/2}}_{\mathscr{U}_{eb}}\mathscr{D}$$

$$\mathscr{U}_{eb}^{\dagger}\mathscr{U}_{eb} = \mathscr{D}^{-1/2}\mathscr{W}^{\dagger}\gamma_{ef}^{\dagger}\gamma_{ef}\mathscr{W}\mathscr{D}^{-1/2} = 1_{bb}$$

Clusterization through a unitary one-electron transformation





Equivalent constructions of the L_f orthonormal **bath** spin-orbitals

Singular value decomposition[1] *of* γ_{ef} **or** ***Block Householder transformation***[2,3]

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[2] *F. Rotella and I. Zambettakis, Appl. Math. Lett.* ***12****, 29 (1999).*

[3] *S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B* ***104****, 035121 (2021).*

Clusterization through a unitary one-electron transformation

$$\gamma = \begin{pmatrix} \gamma_{ff} & \gamma_{ef}^{\dagger} \\ \gamma_{ef} & \gamma_{ee} \end{pmatrix} \qquad \mathcal{U} = \begin{pmatrix} 1_f & 0_{fe} \\ 0_{ef} & \mathcal{U}_{eb} \quad \mathcal{U}_{e\mathscr{E}} \end{pmatrix}$$

REMINDER

$$\gamma_{ef}^{\dagger}\,\mathcal{U}_{e\mathscr{E}} \equiv 0$$

Orthogonality constraint

The only thing we need to remember is that

Environment of the embedding cluster
(usually neglected)

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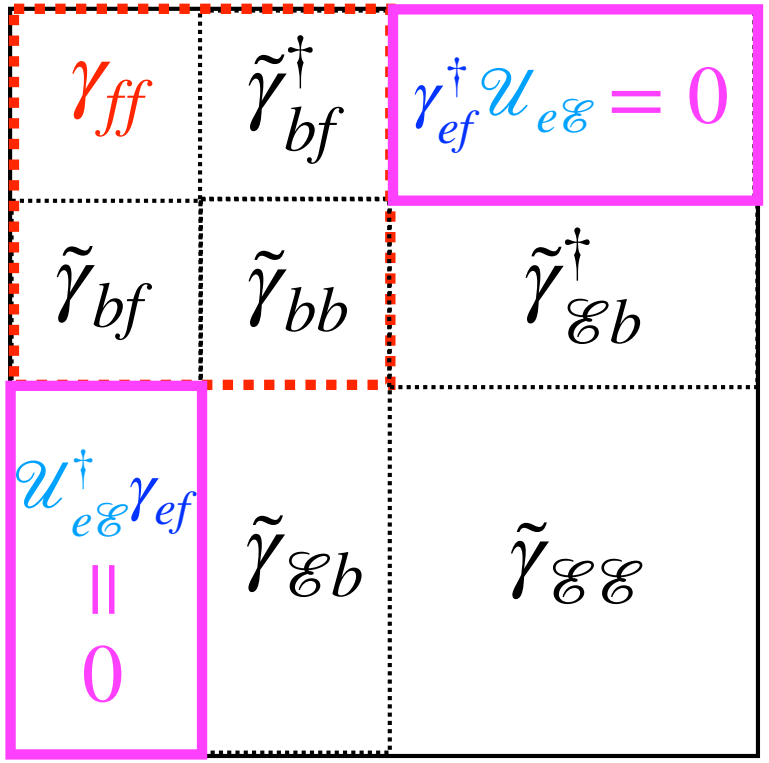
Unitary transformed density matrix

$$\tilde{\gamma} = \mathcal{U}^\dagger \gamma \mathcal{U} \equiv$$



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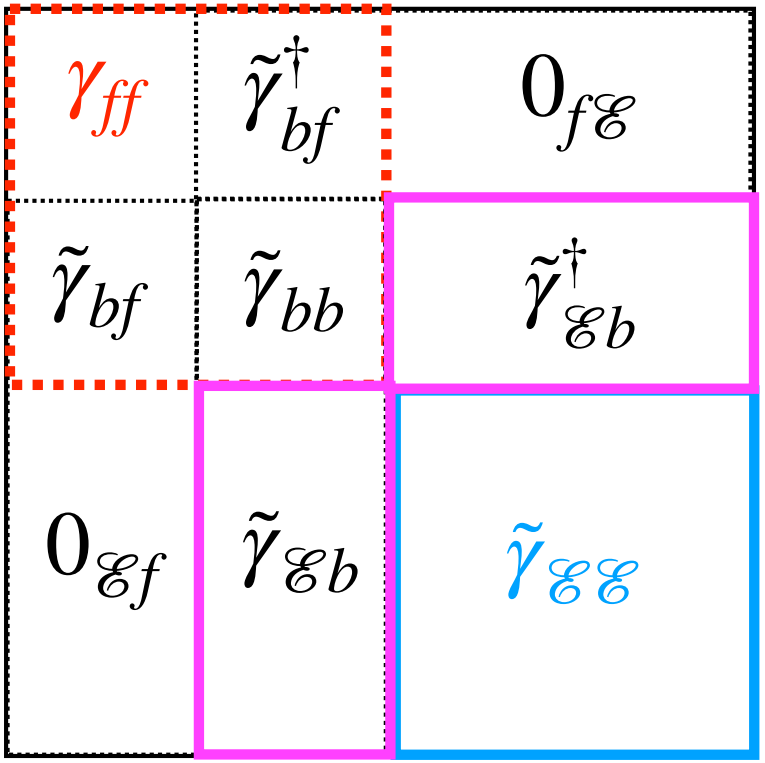
Unitary transformed density matrix

$$\tilde{\gamma} = \mathcal{U}^{\dagger}\gamma\mathcal{U} \equiv$$

"fragment+bath" embedding cluster



Cluster's environment

Entanglement

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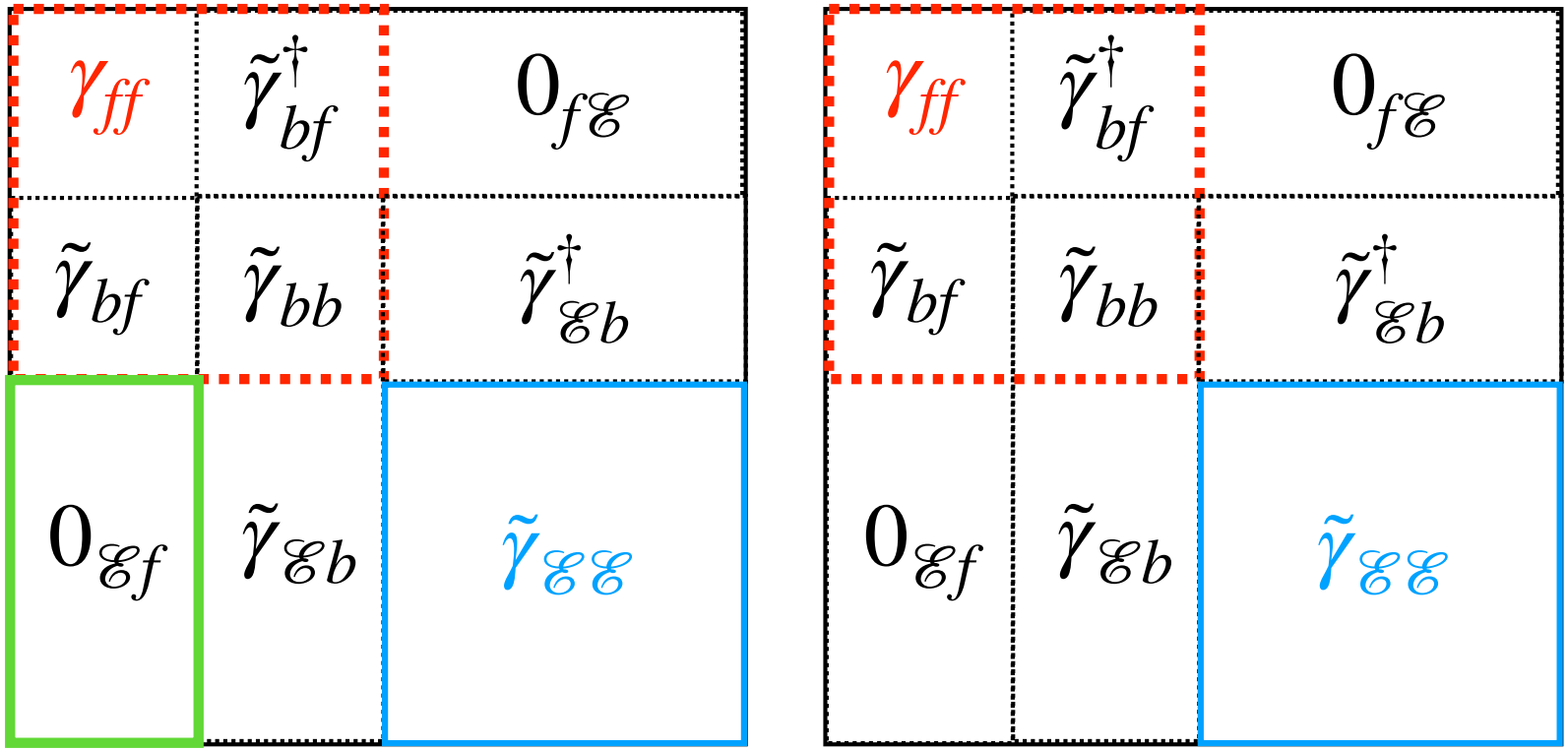
Unitary transformed density matrix

$$\tilde{\gamma}^2 \equiv$$



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Unitary transformed idempotent density matrix

$$\tilde{\gamma}^2 = \tilde{\gamma} = \mathcal{U}^\dagger \gamma \mathcal{U} \equiv$$

γ_{ff}	$\tilde{\gamma}^\dagger_{bf}$	$0_{f\mathscr{E}}$
$\tilde{\gamma}_{bf}$	$\tilde{\gamma}_{bb}$	$\tilde{\gamma}^\dagger_{\mathscr{E}b} = 0$
$0_{\mathscr{E}f}$	$\tilde{\gamma}_{\mathscr{E}b} = 0$	$\tilde{\gamma}_{\mathscr{E}\mathscr{E}}$

$$\tilde{\gamma}_{\mathscr{E}b}\tilde{\gamma}_{bf} \longrightarrow \tilde{\gamma}_{\mathscr{E}b} = 0$$

$$\tilde{\gamma}_{bf}\tilde{\gamma}^\dagger_{bf} = \mathscr{D}$$

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Unitary transformed idempotent density matrix

$$\tilde{\gamma}^2 = \tilde{\gamma} = \mathcal{U}^\dagger \gamma \mathcal{U} \equiv$$

γ_{ff}	$\tilde{\gamma}^\dagger_{bf}$	$0_{f\mathscr{E}}$
$\tilde{\gamma}_{bf}$	$\tilde{\gamma}_{bb}$	$\tilde{\gamma}^\dagger_{\mathscr{E}b} = 0$
$0_{\mathscr{E}f}$	$\tilde{\gamma}_{\mathscr{E}b} \parallel 0$	$\tilde{\gamma}_{\mathscr{E}\mathscr{E}}$

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Disconnected embedding cluster

$$\tilde{\gamma}^2 = \tilde{\gamma} = \mathcal{U}^\dagger \gamma \mathcal{U} \equiv$$

$$\begin{pmatrix} \gamma_{ff} & \tilde{\gamma}_{bf}^\dagger & 0 \\ \tilde{\gamma}_{bf} & \tilde{\gamma}_{bb} & \\ 0 & & \tilde{\gamma}_{\mathscr{E}\mathscr{E}} \end{pmatrix}$$

Cluster's environment

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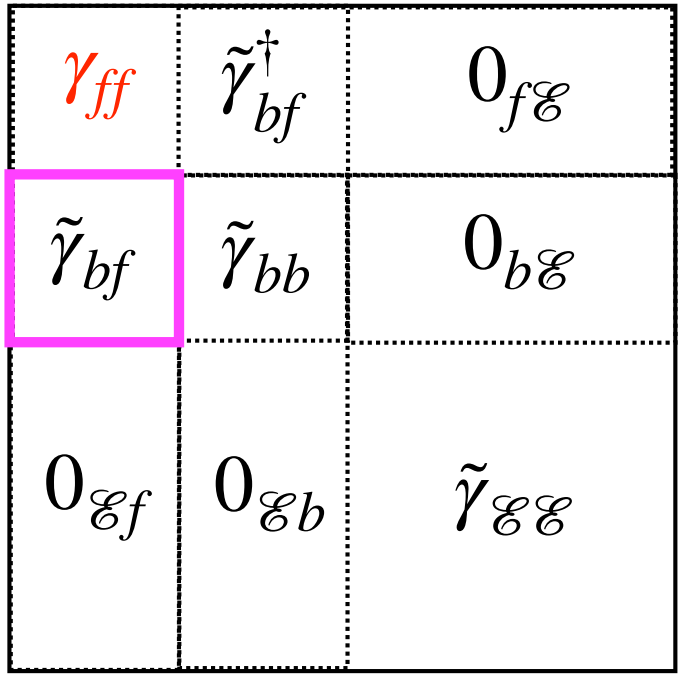
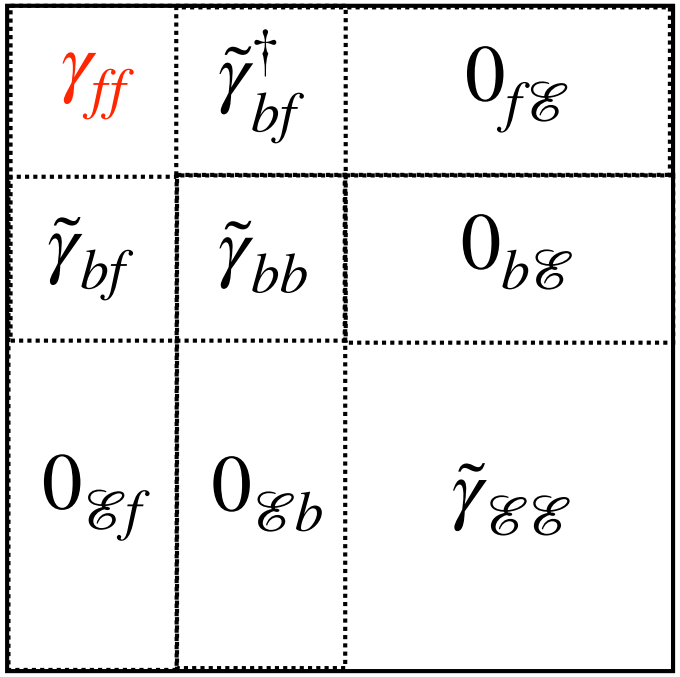
Unitary transformed idempotent density matrix

$$\tilde{\gamma} = \tilde{\gamma}^2 \equiv$$





S. Sekaran, O. Bindech, and E. Fromager, to be submitted *(2022).*

Unitary transformed idempotent density matrix

$$\tilde{\gamma}_{bf}\gamma_{ff}+\tilde{\gamma}_{bb}\tilde{\gamma}_{bf} = \begin{array}{|c|c|c|} \hline \gamma_{ff} & \tilde{\gamma}^{\dagger}_{bf} & 0_{f\mathscr{E}} \\ \hline \tilde{\gamma}_{bf} & \tilde{\gamma}_{bb} & 0_{b\mathscr{E}} \\ \hline 0_{\mathscr{E}f} & 0_{\mathscr{E}b} & \tilde{\gamma}_{\mathscr{E}\mathscr{E}} \\ \hline \end{array} \equiv \tilde{\gamma} = \tilde{\gamma}^2$$

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(L_f L_f)

$$\gamma_{ff}+\tilde{\gamma}_{bf}^{-1}\tilde{\gamma}_{bb}\tilde{\gamma}_{bf} = 1_f$$

$$\mathrm{Tr}[\gamma_{ff}] + \mathrm{Tr}\left[\tilde{\gamma}_{bb}\right] = L_f \rightarrow$$

The embedding cluster contains exactly L_f electrons!

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*Contains **exactly*** $\mathrm{Tr}[\gamma_{ff}] + \mathrm{Tr}\left[\tilde{\gamma}_{bb}\right] = L_f$ *electrons!*

$$\tilde{\gamma}^2 = \tilde{\gamma} = \mathcal{U}^\dagger \gamma \mathcal{U} \equiv$$

$$\begin{pmatrix} \gamma_{ff} & \tilde{\gamma}_{bf}^\dagger & 0 \\ \tilde{\gamma}_{bf} & \tilde{\gamma}_{bb} & \\ 0 & & \tilde{\gamma}_{\mathscr{E}\mathscr{E}} \end{pmatrix}$$

Cluster's environment

S. Sekaran, O. Bindech, and E. Fromager, to be submitted *(2022).*

Approximate embedding of interacting Hamiltonians

$$\hat{H} = \sum_{pq} h_{pq} \hat{c}_p^\dagger \hat{c}_q + \frac{1}{2} \sum_{pqrs} \langle pq \,|\, rs \rangle \hat{c}_p^\dagger \hat{c}_q^\dagger \hat{c}_s \hat{c}_r$$

Original localised representation

$$\hat{d}_j = \sum_{l}^{lattice} \mathcal{U}_{lj}[\gamma_{ef}] \, \hat{c}_l$$

$$= \sum_{pq} \tilde{h}_{pq} \hat{d}_p^\dagger \hat{d}_q + \frac{1}{2} \sum_{pqrs} \widetilde{\langle pq \,|\, rs \rangle} \hat{d}_p^\dagger \hat{d}_q^\dagger \hat{d}_s \hat{d}_r$$

Embedding representation

S. Wouters, C. A. Jiménez-Hoyos, Q. Sun, and G. K.-L. Chan, J. Chem. Theory Comput. ***12****, 2706 (2016).*
S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B ***104****, 035121 (2021).*
S. Sekaran, M. Saubanère, and E. Fromager, Computation **2022***, 10,* 45.

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$$= \sum_{pq}^{\mathscr{C}} \tilde{h}_{pq} \hat{d}_p^\dagger \hat{d}_q$$

$$\hat{h}^{\mathscr{C}}$$

Projection *onto the cluster*

Exact!

Approximate embedding of interacting Hamiltonians

$$\hat{H} = \sum_{pq} h_{pq} \hat{c}_p^\dagger \hat{c}_q + \frac{1}{2} \sum_{pqrs} \langle pq \,|\, rs \rangle \hat{c}_p^\dagger \hat{c}_q^\dagger \hat{c}_s \hat{c}_r$$

Original localised representation

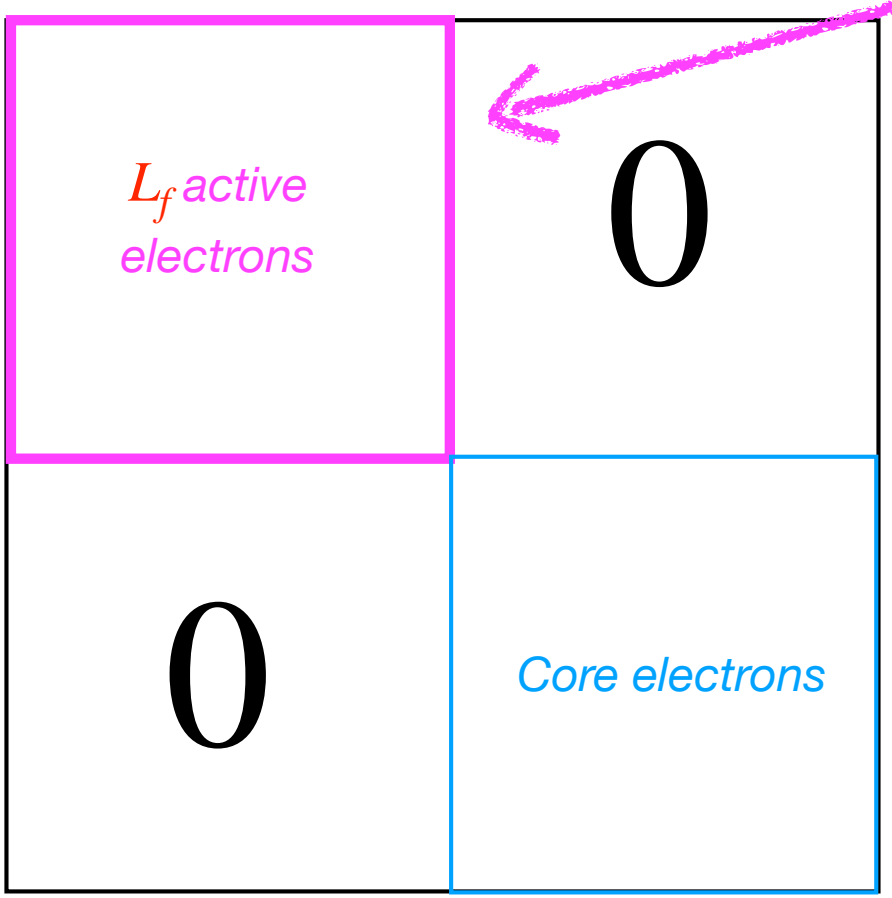
$$\hat{d}_j = \sum_{l}^{lattice} \mathcal{U}_{lj}[\gamma_{ef}] \, \hat{c}_l$$

$$= \underbrace{\sum_{pq}^{\mathscr{C}} \tilde{h}_{pq} \hat{d}_p^\dagger \hat{d}_q}_{\hat{h}^{\mathscr{C}}} + \frac{1}{2} \sum_{pqrs}^{fragment} \widetilde{\langle pq \,|\, rs \rangle} \hat{d}_p^\dagger \hat{d}_q^\dagger \hat{d}_s \hat{d}_r$$

***Projection** onto the cluster*

Approximate!

Approximate embedding of interacting Hamiltonians



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S. Sekaran, M. Saubanère, and E. Fromager, Computation **2022***, 10,* 45.

Approximate embedding of interacting Hamiltonians

Chemical potential on the impurity

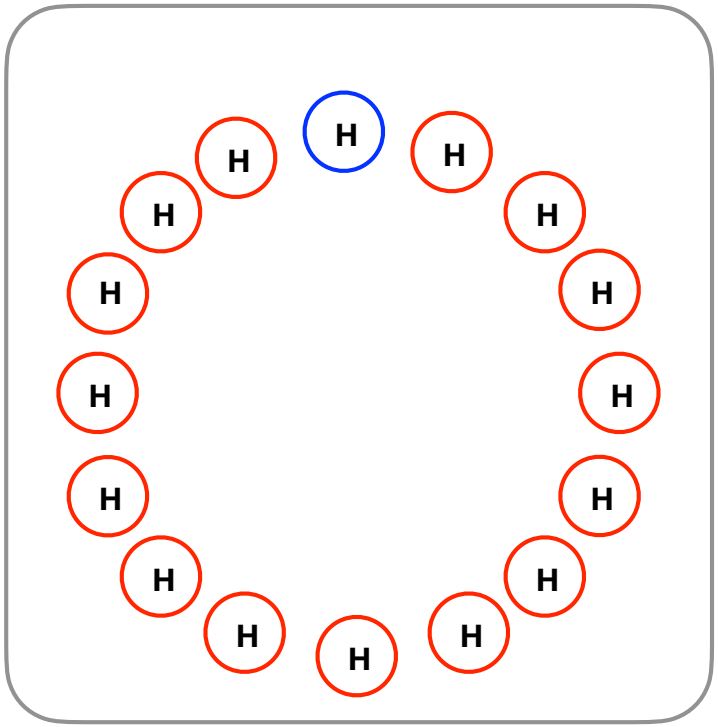
$$\hat{h}^{\mathscr{C}} \xrightarrow{single\ impurity} \hat{h}^{\mathscr{C}} + \langle pp\,|\,pp\rangle\, \hat{c}^{\dagger}_{p\uparrow}\hat{c}^{\dagger}_{p\downarrow}\hat{c}_{p\downarrow}\hat{c}_{p\uparrow} - \tilde{\mu}^{imp} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{\dagger}_{p\sigma}\hat{c}_{p\sigma}$$

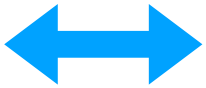
Exact non-interacting embedding

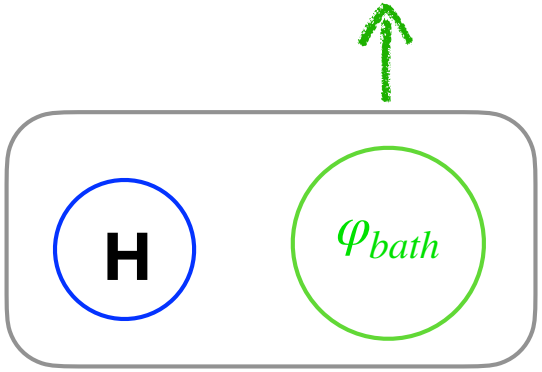
Approximate interacting embedding

S. Wouters, C. A. Jiménez-Hoyos, Q. Sun, and G. K.-L. Chan, J. Chem. Theory Comput. ***12****, 2706 (2016).*
S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B ***104****, 035121 (2021).*
S. Sekaran, M. Saubanère, and E. Fromager, Computation **2022***, 10,* 45.

Hubbard model for rings of hydrogen atoms







Effective
neighbouring atom

Two-electron system

***N*-electron system**

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

G. Knizia and G. K.-L. Chan, Phys. Rev. Lett. ***109****, 186404 (2012).*
S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B ***104****, 035121 (2021).*
S. Sekaran, M. Saubanère, and E. Fromager, Computation **2022***, 10,* 45*.*

Half-filled uniform Hubbard ring with $L = 400$ atomic sites

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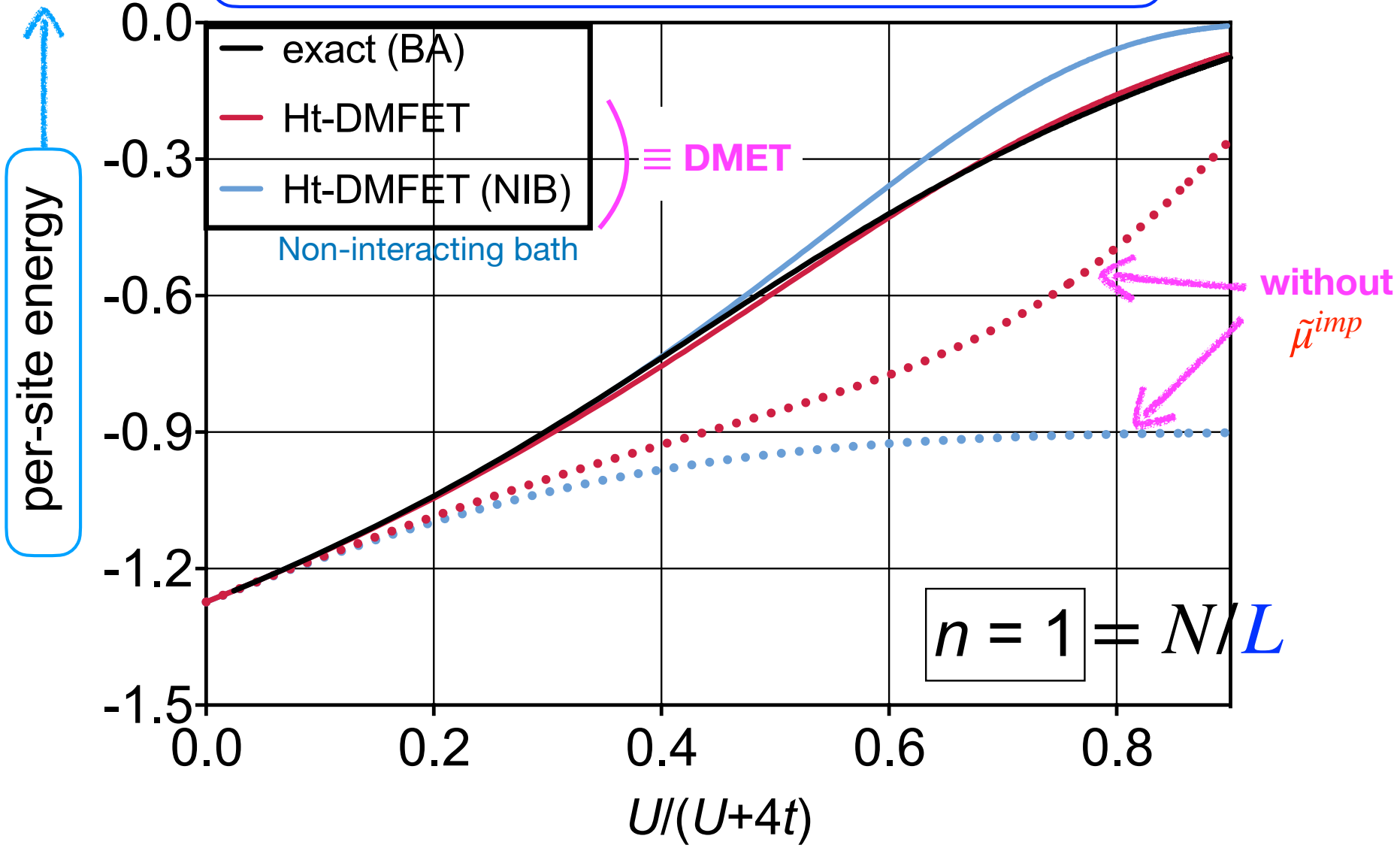

S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B **104**, 035121 (2021).

Half-filled uniform Hubbard ring with $L = 400$ atomic sites

$$E/L$$

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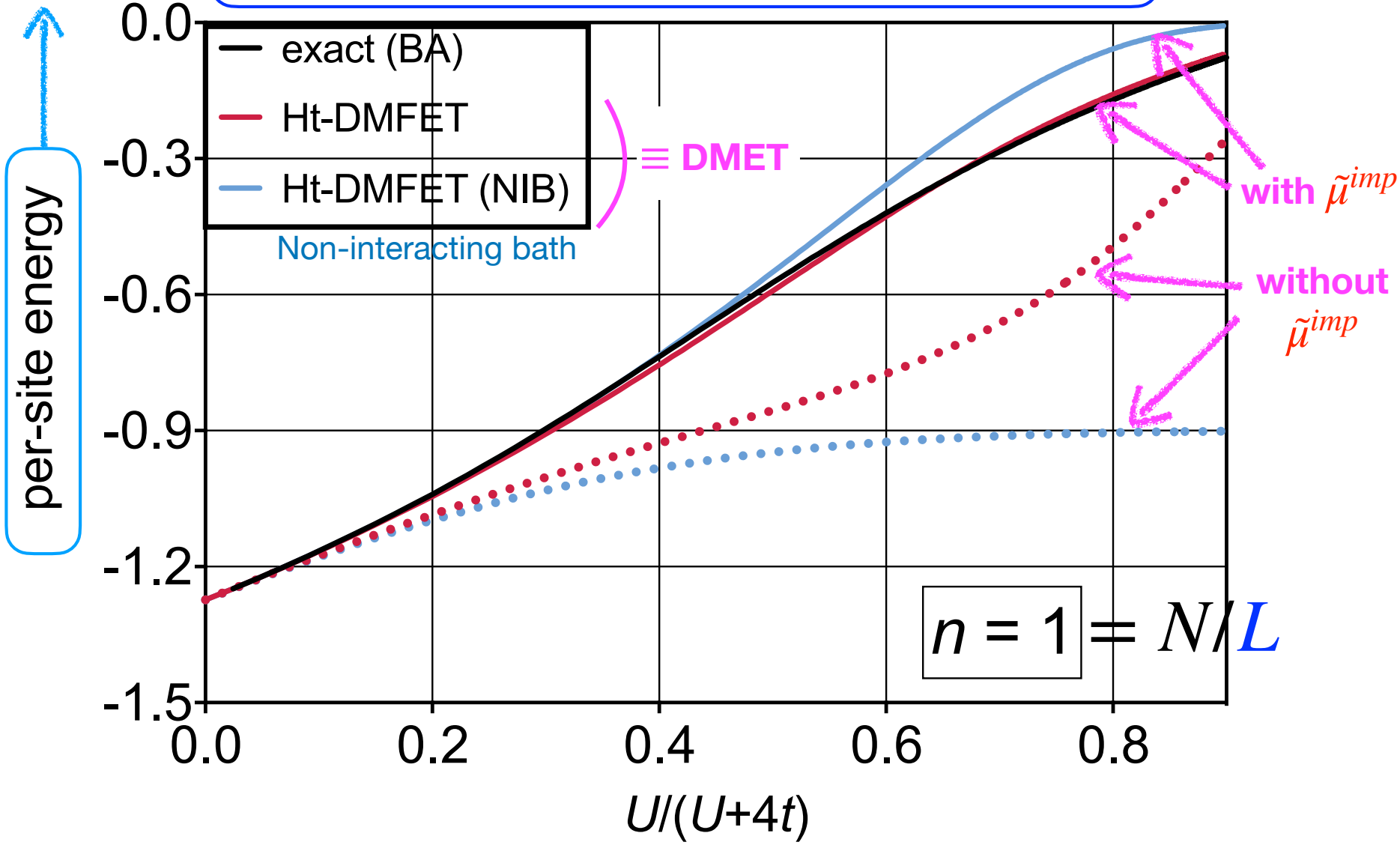
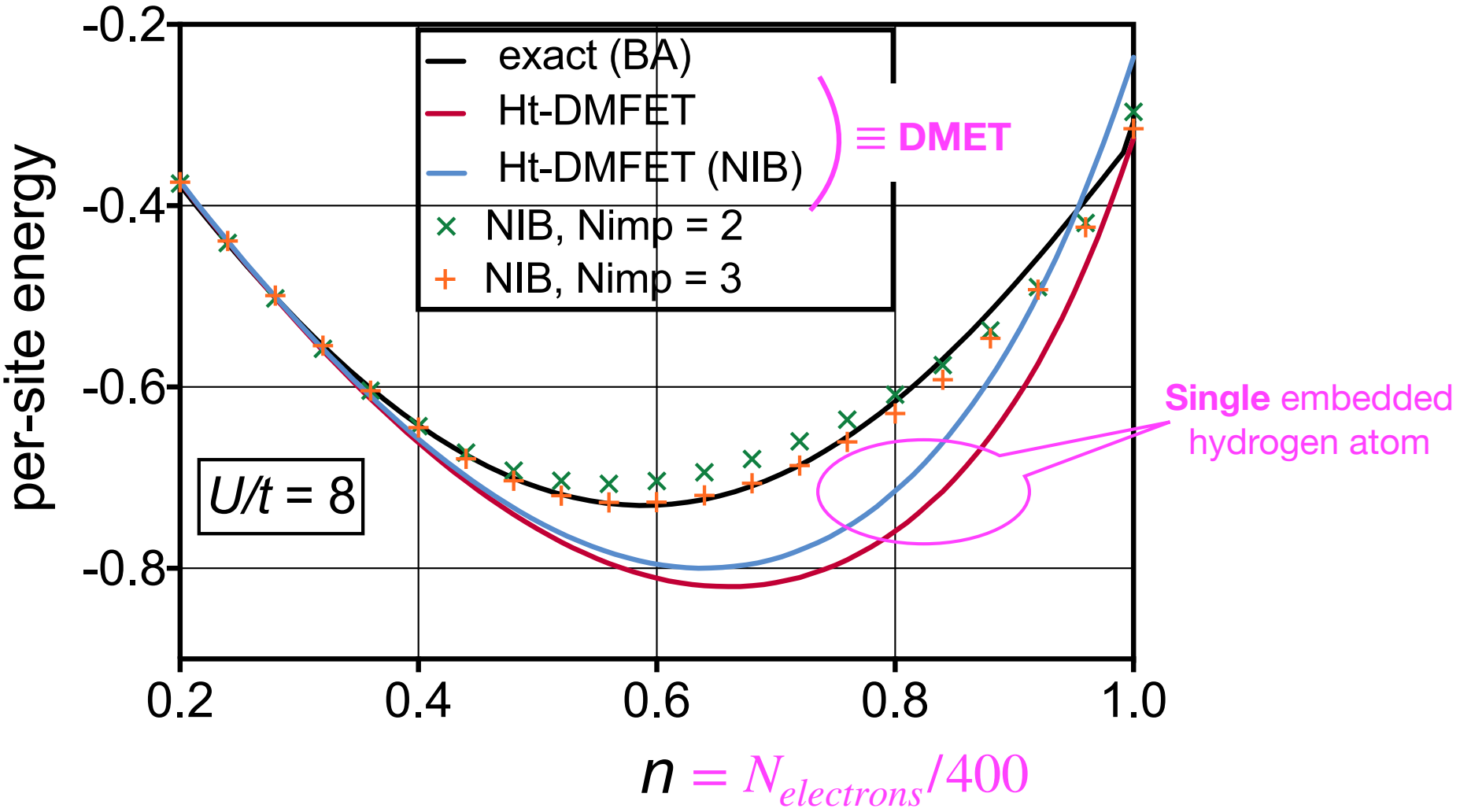


S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B **104**, 035121 (2021).

(Hubbard) model of a stretched 400-atom hydrogen ring



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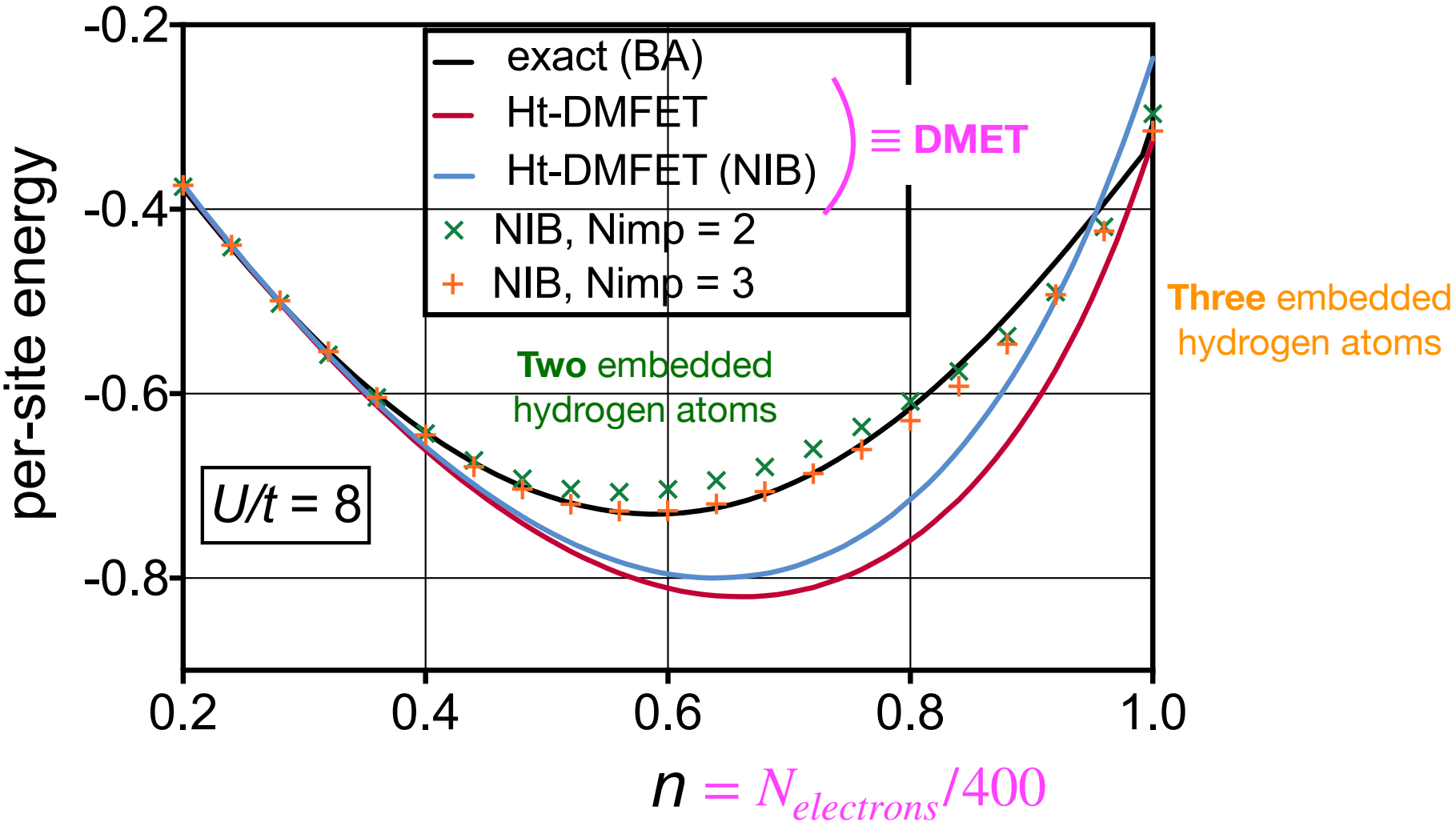


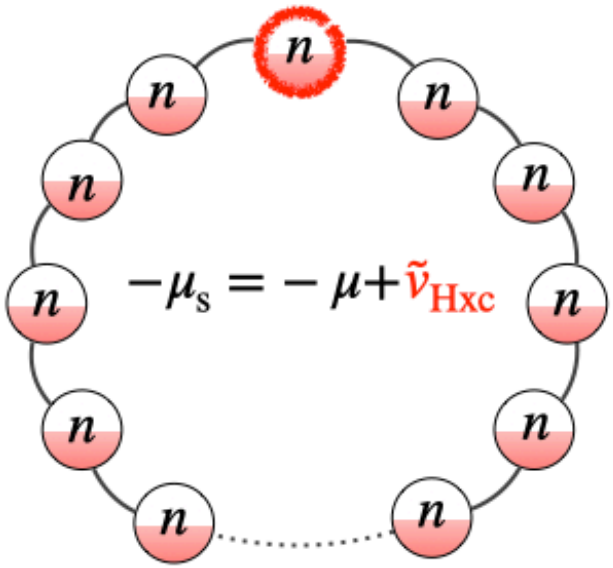
*S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B **104**, 035121 (2021).*

Local potential-functional embedding theory (LPFET)

$$v_{\mathrm{Hxc}}(n) \approx \tilde{\mu}^{\mathrm{imp}}(n)$$

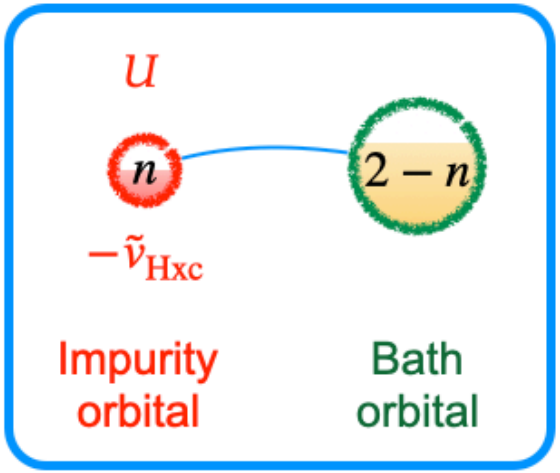
Self-consistency loop

Kohn-Sham lattice



$$n_{\Phi_0^{\mathrm{KS}}[\tilde{v}_{\mathrm{Hxc}}]} = n_{\Psi_0^{cluster}[\tilde{v}_{\mathrm{Hxc}}]}$$

Embedding cluster



S. Sekaran, M. Saubanère, and E. Fromager, Computation **2022**, *10,* 45.

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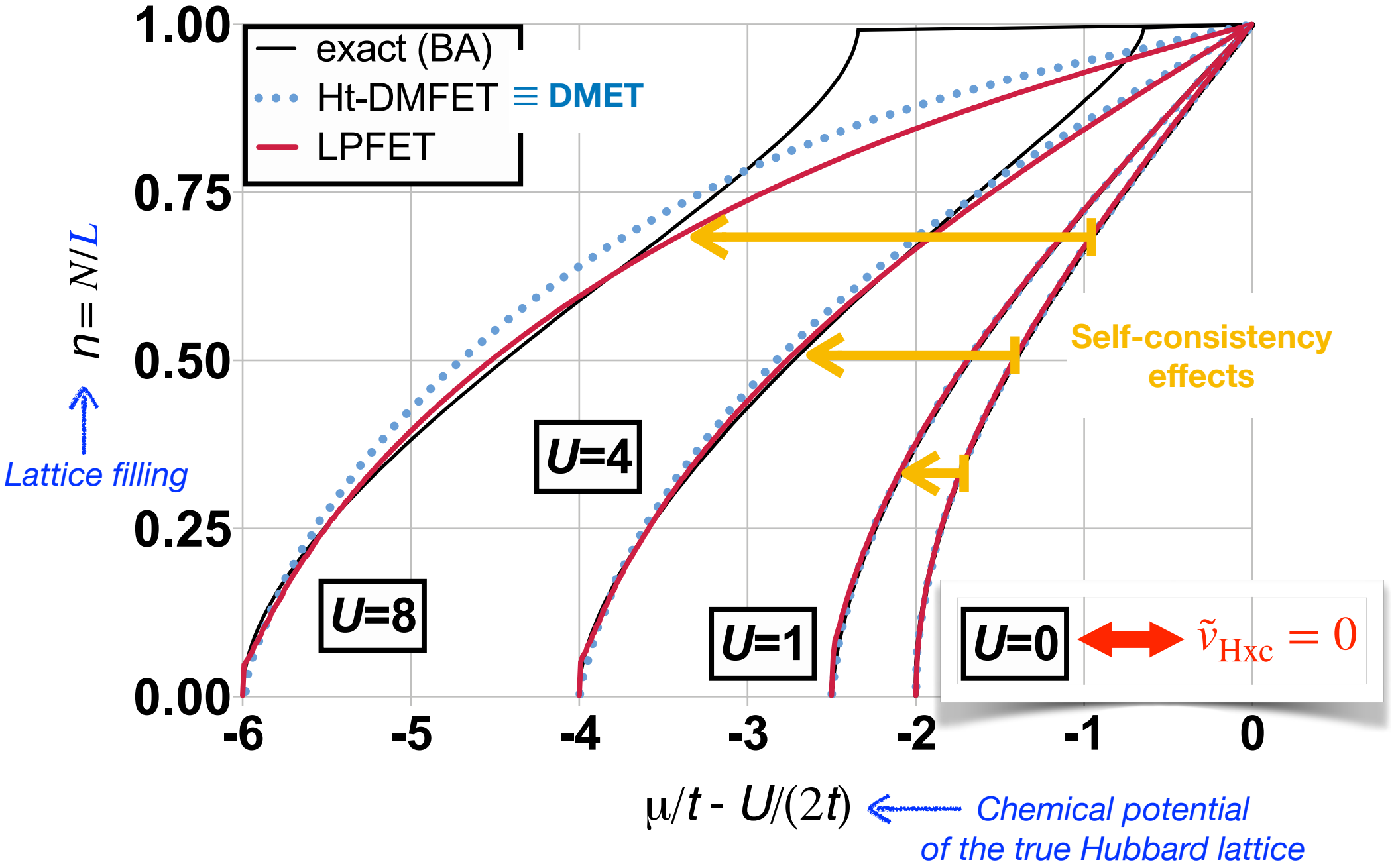

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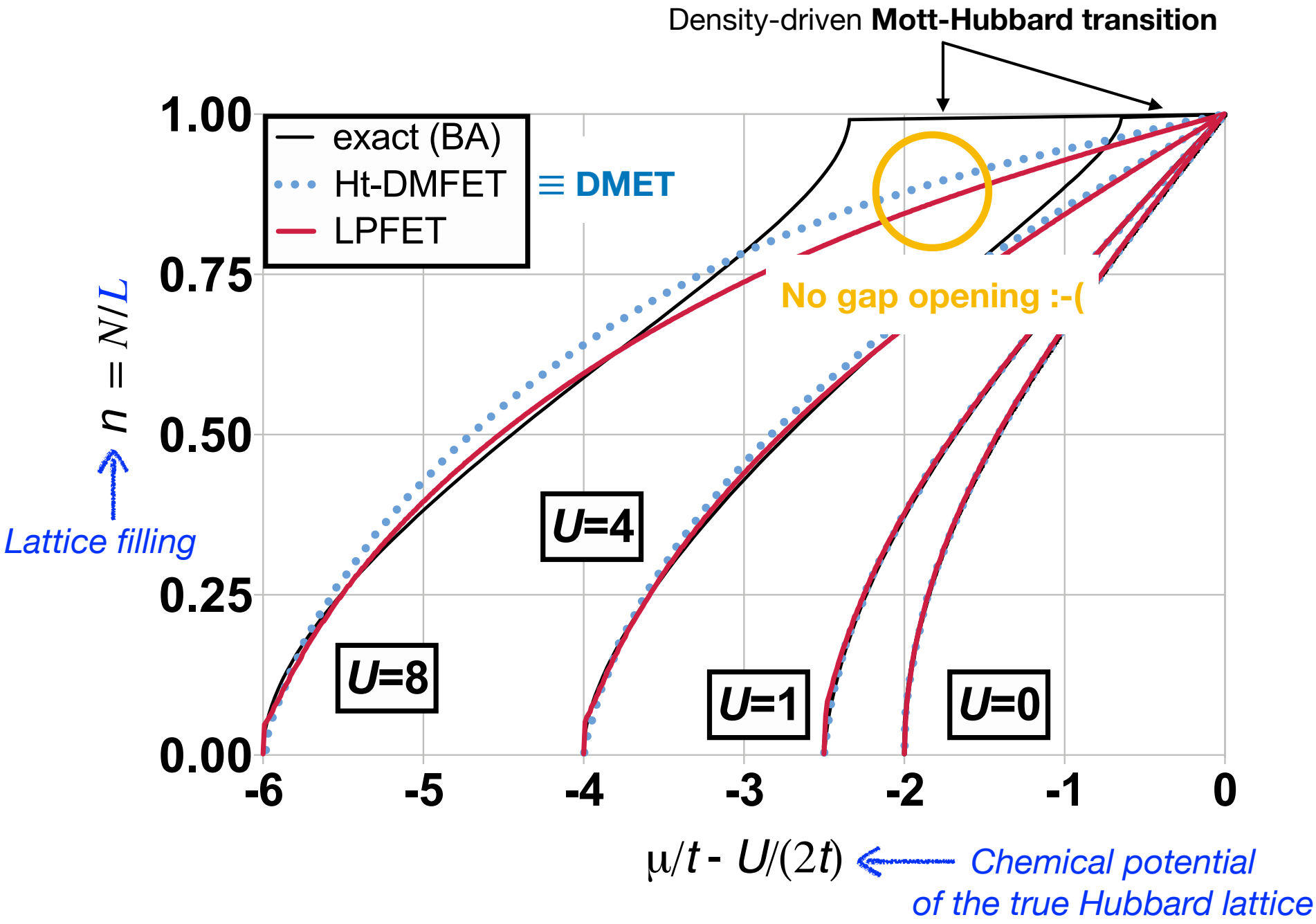
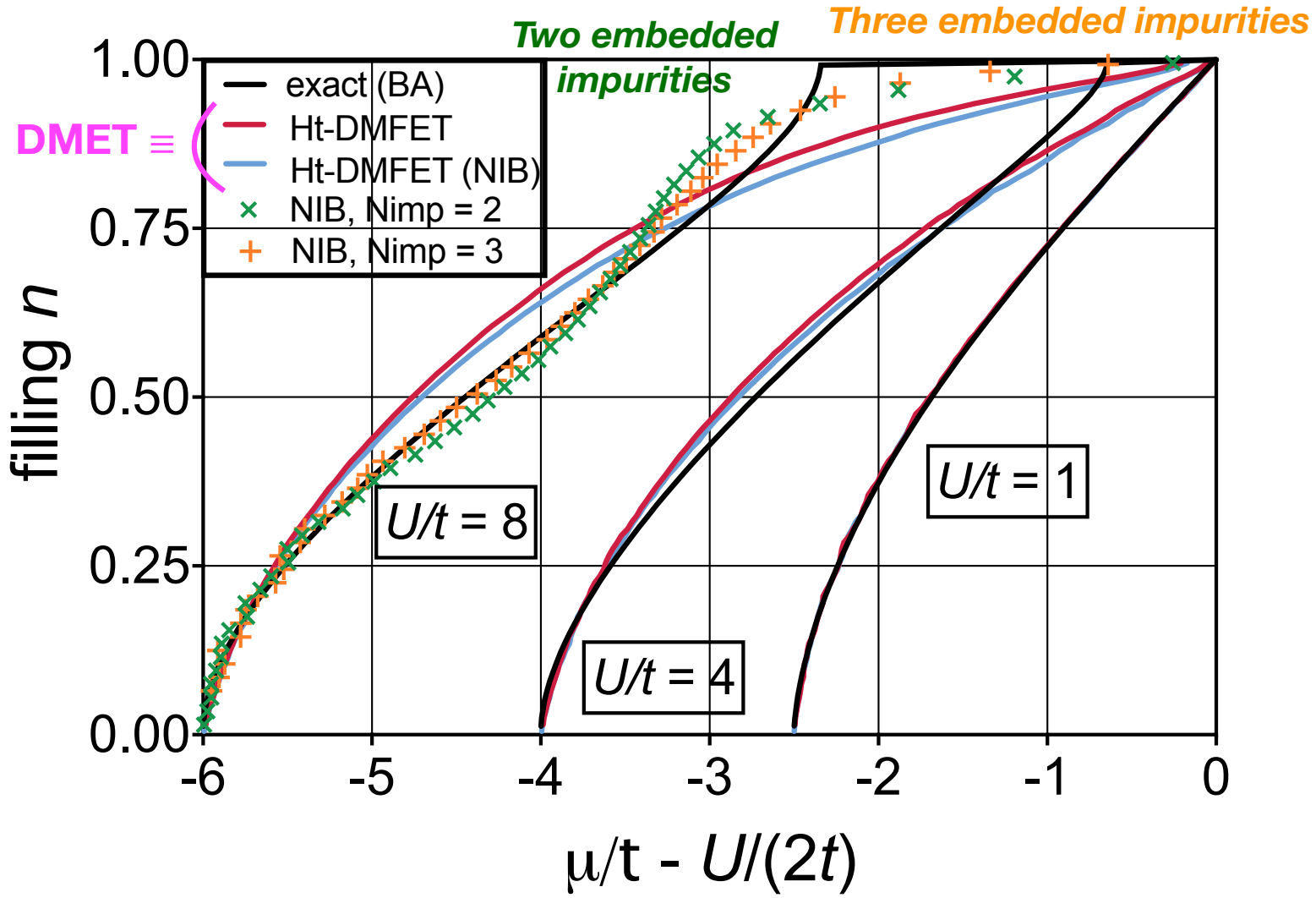


S. Sekaran, M. Saubanère, and E. Fromager, Computation **2022**, *10,* 45.

Mott-Hubbard density-driven transition and multiple impurities

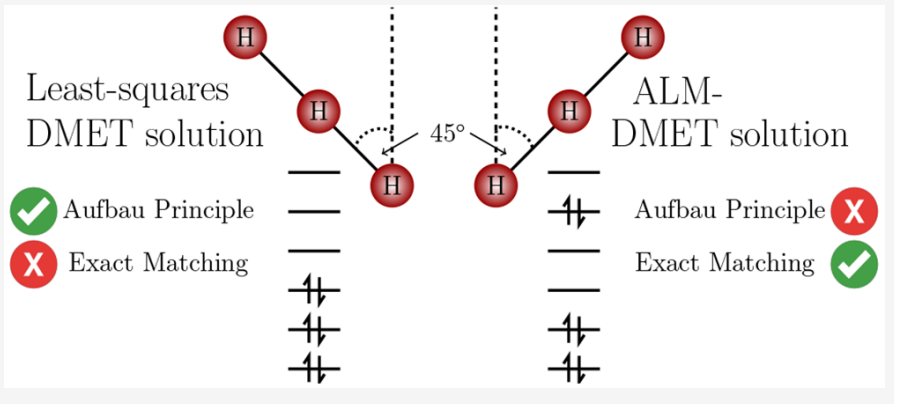


*S. Sekaran, M. Tsuchiizu, M. Saubanère, and E. Fromager, Phys. Rev. B **104**, 035121 (2021).*

Pure State *v*-Representability of Density Matrix Embedding Theory

Fabian M. Faulstich,[⊥] Raehyun Kim,[⊥] Zhi-Hao Cui, Zaiwen Wen, Garnet Kin-Lic Chan, and Lin Lin*

Cite This: *J. Chem. Theory Comput.* 2022, 18, 851−864



Non-interacting full system

$$\gamma = \begin{pmatrix} \gamma_{ff} & \gamma_{ef}^{\dagger} \\ \gamma_{ef} & \gamma_{ee} \end{pmatrix}$$

Idempotent

?

Correlated cluster

$$\begin{pmatrix} \gamma_{ff} & \tilde{\gamma}_{bf}^{\dagger} & & \\ \tilde{\gamma}_{bf} & \tilde{\gamma}_{bb} & & \\ & & & \\ & & & \tilde{\gamma}_{\mathscr{E}\mathscr{E}} \end{pmatrix}$$

Non-idempotent