Wave functions, slave particles and quantum embedding methods for correlated systems

The multi-orbital gGA theory as a Quantum Embedding framework

Lecture notes:
https://www.cond-mat.de/events/correl23/manuscripts/lanata.pdf

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Outline

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A. ***Background notions in many-body theory (board)***

B. ***The GA/gGA wave function: Introduction***

C. ***Derivation gGA method: QE formulation***

D. ***Applications, recent developments and open problems***

Supplementary topics:

- *Spectral properties*
- *Time-dependent extension*
- *DFT+gGA*

Background notions in many-body theory

A. *Functions of Hermitian matrices*

B. *Fock states and representation of Fermionic operators*

C. *Single-particle density matrix for one-body Hamiltonians*

D. *Wick's theorem (for thermal density matrices)*

E. *Many-body reduced density matrices of thermal density matrices for one-body Hamiltonians*

A) Functions of Hermitian matrices

$$H = H^\dagger \xrightarrow{H = UEU^\dagger} f(H) = Uf(E)U^\dagger$$

$$Hv_n = E_n v_n$$

$$f(H)v_n = f(E_n)v_n$$

B) Representation of Fock states and Fermionic operators

Fermionic operators: $\{c^\dagger_\alpha, c_\alpha \,|\, \alpha = 1,\ldots,\nu\}$ *(Subscript combines unit-cell label, orbital, spin…)*

Fock states: $$|\Gamma\rangle = [c^\dagger_1]^{q_1(\Gamma)} \ldots [c^\dagger_\nu]^{q_\nu(\Gamma)} \,|\, 0\rangle$$

$$\Gamma \in \{0,\ldots,2^\nu - 1\}$$

$$\Gamma = \left(q_1(\Gamma), \ldots, q_\nu(\Gamma)\right)$$

Occupation numbers are encoded in binary-representation digits of Γ:

$$\hat{n}_\alpha \,|\, \Gamma\rangle = c^\dagger_\alpha c_\alpha \,|\, \Gamma\rangle = q_\alpha(\Gamma) \,|\, \Gamma\rangle$$

B) Representation of Fock states and Fermionic operators

Fermionic operators: $\{c_\alpha^\dagger, c_\alpha \,|\, \alpha = 1,..,\nu\}$

Fock states: $|\Gamma\rangle = [c_1^\dagger]^{q_1(\Gamma)} \ldots [c_\nu^\dagger]^{q_\nu(\Gamma)} \,|\, 0\rangle$

$\Gamma \in \{0,...,2^\nu - 1\}$

$\Gamma = \big(q_1(\Gamma), \ldots, q_\nu(\Gamma)\big)$

Example for $\nu = 4$:

$\Gamma = 5 = (0101)$

$|\Gamma\rangle = c_3^\dagger c_1^\dagger \,|\, 0\rangle$

B) Representation of Fock states and Fermionic operators

Fermionic operators: $\{c_\alpha^\dagger, c_\alpha \,|\, \alpha = 1,..,\nu\}$

Fock states: $$|\Gamma\rangle = [c_1^\dagger]^{q_1(\Gamma)} \dots [c_\nu^\dagger]^{q_\nu(\Gamma)} \,|\, 0\rangle$$

Matrix representation:

$$[F_\alpha^\dagger]_{\Gamma\Gamma'} = \langle \Gamma \,|\, c_\alpha^\dagger \,|\, \Gamma' \rangle = \delta_{q_\alpha(\Gamma), q_\alpha(\Gamma')+1} \prod_{s \neq \alpha} \delta_{q_s(\Gamma), q_s(\Gamma')} \, (-1)^{\sum_{s=1}^{\alpha-1} q_s(\Gamma)}$$

B) Representation of Fock states and Fermionic operators

Fermionic operators: $\{c_\alpha^\dagger, c_\alpha \,|\, \alpha = 1,\ldots,\nu\}$

Fock states: $|\Gamma\rangle = [c_1^\dagger]^{q_1(\Gamma)} \ldots [c_\nu^\dagger]^{q_\nu(\Gamma)}\,|0\rangle$

Matrix representation: Example $\nu = 2$

$$F_1^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, F_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \; F_2^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}, F_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

C) Single-particle density matrix for one-body Hamiltonians

$$\hat{H} = \sum_{\alpha,\beta=1}^{\nu} h_{\alpha\beta}\, c_{\alpha}^{\dagger} c_{\beta} \qquad \hat{\rho}_T = \frac{e^{-\frac{\hat{H}}{T}}}{\mathrm{Tr}_{\mathscr{H}}\left[e^{-\frac{\hat{H}}{T}}\right]}$$

Trace over $\mathscr{H}$ is a sum over 2^{ν} states

$$\Delta_{\alpha\beta} := \langle c_{\alpha}^{\dagger} c_{\beta} \rangle_T = \mathrm{Tr}_{\mathscr{H}}\left[\hat{\rho}_T\, c_{\alpha}^{\dagger} c_{\beta}\right] = [f_T(h)]_{\beta\alpha}$$

D) Wick's theorem (for thermal density matrices)

$$\hat{H} = \sum_{\alpha,\beta=1}^{\nu} h_{\alpha\beta}\, c_\alpha^\dagger c_\beta \qquad \hat{\rho}_T = \frac{e^{-\frac{\hat{H}}{T}}}{\mathrm{Tr}_{\mathscr{H}}\left[e^{-\frac{\hat{H}}{T}}\right]}$$

Example I:

$$\langle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \rangle_T = \langle c_\alpha^\dagger c_\delta \rangle_T \langle c_\beta^\dagger c_\gamma \rangle_T - \langle c_\alpha^\dagger c_\gamma \rangle_T \langle c_\beta^\dagger c_\delta \rangle_T$$

$$\langle \Psi_0 | c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta | \Psi_0 \rangle = \langle \Psi_0 | c_\alpha^\dagger c_\delta | \Psi_0 \rangle \langle \Psi_0 | c_\beta^\dagger c_\gamma | \Psi_0 \rangle - \langle \Psi_0 | c_\alpha^\dagger c_\gamma | \Psi_0 \rangle \langle \Psi_0 | c_\beta^\dagger c_\delta | \Psi_0 \rangle$$

D) Wick's theorem (for thermal density matrices)

$$\langle c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \rangle_T = \langle c_\alpha^\dagger c_\delta \rangle_T \langle c_\beta^\dagger c_\gamma \rangle_T - \langle c_\alpha^\dagger c_\gamma \rangle_T \langle c_\beta^\dagger c_\delta \rangle_T$$

Example II:

Type I: *Disconnected*

$$\langle \hat{X} c_\alpha^\dagger c_\beta \rangle_T = \langle \hat{X} \rangle_T \langle c_\alpha^\dagger c_\beta \rangle_T + \sum_{\alpha'\beta'} \xi^T_{\alpha'\beta'} \langle c_{\alpha'} c_\alpha^\dagger \rangle_T \langle c_{\beta'}^\dagger c_\beta \rangle_T$$

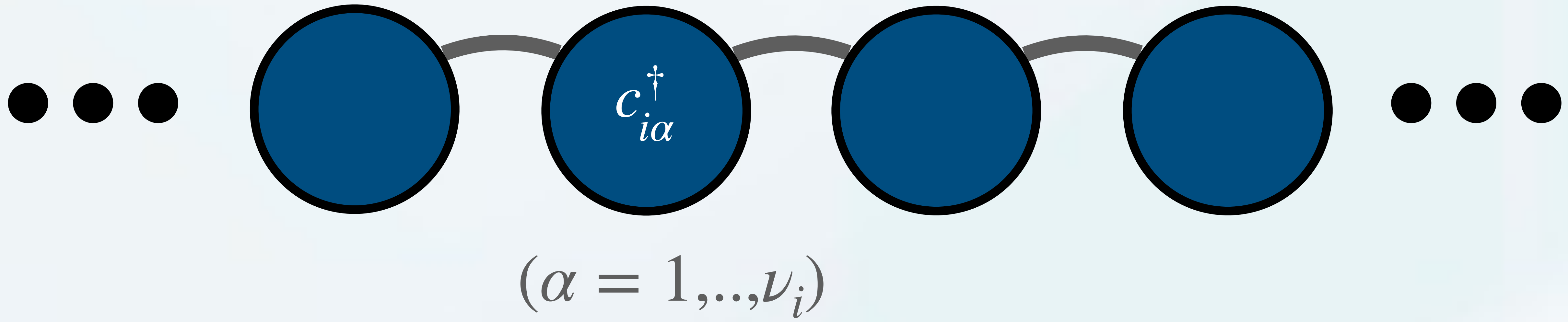
Type II: *Connected*

Depends only on T, α', β', ***not*** on α, β

E) Many-body reduced density matrices of thermal density matrices for one-body Hamiltonians

$$\hat{H} = \sum_{ij} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} h_{ij}^{\alpha\beta} c_{i\alpha}^{\dagger} c_{j\beta}$$

$$\hat{\rho}_T = \frac{e^{-\frac{\hat{H}}{T}}}{\mathrm{Tr}_{\mathscr{H}}\left[e^{-\frac{\hat{H}}{T}}\right]}$$



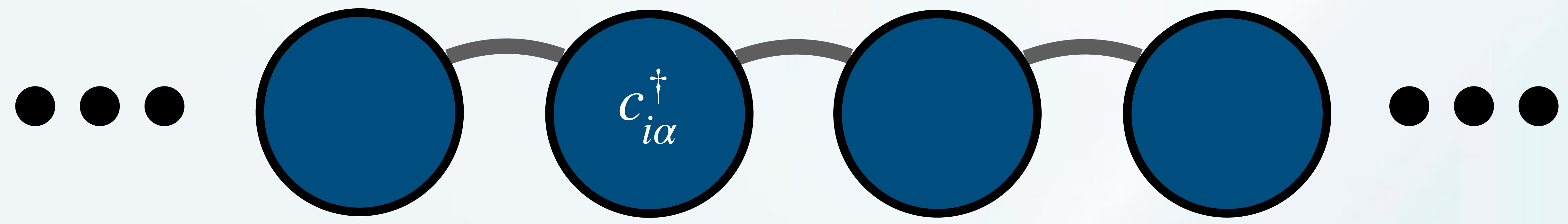
↑

Trace over $\mathscr{H}$ is a sum over $2^{\nu_1} \times 2^{\nu_2} \times \ldots \times 2^{\nu_N}$ states

$$\langle \hat{O}_i \rangle_T = \mathrm{Tr}_{\mathscr{H}}\left[\hat{\rho}_T \hat{O}_i\right] =: \mathrm{Tr}_{\mathscr{H}_i}\left[\hat{P}_i^0 \hat{O}_i\right]$$

← **Trace over $\mathscr{H}_i$ is a sum over 2^{ν_i} states**

E) Many-body reduced density matrices of thermal density matrices for one-body Hamiltonians



$(\alpha = 1,..,\nu_i)$

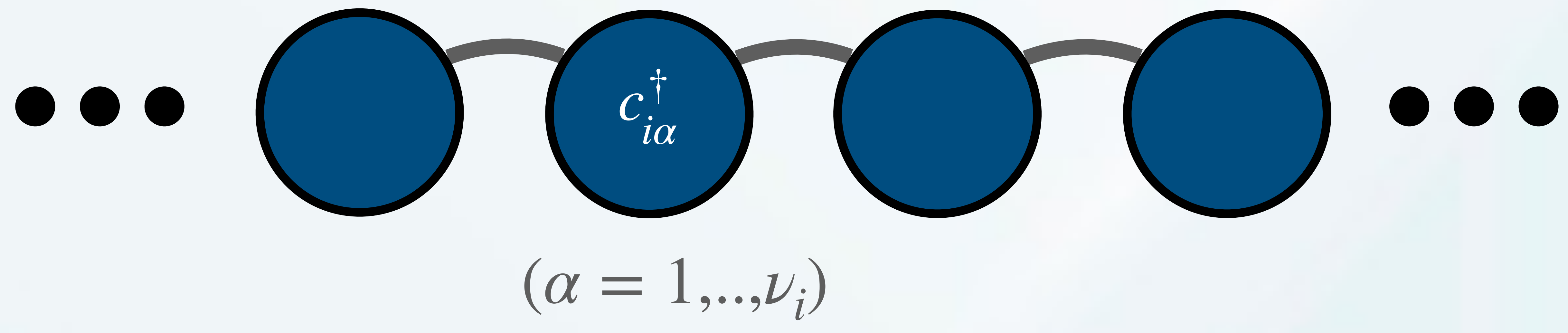
$$\hat{H} = \sum_{ij} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} h_{ij}^{\alpha\beta}\, c^{\dagger}_{i\alpha} c_{j\beta}$$

$$\langle \hat{O}_i \rangle_T = \mathrm{Tr}_{\mathscr{H}} \left[\hat{\rho}_T \hat{O}_i \right] =: \mathrm{Tr}_{\mathscr{H}_i} \left[\hat{P}_i^0 \hat{O}_i \right] \rightarrow \hat{P}_i^0 \propto \exp\left(- \sum_{\alpha,\beta=1}^{\nu_i} [\phi_i]_{\alpha\beta}\, c^{\dagger}_{i\alpha} c_{i\beta} \right)$$

$$\hat{\rho}_T \propto \exp\left(- \frac{\sum_{ij} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} h_{ij}^{\alpha\beta}\, c^{\dagger}_{i\alpha} c_{j\beta}}{T} \right)$$

$$\phi_i = \ln\left(\frac{1 - \Delta_i^T}{\Delta_i^T} \right) \qquad [\Delta_i]_{\alpha\beta} = \langle c^{\dagger}_{i\alpha} c_{j\beta} \rangle_T$$

E) Many-body reduced density matrices of thermal density matrices for one-body Hamiltonians



$$\hat{H} = \sum_{ij} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} h_{ij}^{\alpha\beta}\, c^\dagger_{i\alpha} c_{j\beta}$$

$$\langle \hat{O}_i \rangle_T = \mathrm{Tr}_{\mathscr{H}} \left[\hat{\rho}_T \, \hat{O}_i \right] =: \mathrm{Tr}_{\mathscr{H}_i} \left[\hat{P}^0_i \, \hat{O}_i \right] = \mathrm{Tr} \left[P^0_i \, O_i \right]$$

$$\hat{\rho}_T \propto \exp\left(- \frac{\sum_{ij} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} h_{ij}^{\alpha\beta}\, c^\dagger_{i\alpha} c_{j\beta}}{T} \right)$$

$$P^0_i \propto \exp\left(- \sum_{\alpha,\beta=1}^{\nu_i} [\phi_i]_{\alpha\beta} \, F^\dagger_{i\alpha} F_{i\beta} \right)$$

$$[O_i]_{\Gamma\Gamma'} = \langle \Gamma \,|\, \hat{O}_i \,|\, \Gamma' \rangle$$

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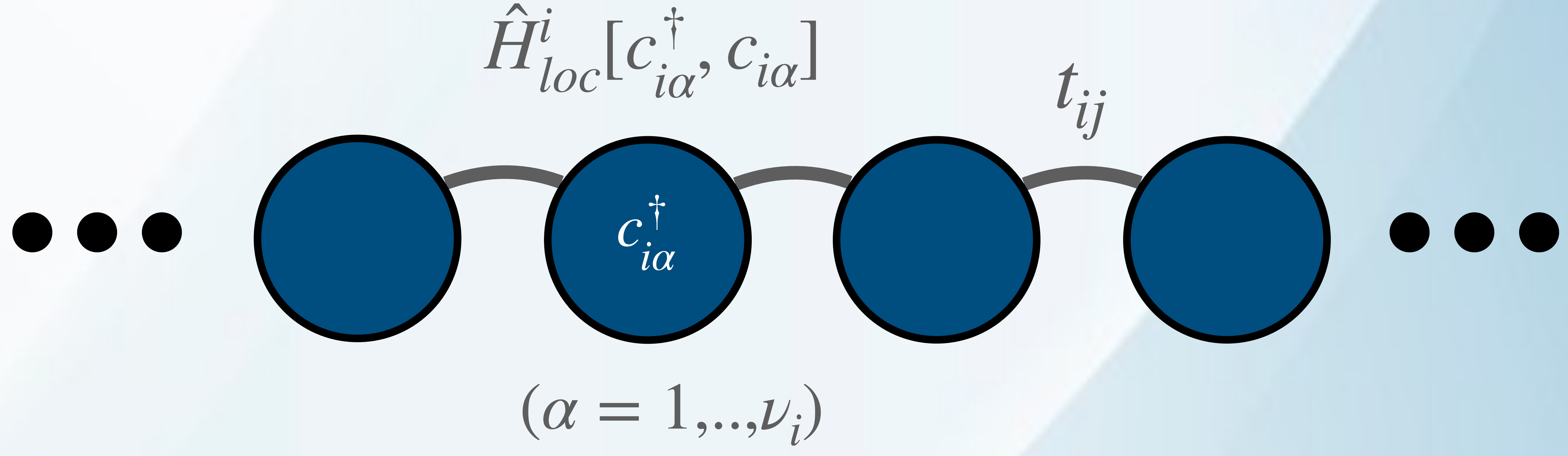
- DFT+gGA

The Hamiltonian:



$$\hat{H} = \sum_{i=1}^{\mathcal{N}} \hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}] + \sum_{i \neq j} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} [t_{ij}]_{\alpha\beta}\, c^\dagger_{i\alpha} c_{j\beta}$$

- i, j : ***Indices of the fragments of the lattice.***
- $\hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}]$: ***Local operator on fragment*** i
- α, β : ***Indices of Fermionic modes within each fragment.***
- $[t_{ij}]_{\alpha\beta}$: ***Matrix elements of the hopping term.***

The gGA variational wave function:

$$|\Psi_G\rangle = \hat{\mathscr{P}}_G|\Psi_0\rangle = \prod_{i=1}^{\mathcal{N}} \hat{\mathscr{P}}_i|\Psi_0\rangle$$

Evaluating and minimizing

$$\langle\Psi_G|\hat{H}|\Psi_G\rangle = \langle\Psi_0|\hat{\mathscr{P}}_G^\dagger \hat{H}\hat{\mathscr{P}}_G|\Psi_0\rangle$$

The gGA variational wave function:

$$|\Psi_G\rangle = \hat{\mathcal{P}}_G |\Psi_0\rangle = \prod_{i=1}^{\mathcal{N}} \hat{\mathcal{P}}_i |\Psi_0\rangle$$

PHYSICAL REVIEW B **96**, 195126 (2017)

Emergent Bloch excitations in Mott matter

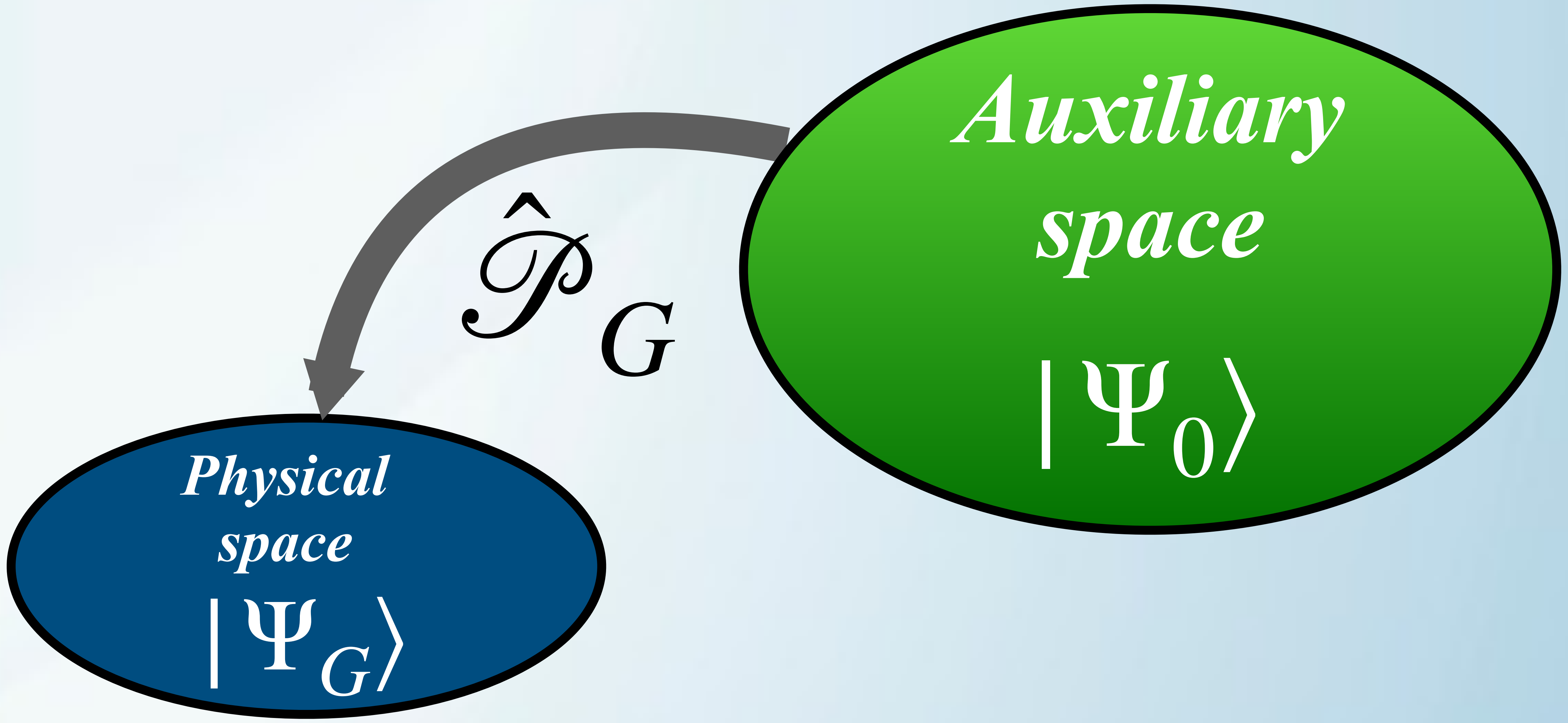
Nicola Lanatà,[1] Tsung-Han Lee,[1] Yong-Xin Yao,[2] and Vladimir Dobrosavljević[1]

PHYSICAL REVIEW B **104**, L081103 (2021)

Letter

Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation

Marius S. Frank,[1] Tsung-Han Lee,[2] Gargee Bhattacharyya,[1] Pak Ki Henry Tsang,[3] Victor L. Quito,[4,3] Vladimir Dobrosavljević,[3] Ove Christiansen,[5] and Nicola Lanatà[1,6,*]

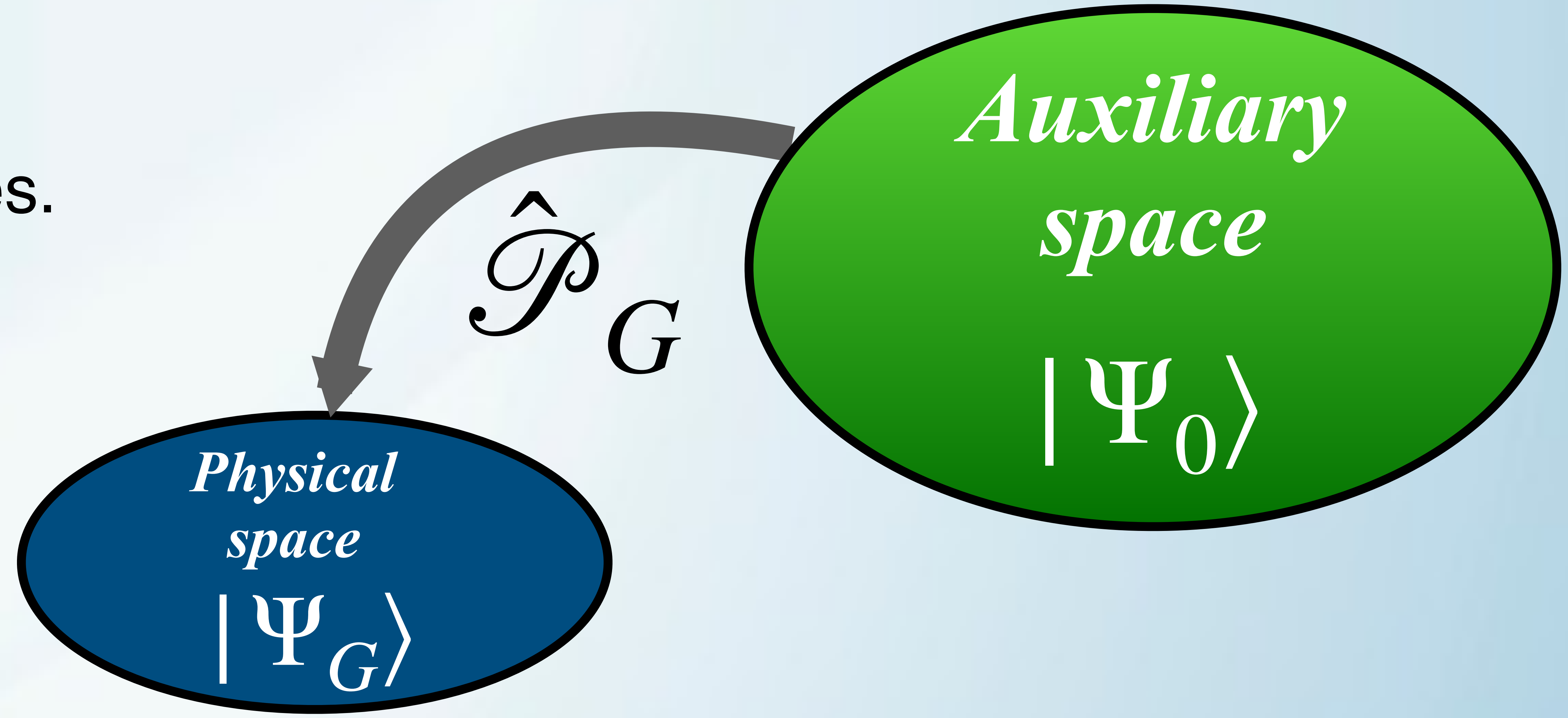


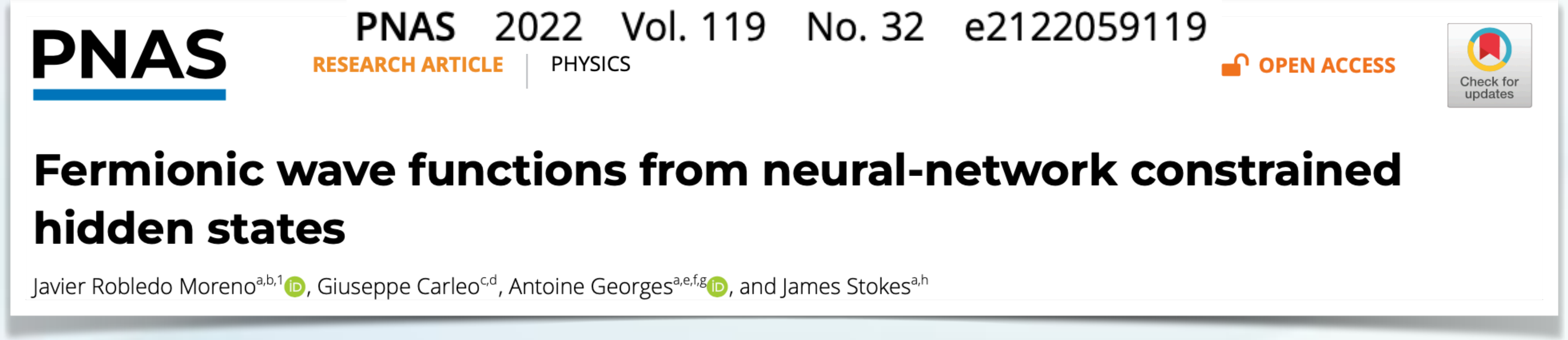
A few related concepts and methods

$$|\Psi_G\rangle = \hat{\mathscr{P}}_G|\Psi_0\rangle = \prod_{i=1}^{\mathscr{N}} \hat{\mathscr{P}}_i|\Psi_0\rangle$$

Suggestive analogies:

- Matrix product states and projected entangled pair states.
- Ancilla qubit techique (S. Sachdev)
- Hidden Fermion (M. Imada)
- Hidden Fermi liquid (P. Anderson)





PNAS 2022 Vol. 119 No. 32 e2122059119
RESEARCH ARTICLE | PHYSICS
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Fermionic wave functions from neural-network constrained hidden states

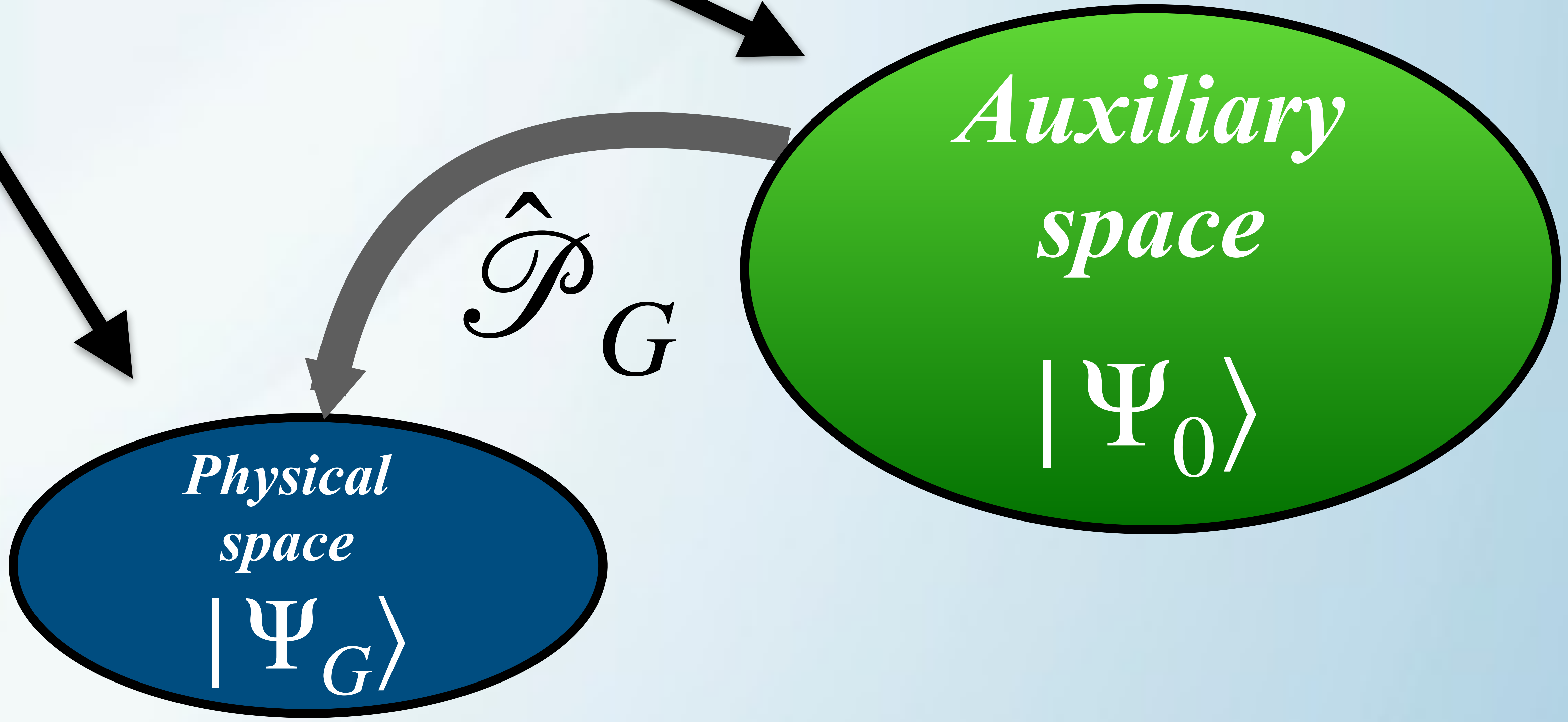
Javier Robledo Moreno[a,b,1], Giuseppe Carleo[c,d], Antoine Georges[a,e,f,g], and James Stokes[a,h]

Our goal is to minimize $\langle\Psi_0|\hat{\mathcal{P}}_G^\dagger \hat{H}\hat{\mathcal{P}}_G|\Psi_0\rangle$ w.r.t. $\{\Lambda_i\}, |\Psi_0\rangle$

$$\hat{\mathcal{P}}_i = \sum_{\Gamma=0}^{2^{\nu_i}-1}\sum_{n=0}^{2^{B\nu_i}-1} [\Lambda_i]_{\Gamma n} |\Gamma,i\rangle\langle n,i|$$

$$|\Gamma,i\rangle = [c^\dagger_{i1}]^{q_1(\Gamma)}\dots[c^\dagger_{i\nu_i}]^{q_{\nu_i}(\Gamma)}|0\rangle$$

$$|n,i\rangle = [f^\dagger_{i1}]^{q_1(n)}\dots[f^\dagger_{iB\nu_i}]^{q_{B\nu_i}(n)}|0\rangle$$



$B \geq 1$ controls the "size" of the auxiliary space

Quantum-embedding formulation

PHYSICAL REVIEW X **5,** 011008 (2015)

Phase Diagram and Electronic Structure of Praseodymium and Plutonium

Nicola Lanatà,[1,*] Yongxin Yao,[2,†] Cai-Zhuang Wang,[2] Kai-Ming Ho,[2] and Gabriel Kotliar[1]

PRL **118,** 126401 (2017) PHYSICAL REVIEW LETTERS week ending 24 MARCH 2017

Slave Boson Theory of Orbital Differentiation with Crystal Field Effects: Application to UO_2

Nicola Lanatà,[1,*] Yongxin Yao,[2,†] Xiaoyu Deng,[3] Vladimir Dobrosavljević,[1] and Gabriel Kotliar[3,4]

PHYSICAL REVIEW B **96**, 195126 (2017)

Emergent Bloch excitations in Mott matter

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PHYSICAL REVIEW B **104**, L081103 (2021)

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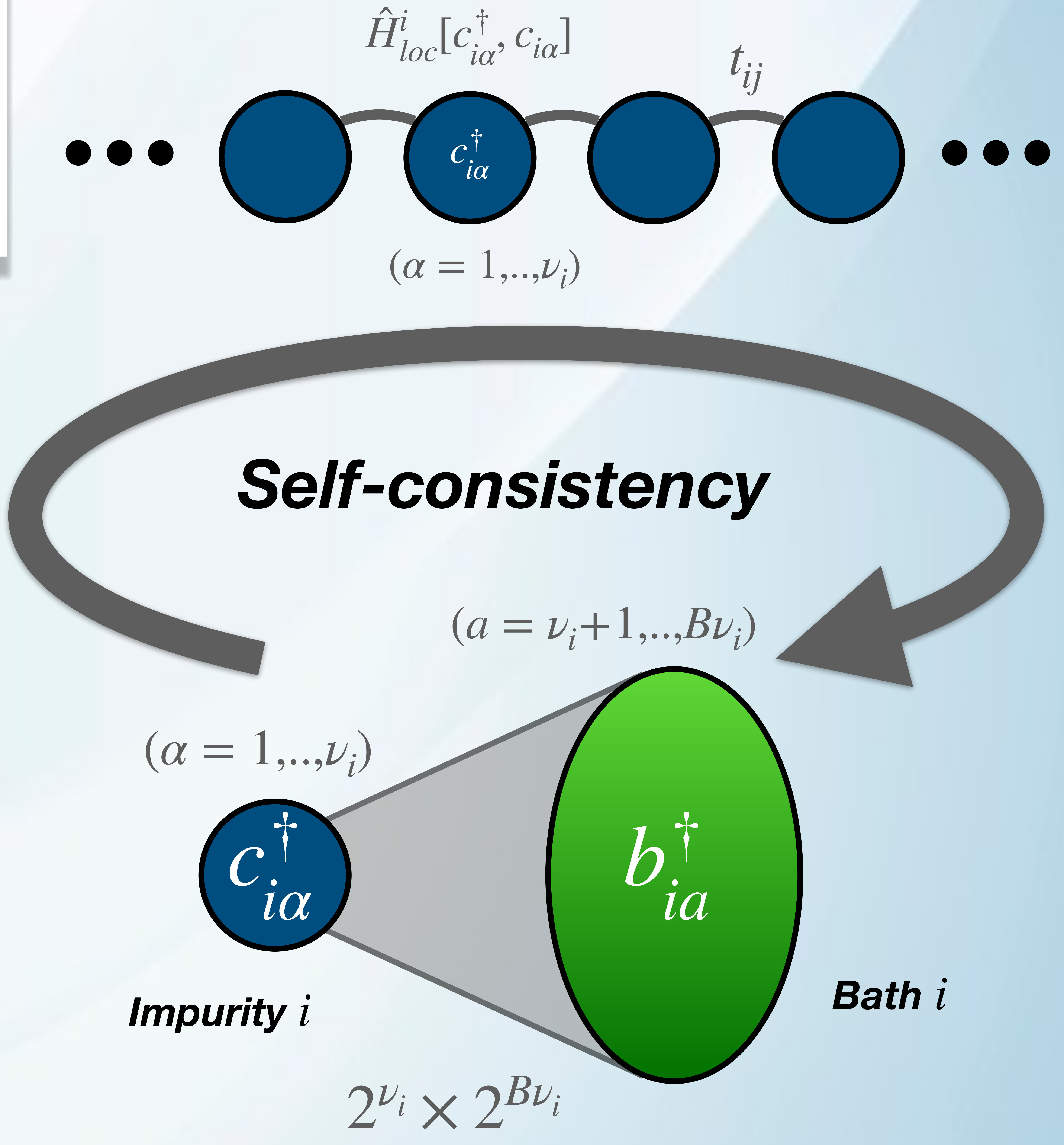


Alternative derivations of gGA equations

$$|\Psi_G\rangle = \hat{\mathcal{P}}_G|\Psi_0\rangle = \prod_{i=1}^{\mathcal{N}} \hat{\mathcal{P}}_i|\Psi_0\rangle$$

Final equations can be also obtained from RISB and DMET principles:

PHYSICAL REVIEW B **105**, 045111 (2022)

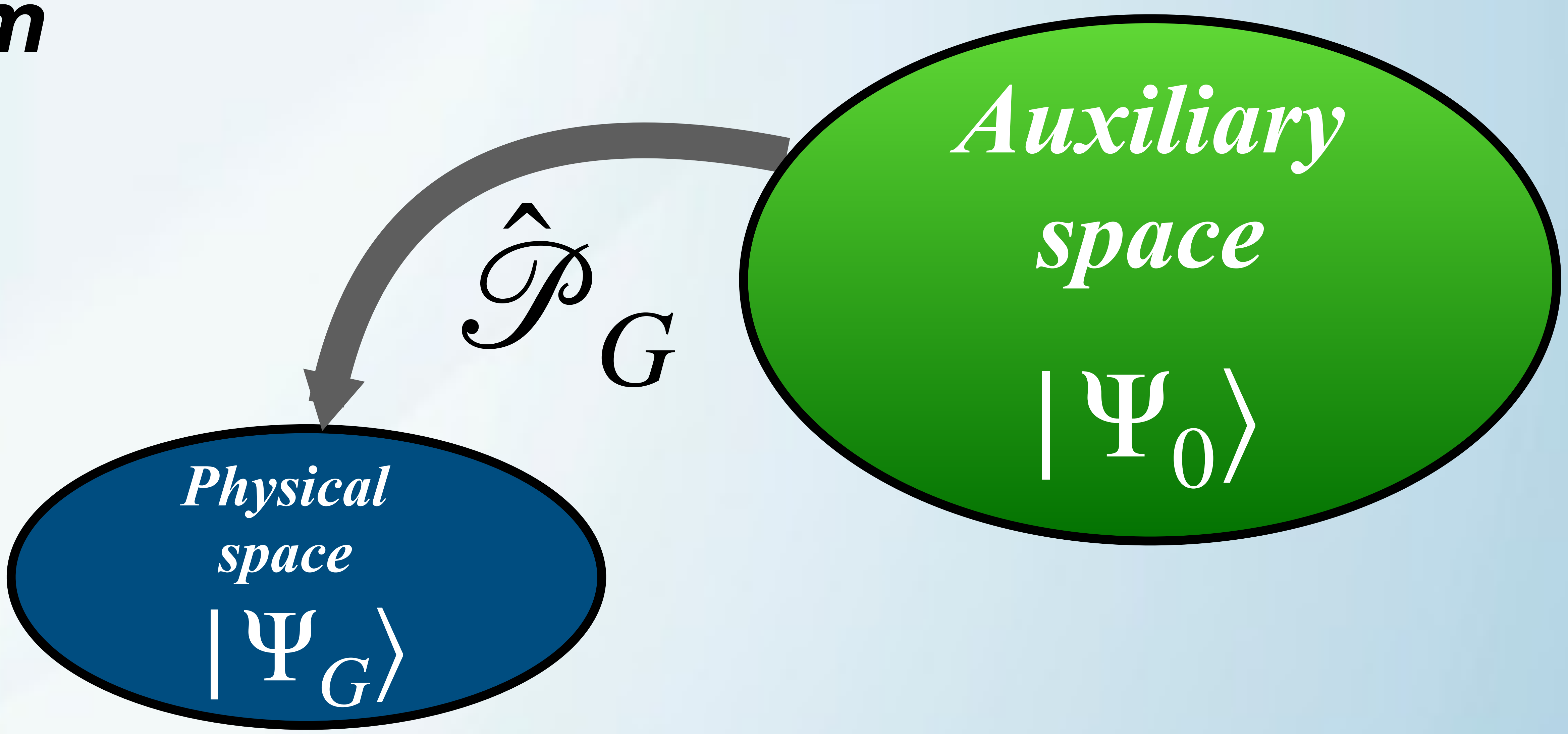
Operatorial formulation of the ghost rotationally invariant slave-boson theory

Nicola Lanatà *

PHYSICAL REVIEW B **108**, 235112 (2023)

Derivation of the ghost Gutzwiller approximation from quantum embedding principles: Ghost density matrix embedding theory

Nicola Lanatà *



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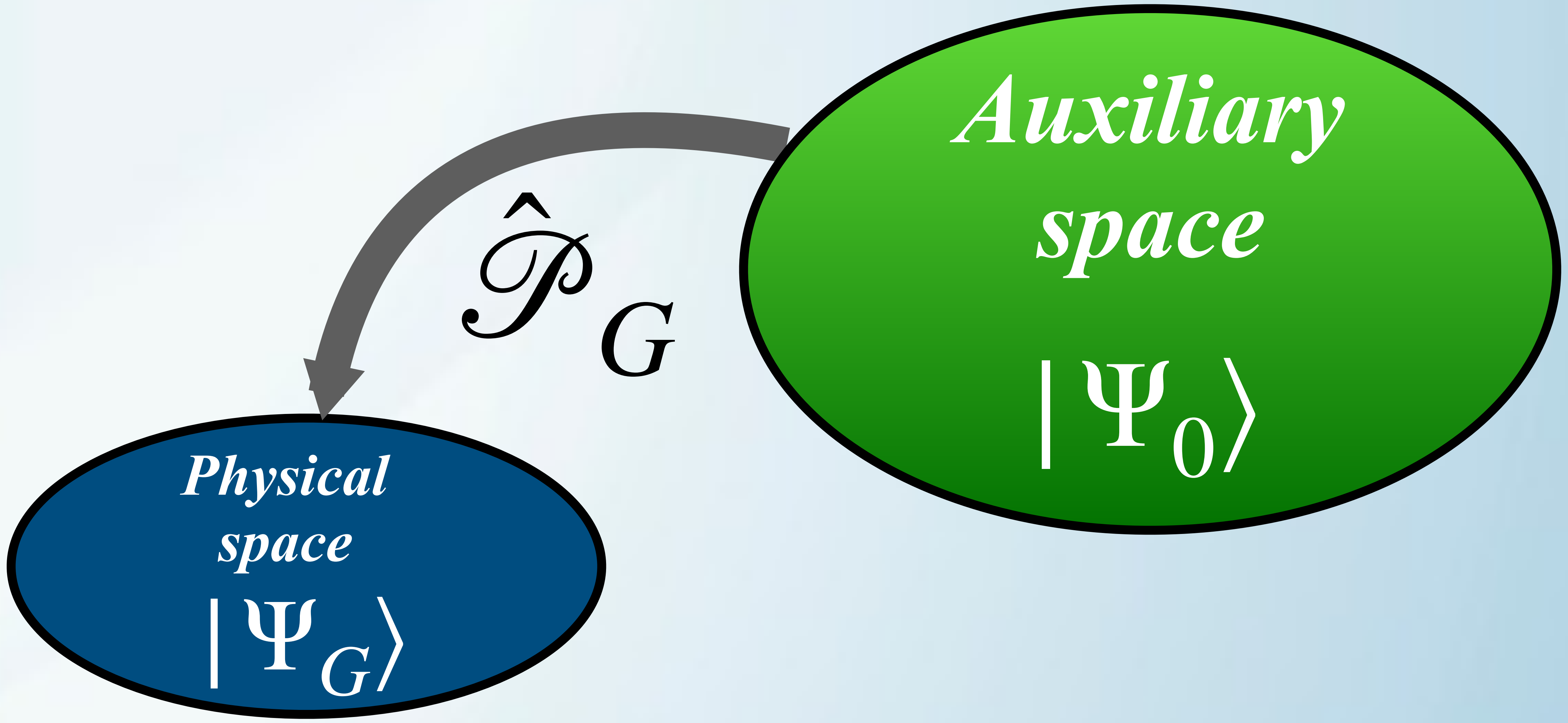
The gGA variational wave function:

$$|\Psi_G\rangle = \hat{\mathscr{P}}_G|\Psi_0\rangle = \prod_{i=1}^{\mathscr{N}} \hat{\mathscr{P}}_i|\Psi_0\rangle$$

$$\hat{\mathscr{P}}_i = \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} [\Lambda_i]_{\Gamma n}|\Gamma, i\rangle\langle n, i|$$

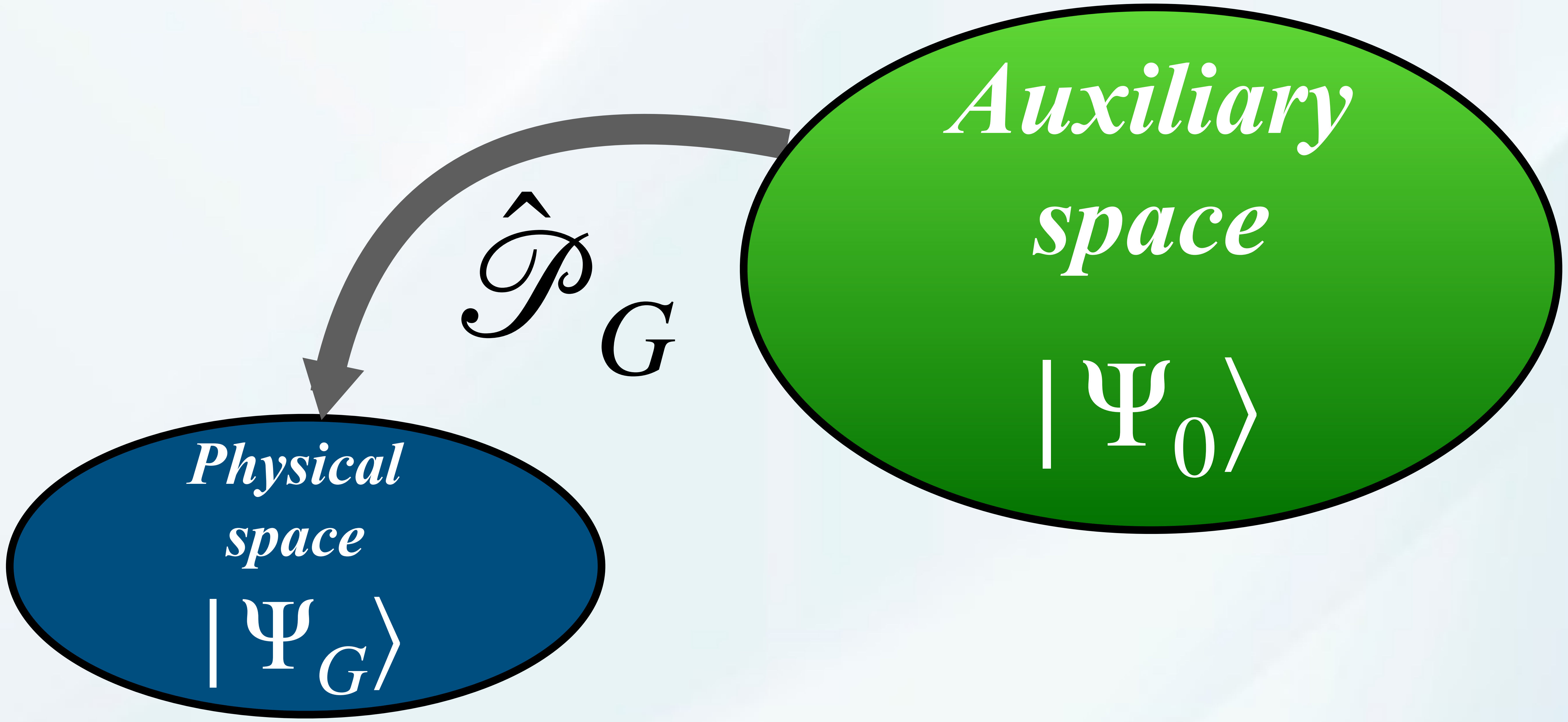
$$|\Gamma, i\rangle = [c_{i1}^\dagger]^{q_1(\Gamma)} \dots [c_{i\nu_i}^\dagger]^{q_{\nu_i}(\Gamma)}|0\rangle$$

$$|n, i\rangle = [f_{i1}^\dagger]^{q_1(n)} \dots [f_{iB\nu_i}^\dagger]^{q_{B\nu_i}(n)}|0\rangle$$



Our goal is to minimize $\langle \Psi_0 | \hat{\mathcal{P}}_G^\dagger \hat{H} \hat{\mathcal{P}}_G | \Psi_0 \rangle$ **w.r.t.** $\{\Lambda_i\}, |\Psi_0\rangle$

$2^{\nu_i} \times 2^{B\nu_i}$



Wick's theorem: $\langle \Psi_0 | f_a^\dagger f_b^\dagger f_c f_d | \Psi_0 \rangle = \langle \Psi_0 | f_a^\dagger f_d | \Psi_0 \rangle \langle \Psi_0 | f_b^\dagger f_c | \Psi_0 \rangle - \langle \Psi_0 | f_a^\dagger f_c | \Psi_0 \rangle \langle \Psi_0 | f_b^\dagger f_d | \Psi_0 \rangle$

$|\Psi_G\rangle$ ***can be treated only numerically in general***

Derivation steps:

1. ***Definition of approximations (GA and G. constraints).***
2. ***Evaluation of*** $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ ***in terms of*** $\{\Lambda_i\}, |\Psi_0\rangle$.
3. ***Definition of slave-boson (SB) amplitudes.***
4. ***Mapping from SB amplitudes to embedding states.***
5. ***Lagrange formulation of the optimization problem.***

Evaluating $\langle \Psi_G | \hat{H} | \Psi_G \rangle = \langle \Psi_0 | \hat{\mathcal{P}}_G^\dagger \hat{H} \hat{\mathcal{P}}_G | \Psi_0 \rangle$

Wick's theorem: $\langle \Psi_0 | c_a^\dagger c_b^\dagger c_c c_d | \Psi_0 \rangle = \langle \Psi_0 | c_a^\dagger c_d | \Psi_0 \rangle \langle \Psi_0 | c_b^\dagger c_c | \Psi_0 \rangle - \langle \Psi_0 | c_a^\dagger c_c | \Psi_0 \rangle \langle \Psi_0 | c_b^\dagger c_d | \Psi_0 \rangle$

Gutzwiller constraints:

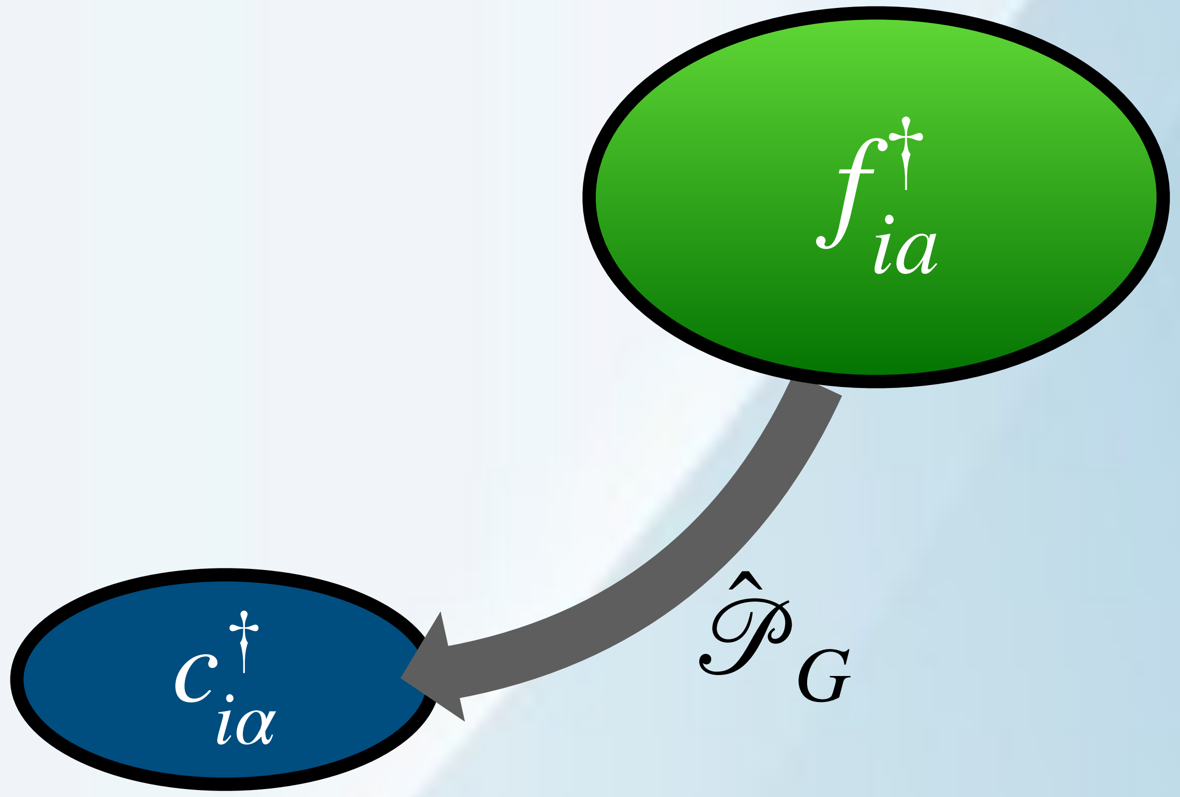
$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i \, f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \qquad \forall \, a, b \in \{1,..,B\nu_i\}$$

Gutzwiller approximation:

We will exploit simplifications that become exact in the limit of ∞-coordination lattices. In this sense, the gGA is a variational approximation to DMFT.

Gutzwiller constraints:



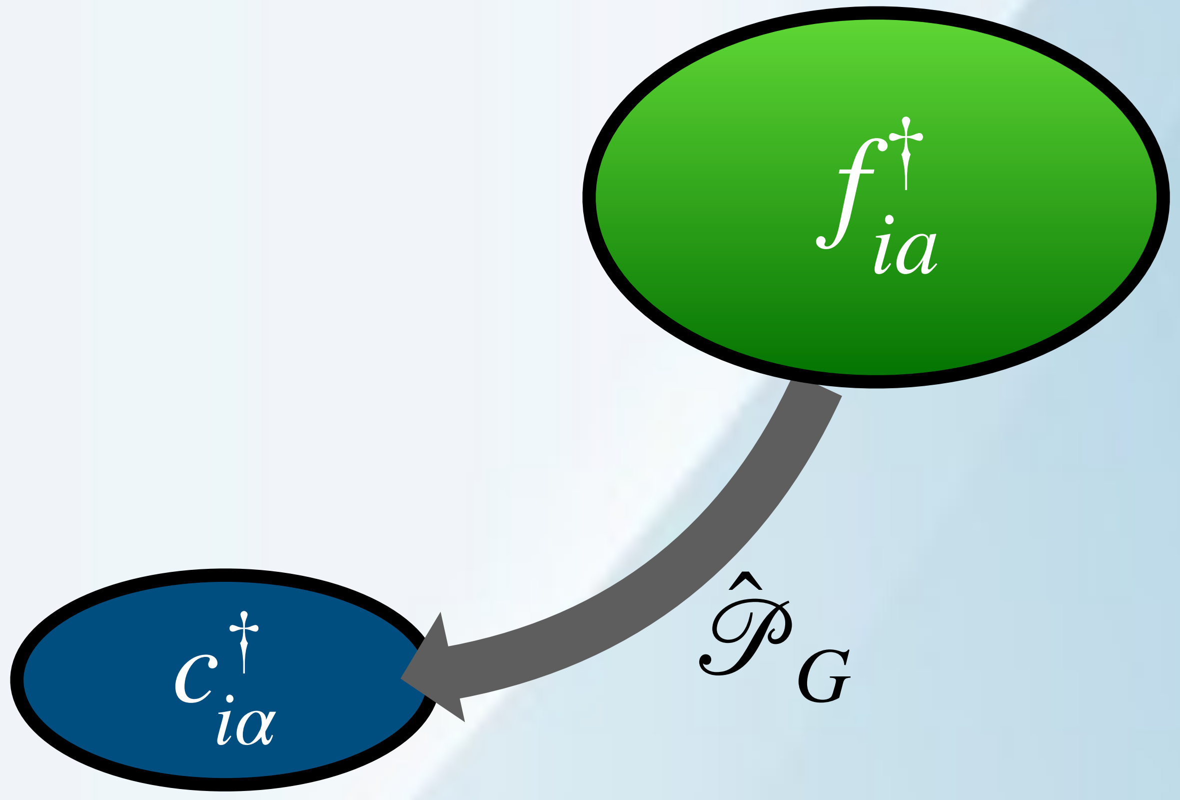
$$\langle \Psi_0 | \hat{\mathcal{P}}^\dagger_i \hat{\mathcal{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Psi_0 | \hat{\mathcal{P}}^\dagger_i \hat{\mathcal{P}}_i \, f^\dagger_{ia} f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f^\dagger_{ia} f_{ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,B\nu_i\}$$

Key consequence:

$$\langle \Psi_0 | \hat{\mathcal{P}}^\dagger_i \hat{\mathcal{P}}_i \, f^\dagger_{ia} f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | \hat{\mathcal{P}}^\dagger_i \hat{\mathcal{P}}_i | \Psi_0 \rangle \langle \Psi_0 | f^\dagger_{ia} f_{ib} | \Psi_0 \rangle$$
$$+ \langle \Psi_0 | \left[\hat{\mathcal{P}}^\dagger_i \hat{\mathcal{P}}_i \right] f^\dagger_{ia} f_{ib} | \Psi_0 \rangle_{2-legs}$$

Gutzwiller constraints:



$$\langle \Psi_0 | \hat{\mathcal{P}}^{\dagger}_i \hat{\mathcal{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

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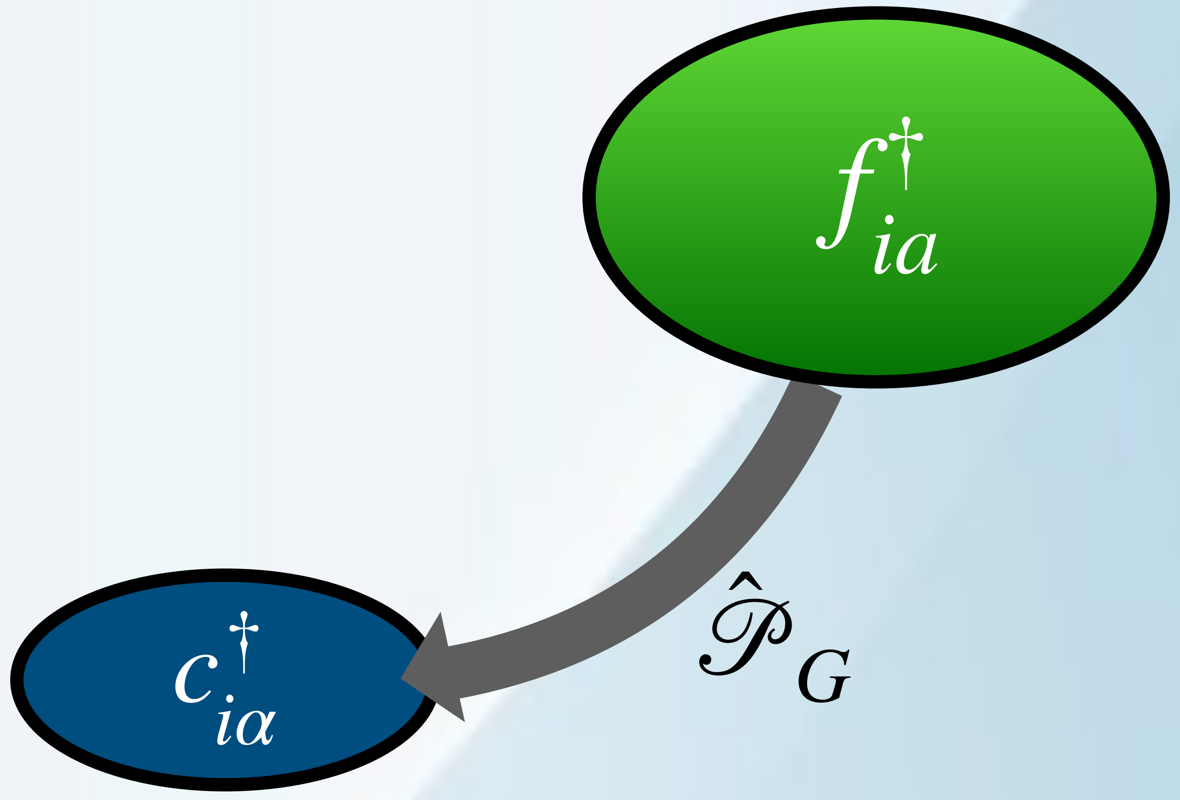
$$+ \langle \Psi_0 | \left[\hat{\mathcal{P}}^{\dagger}_i \hat{\mathcal{P}}_i \right] f^{\dagger}_{ia} f_{ib} | \Psi_0 \rangle_{2-legs}$$

Gutzwiller constraints:



$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i \, f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,B\nu_i\}$$

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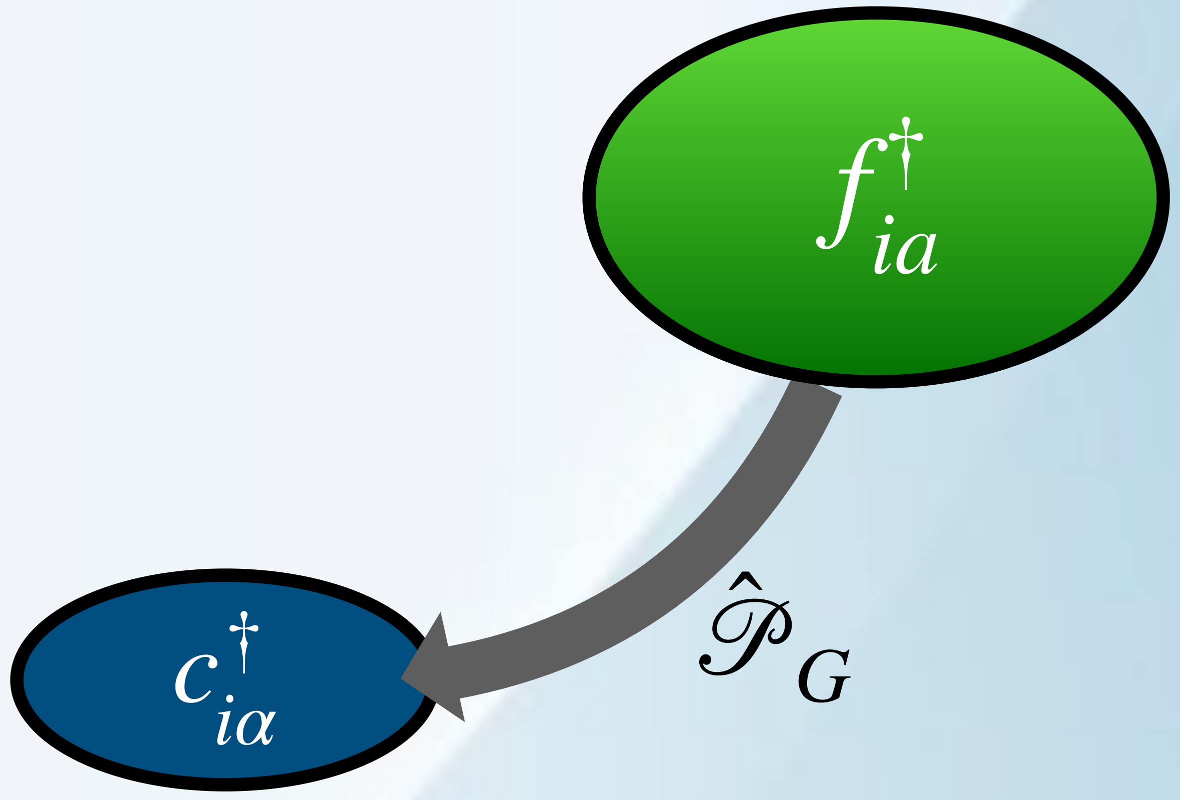
$$+ \langle \Psi_0 | \left[\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i \right] f_{ia}^\dagger f_{ib} | \Psi_0 \rangle_{2-legs}$$

Gutzwiller constraints:



$$\langle \Psi_0 | \hat{\mathscr{P}}_i^{\dagger} \hat{\mathscr{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Psi_0 | \hat{\mathscr{P}}_i^{\dagger} \hat{\mathscr{P}}_i \, f^{\dagger}_{ia} f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f^{\dagger}_{ia} f_{ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,B\nu_i\}$$

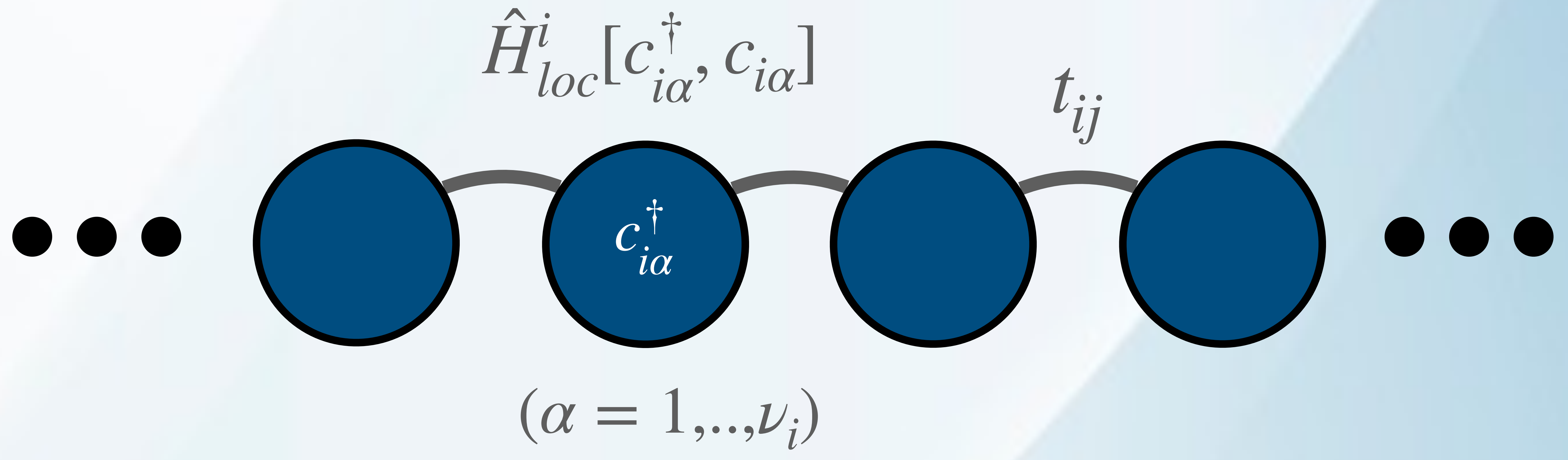
Key consequence:

$$\langle \Psi_0 | \left[\hat{\mathscr{P}}_i^{\dagger} \hat{\mathscr{P}}_i \right] \cdots \, | \Psi_0 \rangle_{2-legs} = 0 \qquad \forall\, a, b$$

Derivation steps:

1. *Definition of approximations (GA and G. constraints).*
2. *Evaluation of* $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ *in terms of* $\{\Lambda_i\}, |\Psi_0\rangle$.
3. *Definition of slave-boson (SB) amplitudes.*
4. *Mapping from SB amplitudes to embedding states.*
5. *Lagrange formulation of the optimization problem.*

The Hamiltonian:



$$\hat{H} = \sum_{i=1}^{\mathcal{N}} \hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}] + \sum_{i\neq j} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} [t_{ij}]_{\alpha\beta}\, c^\dagger_{i\alpha} c_{j\beta}$$

- i, j : ***Indices of the fragments of the lattice.***
- $\hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}]$: ***Local operator on fragment*** i
- α, β : ***Indices of Fermionic modes within each fragment.***
- $[t_{ij}]_{\alpha\beta}$: ***Matrix elements of the hopping term.***

Local operators:

$$\langle \Psi_G | \hat{H}^i_{loc} | \Psi_G \rangle = \langle \Psi_0 | \left(\prod_{k=1}^{\mathcal{N}} \hat{\mathcal{P}}^\dagger_k \right) \hat{H}^i_{loc} \left(\prod_{k=1}^{\mathcal{N}} \hat{\mathcal{P}}_k \right) | \Psi_0 \rangle$$

$$= \langle \Psi_0 | \left(\prod_{k \neq i} \hat{\mathcal{P}}^\dagger_k \hat{\mathcal{P}}_k \right) \left(\hat{\mathcal{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathcal{P}}_i \right) | \Psi_0 \rangle$$

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$$= \langle \Psi_0 | \left(\hat{\mathcal{P}}^\dagger_k \hat{\mathcal{P}}_k \right) \left[\prod_{k' \neq i,k} \hat{\mathcal{P}}^\dagger_{k'} \hat{\mathcal{P}}_{k'} \right] \left(\hat{\mathcal{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathcal{P}}_i \right) | \Psi_0 \rangle$$

Local operators: (disconnected terms)

$$\langle\Psi_0|\left(\hat{\mathcal{P}}_k^\dagger\hat{\mathcal{P}}_k\right)\left(\prod_{k'\neq i,k}\hat{\mathcal{P}}_{k'}^\dagger\hat{\mathcal{P}}_{k'}\right)\left(\hat{\mathcal{P}}_i^\dagger\hat{H}^i_{loc}\hat{\mathcal{P}}_i\right)|\Psi_0\rangle$$

$$=\underbrace{\langle\Psi_0|\left(\hat{\mathcal{P}}_k^\dagger\hat{\mathcal{P}}_k\right)|\Psi_0\rangle}_{=1}\times\langle\Psi_0|\left(\prod_{k'\neq i,k}\hat{\mathcal{P}}_{k'}^\dagger\hat{\mathcal{P}}_{k'}\right)\left(\hat{\mathcal{P}}_i^\dagger\hat{H}^i_{loc}\hat{\mathcal{P}}_i\right)|\Psi_0\rangle$$

(G. constraints)

Local operators: (disconnected terms)

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$$=\langle\Psi_0|\left(\hat{\mathscr{P}}_k^\dagger\hat{\mathscr{P}}_k\right)|\Psi_0\rangle\times\langle\Psi_0|\left(\prod_{k'\neq i,k}\hat{\mathscr{P}}_{k'}^\dagger\hat{\mathscr{P}}_{k'}\right)\left(\hat{\mathscr{P}}_i^\dagger\hat{H}_{loc}^i\hat{\mathscr{P}}_i\right)|\Psi_0\rangle$$

$$=\langle\Psi_0|\left(\prod_{k'\neq i,k}\hat{\mathscr{P}}_{k'}^\dagger\hat{\mathscr{P}}_{k'}\right)\left(\hat{\mathscr{P}}_i^\dagger\hat{H}_{loc}^i\hat{\mathscr{P}}_i\right)|\Psi_0\rangle$$

Local operators: (connected terms 2 legs)

$$\langle \Psi_0 | \left(\hat{\mathscr{P}}^\dagger_k \hat{\mathscr{P}}_k \right) \left[\prod_{k' \neq i,k} \hat{\mathscr{P}}^\dagger_{k'} \hat{\mathscr{P}}_{k'} \right] \left(\hat{\mathscr{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathscr{P}}_i \right) | \Psi_0 \rangle \quad = 0$$

$$\langle \Psi_0 | \left[\hat{\mathscr{P}}^\dagger_i \hat{\mathscr{P}}_i \right] \cdots \ | \Psi_0 \rangle_{2-legs} = 0 \qquad \forall\, a, b$$

(G. constraints)

Local operators: (connected terms >2 legs)

$$\langle \Psi_0 | \left(\hat{\mathscr{P}}_k^\dagger \hat{\mathscr{P}}_k \right) \left(\prod_{k' \neq i,k} \hat{\mathscr{P}}_{k'}^\dagger \hat{\mathscr{P}}_{k'} \right) \left(\hat{\mathscr{P}}_i^\dagger \hat{H}_{loc}^i \hat{\mathscr{P}}_i \right) | \Psi_0 \rangle \quad = 0$$

(G. Approximation)

(Exact in limit of ∞ dimension)

Local operators:

$$\langle \Psi_G | \hat{H}^i_{loc} | \Psi_G \rangle = \langle \Psi_0 | \left(\hat{\mathcal{P}}^\dagger_k \hat{\mathcal{P}}_k \right) \left(\prod_{k' \neq i,k} \hat{\mathcal{P}}^\dagger_{k'} \hat{\mathcal{P}}_{k'} \right) \left(\hat{\mathcal{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathcal{P}}_i \right) | \Psi_0 \rangle$$

(GA and G. constraints) $\approx \langle \Psi_0 | \left(\prod_{k' \neq i,k} \hat{\mathcal{P}}^\dagger_{k'} \hat{\mathcal{P}}_{k'} \right) \left(\hat{\mathcal{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathcal{P}}_i \right) | \Psi_0 \rangle$

Local operators:

$$\langle \Psi_G | \hat{H}^i_{loc} | \Psi_G \rangle = \langle \Psi_0 | \left(\hat{\mathscr{P}}^\dagger_k \hat{\mathscr{P}}_k \right) \left(\prod_{k' \neq i,k} \hat{\mathscr{P}}^\dagger_{k'} \hat{\mathscr{P}}_{k'} \right) \left(\hat{\mathscr{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathscr{P}}_i \right) | \Psi_0 \rangle$$

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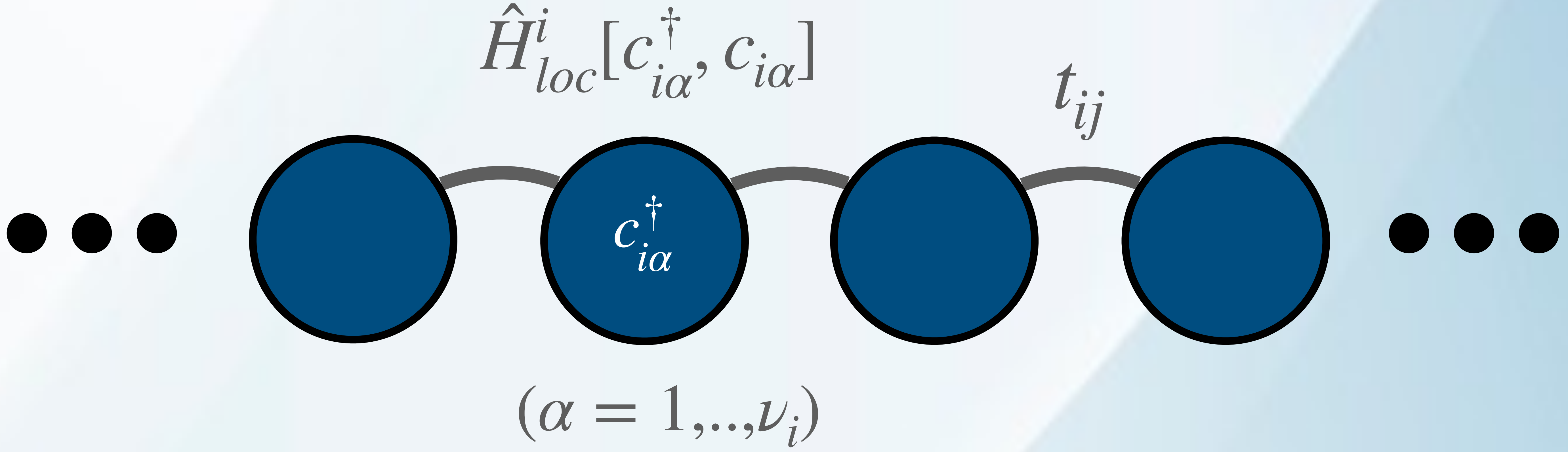
$$\approx \langle \Psi_0 | \hat{\mathscr{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathscr{P}}_i | \Psi_0 \rangle$$

The Hamiltonian:



$$\hat{H} = \sum_{i=1}^{\mathcal{N}} \hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}] + \sum_{i \neq j} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} [t_{ij}]_{\alpha\beta}\, c^\dagger_{i\alpha} c_{j\beta}$$

- i, j : ***Indices of the fragments of the lattice.***
- $\hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}]$: ***Local operator on fragment*** i
- α, β : ***Indices of Fermionic modes within each fragment.***
- $[t_{ij}]_{\alpha\beta}$: ***Matrix elements of the hopping term.***

Non-Local 1-body operators, i.e., $i \neq j$:

$$\langle \Psi_G | c^\dagger_{i\alpha} c_{j\beta} | \Psi_G \rangle = \langle \Psi_0 | \left(\prod_{k=1}^{\mathcal{N}} \hat{\mathcal{P}}^\dagger_k \right) c^\dagger_{i\alpha} c_{j\beta} \left(\prod_{k=1}^{\mathcal{N}} \hat{\mathcal{P}}_k \right) | \Psi_0 \rangle$$

$$= \langle \Psi_0 | \left[\prod_{k \neq i,j} \hat{\mathcal{P}}^\dagger_k \hat{\mathcal{P}}_k \right] \left(\hat{\mathcal{P}}^\dagger_i c^\dagger_{i\alpha} \hat{\mathcal{P}}_i \right) \left(\hat{\mathcal{P}}^\dagger_j c_{j\beta} \hat{\mathcal{P}}_j \right) | \Psi_0 \rangle$$

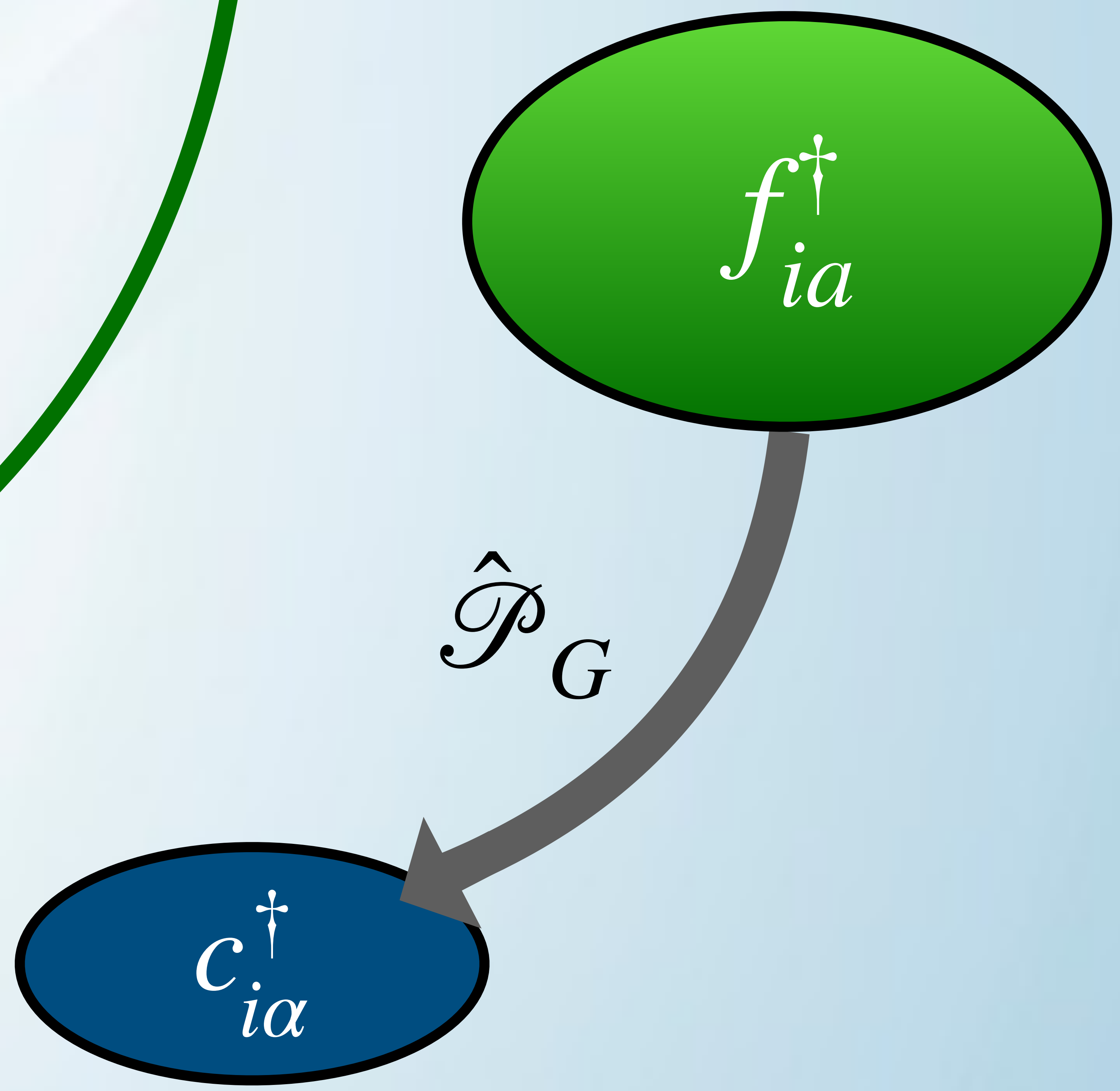
(GA and G. constraints) $\approx \langle \Psi_0 | \left(\hat{\mathcal{P}}^\dagger_i c^\dagger_{i\alpha} \hat{\mathcal{P}}_i \right) \left(\hat{\mathcal{P}}^\dagger_j c_{j\beta} \hat{\mathcal{P}}_j \right) | \Psi_0 \rangle$

Non-Local 1-body operators, i.e., $i \neq j$:

$$\langle \Psi_G | c^\dagger_{i\alpha} c_{j\beta} | \Psi_G \rangle \approx \langle \Psi_0 | \left(\hat{\mathscr{P}}^\dagger_i c^\dagger_{i\alpha} \hat{\mathscr{P}}_i \right) \left(\hat{\mathscr{P}}^\dagger_j c_{j\beta} \hat{\mathscr{P}}_j \right) | \Psi_0 \rangle$$

Constructed with $\{f_{ia}, f^\dagger_{ia}\}$ operators

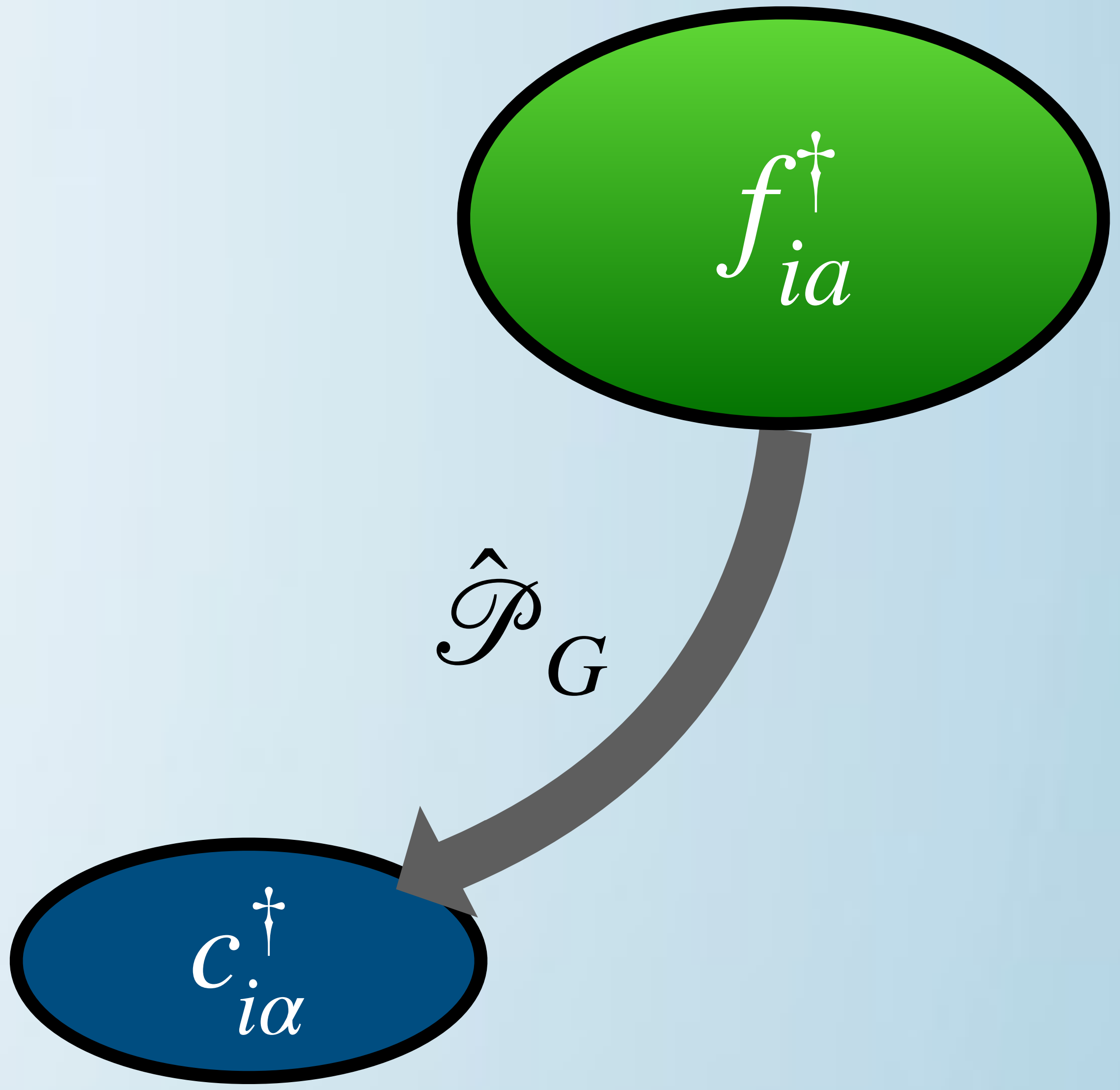
Constructed with $\{f_{ja}, f^\dagger_{ja}\}$ operators



Non-Local 1-body operators, i.e., $i \neq j$:

$$\langle \Psi_G | c^\dagger_{i\alpha} c_{j\beta} | \Psi_G \rangle \approx \langle \Psi_0 | \left(\hat{\mathscr{P}}_i^\dagger c^\dagger_{i\alpha} \hat{\mathscr{P}}_i \right) \left(\hat{\mathscr{P}}_j^\dagger c_{j\beta} \hat{\mathscr{P}}_j \right) | \Psi_0 \rangle$$

$$= \sum_{a=1}^{B\nu_i} \sum_{b=1}^{B\nu_j} \langle \Psi_0 | \left([\mathscr{R}_i]_{a\alpha} f^\dagger_{ia} \right) \left([\mathscr{R}_j]^\dagger_{\beta b} f_{jb} \right) | \Psi_0 \rangle$$



Where $\mathscr{R}_i$ is determined by:

$$\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger c^\dagger_{i\alpha} \hat{\mathscr{P}}_i f_{ia} | \Psi_0 \rangle = \sum_{b=1}^{B\nu_i} [\mathscr{R}_i]_{ba} \langle \Psi_0 | f^\dagger_{ib} f_{ia} | \Psi_0 \rangle$$

Variational energy:

$$\hat{H} = \sum_{i=1}^{\mathcal{N}} \hat{H}^{i}_{loc}[c^{\dagger}_{i\alpha}, c_{i\alpha}] + \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} [t_{ij}]_{\alpha\beta}\, c^{\dagger}_{i\alpha} c_{j\beta}$$

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}^{\dagger}_j\right]_{ab} \langle \Psi_0 | f^{\dagger}_{ia} f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \langle \Psi_0 | \hat{\mathcal{P}}^{\dagger}_i \hat{H}^{i}_{loc}[c^{\dagger}_{i\alpha}, c_{i\alpha}]\, \hat{\mathcal{P}}_i | \Psi_0 \rangle$$

Where: $\langle \Psi_0 | \hat{\mathcal{P}}^{\dagger}_i c^{\dagger}_{i\alpha} \hat{\mathcal{P}}_i f_{ia} | \Psi_0 \rangle = \sum_{b=1}^{B\nu_i} [\mathcal{R}_i]_{b\alpha} \langle \Psi_0 | f^{\dagger}_{ib} f_{ia} | \Psi_0 \rangle$

$$\begin{cases} \langle \Psi_0 | \hat{\mathcal{P}}^{\dagger}_i \hat{\mathcal{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1 \\ \langle \Psi_0 | \hat{\mathcal{P}}^{\dagger}_i \hat{\mathcal{P}}_i\, f^{\dagger}_{ia} f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f^{\dagger}_{ia} f_{ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,B\nu_i\} \end{cases}$$

Derivation steps:

1. *Definition of approximations (GA and G. constraints).*

2. *Evaluation of* $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ *in terms of* $\{\Lambda_i\}, |\Psi_0\rangle$.

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4. *Mapping from SB amplitudes to embedding states.*

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(Connection with RISB)

Variational energy:

$$\mathscr{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathscr{R}_i t_{ij} \mathscr{R}_j^\dagger\right]_{ab} \langle \Psi_0 | f_{ia}^\dagger f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \boxed{\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \hat{H}_{loc}^i [c_{i\alpha}^\dagger, c_{i\alpha}] \hat{\mathscr{P}}_i | \Psi_0 \rangle}$$

Where: $$\boxed{\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathscr{P}}_i f_{ia} | \Psi_0 \rangle} = \sum_{b=1}^{B\nu_i} [\mathscr{R}_i]_{b\alpha} \boxed{\langle \Psi_0 | f_{ib}^\dagger f_{ia} | \Psi_0 \rangle}$$

$$\begin{cases} \boxed{\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \hat{\mathscr{P}}_i | \Psi_0 \rangle} = \langle \Psi_0 | \Psi_0 \rangle = 1 \\ \boxed{\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \hat{\mathscr{P}}_i \, f_{ia}^\dagger f_{ib} | \Psi_0 \rangle} = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,B\nu_i\} \end{cases}$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger\hat{\mathscr{P}}_i|\Psi_0\rangle = \mathrm{Tr}\left[P_i^0\Lambda_i^\dagger\Lambda_i\right] = 1$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger\hat{\mathscr{P}}_i\, f_{ia}^\dagger f_{ib}|\Psi_0\rangle = \mathrm{Tr}\left[P_i^0\Lambda_i^\dagger\Lambda_i\tilde{F}_{ia}^\dagger\tilde{F}_{ib}\right] = \langle\Psi_0|f_{ia}^\dagger f_{ib}|\Psi_0\rangle =: [\Delta_i]_{ab}$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger\,\hat{H}_{loc}^i[c_{i\alpha}^\dagger, c_{i\alpha}]\,\hat{\mathscr{P}}_i|\Psi_0\rangle = \mathrm{Tr}\left[P_i^0\Lambda_i^\dagger\hat{H}_{loc}^i\left[F_{i\alpha}^\dagger, F_{i\alpha}\right]\Lambda_i\right]$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger c_{i\alpha}^\dagger\hat{\mathscr{P}}_i f_{ia}|\Psi_0\rangle = \mathrm{Tr}\left[P_i^0\Lambda_i^\dagger F_{i\alpha}^\dagger\Lambda_i\tilde{F}_{ia}\right] = \sum_{b=1}^{B\nu_i}[\mathscr{R}_i]_{ba}\,[\Delta_i]_{ba}$$

Where:

$$P_i^0 \propto \exp\left\{-\sum_{a,b=1}^{B\nu_i}\left[\ln\left(\frac{\mathbf{1}-\Delta_i^T}{\Delta_i^T}\right)\right]_{ab}\tilde{F}_{ia}^\dagger\tilde{F}_{ib}\right\}$$

$$[F_{i\alpha}]_{\Gamma\Gamma'} = \langle\Gamma, i|c_{i\alpha}|\Gamma', i\rangle$$

$$[\tilde{F}_{ia}]_{nn'} = \langle n, i|f_{ia}|n', i\rangle$$

$$\hat{\mathscr{P}}_i = \sum_{\Gamma=0}^{2^{\nu_i}-1}\sum_{n=0}^{2^{B\nu_i}-1}[\Lambda_i]_{\Gamma n}|\Gamma, i\rangle\langle n, i|$$

$$|\Gamma, i\rangle = [c_{i1}^\dagger]^{q_1(\Gamma)}\ldots[c_{i\nu_i}^\dagger]^{q_{\nu_i}(\Gamma)}|0\rangle$$

$$|n, i\rangle = [f_{i1}^\dagger]^{q_1(n)}\ldots[f_{iB\nu_i}^\dagger]^{q_{B\nu_i}(n)}|0\rangle$$

$$\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \hat{\mathscr{P}}_i | \Psi_0 \rangle = \mathrm{Tr}\left[P_i^0 \Lambda_i^\dagger \Lambda_i\right] = 1$$

$$\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \hat{\mathscr{P}}_i \, f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \mathrm{Tr}\left[P_i^0 \Lambda_i^\dagger \Lambda_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib}\right] = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle =: [\Delta_i]_{ab}$$

$$\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \, \hat{H}^i_{loc}[c_{i\alpha}^\dagger, c_{i\alpha}] \, \hat{\mathscr{P}}_i | \Psi_0 \rangle = \mathrm{Tr}\left[P_i^0 \Lambda_i^\dagger \hat{H}^i_{loc}\left[F_{i\alpha}^\dagger, F_{i\alpha}\right] \Lambda_i\right]$$

$$\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathscr{P}}_i f_{ia} | \Psi_0 \rangle = \mathrm{Tr}\left[P_i^0 \Lambda_i^\dagger F_{i\alpha}^\dagger \Lambda_i \tilde{F}_{ia}\right] = \sum_{b=1}^{B\nu_i} [\mathscr{R}_i]_{ba} \, [\Delta_i]_{ba}$$

$$P_i^0 \propto \exp\left\{ - \sum_{a,b=1}^{B\nu_i} \left[\ln\left(\frac{\mathbf{1} - \Delta_i^T}{\Delta_i^T} \right) \right]_{ab} \tilde{F}_{ia}^\dagger \tilde{F}_{ib} \right\}$$

Matrix of SB amplitudes:

$$\phi_i = \Lambda_i \sqrt{P_i^0}$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger\hat{\mathscr{P}}_i|\Psi_0\rangle = \mathrm{Tr}\left[\phi_i^\dagger\phi_i\right] = 1$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger\hat{\mathscr{P}}_i\, f_{ia}^\dagger f_{ib}|\Psi_0\rangle = \mathrm{Tr}\left[\phi_i^\dagger\phi_i\tilde{F}_{ia}^\dagger\tilde{F}_{ib}\right] = \langle\Psi_0|f_{ia}^\dagger f_{ib}|\Psi_0\rangle =: [\Delta_i]_{ab}$$

$$\langle\Psi_0|\hat{\mathscr{P}}_i^\dagger\,\hat{H}^i_{loc}[c_{i\alpha}^\dagger, c_{i\alpha}]\,\hat{\mathscr{P}}_i|\Psi_0\rangle = \mathrm{Tr}\left[\phi_i\phi_i^\dagger\hat{H}^i_{loc}[F_{i\alpha}^\dagger, F_{i\alpha}]\right]$$

$$\mathrm{Tr}\left[\phi_i^\dagger F_{i\alpha}^\dagger\phi_i\tilde{F}_{ia}\right] = \sum_{c=1}^{B\nu_i}[\mathscr{R}_i]_{c\alpha}\,[\Delta_i(\mathbf{1}-\Delta_i)]^{\frac{1}{2}}_{ca}$$

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$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}^\dagger_j\right]_{ab} \langle \Psi_0 | f^\dagger_{ia} f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \mathrm{Tr}\left[\phi_i \phi^\dagger_i \hat{H}^i_{loc}[F^\dagger_{i\alpha}, F_{i\alpha}]\right]$$

Where: $\mathrm{Tr}\left[\phi^\dagger_i F^\dagger_{i\alpha} \phi_i \tilde{F}_{ia}\right] = \sum_{c=1}^{B\nu_i} [\mathcal{R}_i]_{c\alpha} \left[\Delta_i(\mathbf{1} - \Delta_i)\right]^{\frac{1}{2}}_{ca}$

$$\begin{cases} \mathrm{Tr}\left[\phi^\dagger_i \phi_i\right] = 1 \\ \mathrm{Tr}\left[\phi^\dagger_i \phi_i \tilde{F}^\dagger_{ia} \tilde{F}_{ib}\right] = \langle \Psi_0 | f^\dagger_{ia} f_{ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,B\nu_i\} \end{cases}$$

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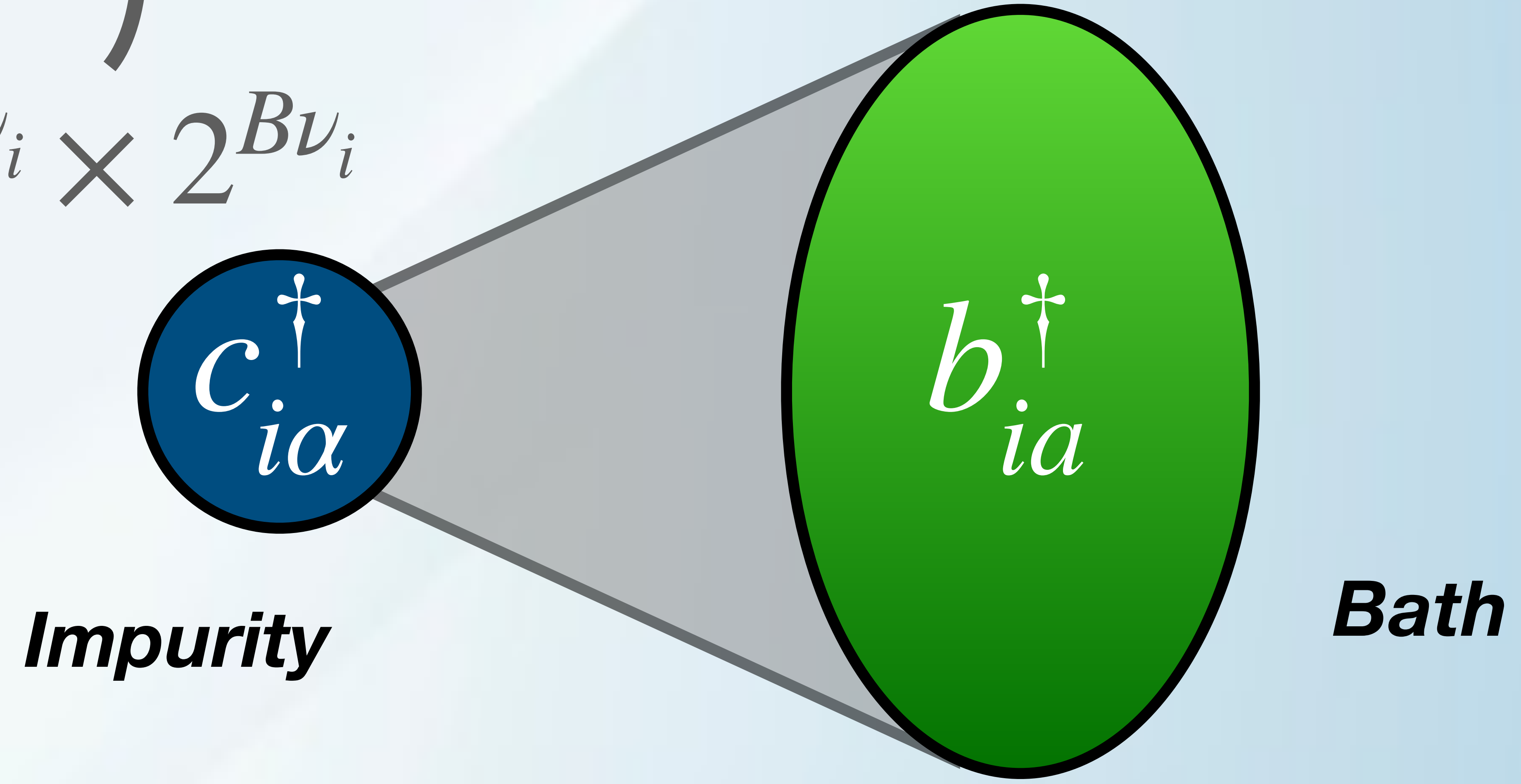
(Connection with QE theories and DMET)

Quantum-embedding formulation

$$[\phi_i]_{\Gamma n} \longrightarrow |\Phi_i\rangle = \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} [\phi_i]_{\Gamma n} |\Gamma; i\rangle \otimes |n; i\rangle$$

$2^{\nu_i} \times 2^{B\nu_i}$

$2^{\nu_i} \times 2^{B\nu_i}$



A useful trick: interpret the variational parameters $\phi_i = \Lambda_i \sqrt{P_i^0}$ as coefficients parametrizing an AIM state

$$|\Gamma, i\rangle = [c^\dagger_{i1}]^{q_1(\Gamma)} \dots [c^\dagger_{i\nu_i}]^{q_{\nu_i}(\Gamma)} |0\rangle$$

$$|n, i\rangle = [b^\dagger_{i1}]^{q_1(n)} \dots [b^\dagger_{iB\nu_i}]^{q_{B\nu_i}(n)} |0\rangle$$

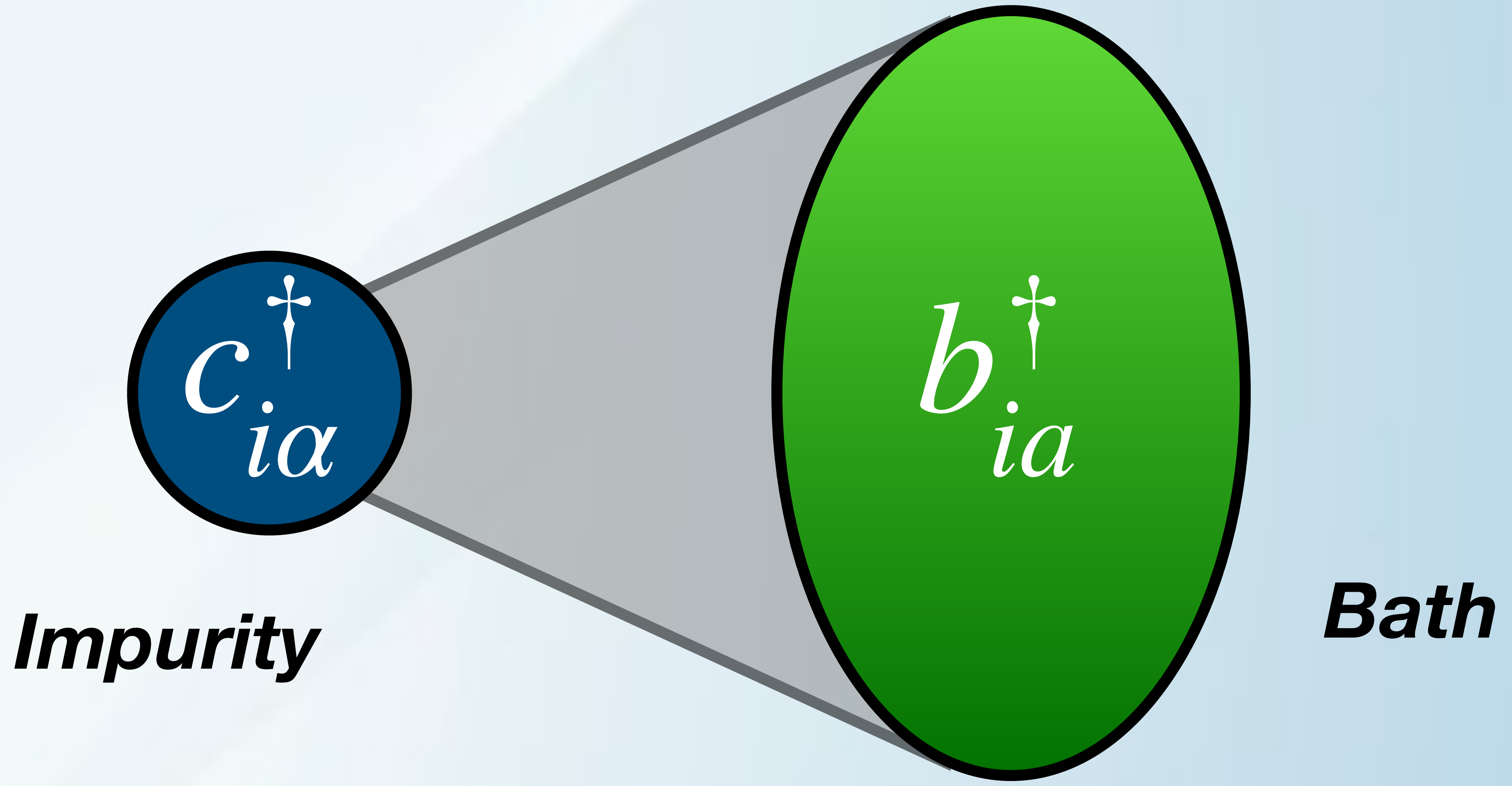
Quantum-embedding formulation

$$2^{\nu_i} \times 2^{B\nu_i}$$

$$[\phi_i]_{\Gamma n} \longrightarrow |\Phi_i\rangle = \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2} N(n)(N(n)-1)} [\phi_i]_{\Gamma n} |\Gamma; i\rangle \otimes U_{PH} |n; i\rangle$$

$$2^{\nu_i} \times 2^{B\nu_i}$$

$$N(n) = \sum_{a=1}^{B\nu_i} q_a(n)$$



If $|\Psi_G\rangle$ *eigenstate of number operator:*

$$\left[\sum_{\alpha=1}^{\nu_i} c^\dagger_\alpha c_\alpha + \sum_{a=1}^{B\nu_i} b^\dagger_a b_a\right] |\Phi_i\rangle = \frac{B+1}{2} \nu_i |\Phi_i\rangle$$

$$|\Gamma, i\rangle = [c^\dagger_{i1}]^{q_1(\Gamma)} \dots [c^\dagger_{i\nu_i}]^{q_{\nu_i}(\Gamma)} |0\rangle$$

$$|n, i\rangle = [b^\dagger_{i1}]^{q_1(n)} \dots [b^\dagger_{iB\nu_i}]^{q_{B\nu_i}(n)} |0\rangle$$

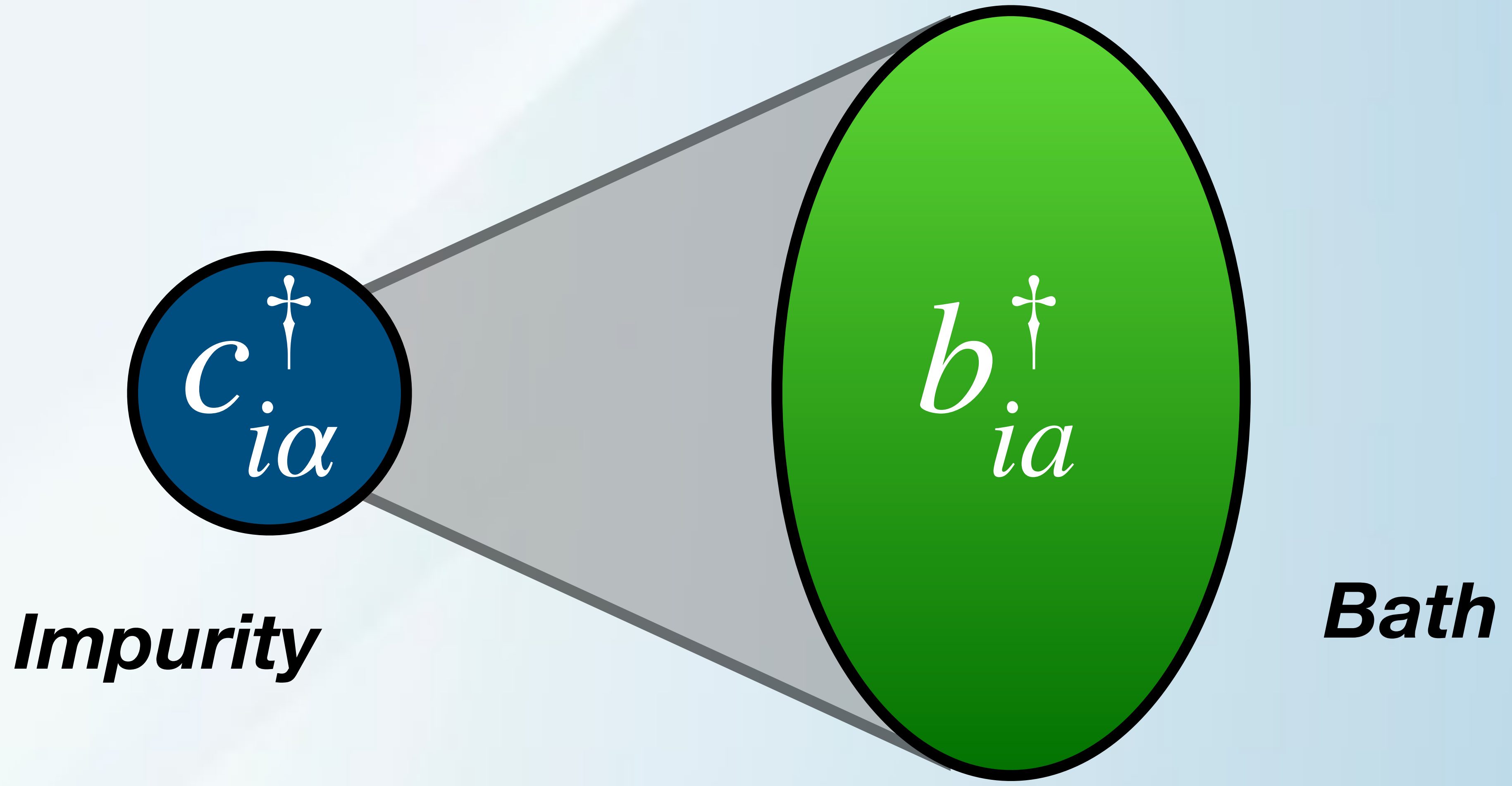
Quantum-embedding formulation

$$[\phi_i]_{\Gamma n} \longrightarrow |\Phi_i\rangle = \sum_{\Gamma=0}^{2^{\nu_i}-1}\sum_{n=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2}N(n)(N(n)-1)}[\phi_i]_{\Gamma n}\,|\Gamma;i\rangle \otimes U_{PH}\,|n;i\rangle$$

$2^{\nu_i}\times 2^{B\nu_i}$

$2^{\nu_i}\times 2^{B\nu_i}$

$$\mathrm{Tr}\left[\phi_i^\dagger \phi_i F_{ia}^\dagger F_{ib}\right] = \langle\Phi_i|\, b_{ib} b_{ia}^\dagger \,|\Phi_i\rangle = [\Delta_i]_{ab}$$



$$\mathrm{Tr}\left[\phi_i \phi_i^\dagger \hat{H}^i_{loc}[F^\dagger_{i\alpha}, F_{i\alpha}]\right] = \langle\Phi_i|\,\hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}]\,|\Phi_i\rangle$$

$$\mathrm{Tr}\left[\phi_i^\dagger F^\dagger_{i\alpha} \phi_i F_{ia}\right] = \langle\Phi_i|\, c^\dagger_{i\alpha} b_{ia} \,|\Phi_i\rangle$$

Variational energy:

$$\hat{H} = \sum_{i=1}^{\mathcal{N}} \hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}] + \sum_{i\neq j} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} [t_{ij}]_{\alpha\beta}\, c^\dagger_{i\alpha} c_{j\beta}$$

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}^\dagger_j\right]_{ab} \langle \Psi_0 | f^\dagger_{ia} f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \langle \Phi_i | \hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}] | \Phi_i \rangle$$

Where:

$$\langle \Phi_i | c^\dagger_{i\alpha} b_{ia} | \Phi_i \rangle = \sum_{a=1}^{B\nu_i} [\mathcal{R}_i]_{a\alpha} [\Delta_i (\mathbf{1} - \Delta_i)]^{\frac{1}{2}}_{ab}$$

$$\langle \Phi_i | \Phi_i \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Phi_i | b^\dagger_{ib} b_{ia} | \Phi_i \rangle = \langle \Psi_0 | f^\dagger_{ia} f_{ib} | \Psi_0 \rangle = [\Delta_i]_{ab}\,, \quad \forall a, b = 1, \ldots, B\nu_i$$

Derivation steps:

1. ***Definition of approximations (GA and G. constraints).***
2. ***Evaluation of*** $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ ***in terms of*** $\{\Lambda_i\}, |\Psi_0\rangle$.
3. ***Definition of slave-boson (SB) amplitudes.***
4. ***Mapping from SB amplitudes to embedding states.***
5. ***Lagrange formulation of the optimization problem.***

Variational energy:

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}_j^\dagger\right]_{ab} \langle \Psi_0 | f_{ia}^\dagger f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \langle \Phi_i | \hat{H}^i_{loc}[c_{i\alpha}^\dagger, c_{i\alpha}] | \Phi_i \rangle$$

Where: $\langle \Phi_i | c_{i\alpha}^\dagger b_{ia} | \Phi_i \rangle = \sum_{a=1}^{B\nu_i} [\mathcal{R}_i]_{a\alpha} [\Delta_i(\mathbf{1} - \Delta_i)]^{\frac{1}{2}}_{ab}$

$$\langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Phi_i | \Phi_i \rangle = 1$$

$$\langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle =: [\Delta_i]_{ab}$$

$$\langle \Phi_i | b_{ib} b_{ia}^\dagger | \Phi_i \rangle = [\Delta_i]_{ab}$$

Variational energy:

$$\mathscr{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathscr{R}_i t_{ij} \mathscr{R}_j^\dagger\right]_{ab} \langle \Psi_0 | f_{ia}^\dagger f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \langle \Phi_i | \hat{H}^i_{loc}[c_{i\alpha}^\dagger, c_{i\alpha}] | \Phi_i \rangle$$

Where: $$\langle \Phi_i | c_{i\alpha}^\dagger b_{ia} | \Phi_i \rangle = \sum_{a=1}^{B\nu_i} [\mathscr{R}_i]_{a\alpha} [\Delta_i(\mathbf{1} - \Delta_i)]^{\frac{1}{2}}_{ab}$$

$[\mathscr{R}_i]_{a\alpha} \leftarrow [\mathscr{D}_i]_{a\alpha}$

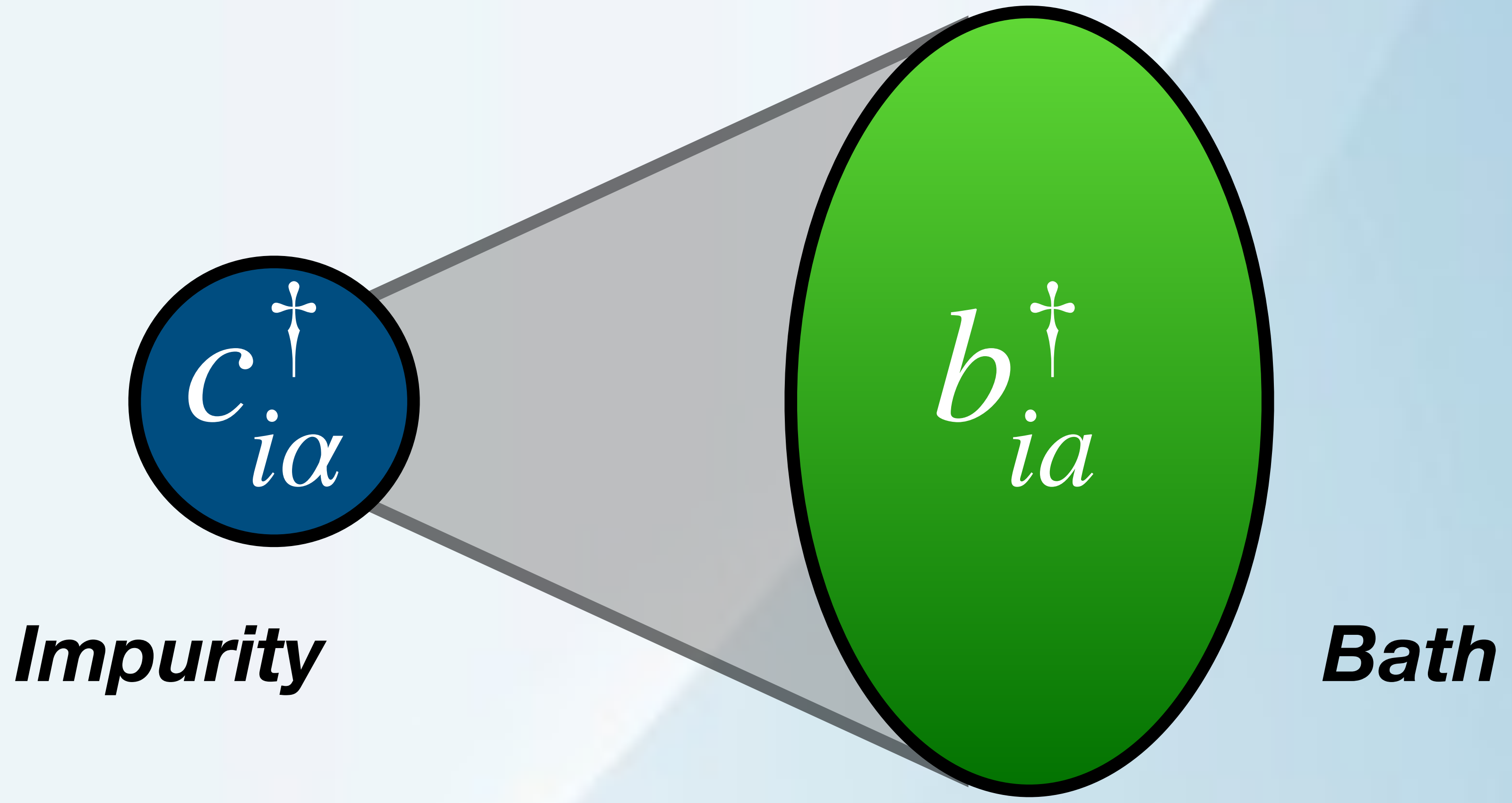
$\langle \Psi_0 | \Psi_0 \rangle = 1 \leftarrow E$

$\langle \Phi_i | \Phi_i \rangle = 1 \leftarrow E_i^c$

$\langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle =: [\Delta_i]_{ab} \leftarrow [\lambda_i]_{ab}$

$\langle \Phi_i | b_{ib} b_{ia}^\dagger | \Phi_i \rangle = [\Delta_i]_{ab} \leftarrow [\lambda_i^c]_{ab}$

Lagrange function:

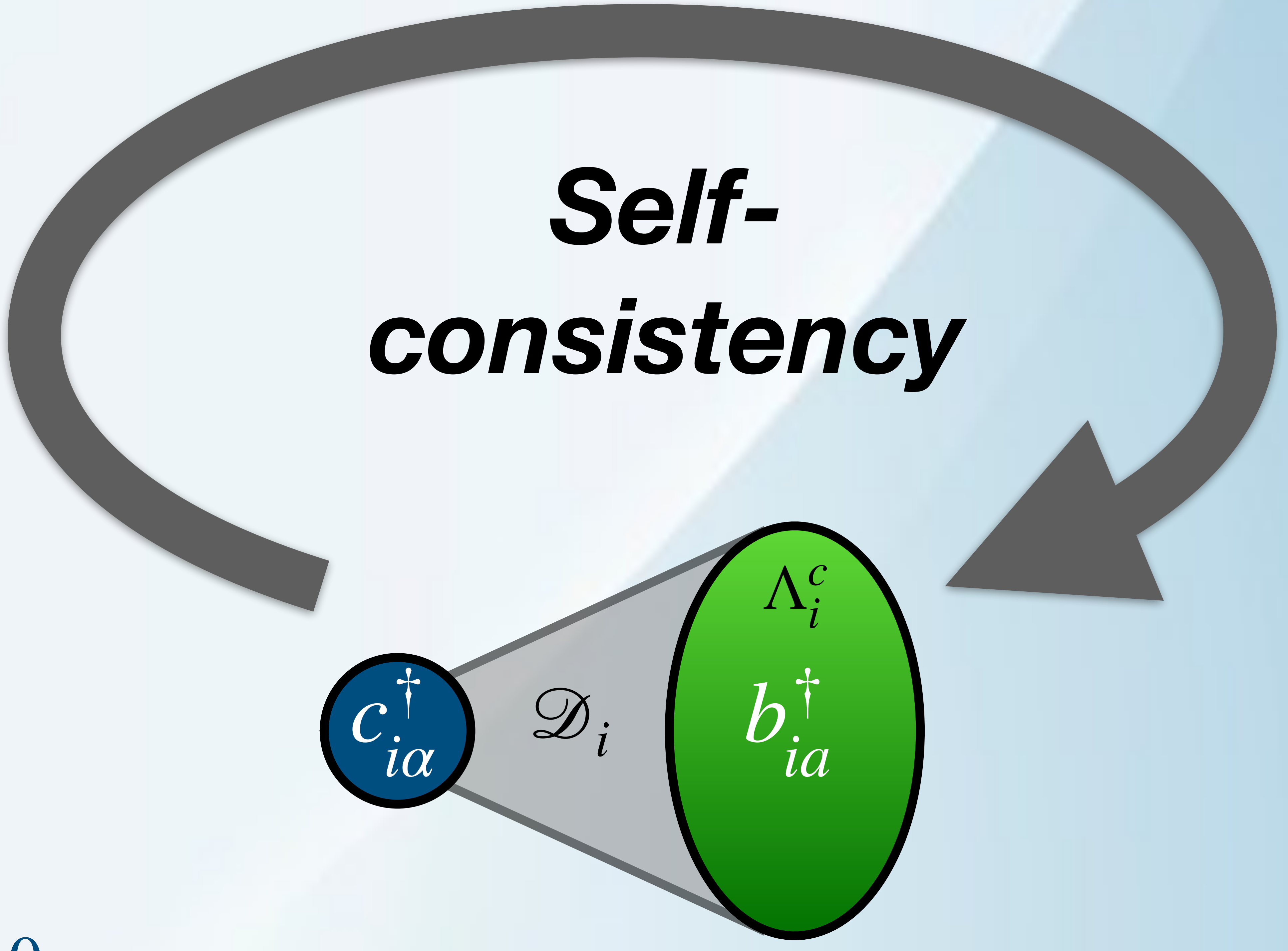


$$\mathscr{L} = \langle \Psi_0 | \hat{H}_{qp}[\mathscr{R}, \lambda] | \Psi_0 \rangle + E \left(1 - \langle \Psi_0 | \Psi_0 \rangle \right)$$
$$+ \sum_{i=1}^{\mathcal{N}} \left[\langle \Phi_i | \hat{H}_i^{emb}[\mathscr{D}_i, \lambda_i^c] | \Phi_i \rangle + E_i^c \left(\mathbf{1} - \langle \Phi_i | \Phi_i \rangle \right) \right]$$
$$- \sum_{i=1}^{\mathcal{N}} \left[\sum_{a,b=1}^{B\nu_i} \left([\lambda_i]_{ab} + [\lambda_i^c]_{ab} \right) [\Delta_i]_{ab} + \sum_{c,a=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \left([\mathscr{D}_i]_{a\alpha} [\mathscr{R}_i]_{c\alpha} [\Delta_i(\mathbf{1} - \Delta_i)]^{\frac{1}{2}}_{ca} + \text{c.c.} \right) \right]$$

$$\hat{H}_{qp}[\mathscr{R}, \Lambda] = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathscr{R}_i t_{ij} \mathscr{R}_j^\dagger \right]_{ab} f^\dagger_{ia} f_{jb} + \sum_{i=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} [\lambda_i]_{ab} f^\dagger_{ia} f_{ib}$$

$$\hat{H}^i_{emb}[\mathscr{D}_i, \Lambda_i^c] = \hat{H}^i_{loc} \left[c_{i\alpha}, c^\dagger_{i\alpha} \right] + \sum_{a=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \left([\mathscr{D}_i]_{a\alpha} c^\dagger_{i\alpha} b_{ia} + \text{H.c.} \right) + \sum_{a,b=1}^{B\nu_i} [\lambda_i^c]_{ab} b_{ib} b^\dagger_{ia}$$

Lagrange equations:



$$\left[\Pi_i f\left(\mathscr{R} t \mathscr{R}^{\dagger} + \lambda\right) \Pi_i\right]_{ba} = \left[\Delta_i\right]_{ab}$$

$$\left[\Pi_i t \mathscr{R}^{\dagger} f\left(\mathscr{R} t \mathscr{R}^{\dagger} + \lambda\right) \Pi_i\right]_{\alpha a} = \sum_{c=1}^{B\nu_i} \left[\mathscr{D}_i\right]_{c\alpha} \left[\Delta_i \left(1 - \Delta_i\right)\right]^{\frac{1}{2}}_{ac}$$

$$\sum_{c,b=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \frac{\partial}{\partial \left[d^0_i\right]_s} \left(\left[\Delta_i \left(1 - \Delta_i\right)\right]^{\frac{1}{2}}_{cb} \left[\mathscr{D}_i\right]_{b\alpha} \left[\mathscr{R}_i\right]_{c\alpha} + \mathrm{c.c.} \right) + \left[l_i + l^c_i\right]_s = 0$$

$$\hat{H}^i_{emb}[\mathscr{D}_i, \lambda^c_i] \, |\Phi_i\rangle = E^c_i \, |\Phi_i\rangle \quad \longrightarrow \quad |\Phi_i\rangle$$

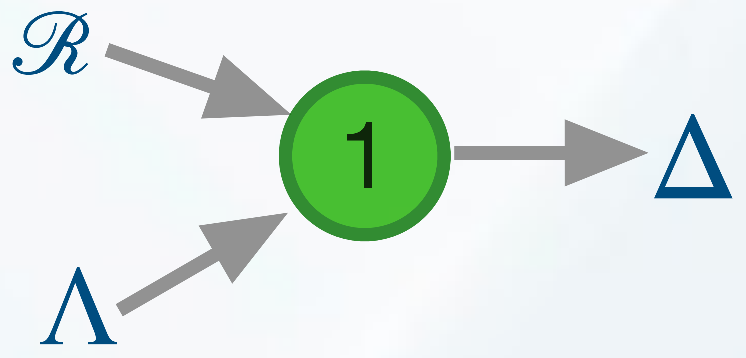
$$\langle \Phi_i | c^{\dagger}_{i\alpha} b_{ia} | \Phi_i \rangle - \sum_{c=1}^{B\nu_i} \left[\Delta_i \left(1 - \Delta_i\right)\right]^{\frac{1}{2}}_{ca} \left[\mathscr{R}_i\right]_{c\alpha} = 0$$

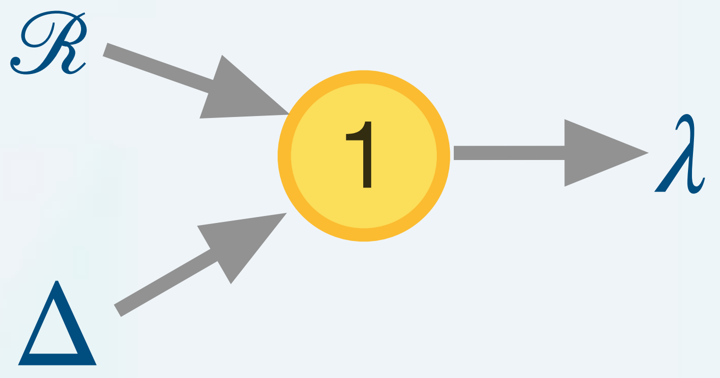
$$\langle \Phi_i | b_{ib} b^{\dagger}_{ia} | \Phi_i \rangle - \left[\Delta_i\right]_{ab} = 0$$

$$\begin{cases} \Delta_i = \sum_{s=1}^{(B\nu_i)^2} \left[d^0_i\right]_s \left[h^T_i\right]_s \\ \lambda_i = \sum_{s=1}^{(B\nu_i)^2} \left[l_i\right]_s \left[h_i\right]_s \\ \lambda^c_i = \sum_{s=1}^{(B\nu_i)^2} \left[l^c_i\right]_s \left[h_i\right]_s \end{cases}$$

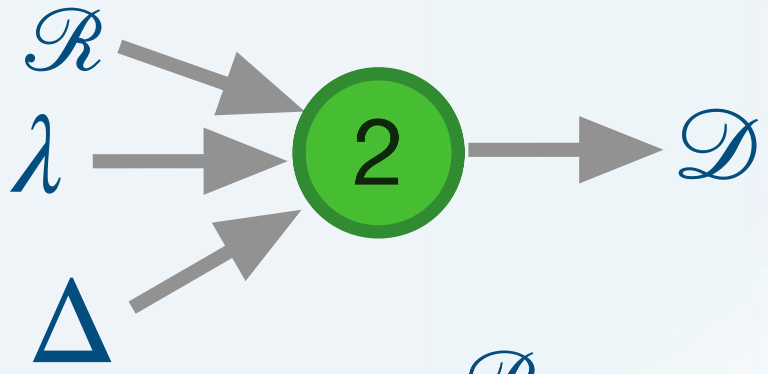
Lagrange equations:

$$\left[\Pi_i f\left(\mathcal{R} t \mathcal{R}^\dagger + \lambda\right)\Pi_i\right]_{ba} = \left[\Delta_i\right]_{ab}$$

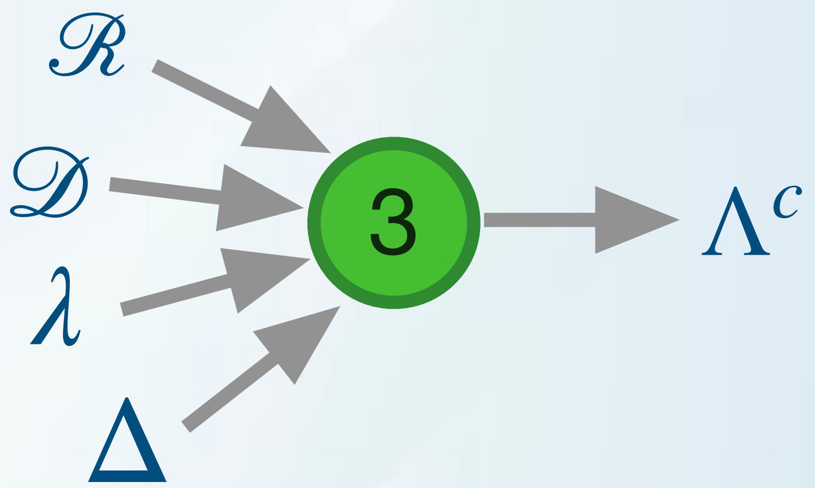


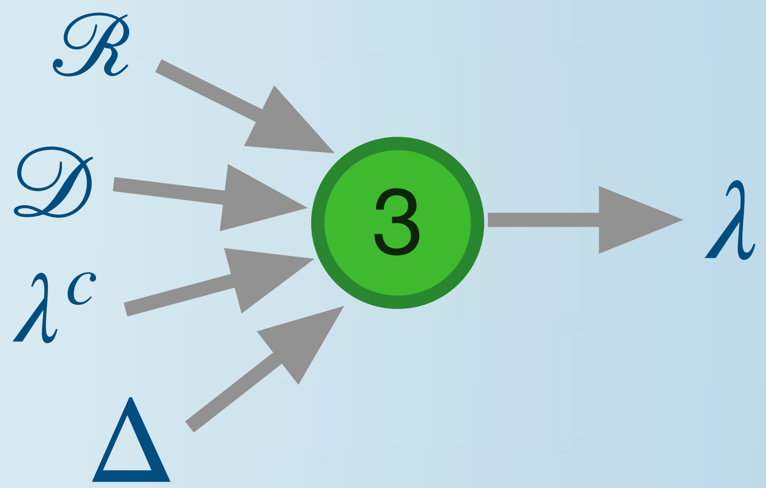


$$\left[\Pi_i t\mathcal{R}^\dagger f\left(\mathcal{R}t\mathcal{R}^\dagger+\lambda\right)\Pi_i\right]_{\alpha a} = \sum_{c=1}^{B\nu_i} \left[\mathcal{D}_i\right]_{c\alpha}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}_{ac}$$



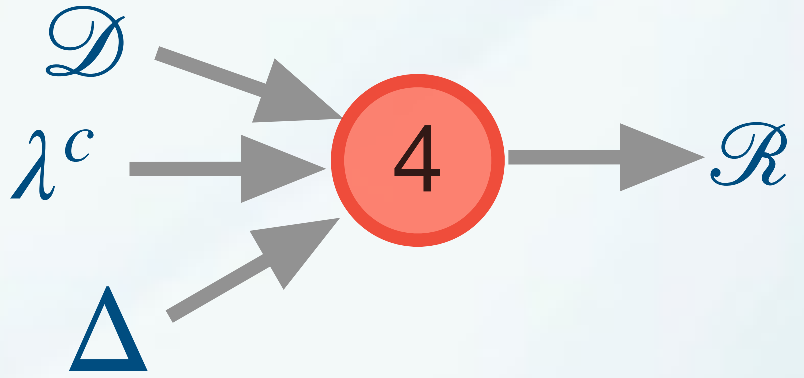
$$\sum_{c,b=1}^{B\nu_i}\sum_{\alpha=1}^{\nu_i}\frac{\partial}{\partial \left[d_i^0\right]_s}\left(\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}_{cb}\left[\mathcal{D}_i\right]_{b\alpha}\left[\mathcal{R}_i\right]_{c\alpha} + \text{c.c.}\right) + \left[l_i + l_i^c\right]_s = 0$$



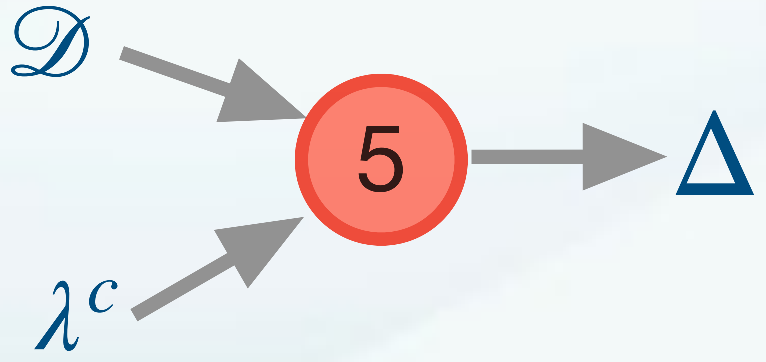


$$\hat{H}^i_{emb}\left[\mathcal{D}_i,\lambda_i^c\right]|\Phi_i\rangle = E_i^c|\Phi_i\rangle \longrightarrow |\Phi_i\rangle$$

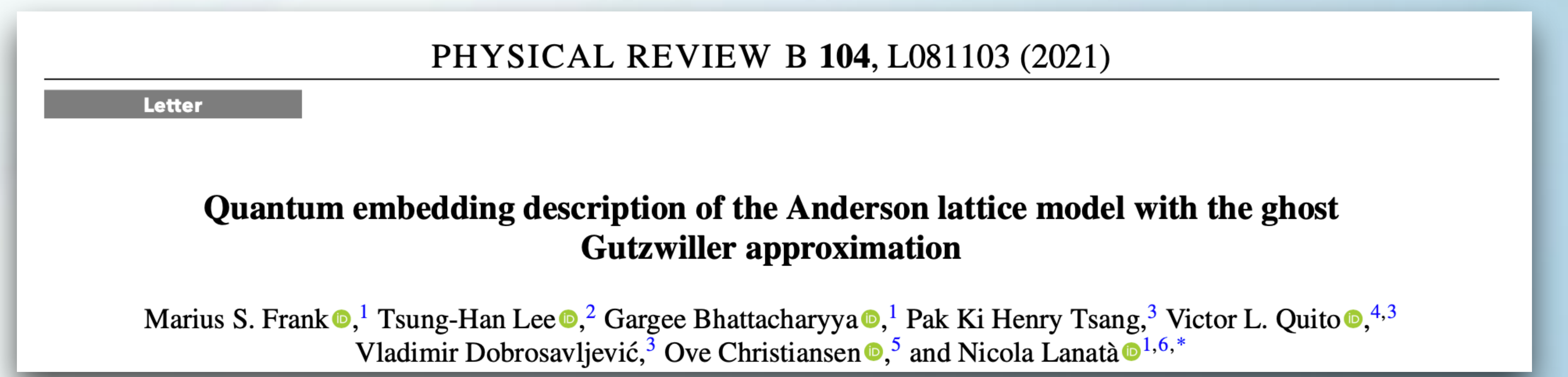
$$\langle\Phi_i|c^\dagger_{i\alpha}b_{ia}|\Phi_i\rangle - \sum_{c=1}^{B\nu_i}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}_{ca}\left[\mathcal{R}_i\right]_{c\alpha}=0$$



$$\langle\Phi_i|b_{ib}b^\dagger_{ia}|\Phi_i\rangle - \left[\Delta_i\right]_{ab}=0$$



Lagrange equations:



PHYSICAL REVIEW B **104**, L081103 (2021)

Letter

Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation

Marius S. Frank,[1] Tsung-Han Lee,[2] Gargee Bhattacharyya,[1] Pak Ki Henry Tsang,[3] Victor L. Quito,[4,3] Vladimir Dobrosavljević,[3] Ove Christiansen,[5] and Nicola Lanatà[1,6,*]

Lagrange equations:

PHYSICAL REVIEW B **96**, 235139 (2017)

Dynamical mean-field theory, density-matrix embedding theory, and rotationally invariant slave bosons: A unified perspective

Thomas Ayral,[1] Tsung-Han Lee,[1] and Gabriel Kotliar[1,2]

<u>Summary</u>: Connection between different theoretical frameworks (gGA, DMFT, RISB, DMET)

$$\langle \Psi_G | \hat{H} | \Psi_G \rangle = \langle \Psi_0 | \hat{\mathscr{P}}_G^\dagger \hat{H} \hat{\mathscr{P}}_G | \Psi_0 \rangle$$

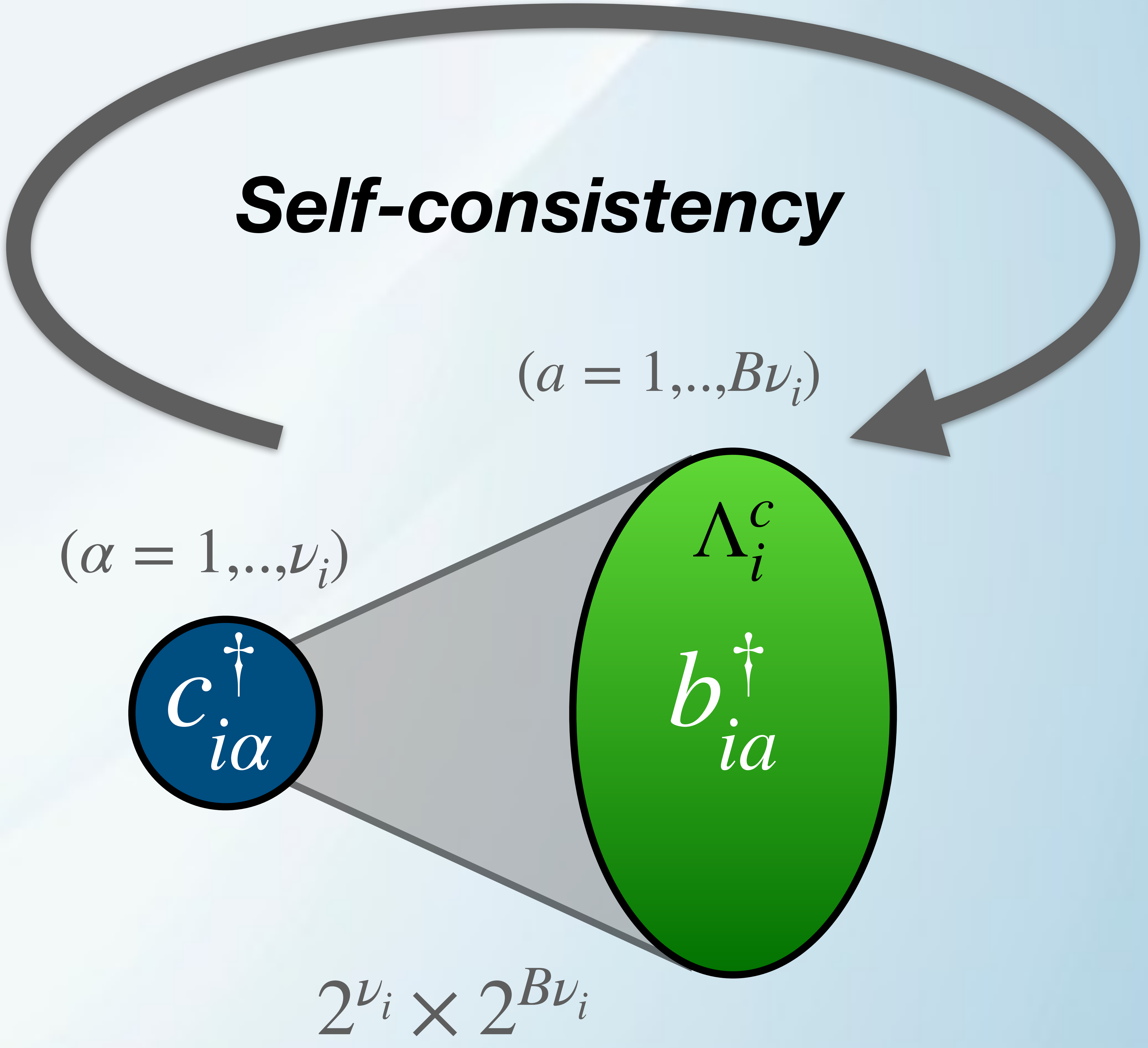
gGA (variational)

$$[\Lambda_i]_{\Gamma n} \rightarrow [\phi_i]_{\Gamma n} \rightarrow |\Phi_i\rangle$$

$d \rightarrow \infty$ (DMFT)

(gRISB)

Quantum Embedding (gDMET)



Outline

A. Background notions in many-body theory (board)

B. The GA/gGA wave function: Introduction

C. Derivation gGA method: QE formulation

D. Applications, recent developments and open problems

Supplementary topics:

- Spectral properties

- Time-dependent extension

- DFT+gGA

Applications, recent developments and open problems

1. Single-band Hubbard model

2. Single-band Anderson Lattice model

3. Three-band Hubbard model

4. Real materials: DFT+gGA (NiO)

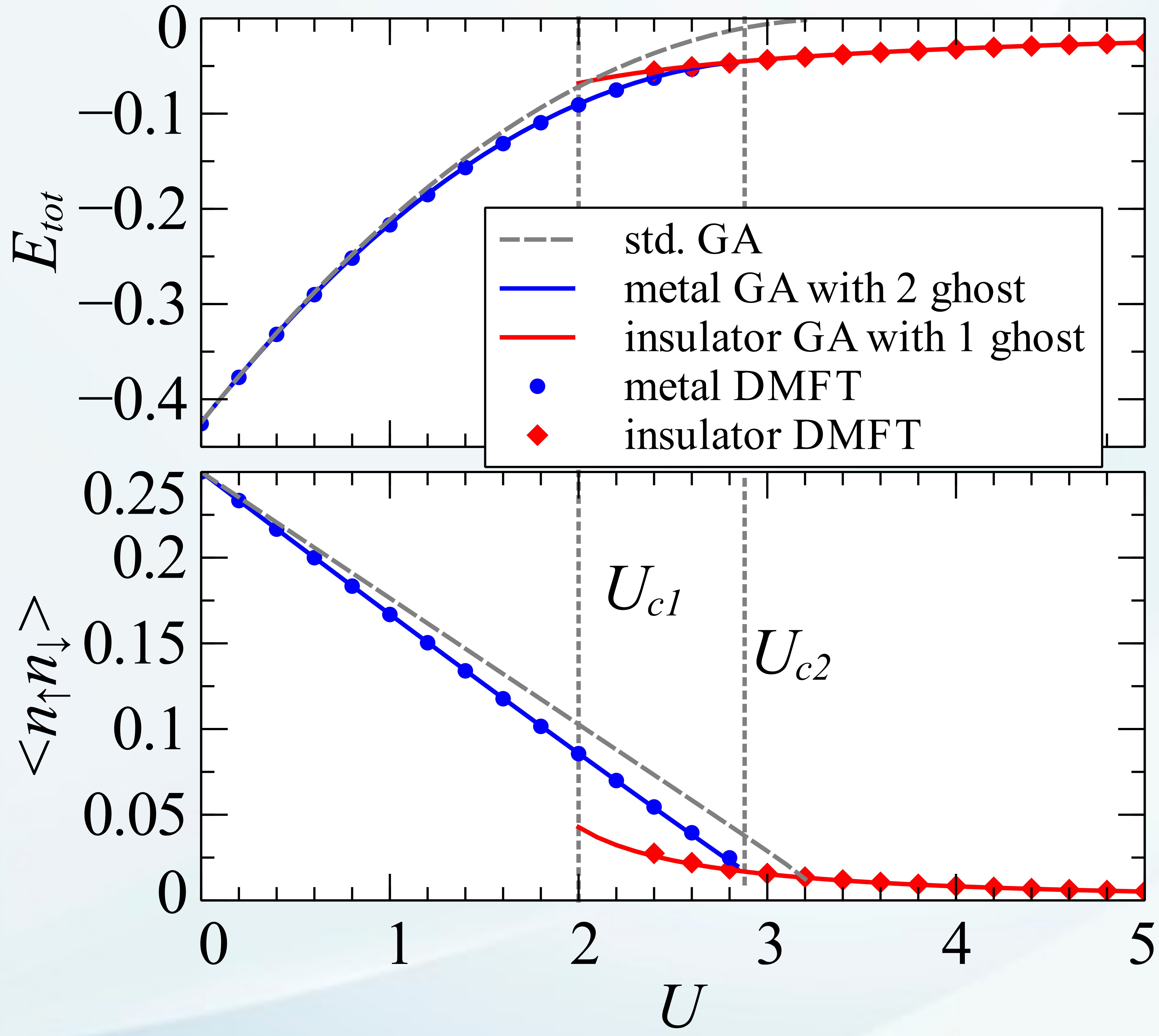
5. Extensions and future applications

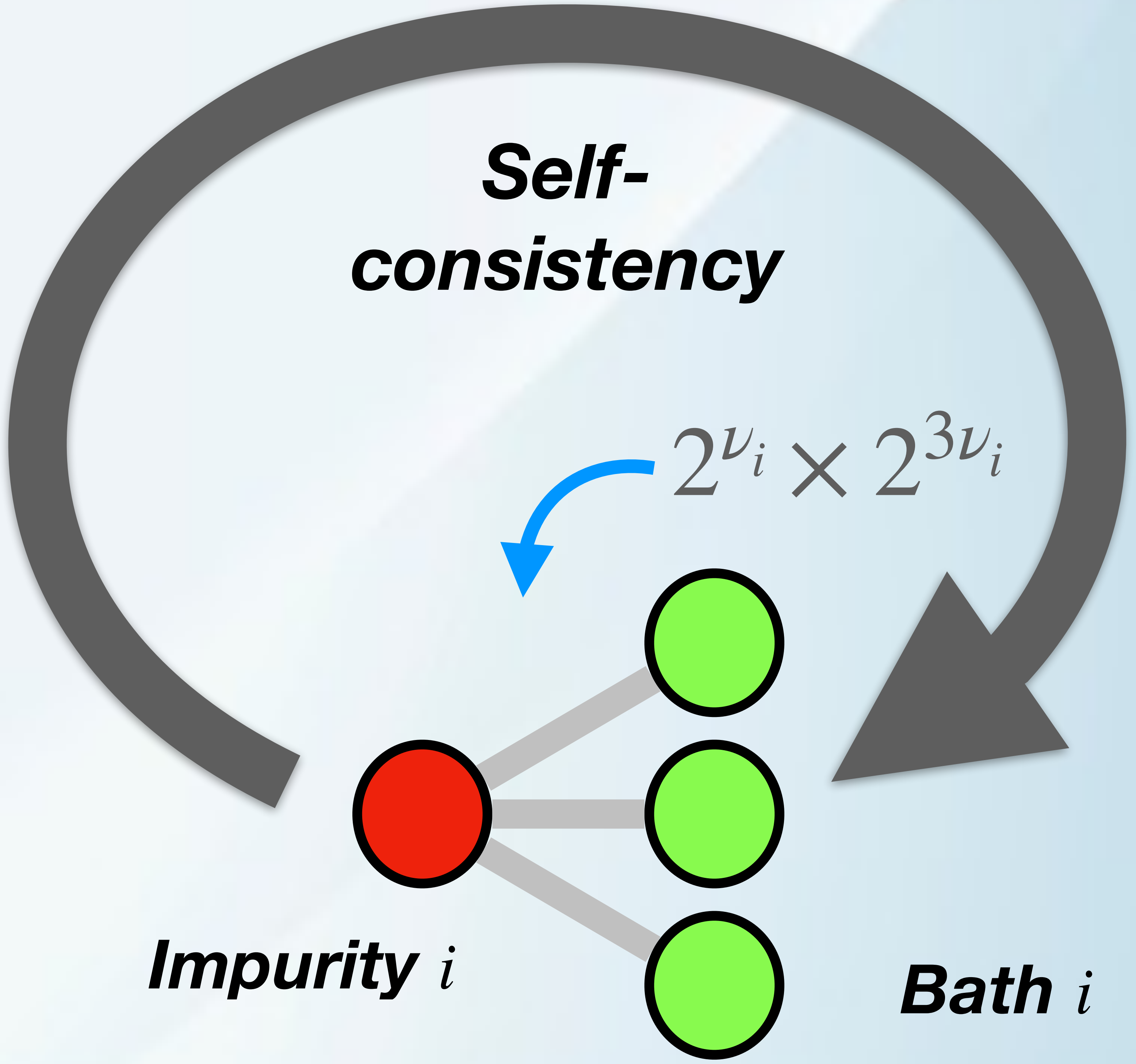
1-Band Hubbard model:

PHYSICAL REVIEW B **96**, 195126 (2017)

Emergent Bloch excitations in Mott matter

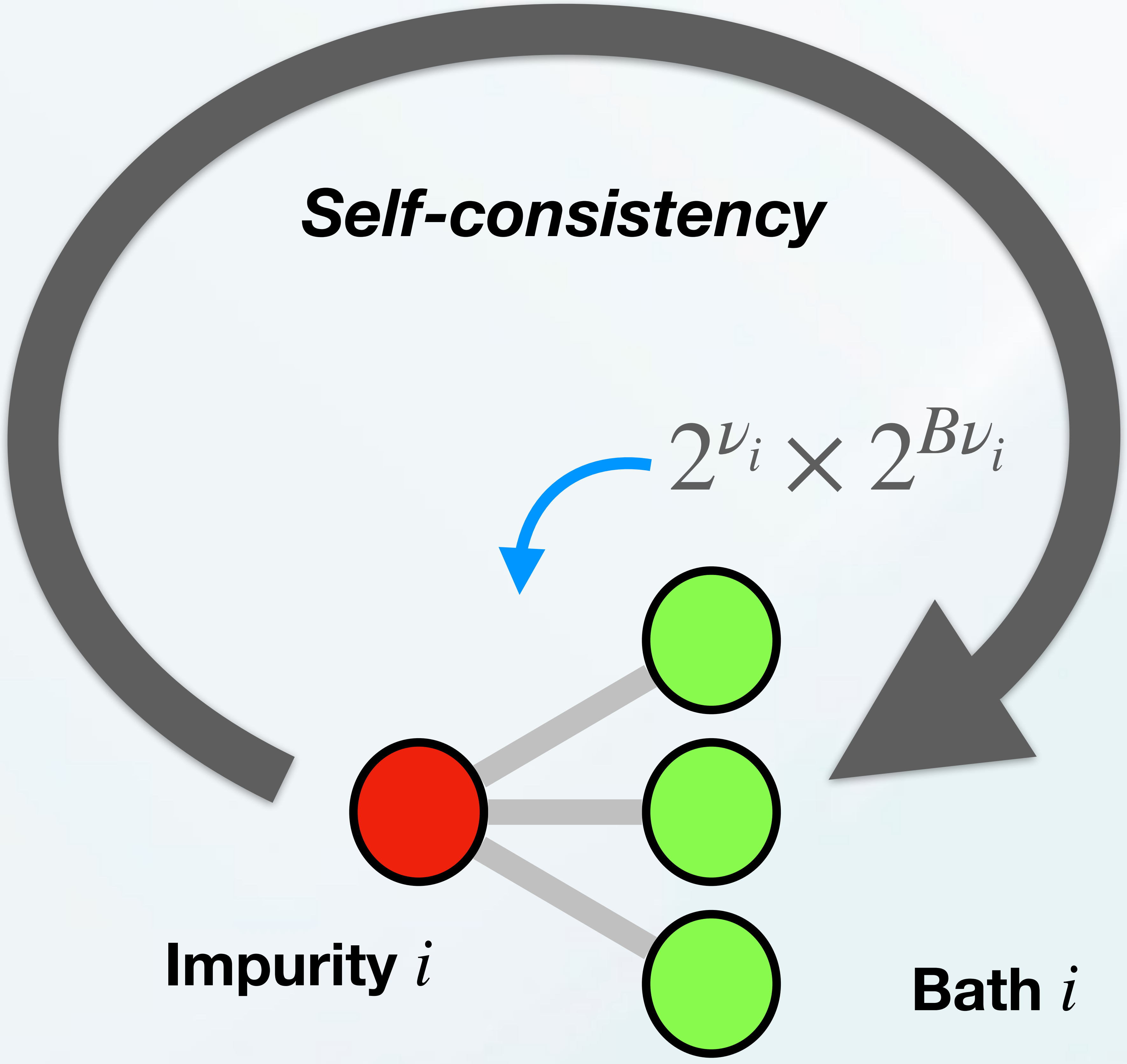
Nicola Lanatà,[1] Tsung-Han Lee,[1] Yong-Xin Yao,[2] and Vladimir Dobrosavljević[1]





$$\hat{H} = \sum_{RR'} \sum_{\sigma} t_{RR'} \, c^\dagger_{R\sigma} c_{R'\sigma} + \sum_{R\sigma} U \, \hat{n}_{R\uparrow} \hat{n}_{R\downarrow}$$

1-Band Hubbard model:

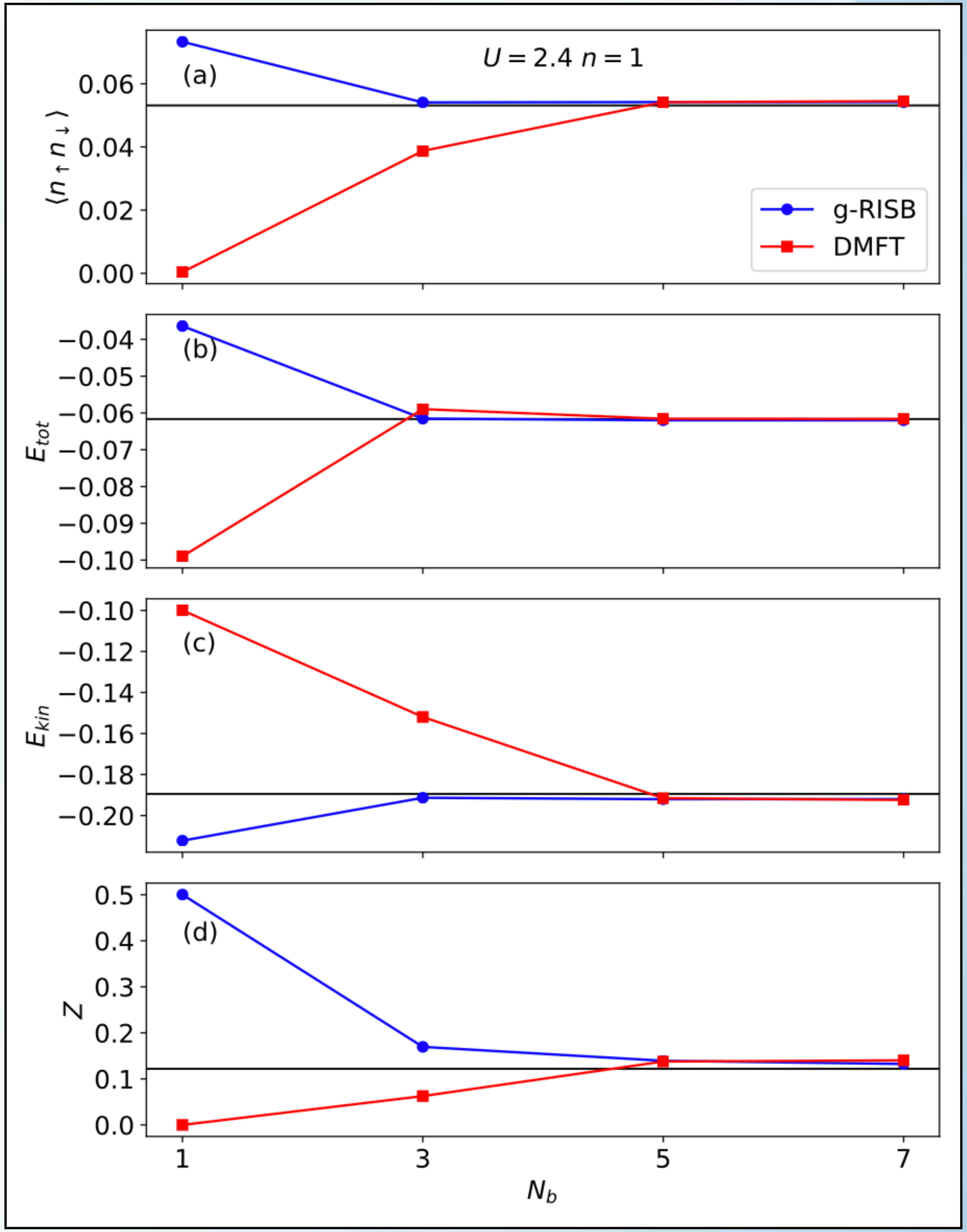


PHYSICAL REVIEW B **107**, L121104 (2023)

Letter

Accuracy of ghost rotationally invariant slave-boson and dynamical mean field theory as a function of the impurity-model bath size

Tsung-Han Lee[1,*] Nicola Lanatà[2] and Gabriel Kotliar[1,3]



1-Band Hubbard model:

PHYSICAL REVIEW B **107**, L121104 (2023)

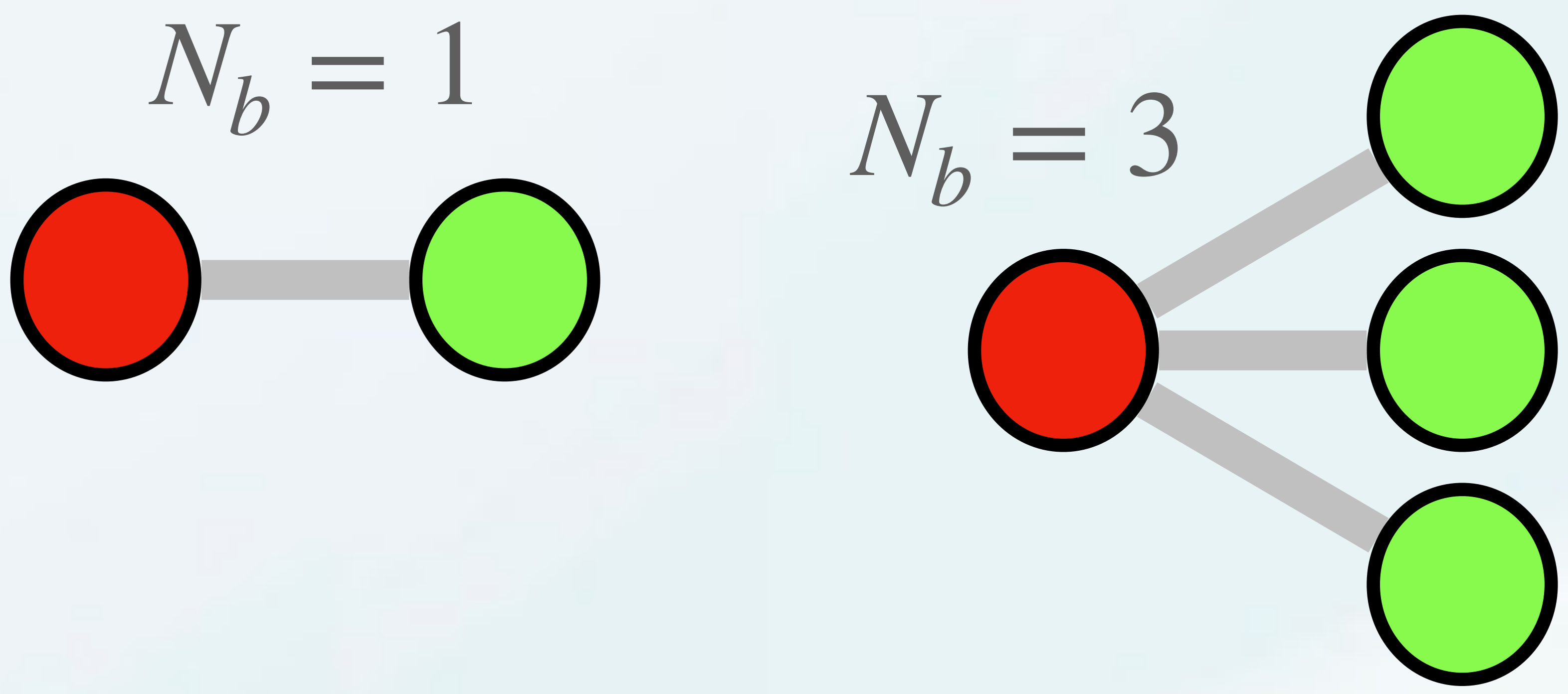
Letter

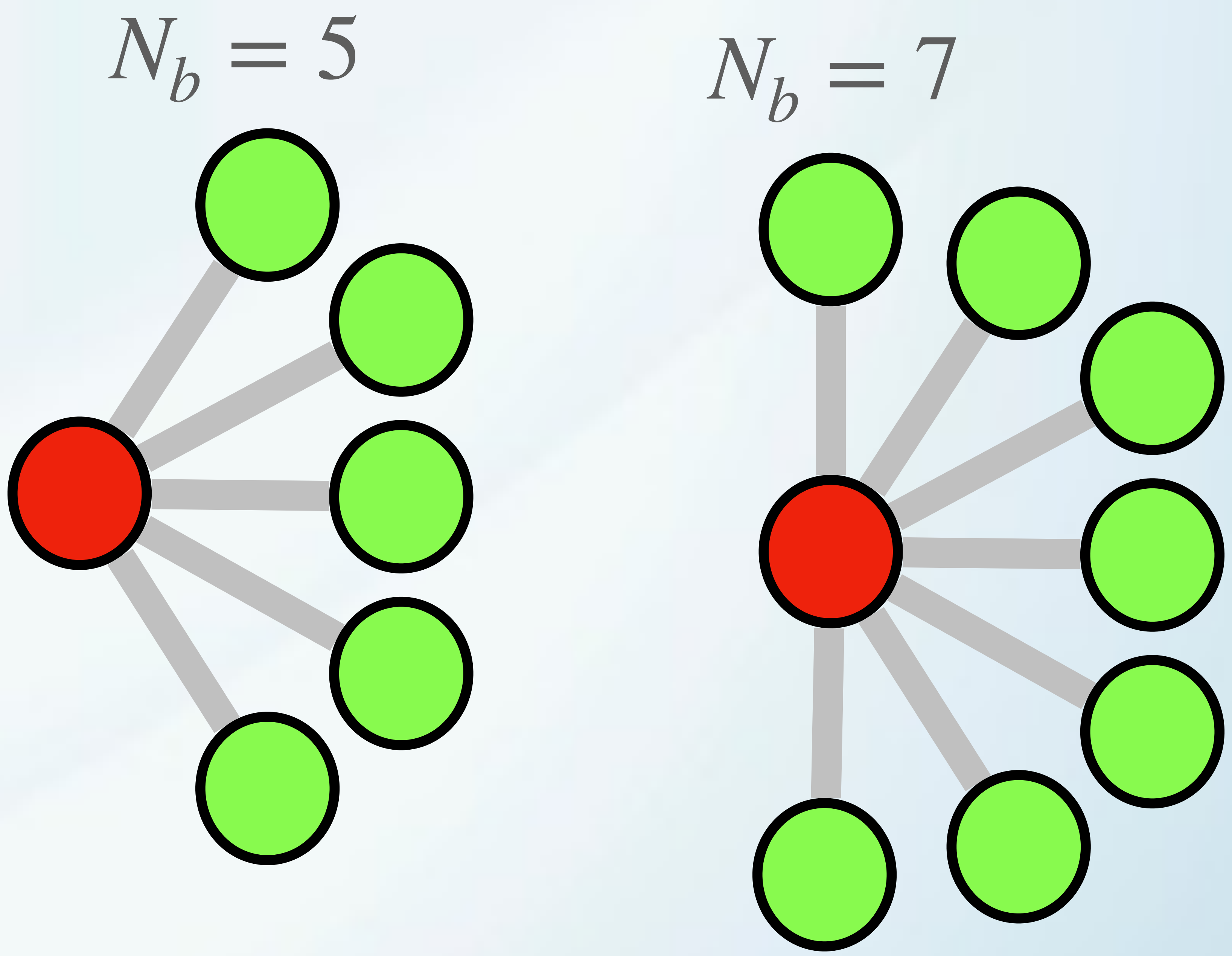
Accuracy of ghost rotationally invariant slave-boson and dynamical mean field theory as a function of the impurity-model bath size

Tsung-Han Lee[1,*] Nicola Lanatà[2] and Gabriel Kotliar[1,3]

TABLE I. The g-RISB total energy at $U = 2.4$ and filling $n = 1$ and $n = 0.75$ with different numbers of bath orbitals N_b. The DMFT energy at $\beta = 200$ with the CTQMC solver is shown for comparison.

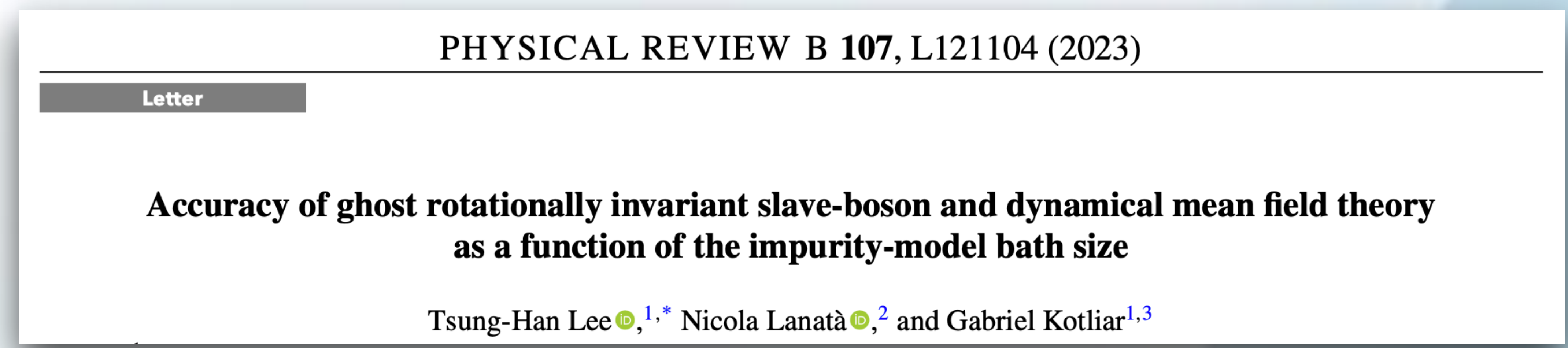
n	$N_b = 1$	$N_b = 3$	$N_b = 5$	$N_b = 7$	CTQMC
1	−0.03637	−0.06155	−0.06189	−0.06199	-0.0621 ± 0.0001
0.75	−0.21829	−0.23158	−0.23189	−0.23190	-0.2319 ± 0.0001





***Variational*: Energy decreases as we increase N_b**

1-Band Hubbard model:


PHYSICAL REVIEW B 107, L121104 (2023)

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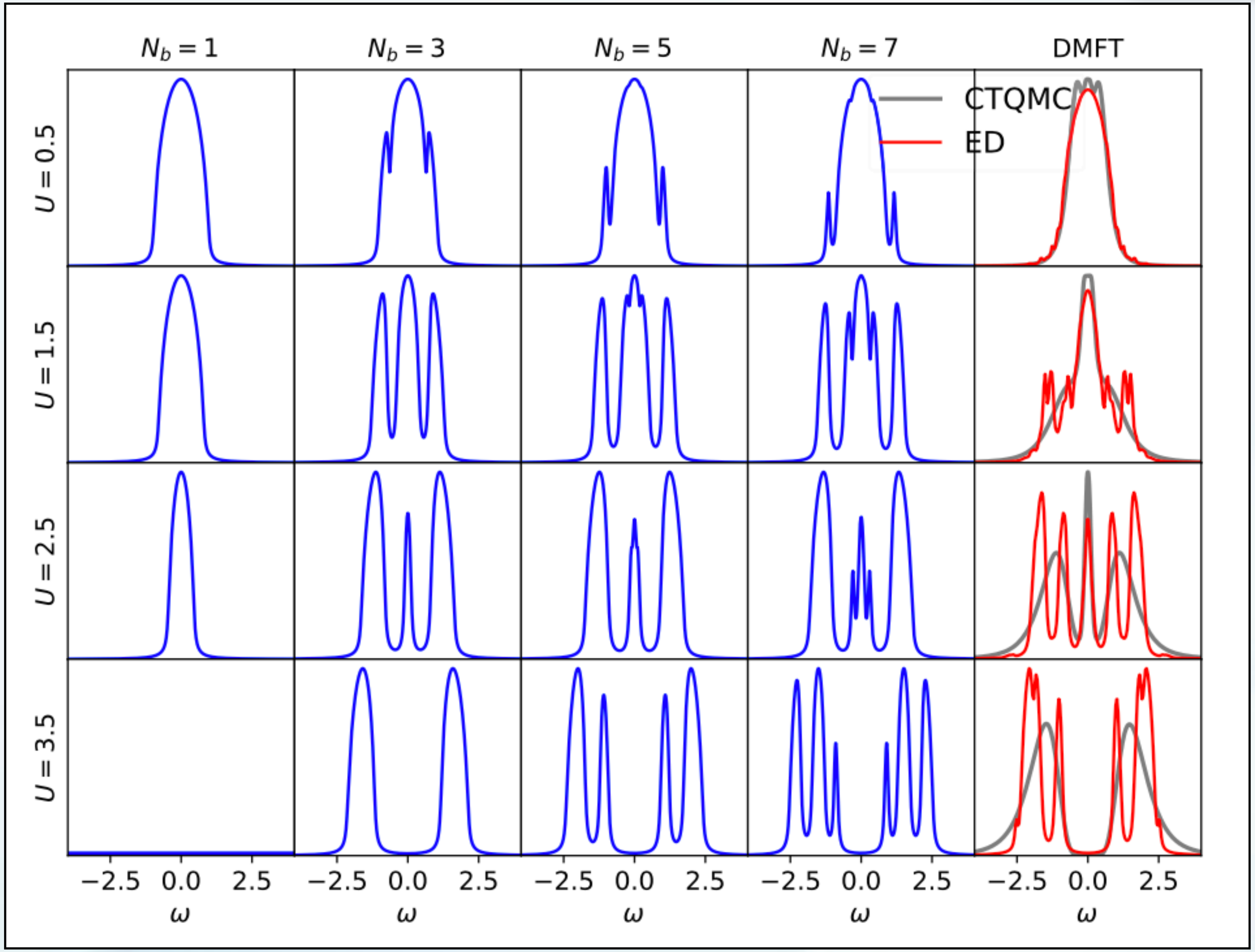
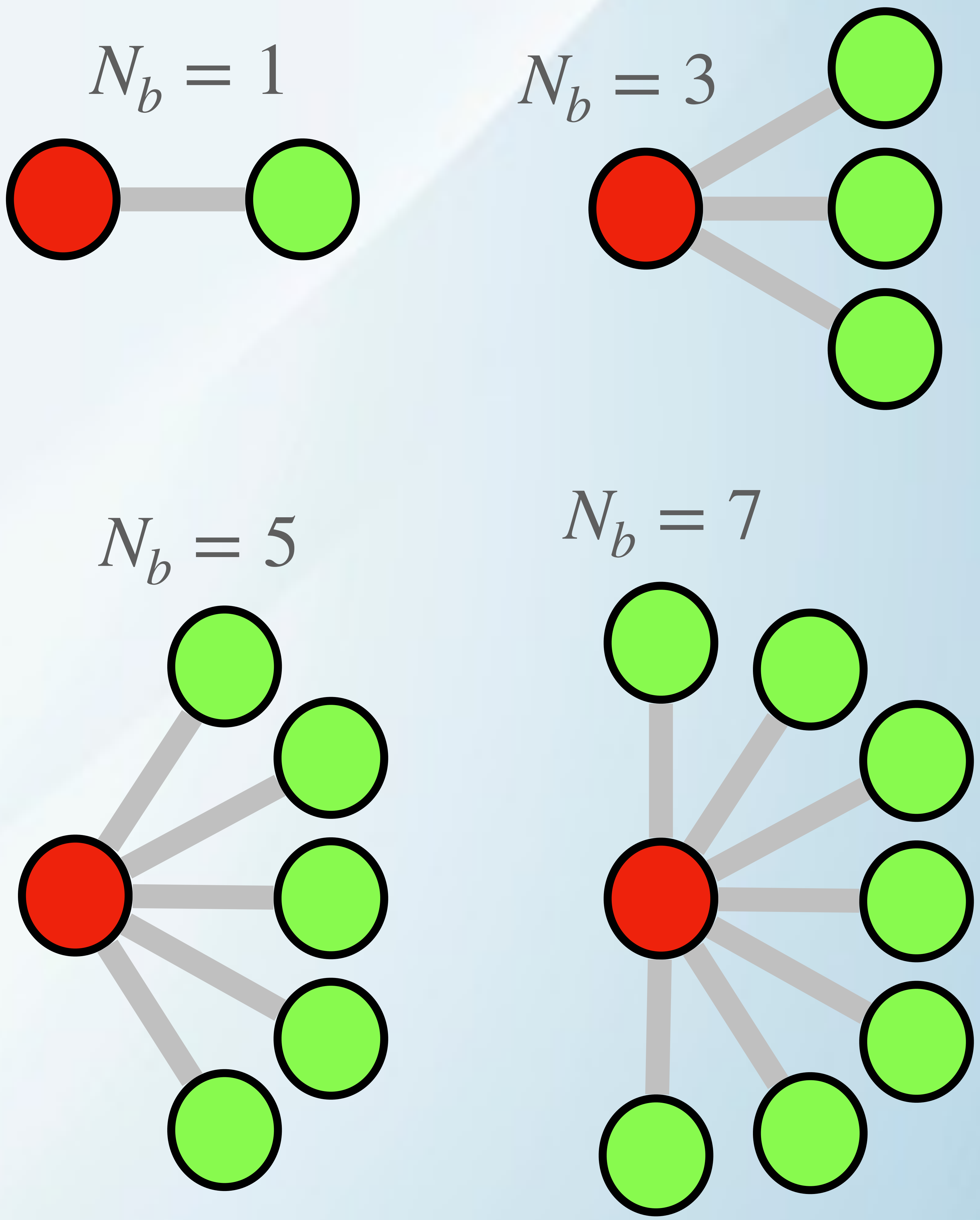
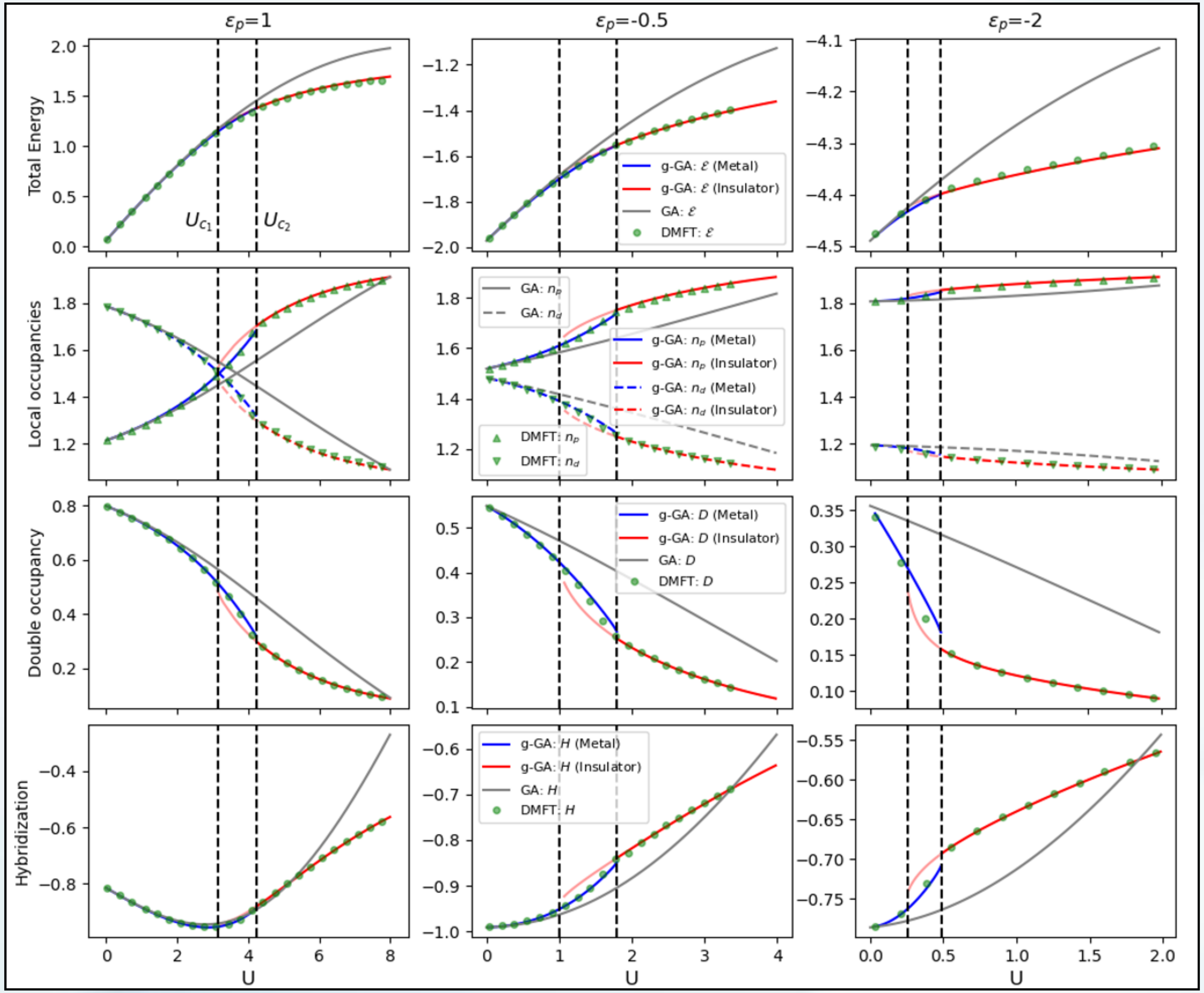
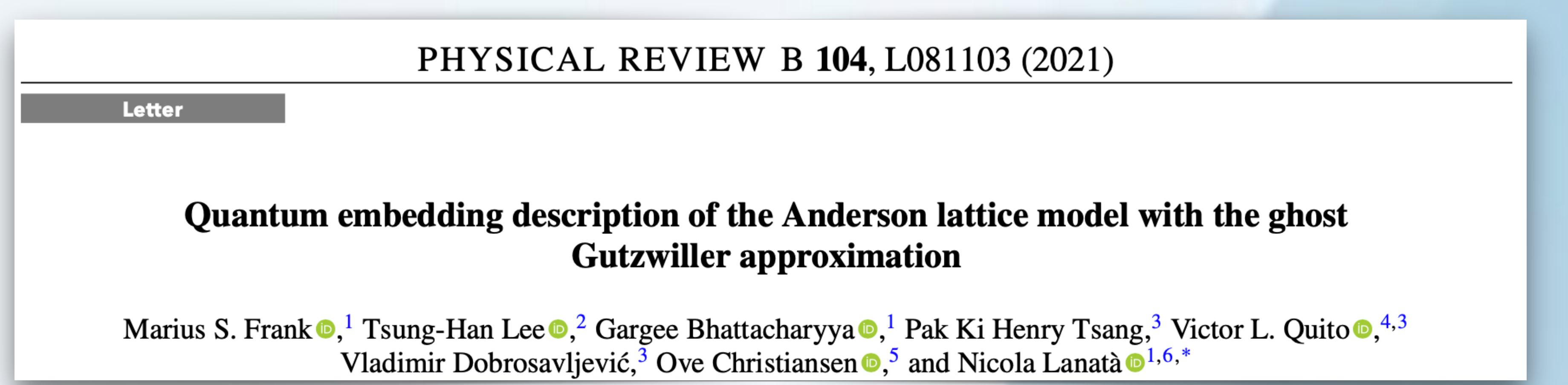
Tsung-Han Lee[1,*] Nicola Lanatà[2] and Gabriel Kotliar[1,3]





1-Band Anderson Lattice Model




PHYSICAL REVIEW B **104**, L081103 (2021)

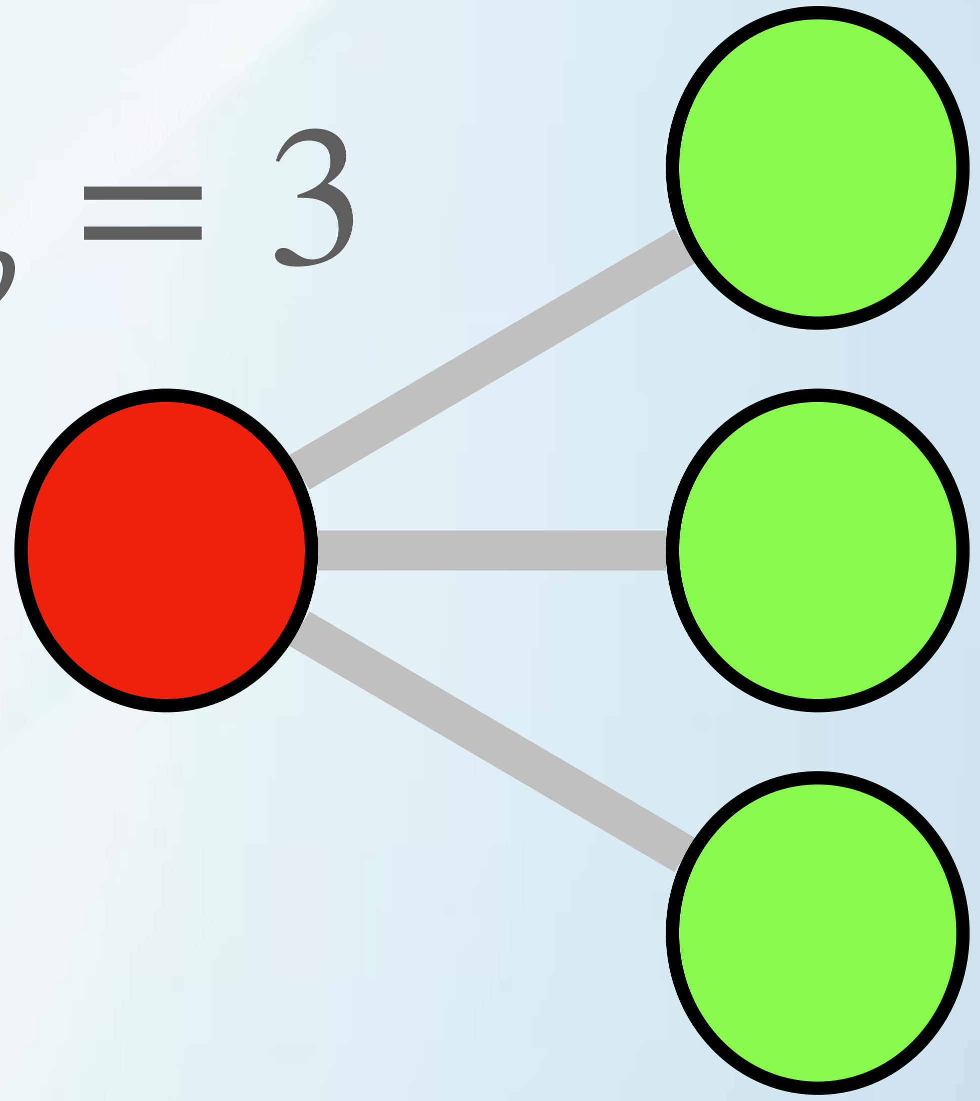
Letter

Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation

Marius S. Frank,[1] Tsung-Han Lee,[2] Gargee Bhattacharyya,[1] Pak Ki Henry Tsang,[3] Victor L. Quito,[4,3] Vladimir Dobrosavljević,[3] Ove Christiansen,[5] and Nicola Lanatà[1,6,*]

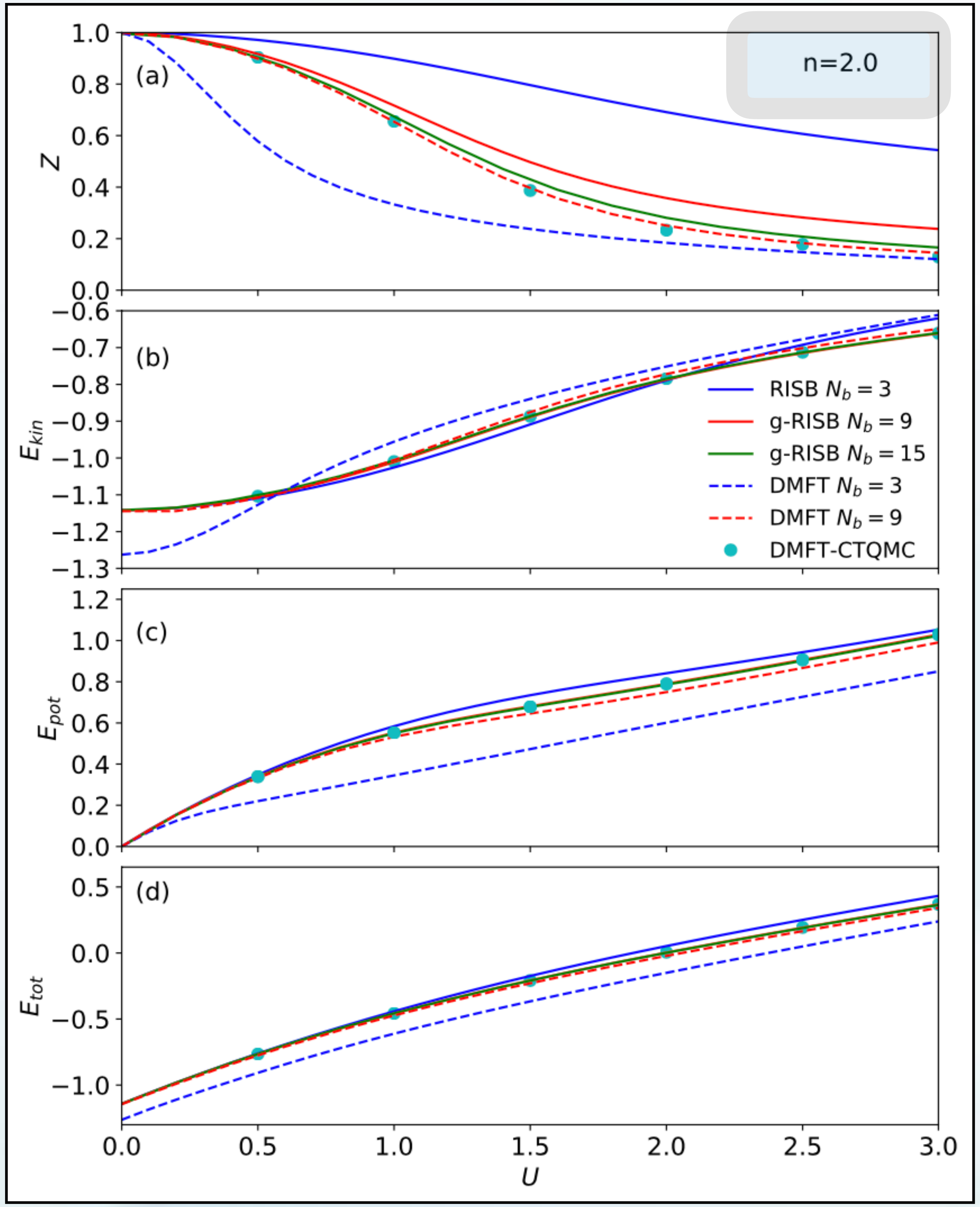
$$\hat{H} = \sum_{ij}\sum_{\sigma}(t_{ij} + \delta_{ij}\epsilon_p)\, p^\dagger_{i\sigma} p_{j\sigma} + \sum_i \frac{U}{2}(\hat{n}_{di} - 1)^2 + V\sum_{i\sigma}\left(p^\dagger_{i\sigma} d_{i\sigma} + \text{H.c.}\right) - \mu \sum_i \hat{N}_i$$

$N_b = 3$



Ghost extension *necessary* to capture interplay between Mott physics and hybridization between correlated and itinerant degrees of freedom

3-Band Hubbard model:



PHYSICAL REVIEW B **108**, 245147 (2023)

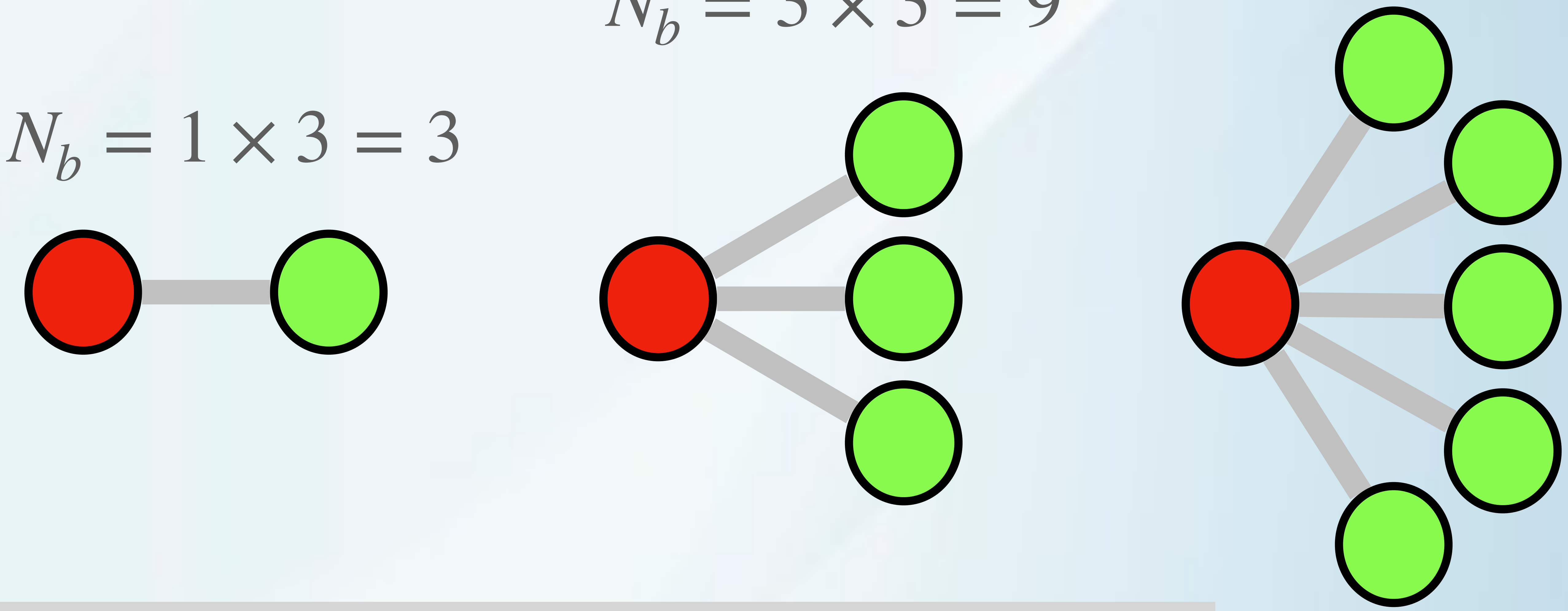
Accuracy of ghost-rotationally-invariant slave-boson theory for multiorbital Hubbard models and realistic materials

Tsung-Han Lee,[1,2,*] Corey Melnick,[3] Ran Adler,[1] Nicola Lanatà,[4,5] and Gabriel Kotliar[1,3]

$N_b = 3 \times 5 = 15$

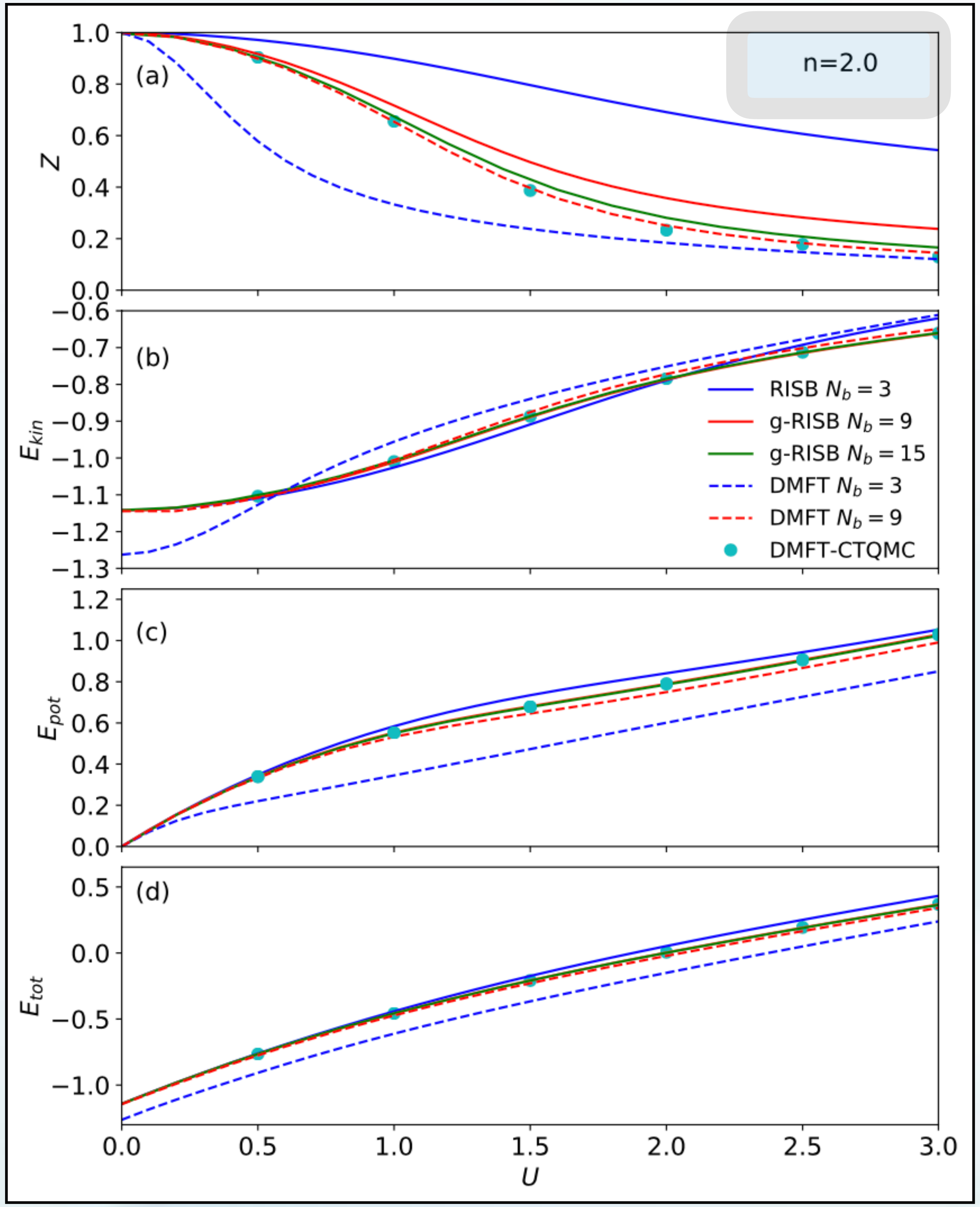
$N_b = 3 \times 3 = 9$

$N_b = 1 \times 3 = 3$



$$H^{\text{int}}_{\mathbf{R}}[\{c^\dagger_{\mathbf{R}l\sigma}, c_{\mathbf{R}l\sigma}\}] = U \sum_l n_{\mathbf{R}l\uparrow} n_{\mathbf{R}l\downarrow} + U' \sum_{l<l',\sigma} n_{\mathbf{R}l\sigma} n_{\mathbf{R}l'\bar{\sigma}} + (U' - J) \sum_{l<l',\sigma} n_{\mathbf{R}l\sigma} n_{\mathbf{R}l'\sigma} - J \sum_{l<l'} (c^\dagger_{\mathbf{R}l\uparrow} c_{\mathbf{R}l\downarrow} c^\dagger_{\mathbf{R}l'\downarrow} c_{\mathbf{R}l'\uparrow} + c^\dagger_{\mathbf{R}l\uparrow} c^\dagger_{\mathbf{R}l\downarrow} c_{\mathbf{R}l'\uparrow} c_{\mathbf{R}l'\downarrow} + \text{H.c.}).$$

3-Band Hubbard model:



PHYSICAL REVIEW B **108**, 245147 (2023)

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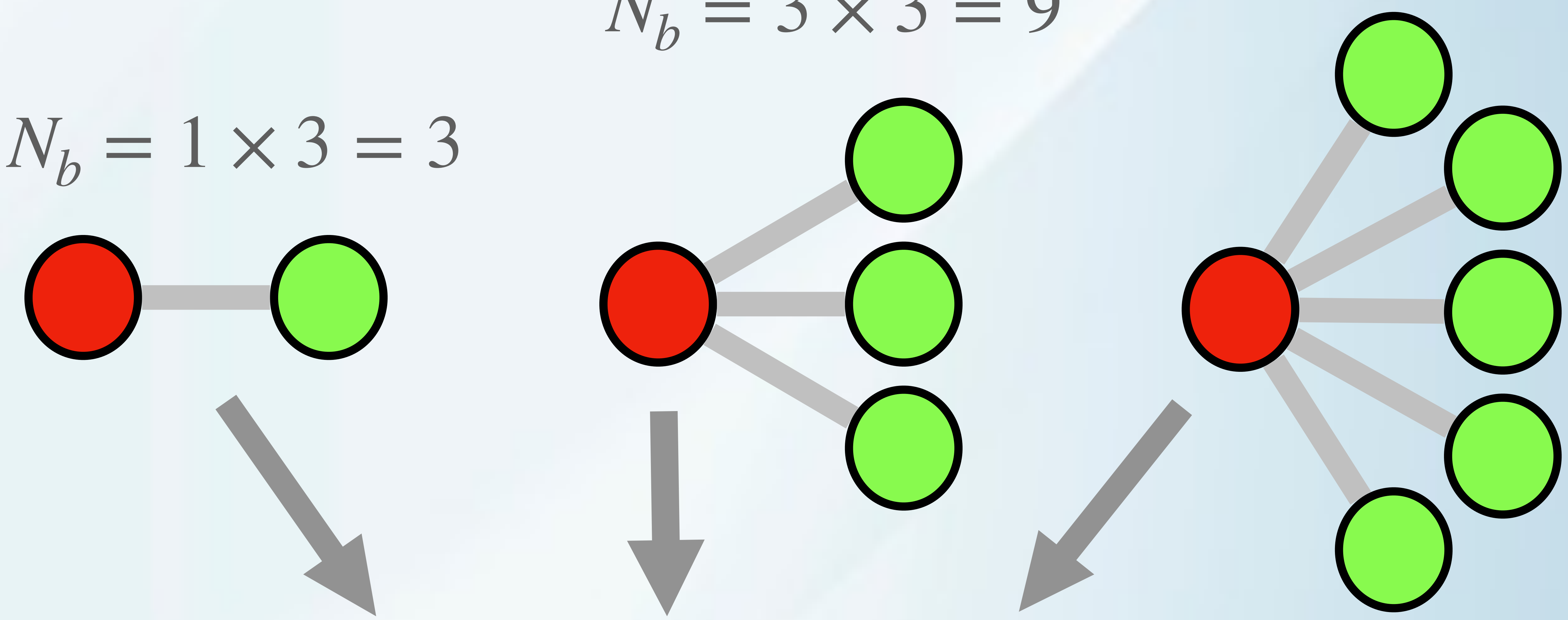
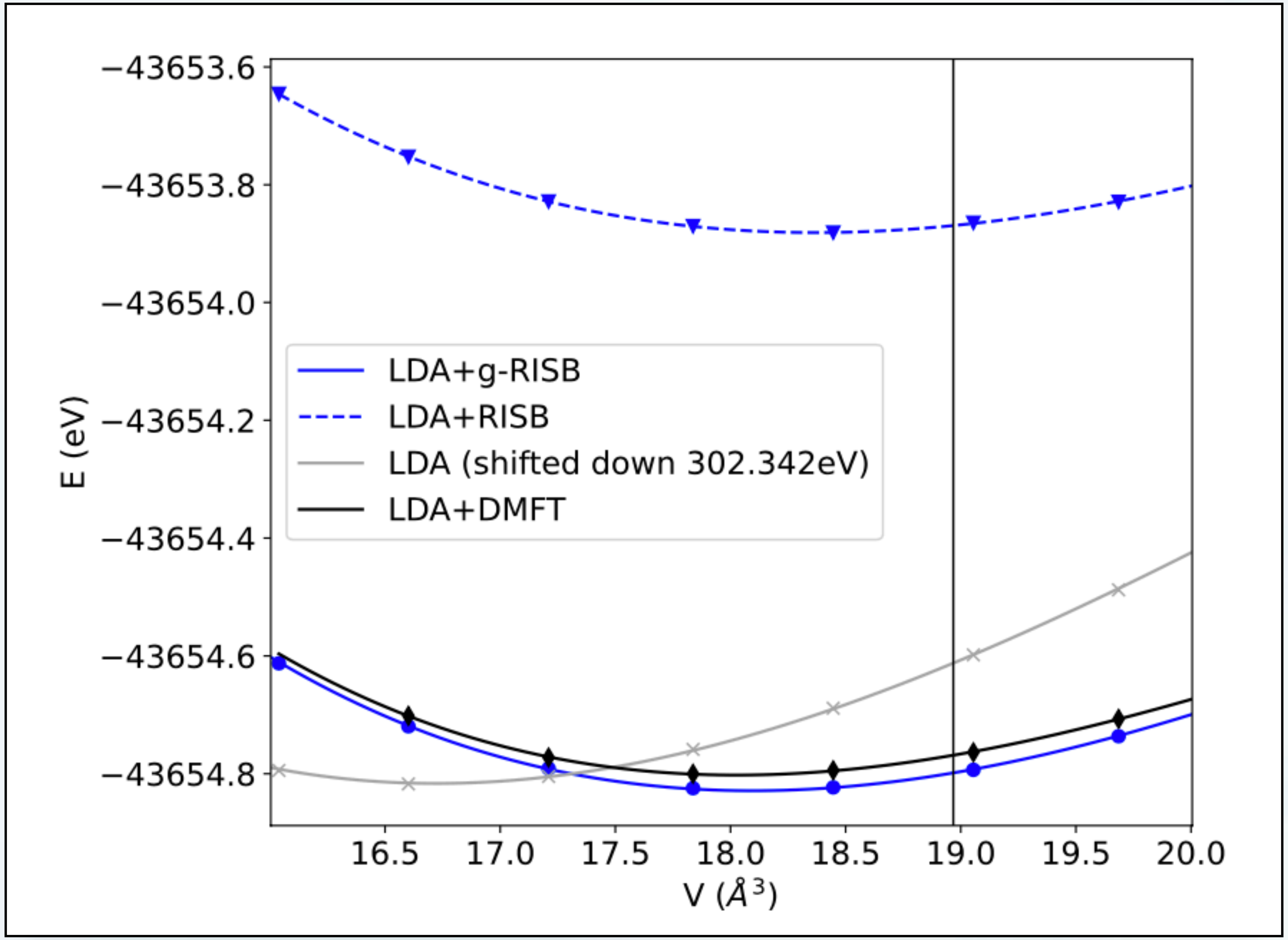
Tsung-Han Lee,[1,2,*] Corey Melnick,[3] Ran Adler,[1] Nicola Lanatà,[4,5] and Gabriel Kotliar[1,3]



Total energy

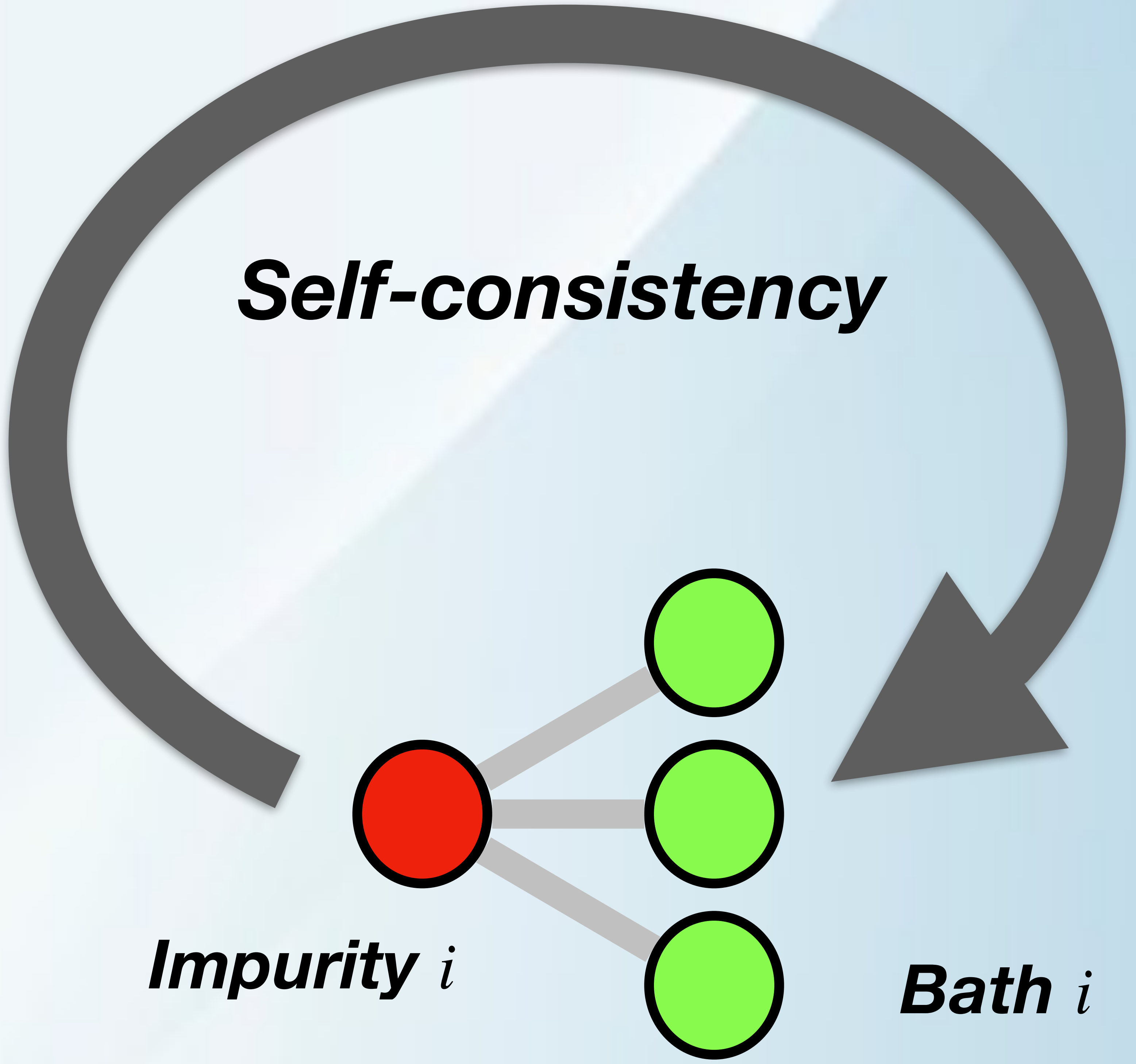
n	U	$N_b = 3$	$N_b = 9$	$N_b = 15$	DMFT-CTQMC
3.0	1.0	0.412	0.389	0.388	0.389
3.0	2.5	1.875	1.774	1.773	1.772
2.0	1.5	-0.174	-0.208	-0.209	-0.208
2.0	2.5	0.2506	0.192	0.189	0.193

Benchmark calculations NiO (DFT+gGA):



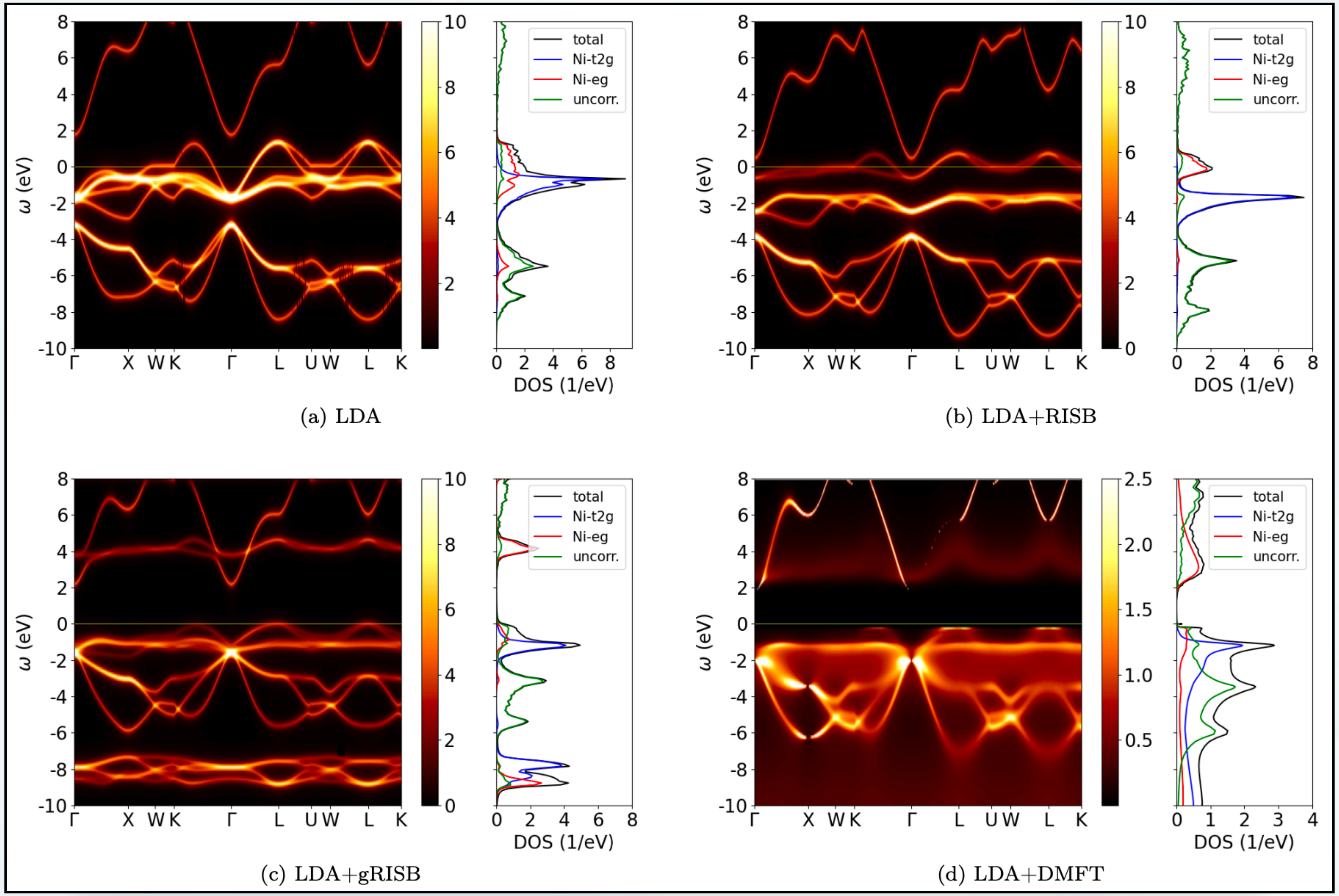
Charge self-consistent density functional theory plus ghost rotationally-invariant slave-boson theory for correlated materials

Tsung-Han Lee[1,2], Corey Melnick[3], Ran Adler[1], Xue Sun[1], Yongxin Yao[4], Nicola Lanatà[5,6], Gabriel Kotliar[1,3]



- - DFT+gGA written by Tsung-Han Lee, built on ComRISB DFT+GA code by Yongxin Yao et. al
- - DFT+DMFT (CTQMC) generated using Kristjan Haule's code https://www.physics.rutgers.edu/~haule/

Benchmark calculations NiO (DFT+gGA):



(a) LDA
(b) LDA+RISB
(c) LDA+gRISB
(d) LDA+DMFT

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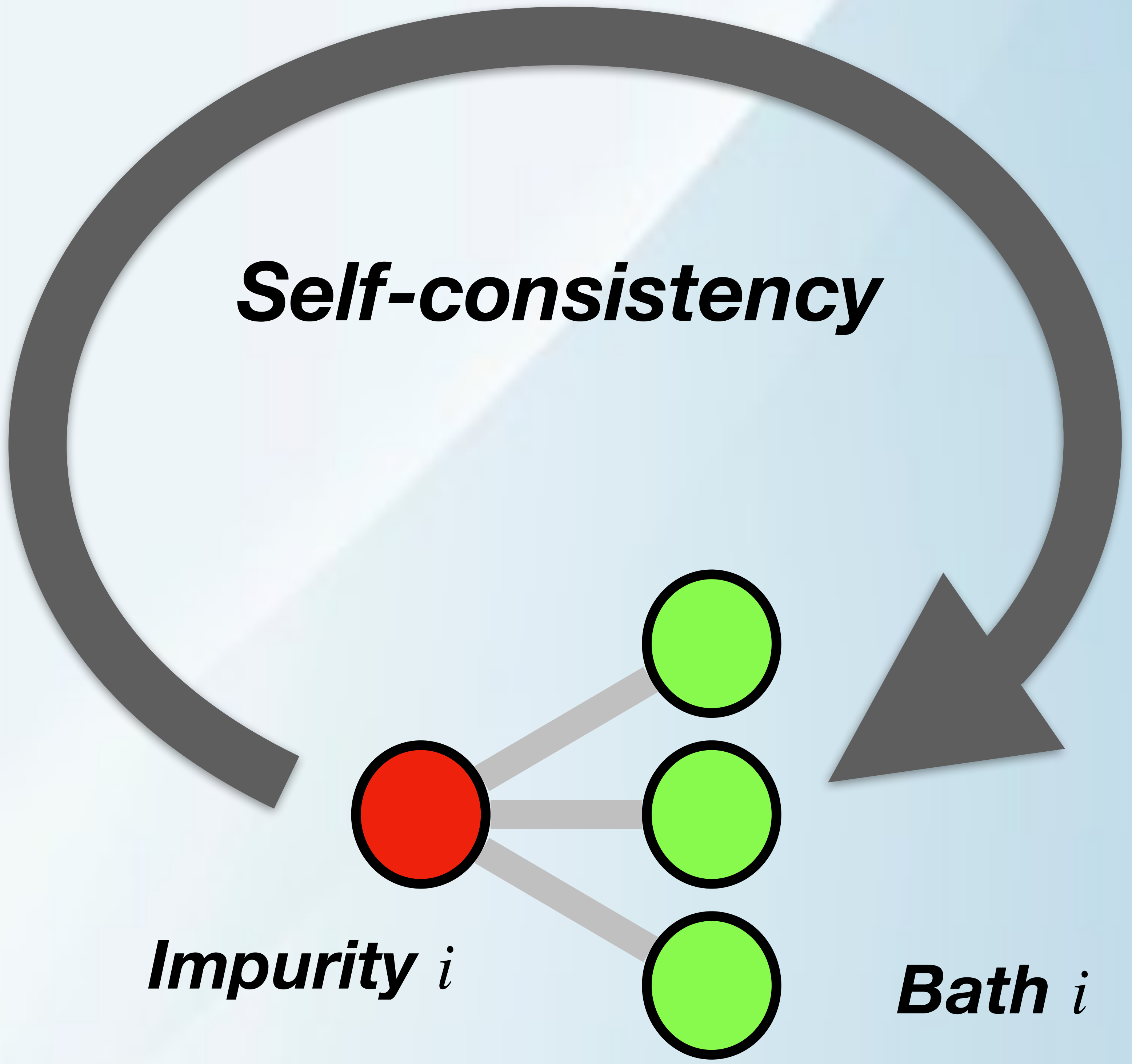

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- - DFT+DMFT (CTQMC) generated using Kristjan Haule's code https://www.physics.rutgers.edu/~haule/

Key features of gGA:

1. *Less computationally demanding than DMFT*

2. *Practically as accurate as DMFT for ground-state properties (with “ghost” extension)*

3. *Variational (T=0)*

3. *Flexible (e.g., possible extension to non-equilibrium dynamics)*

Implementations

1. ***ComRISB (only GA for now):***
   https://www.bnl.gov/comscope/software/downloads.php
   For further inquiries, contact Yongxin Yao at ykent@iastate.edu.

2. ***Portobello (GA/gGA):***
   Computer Physics Communications 294, 108907 (2024), ISSN 0010- 4655

3. ***Pedagogical gGA code for 1-band Hubbard Model:***
   https://gitlab.com/collaborations3/g-ga-hubbard
   For further inquiries, contact Marius Frank at marius.frank@chem.au.dk.

4. ***Implementation within TRIQS under development***

Potential extensions and Perspectives

1. *Efficient impurity solvers for ground state:*

- *Matrix Product States*
- *Variational Quantum Eigensolvers*
- *Neural Network States*
- *Machine Learning*

PHYSICAL REVIEW RESEARCH **6**, 013242 (2024)

Active learning approach to simulations of strongly correlated matter with the ghost Gutzwiller approximation

Marius S. Frank,[1] Denis G. Artiukhin,[2] Tsung-Han Lee,[3] Yongxin Yao,[4,5] Kipton Barros,[6] Ove Christiansen,[7] and Nicola Lanatà[8,9,*]

2. *Extensions based on RISB/DMET perspectives:*

- *Gaussian fluctuations, non-local interactions …*

3. ***Applications:*** *Structure prediction, Catalysis, Quantum dynamics (td-gGA) …*

Outline

A. Background notions in many-body theory (board)

B. The GA/gGA wave function: Introduction

C. Derivation gGA method: QE formulation

D. Applications, recent developments and open problems

Supplementary topics:

- Spectral properties

- Time-dependent extension

- DFT+gGA

THANK YOU FOR YOUR ATTENTION !!!

Supplemental topic 1: Spectral properties

Spectral properties

$$\mathscr{L} = \langle\Psi_0|\hat{H}_{qp}[\mathscr{R},\lambda]|\Psi_0\rangle + E\left(1 - \langle\Psi_0|\Psi_0\rangle\right)$$
$$+ \sum_{i=1}^{\mathcal{N}} \left[\langle\Phi_i|\hat{H}_i^{emb}[\mathscr{D}_i,\lambda_i^c]|\Phi_i\rangle + E_i^c\left(\mathbf{1} - \langle\Phi_i|\Phi_i\rangle\right)\right]$$
$$- \sum_{i=1}^{\mathcal{N}} \left[\sum_{a,b=1}^{B\nu_i}\left([\lambda_i]_{ab} + [\lambda_i^c]_{ab}\right)[\Delta_i]_{ab} + \sum_{c,a=1}^{B\nu_i}\sum_{\alpha=1}^{\nu_i}\left([\mathscr{D}_i]_{a\alpha}[\mathscr{R}_i]_{c\alpha}\left[\Delta_i(\mathbf{1}-\Delta_i)\right]^{\frac{1}{2}}_{ca} + \text{c.c.}\right)\right]$$

Iteratively calculated ground state $|\Psi_0\rangle$ *of* $\hat{H}_{qp}$*, but its excited states* $\xi_n^\dagger|\Psi_0\rangle$ *also correspond to a saddle point !*

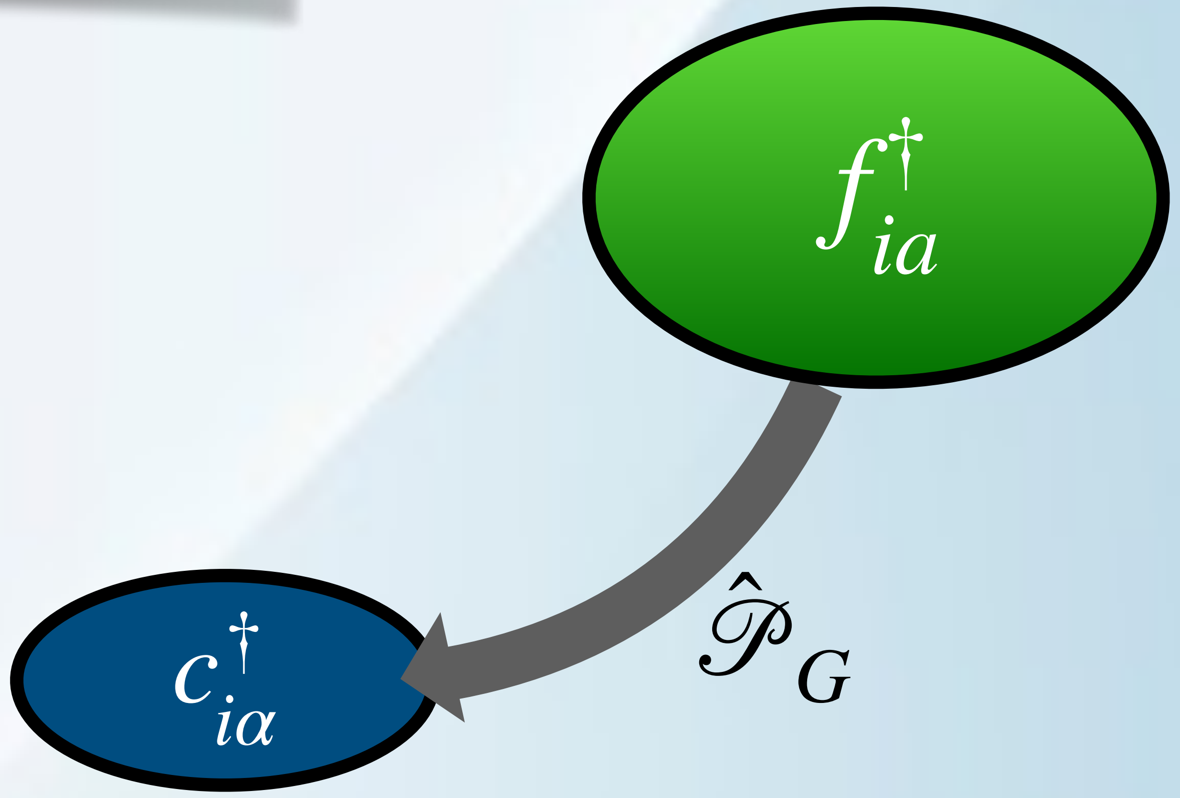
$$\hat{H}_{qp}[\mathscr{R},\Lambda] = \sum_{i,j=1}^{\mathcal{N}}\sum_{a,b=1}^{B\nu_i}\left[\mathscr{R}_i t_{ij} \mathscr{R}_j^\dagger\right]_{ab} f_{ia}^\dagger f_{jb} + \sum_{i=1}^{\mathcal{N}}\sum_{a,b=1}^{B\nu_i}[\lambda_i]_{ab} f_{ia}^\dagger f_{ib}$$

$$\hat{H}^i_{emb}[\mathscr{D}_i,\Lambda_i^c] = \hat{H}^i_{loc}\left[c_{i\alpha}, c_{i\alpha}^\dagger\right] + \sum_{a=1}^{B\nu_i}\sum_{\alpha=1}^{\nu_i}\left([\mathscr{D}_i]_{a\alpha} c_{i\alpha}^\dagger b_{ia} + \text{H.c.}\right) + \sum_{a,b=1}^{B\nu_i}[\lambda_i^c]_{ab} b_{ib} b_{ia}^\dagger$$

Spectral properties

Ground state: $|\Psi_G\rangle = \mathscr{P}\,|\Psi_0\rangle$

Excited states: $|\Psi^n_G\rangle = \mathscr{P}\,\xi^\dagger_n\,|\Psi_0\rangle$



$$A_{i\alpha,j\beta}(\omega) = \langle\Psi_G|\,c_{i\alpha}\,\delta(\omega - \hat{H})\,c^\dagger_{j\beta}\,|\Psi_G\rangle + \langle\Psi_G|\,c^\dagger_{j\beta}\,\delta(\omega + \hat{H})\,c_{i\alpha}\,|\Psi_G\rangle$$

PHYSICAL REVIEW B **67**, 075103 (2003)

Landau-Gutzwiller quasiparticles

Jörg Bünemann
Oxford University, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, United Kingdom

Florian Gebhard
Fachbereich Physik, Philipps–Universität Marburg, D-35032 Marburg, Germany

Rüdiger Thul
Abteilung Theorie, Hahn-Meitner-Institut Berlin, D–14109 Berlin, Germany

PHYSICAL REVIEW B **96**, 195126 (2017)

Emergent Bloch excitations in Mott matter

Nicola Lanatà,[1] Tsung-Han Lee,[1] Yong-Xin Yao,[2] and Vladimir Dobrosavljević[1]

PHYSICAL REVIEW B **104**, L081103 (2021)

Letter

Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation

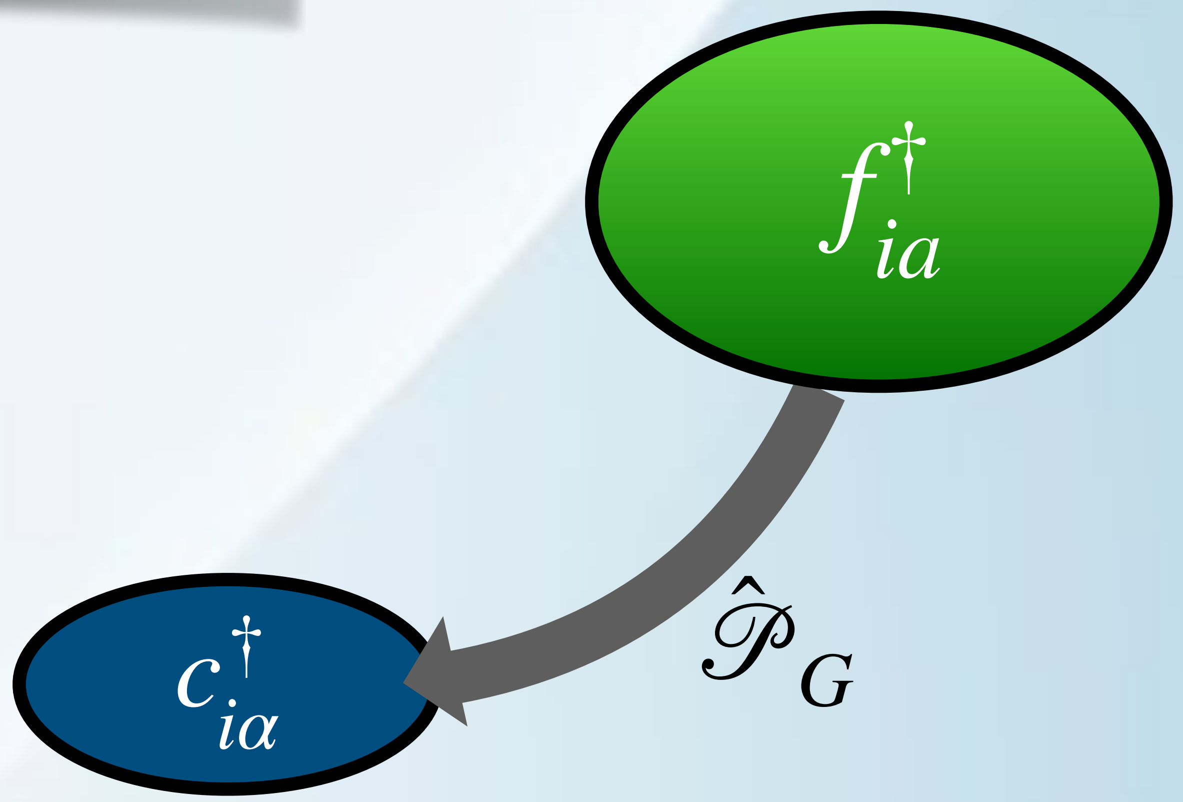
Marius S. Frank,[1] Tsung-Han Lee,[2] Gargee Bhattacharyya,[1] Pak Ki Henry Tsang,[3] Victor L. Quito,[4,3] Vladimir Dobrosavljević,[3] Ove Christiansen,[5] and Nicola Lanatà[1,6,*]

PHYSICAL REVIEW B **108**, 245147 (2023)

Accuracy of ghost-rotationally-invariant slave-boson theory for multiorbital Hubbard models and realistic materials

Tsung-Han Lee,[1,2,*] Corey Melnick,[3] Ran Adler,[1] Nicola Lanatà,[4,5] and Gabriel Kotliar[1,3]

Spectral properties



Ground state: $|\Psi_G\rangle = \mathscr{P}|\Psi_0\rangle$

Excited states: $|\Psi_G^n\rangle = \mathscr{P}\,\xi_n^\dagger|\Psi_0\rangle$

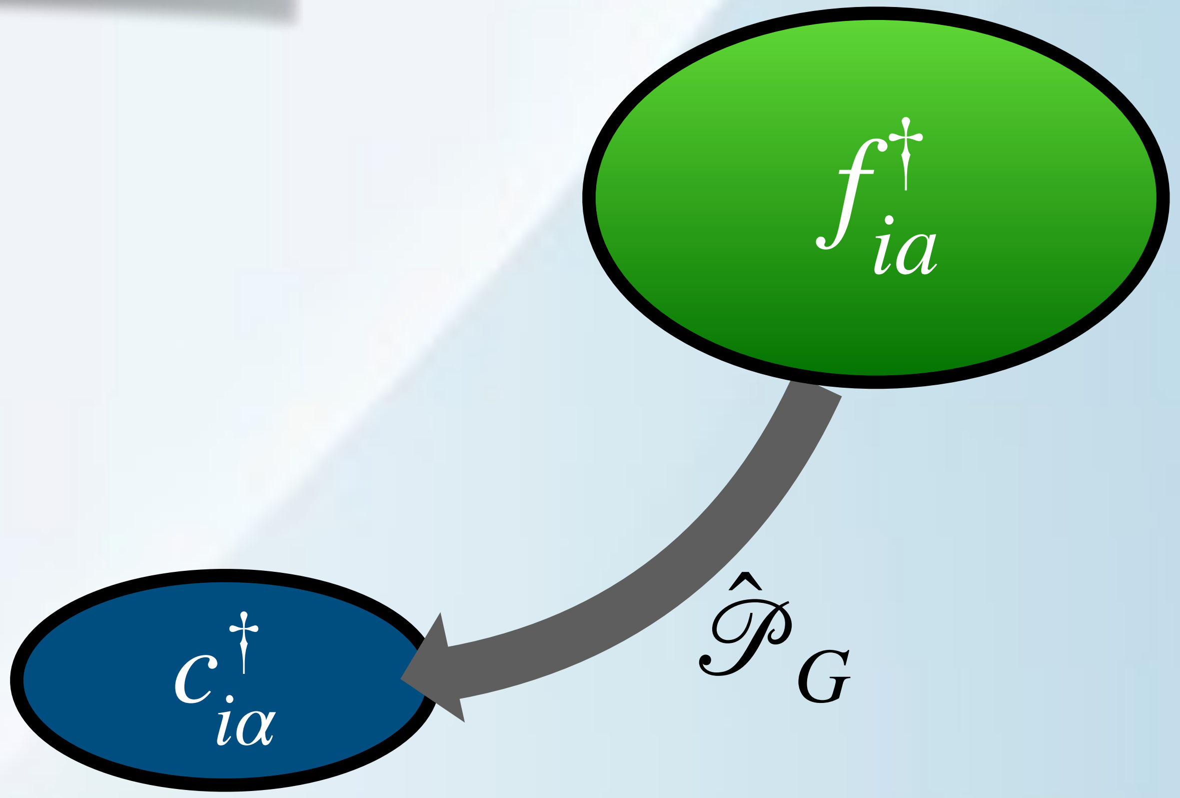
$$A_{i\alpha,j\beta}(\omega) = \langle\Psi_G|c_{i\alpha}\delta(\omega - \hat{H})c_{j\beta}^\dagger|\Psi_G\rangle + \langle\Psi_G|c_{j\beta}^\dagger\delta(\omega + \hat{H})\,c_{i\alpha}|\Psi_G\rangle$$

$$\mathscr{G}(\omega) = \int_{-\infty}^{\infty} d\epsilon\,\frac{A(\epsilon)}{\omega - \epsilon} \simeq \mathscr{R}^\dagger\frac{1}{\omega - [\mathscr{R}t\mathscr{R}^\dagger + \lambda]}\mathscr{R} =: \frac{1}{\omega - t_{loc} - \Sigma(\omega)}$$

Spectral properties

Ground state: $|\Psi_G\rangle = \mathscr{P}\,|\Psi_0\rangle$

Excited states: $|\Psi_G^n\rangle = \mathscr{P}\,\xi_n^\dagger\,|\Psi_0\rangle$



$$A_{i\alpha,j\beta}(\omega) = \langle\Psi_G|\,c_{i\alpha}\,\delta(\omega-\hat{H})\,c_{j\beta}^\dagger\,|\Psi_G\rangle + \langle\Psi_G|\,c_{j\beta}^\dagger\,\delta(\omega+\hat{H})\,c_{i\alpha}\,|\Psi_G\rangle$$

$$[\Sigma_i(\omega)]_{\alpha\beta} = [a_i]_{\alpha\beta} + \sum_n \frac{[b_{in}]_{\alpha\beta}}{\omega + i0^+ - p_n}$$

Supplemental topic 2: Time-dependent gGA

Time-dependent gGA

Our goal is to extremize w.r.t. $\{\Lambda_i\}, |\Psi_0\rangle$:

$$S = \int_{t_i}^{t_f} dt \, \langle \Psi_G(t) | \, i\partial_t - \hat{H} \, | \Psi_G(t) \rangle$$

PRL **105,** 076401 (2010) PHYSICAL REVIEW LETTERS week ending 13 AUGUST 2010

Time-Dependent Mean Field Theory for Quench Dynamics in Correlated Electron Systems

Marco Schiró[1] and Michele Fabrizio[1,2]

PHYSICAL REVIEW RESEARCH **5,** L032023 (2023)

Letter

Time-dependent ghost Gutzwiller nonequilibrium dynamics

Daniele Guerci,[1] Massimo Capone,[2,3] and Nicola Lanatà[4,1,*]

$$\hat{H} = \frac{U}{2}\sum_i (\hat{n}_i - 1)^2 - J\sum_{\langle i,j\rangle}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{i\sigma}c_{j\sigma} + \mathrm{H.c.})$$

$$\mathcal{L} = \frac{1}{\mathcal{N}}\langle\Psi_0|i\partial_t - \hat{H}_{\mathrm{qp}}|\Psi_0\rangle + \langle\Phi|i\partial_t - \hat{H}_{\mathrm{emb}}|\Phi\rangle$$
$$+ \Bigg[\sum_{\sigma=\uparrow,\downarrow}\sum_{a,b=1}^{\mathcal{B}}\Lambda^c_{ab}\Delta_{ab}$$
$$+ \sum_{\sigma=\uparrow,\downarrow}\sum_{c,a=1}^{\mathcal{B}}\left(\mathcal{D}_a\mathcal{R}_c[\Delta(1-\Delta)]^{\frac{1}{2}}_{ca} + \mathrm{c.c.}\right)\Bigg]$$

$$\hat{H} = \frac{U}{2}\sum_i (\hat{n}_i - 1)^2 - J\sum_{\langle i,j\rangle}\sum_{\sigma=\uparrow,\downarrow}(c^\dagger_{i\sigma}c_{j\sigma} + \mathrm{H.c.})$$

PHYSICAL REVIEW RESEARCH **5**, L032023 (2023)

Letter

Time-dependent ghost Gutzwiller nonequilibrium dynamics

Daniele Guerci,[1] Massimo Capone,[2,3] and Nicola Lanatà[4,1,*]

PRL **103**, 056403 (2009) PHYSICAL REVIEW LETTERS week ending 31 JULY 2009

Thermalization after an Interaction Quench in the Hubbard Model

Martin Eckstein,[1] Marcus Kollar,[1] and Philipp Werner[2]

Supplemental topic 3: DFT+gGA

DFT+gGA

$$\mathcal{L}_N^{\mathrm{DFT+gRISB}}\left[\rho(\mathbf{r}), \mathcal{J}(\mathbf{r}), \mu, V_i^0, N_i^0\right] = \mathcal{L}_{\mathrm{gRISB}}\left[\mathcal{J}(\mathbf{r}), \mu\right] - \int d\mathbf{r}\, \rho(\mathbf{r})\mathcal{J}(\mathbf{r}) + E_{\mathrm{Hxc}}[\rho(\mathbf{r})] + E_{\text{ion-ion}} + E_{\mathrm{ion}}[\rho(\mathbf{r})] + \sum_i E_{\mathrm{dc}}^i\left[N_i^0\right] - \sum_i V_i^0 N_i^0 + \mu N$$

$$\hat{H}_{\mathrm{KSH}} = \int dx\, \hat{\Psi}^\dagger(x)\, \hat{P}\left[-\hat{\nabla}^2 + \mathcal{J}(\hat{x}) - \mu\right]\hat{P}\,\hat{\Psi}(x) + \sum_{\mathbf{R},i}\left(\hat{H}_i^{\mathrm{int}}[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}] + V_i^0 \sum_\alpha c^\dagger_{\mathbf{R}i\alpha} c_{\mathbf{R}i\alpha}\right)$$

$$c_{\mathbf{R}i\alpha} = \int dx\, \phi^*_{\mathbf{R}i\alpha}(x)\hat{\Psi}(x)$$

$$\phi_{\mathbf{R}i\alpha}(\mathbf{r}) = \mathcal{N}^{-1}\sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{R}}\phi_{\mathbf{k}i\alpha}(x)$$

DFT+gGA

$$\mathcal{J}(\mathbf{r}) = \frac{\delta H^{\mathrm{LDA}}_{\mathrm{Hxc}}[\rho(\mathbf{r})]}{\delta\rho(\mathbf{r})} + \frac{\delta E_{\mathrm{ion}}[\rho(\mathbf{r})]}{\delta\rho(\mathbf{r})},$$

$$\frac{1}{\mathcal{N}}\sum_{\mathbf{k}} \langle f^\dagger_{\mathbf{k}ia} f_{\mathbf{k}ib}\rangle_0 = [\Delta_i]_{ab}\,,$$

$$\rho(\mathbf{r}) = \langle \hat{\Psi}^\dagger_{\mathrm{u}}(\mathbf{r})\hat{\Psi}_{\mathrm{u}}(\mathbf{r})\rangle_0 + \langle \hat{\Psi}^\dagger_{\mathrm{c}}(\mathbf{r})\hat{\Psi}_{\mathrm{c}}(\mathbf{r})\rangle_0 + \left(\langle \hat{\Psi}^\dagger_{\mathrm{c}}(\mathbf{r})\hat{\Psi}_{\mathrm{u}}(\mathbf{r})\rangle_0 + \mathrm{H.c.}\right)$$

$$+\frac{1}{\mathcal{N}}\sum_{i}\sum_{\mathbf{k}}\sum_{\alpha\beta} \phi^*_{\mathbf{k}i\alpha}(\mathbf{r}) \left(\langle\Phi_i|c^\dagger_{i\alpha}c_{i\beta}|\Phi_i\rangle - \sum_{ab}[R^\dagger_i]_{\alpha a}\,[\Delta_i]_{ab}\,[R_i]_{b\beta}\right)\phi_{\mathbf{k}i\beta}(\mathbf{r}),$$

$$\int dx \frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\sum_{b}\sum_{i'} \phi^*_{\mathbf{k}i\alpha}(x)\hat{P}\left[-\nabla^2 + J(\hat{x}) - \mu\right]\hat{P}\phi_{\mathbf{k}i'\beta}(x)[R^\dagger_i]_{\beta b}\langle f^\dagger_{\mathbf{k}ia} f_{\mathbf{k}i'b}\rangle_0$$

$$+\int dx \frac{1}{\mathcal{N}}\sum_{\mathbf{k}} \phi^*_{\mathbf{k}i\alpha}(x)\hat{P}\left[-\nabla^2 + J(\hat{x})\right]\hat{P}\langle f^\dagger_{\mathbf{k}ia}\hat{\Psi}_{\mathrm{u}}(x)\rangle_T = \sum_c [D_i]_{c\alpha}\left[\Delta_i(1-\Delta_i)\right]^{\frac{1}{2}}_{ac},$$

$$\int dx \left[\langle \hat{\Psi}^\dagger_{\mathrm{u}}(x)\hat{\Psi}_{\mathrm{u}}(x)\rangle_0 + \langle \hat{\Psi}^\dagger_{\mathrm{c}}(x)\hat{\Psi}_{\mathrm{c}}(x)\rangle_0\right] = N + \sum_i m_i,$$

$$\sum_{cd\alpha}\frac{\partial}{\partial d_{i,s}}\left(\left[\Delta_i(1-\Delta_i)\right]^{\frac{1}{2}}_{cd}[D_i]_{d\alpha}\,[R_i]_{c\alpha} + \mathrm{c.c.}\right) + l_{i,s} + l^c_{i,s} = 0,$$

$$\hat{H}^{\mathrm{emb}}_i|\Phi_i\rangle = E^c_i|\Phi_i\rangle,$$

$$\langle\Phi_i|c^\dagger_{i\alpha}b_{ia}|\Phi_i\rangle - \sum_c \left[\Delta_i(1-\Delta_i)\right]^{\frac{1}{2}}_{ac}[R_i]_{c\alpha} = 0,$$

$$\langle\Phi_i|b_{ib}b^\dagger_{ia}|\Phi_i\rangle - [\Delta_i]_{ab} = 0,$$

$$\hat{\Psi}_{\mathrm{u}}(x) = \left[\hat{I} - \sum_{\mathbf{k}i\alpha}|\phi_{\mathbf{k}i\alpha}\rangle\langle\phi_{\mathbf{k}i\alpha}|\right]\hat{\Psi}(x)$$

$$\hat{\Psi}_{\mathrm{c}}(x) = \sum_{\mathbf{k}ia} f_{\mathbf{k}ia}\sum_{\alpha}[R^\dagger_i]_{a\alpha}\phi_{\mathbf{k}i\alpha}(x)\,,$$