Slave Boson theories of multi-orbital correlated systems

The multi-orbital <u>gGA</u> theory as a Quantum Embedding framework

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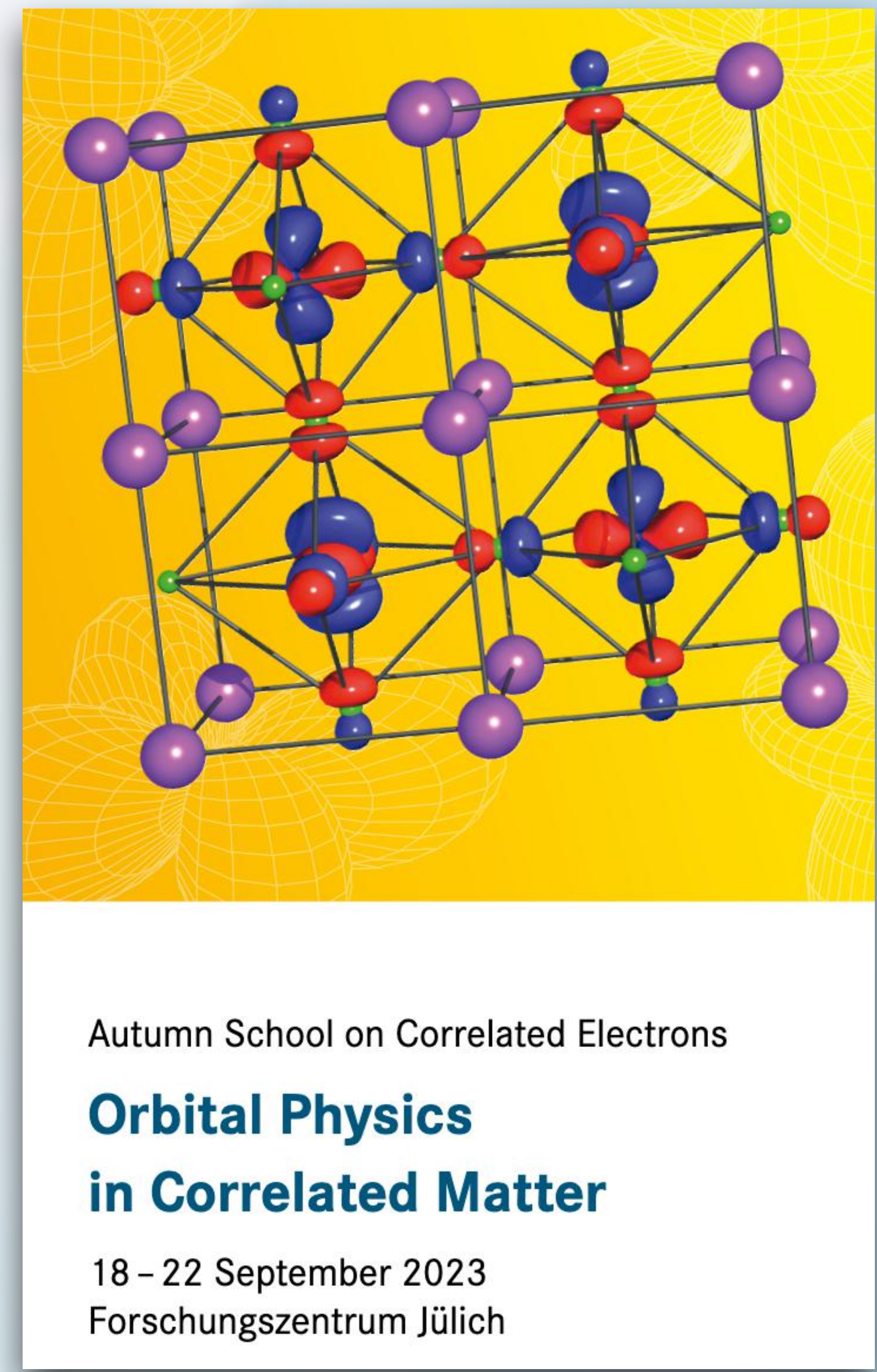
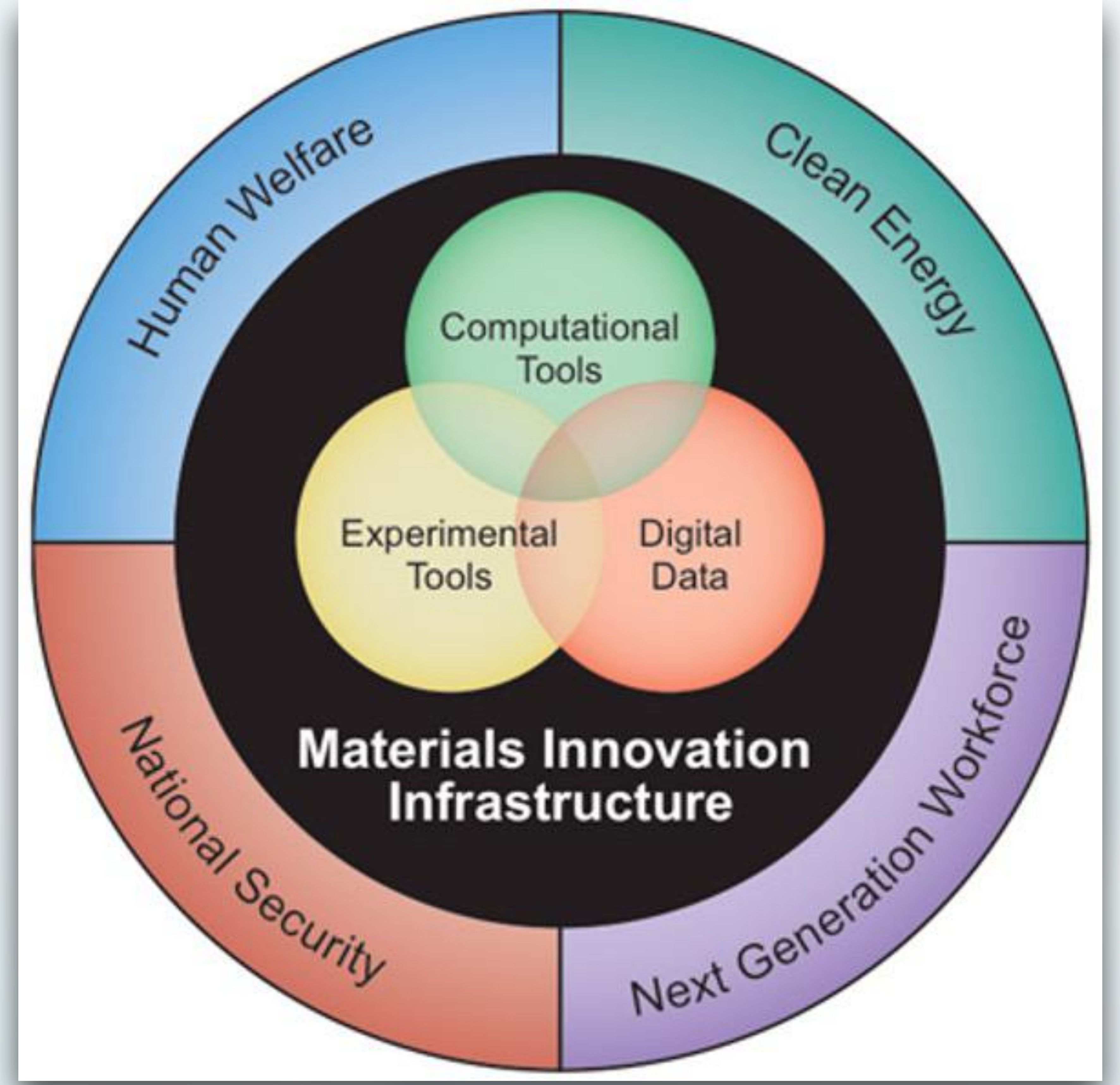


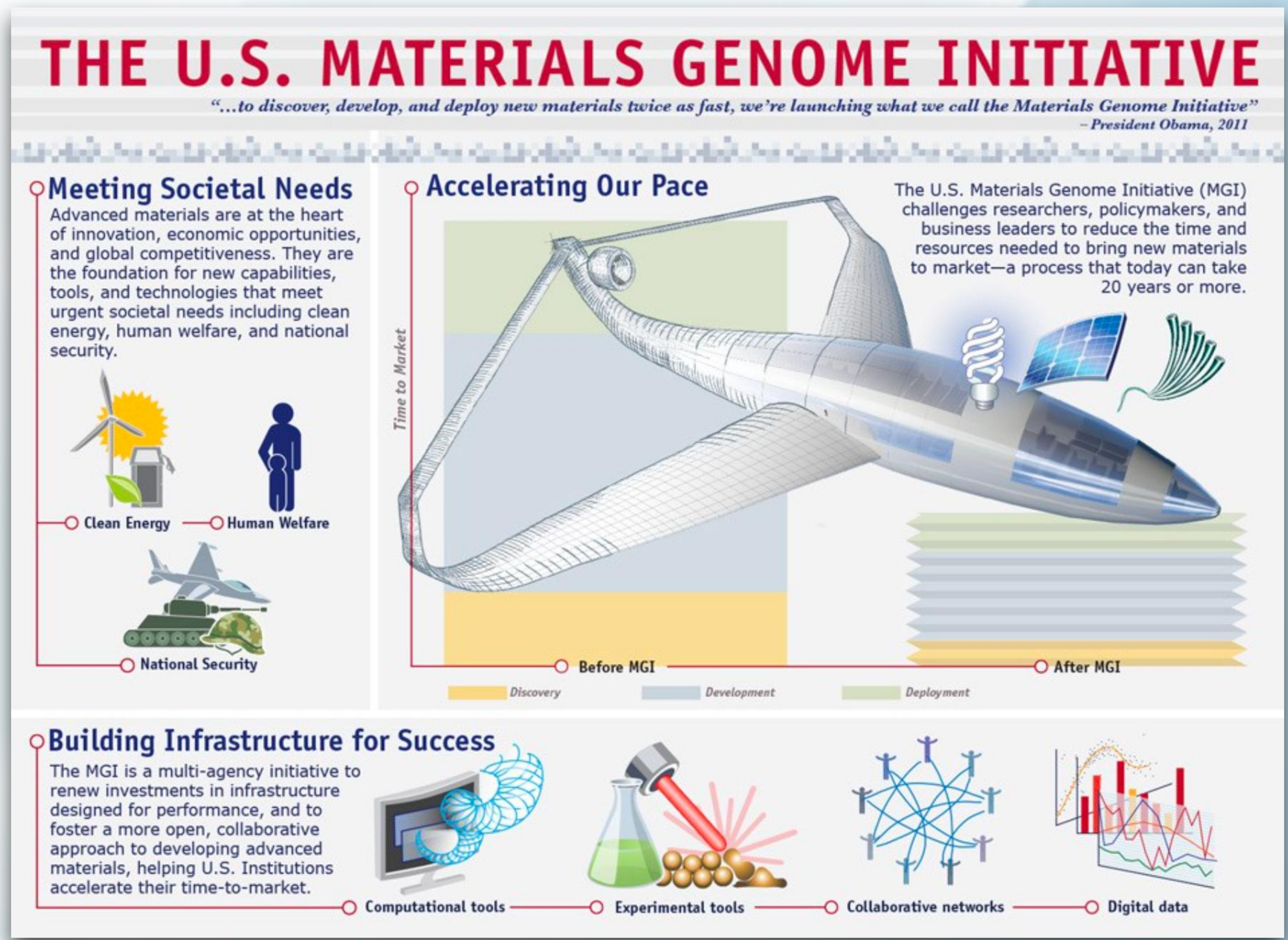
Why useful?

1. *Less computationally demanding than DMFT, with comparable accuracy (with “ghost” extension).*
2. *Variational ($T=0$).*
3. *Computationally convenient extension to non-equilibrium problems.*

Why is computational speed important?

Exploring large chemical spaces





Outline

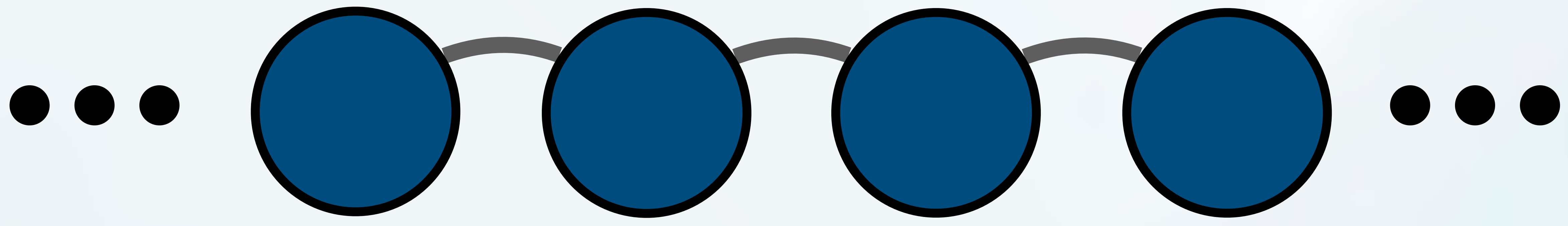
A. Quantum Embedding (QE) methods.

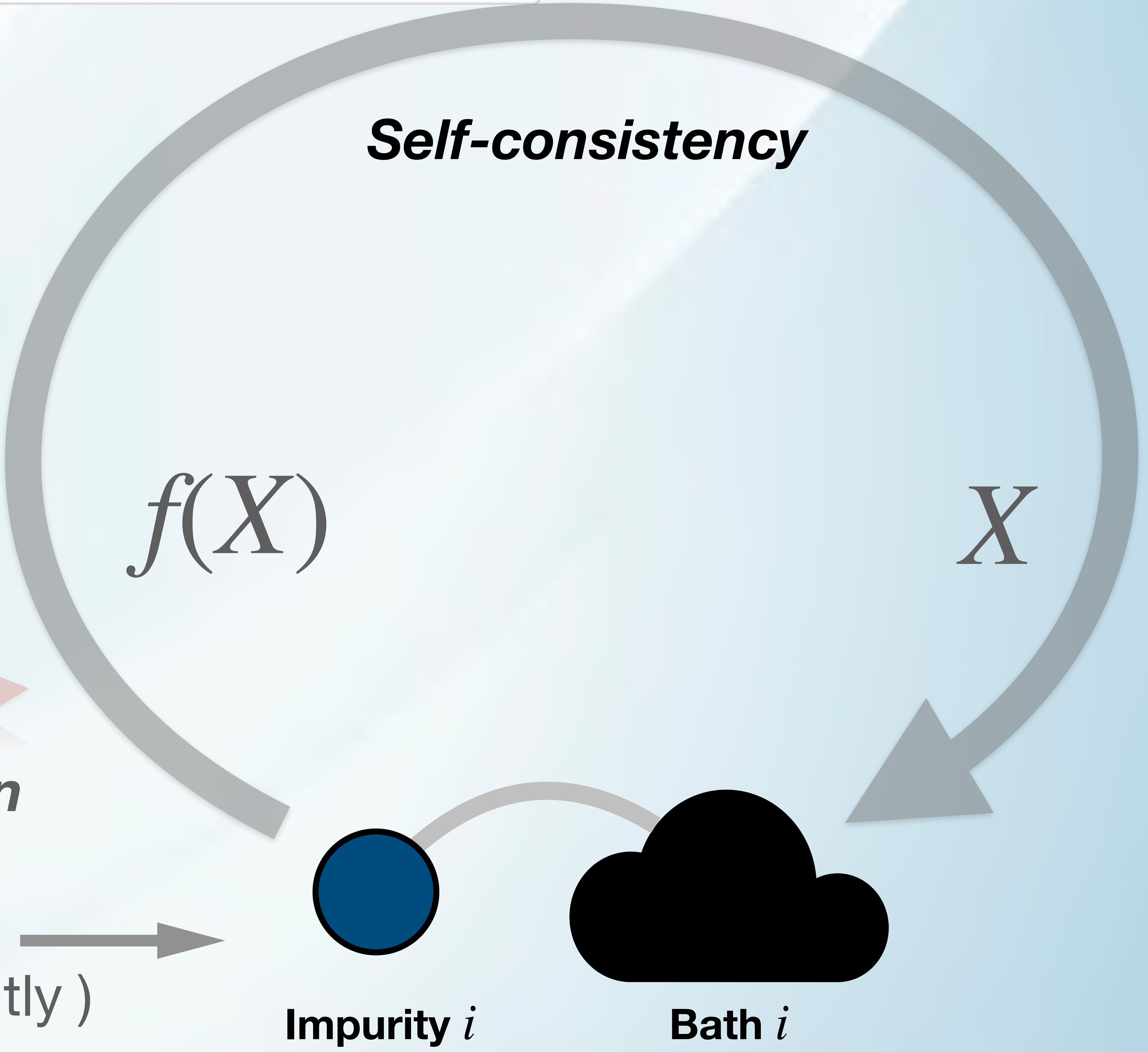
B. gGA method (multi-orbital models): *QE formulation*.

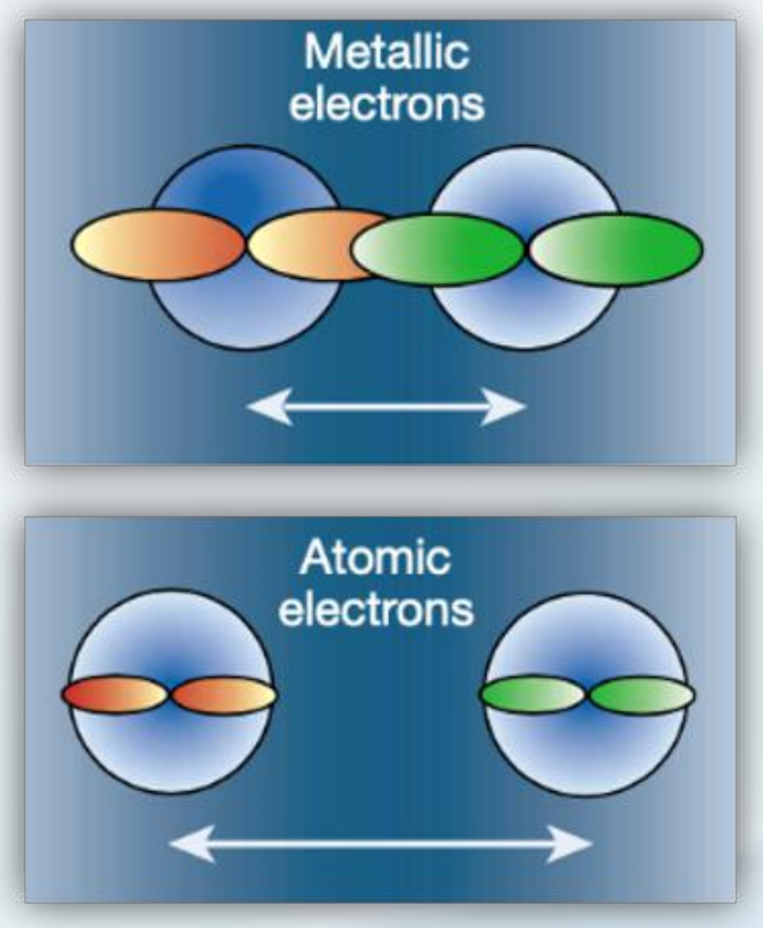
Supplementary topics:

- Spectral properties
- Examples of applications.
- Recent formalism extensions and open problems.

Algorithmic structure of QE methods
(DMFT, DMET, GA, gGA,…)







Embedding Hamiltonian
or impurity model
(Atomic energy scales
of fragment included explicitly)

Example: DMFT

Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions

Antoine Georges

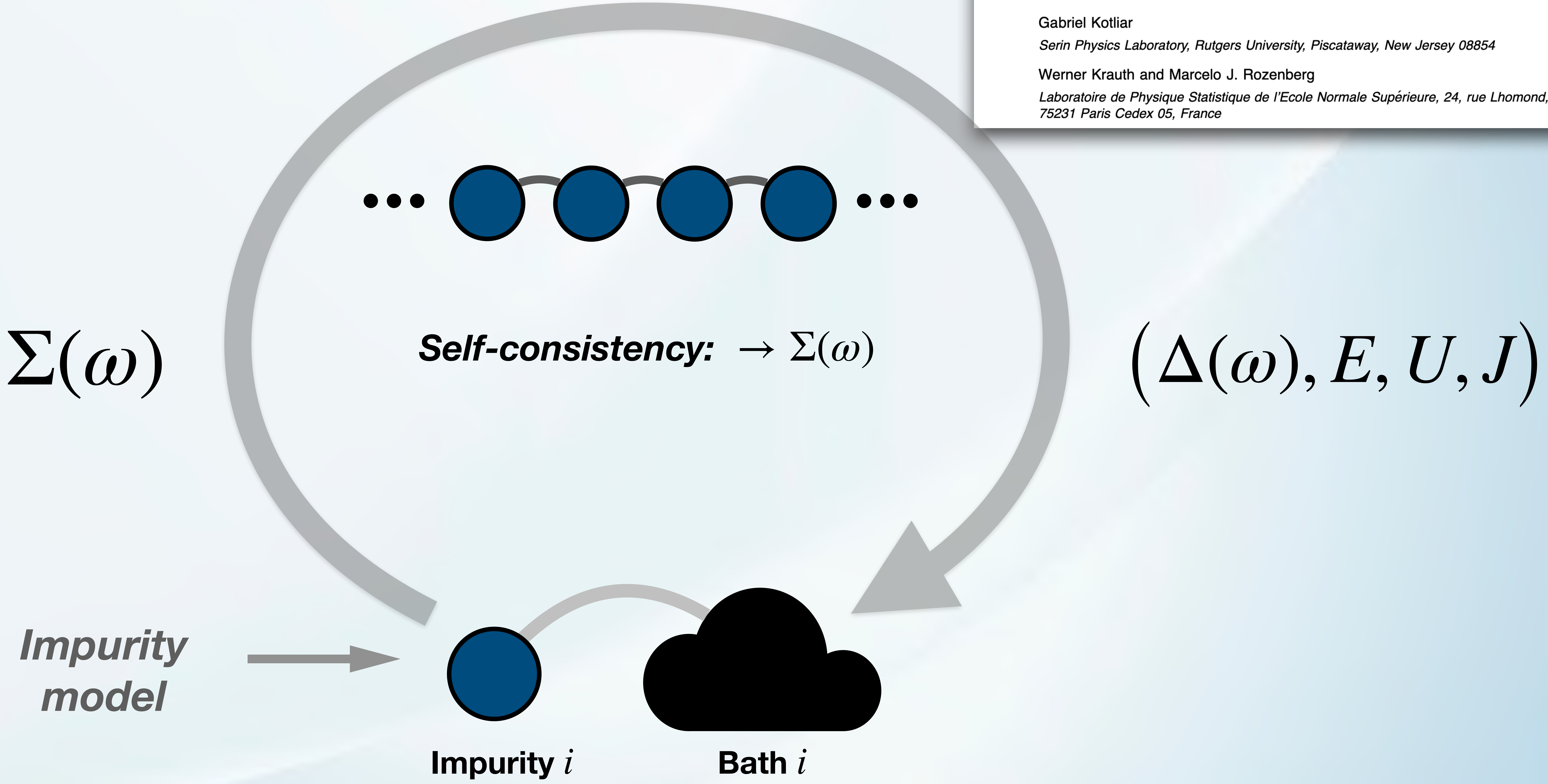
Laboratoire de Physique Théorique de l'Ecole Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France

Gabriel Kotliar

Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08854

Werner Krauth and Marcelo J. Rozenberg

Laboratoire de Physique Statistique de l'Ecole Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France



GA/RISB (QE formulation)

PHYSICAL REVIEW X 5, 011008 (2015)

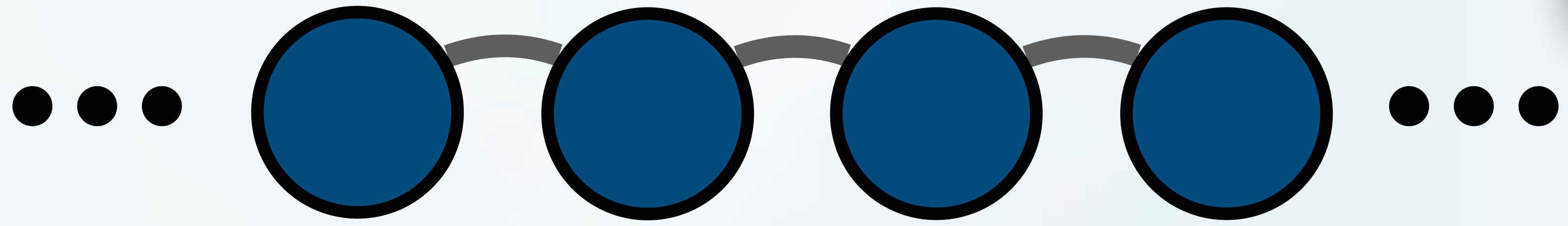
Phase Diagram and Electronic Structure of Praseodymium and Plutonium

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]



$$\begin{bmatrix} \langle c^\dagger_\alpha c_\beta \rangle & \langle c^\dagger_\alpha b_a \rangle \\ \langle b^\dagger_a c_\alpha \rangle & \langle b^\dagger_a b_b \rangle \end{bmatrix}$$

Self-consistency: $\rightarrow \begin{bmatrix} \langle c^\dagger_\alpha c_\beta \rangle & \langle c^\dagger_\alpha b_a \rangle \\ \langle b^\dagger_a c_\alpha \rangle & \langle b^\dagger_a b_b \rangle \end{bmatrix}$

$$\left(D, \Lambda^c, E, U, J\right)$$

$\mathscr{D}$

Embedding Hamiltonian

E, U, J Λ^c

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

gGA/gRISB (QE formulation)

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]

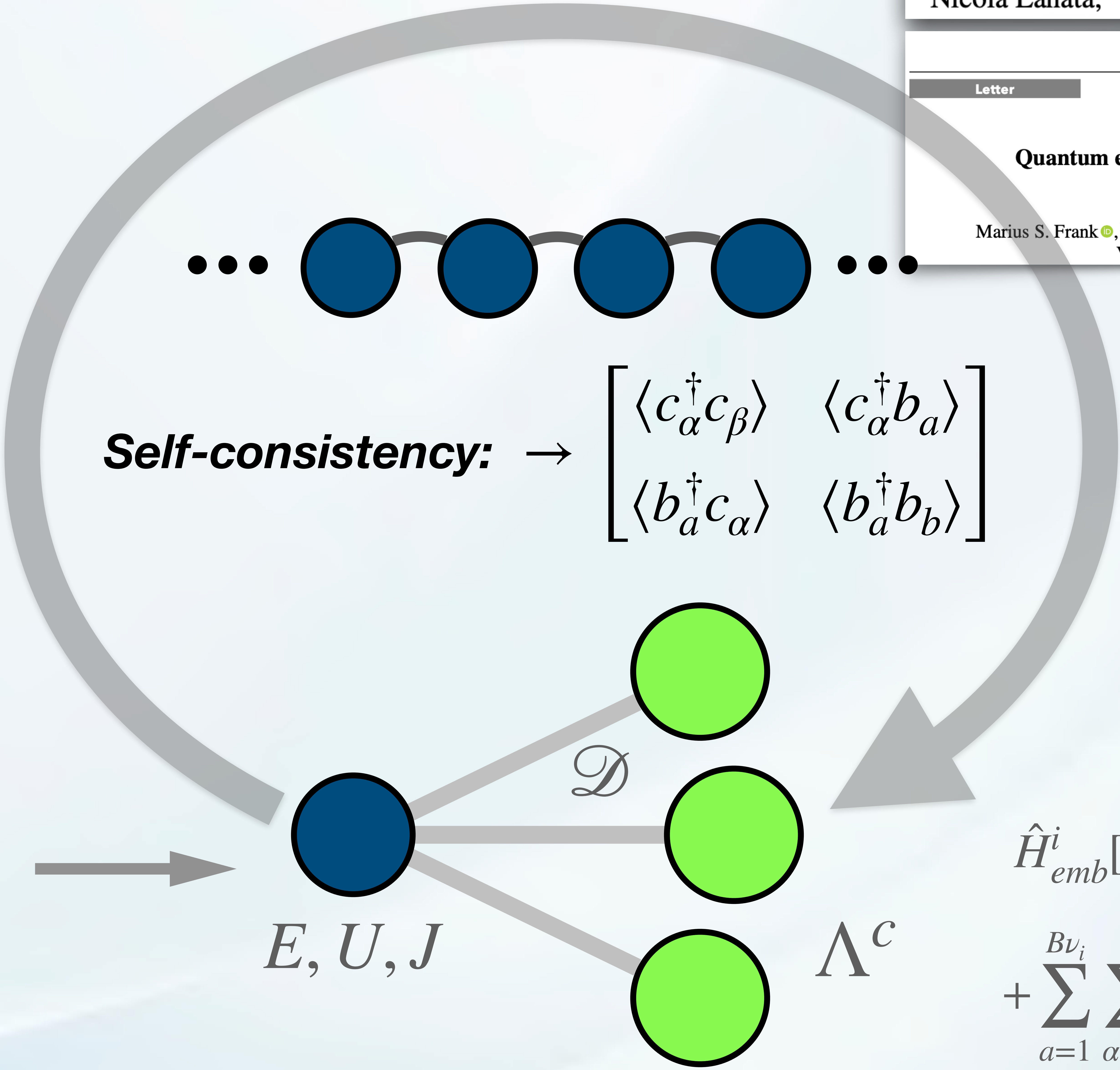
PHYSICAL REVIEW B **104**, L081103 (2021)

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,*]

$$\begin{bmatrix} \langle c^\dagger_\alpha c_\beta\rangle & \langle c^\dagger_\alpha b_a\rangle \\ \langle b^\dagger_a c_\alpha\rangle & \langle b^\dagger_a b_b\rangle \end{bmatrix}$$



$$\left(D, \Lambda^c, E, U, J\right)$$

Embedding Hamiltonian

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

Outline

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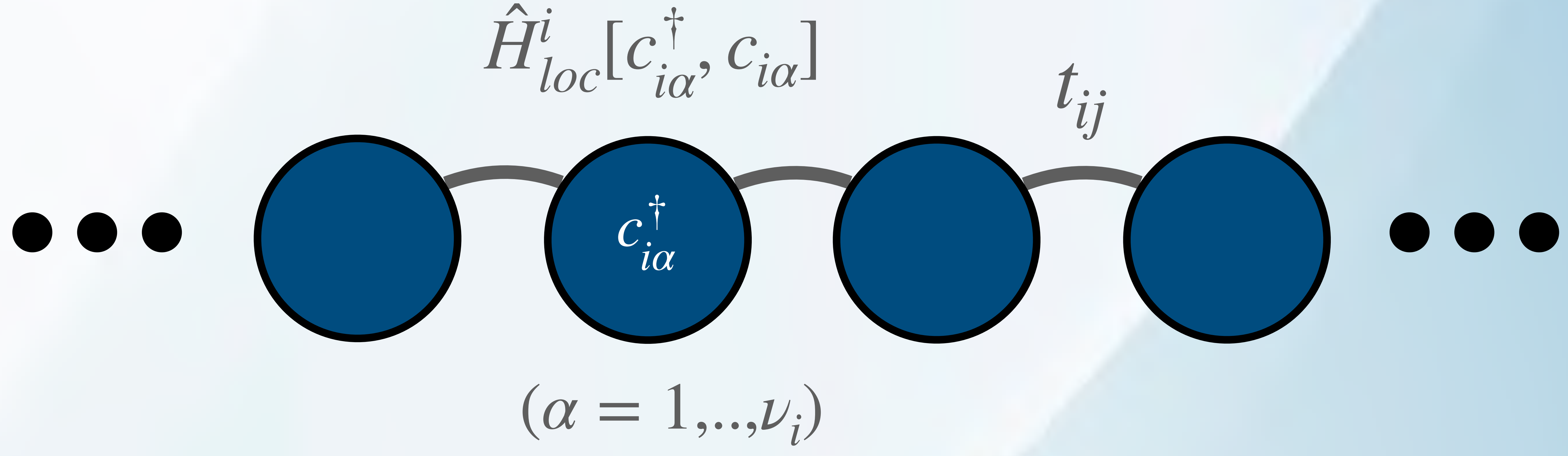
B. **gGA method (multi-orbital models): *QE formulation*.**

Supplementary topics:

- Spectral properties
- Examples of applications.
- Recent formalism extensions and open problems.

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:

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

Evaluating and minimizing

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

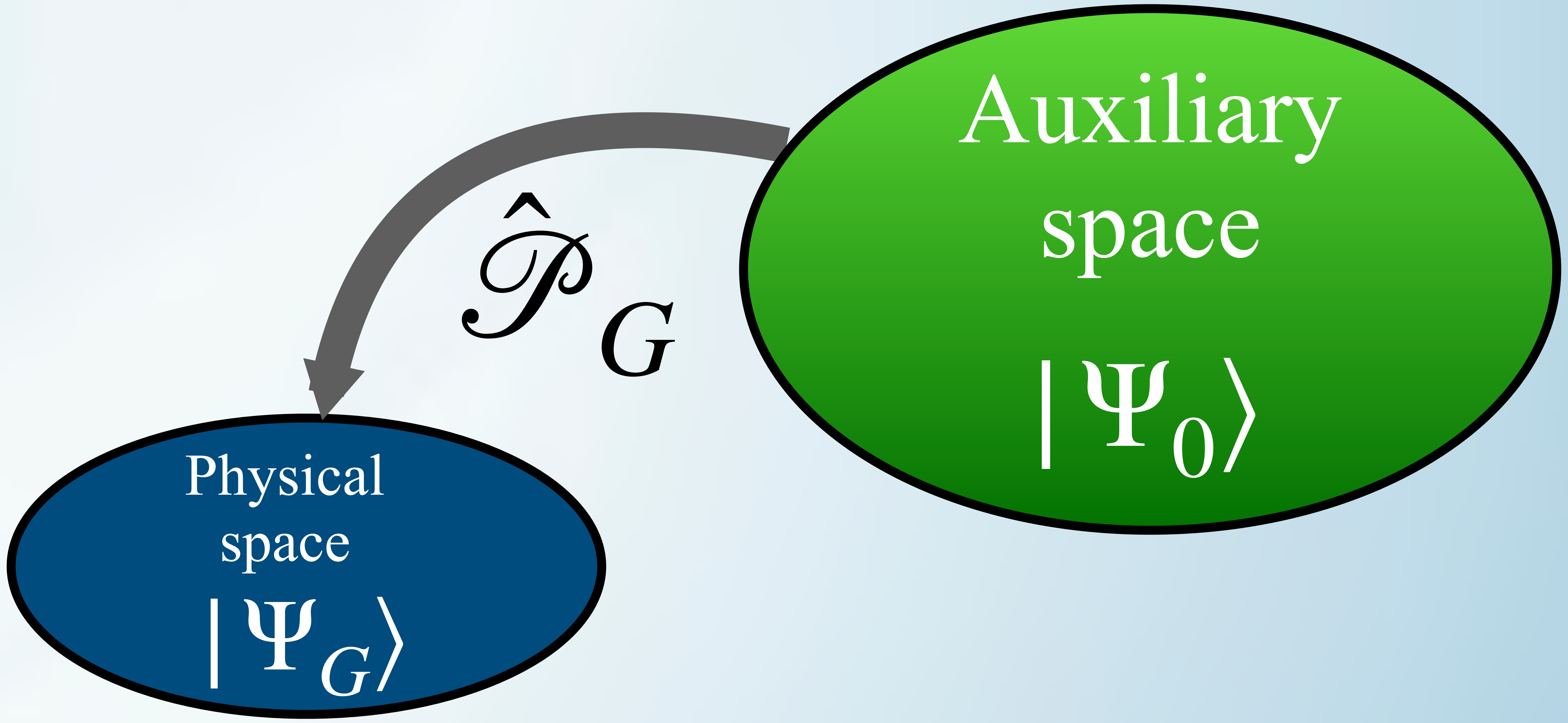
The gGA variational wave function:

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

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

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

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

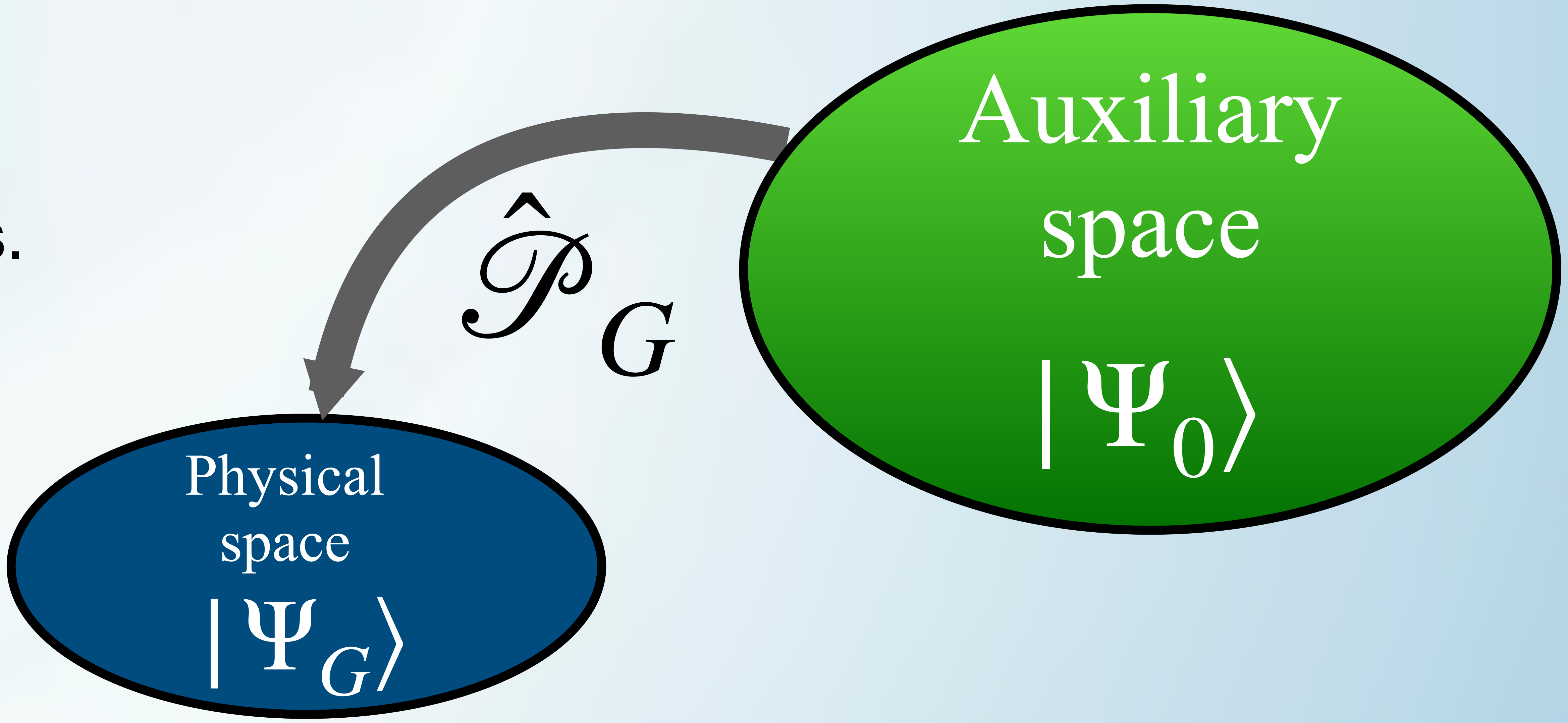


The gGA variational wave function:

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

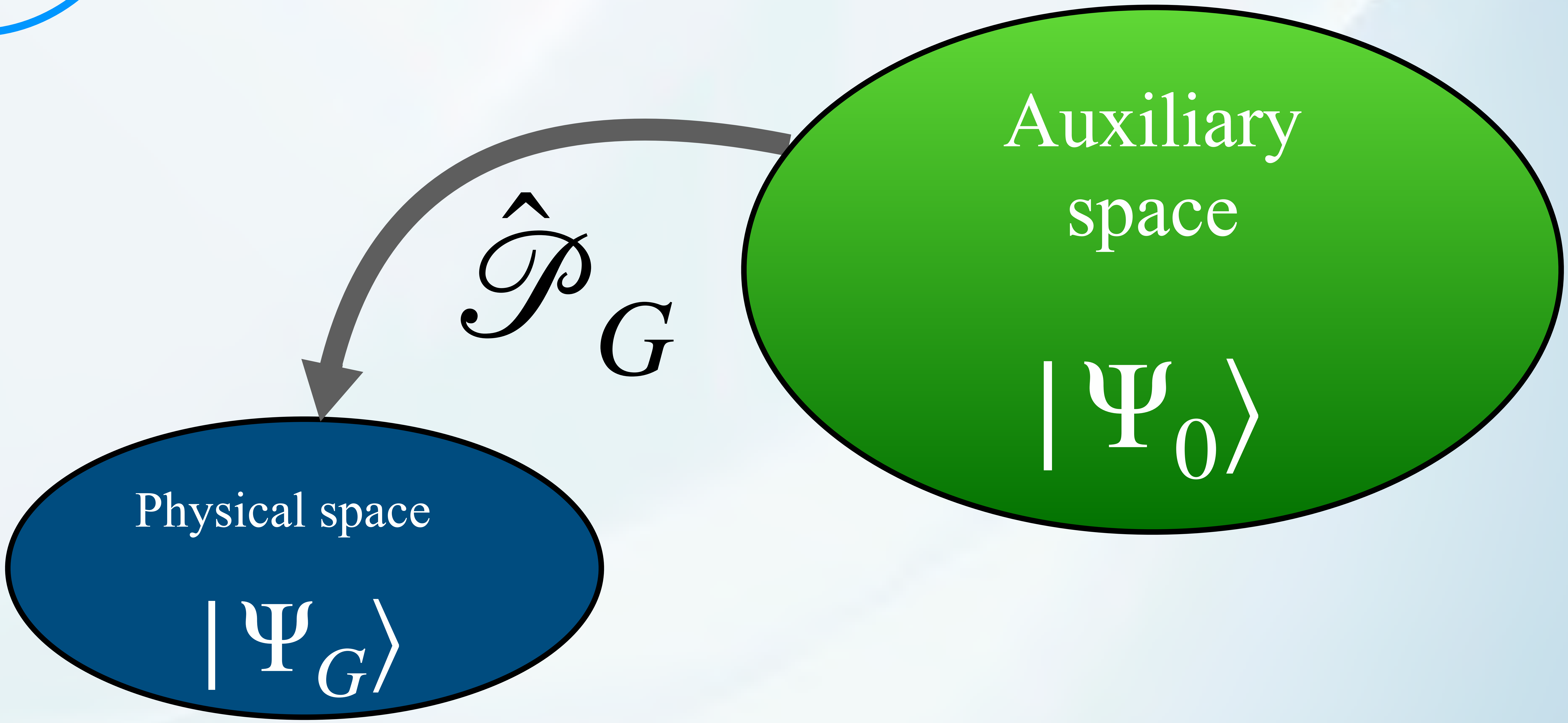
Suggestive analogies:

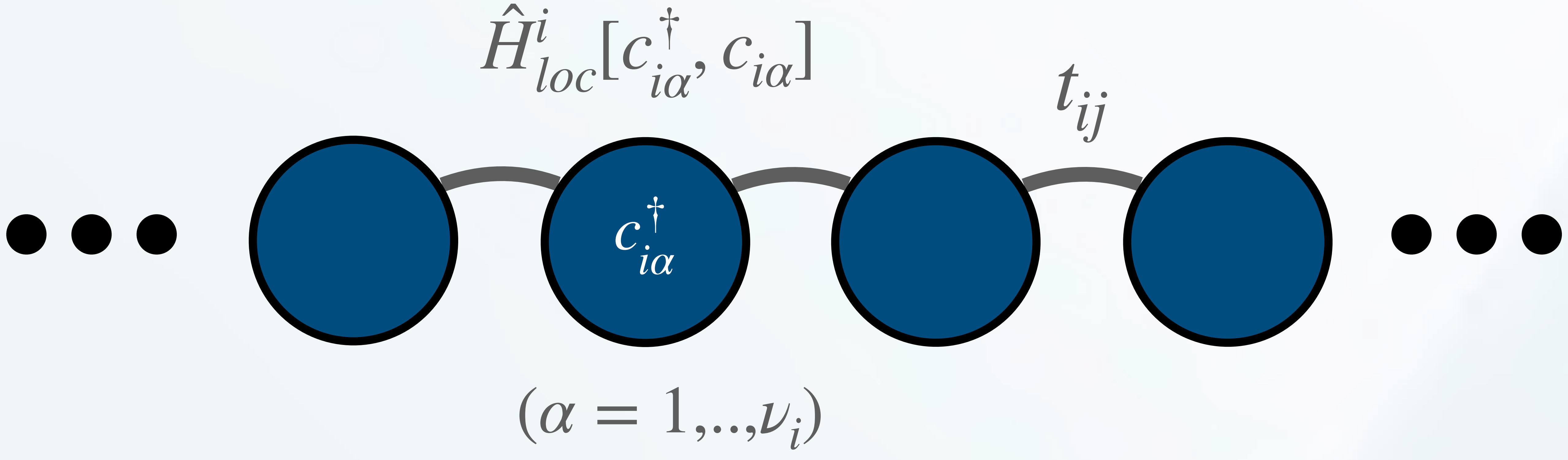
- Matrix product states and projected entangled pair states.
- Ancilla qubit techique (S. Sachdev)
- Hidden Fermion (M. Imada)
- Hidden Fermi liquid (P. Anderson)



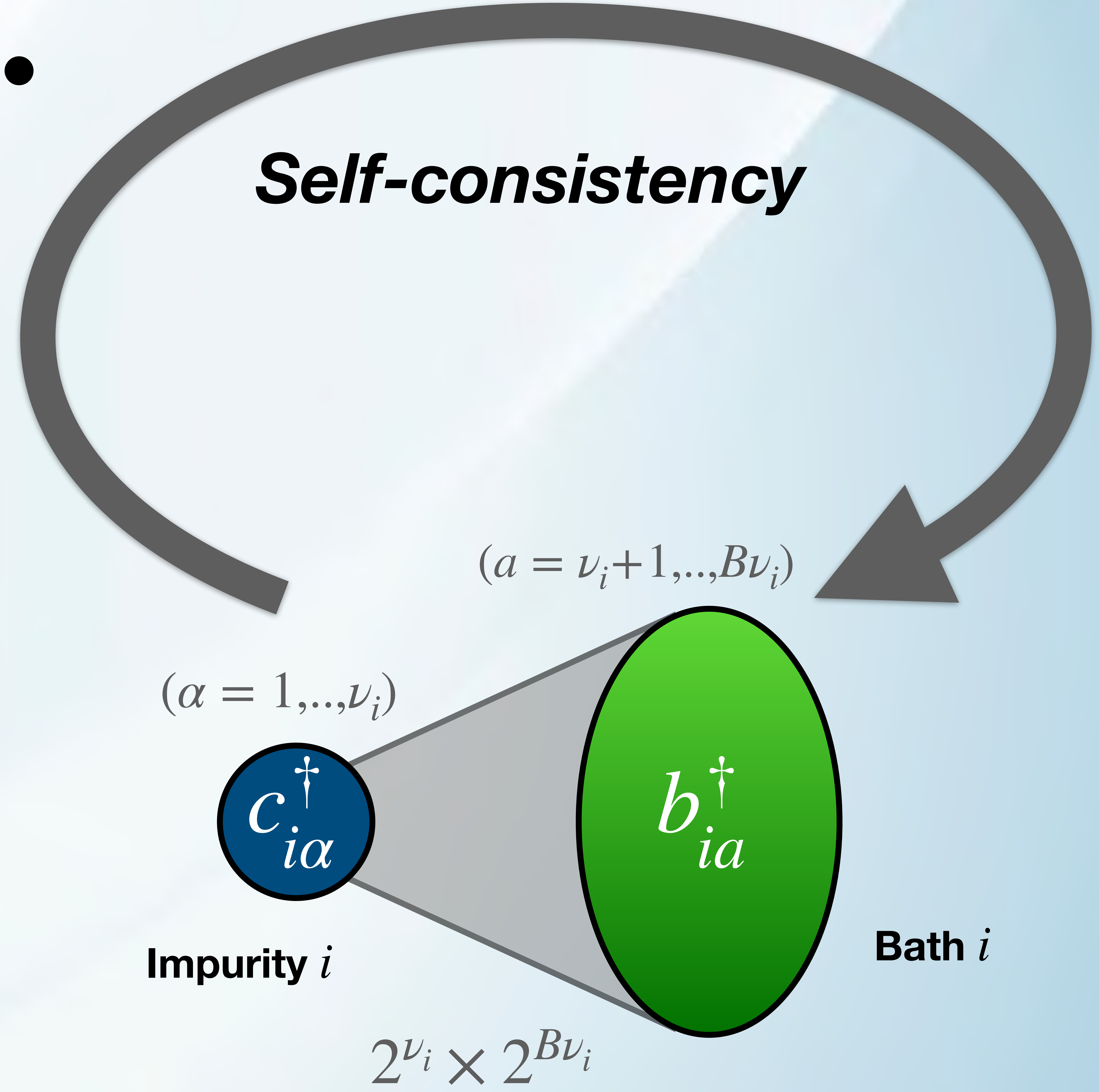
Our goal is to minimize $\langle \Psi_0 | \hat{\mathscr{P}}_G^\dagger \hat{H} \hat{\mathscr{P}}_G | \Psi_0 \rangle$ **w.r.t.** $\{\hat{\Lambda}_i\}, |\Psi_0\rangle$

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





Quantum-embedding formulation

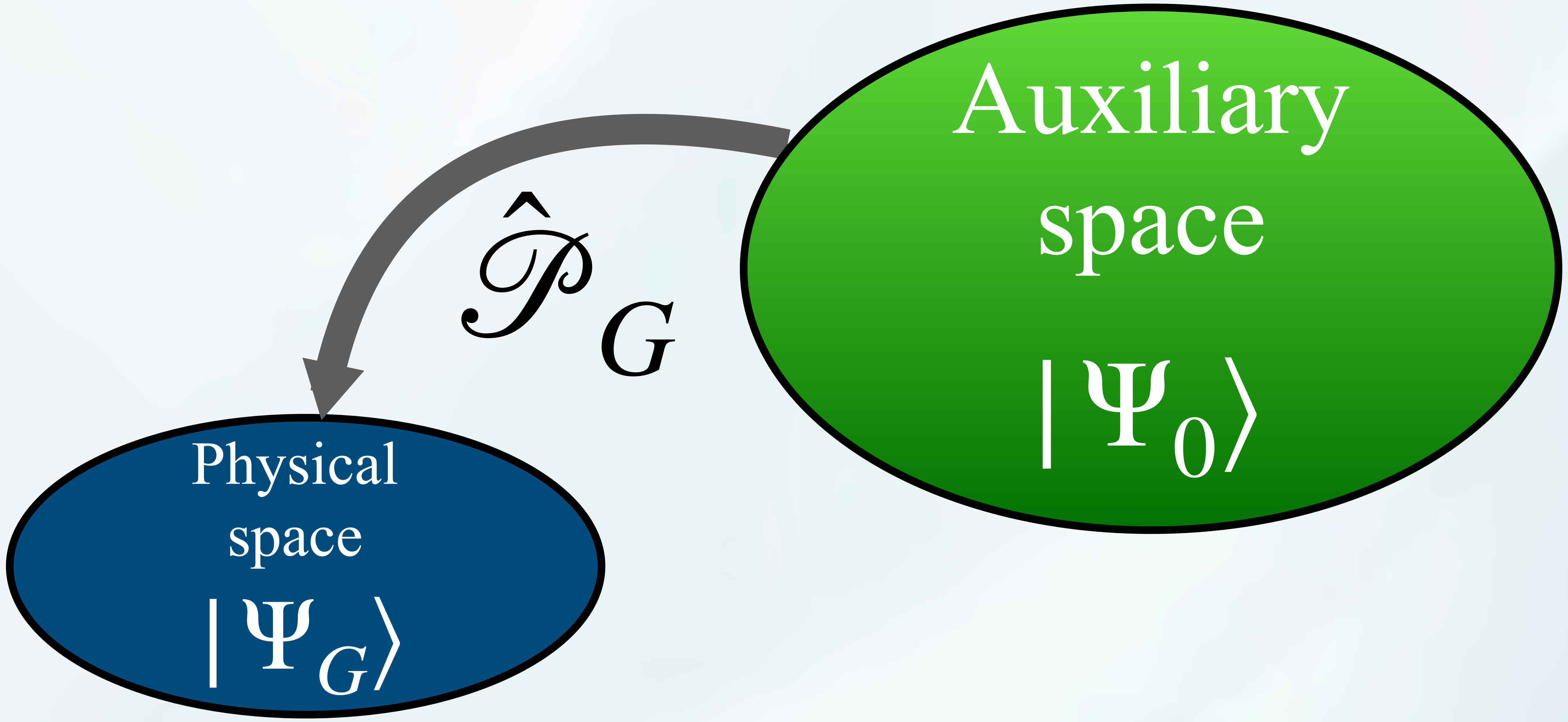


Necessary steps:

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

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

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



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

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

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

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:

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

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

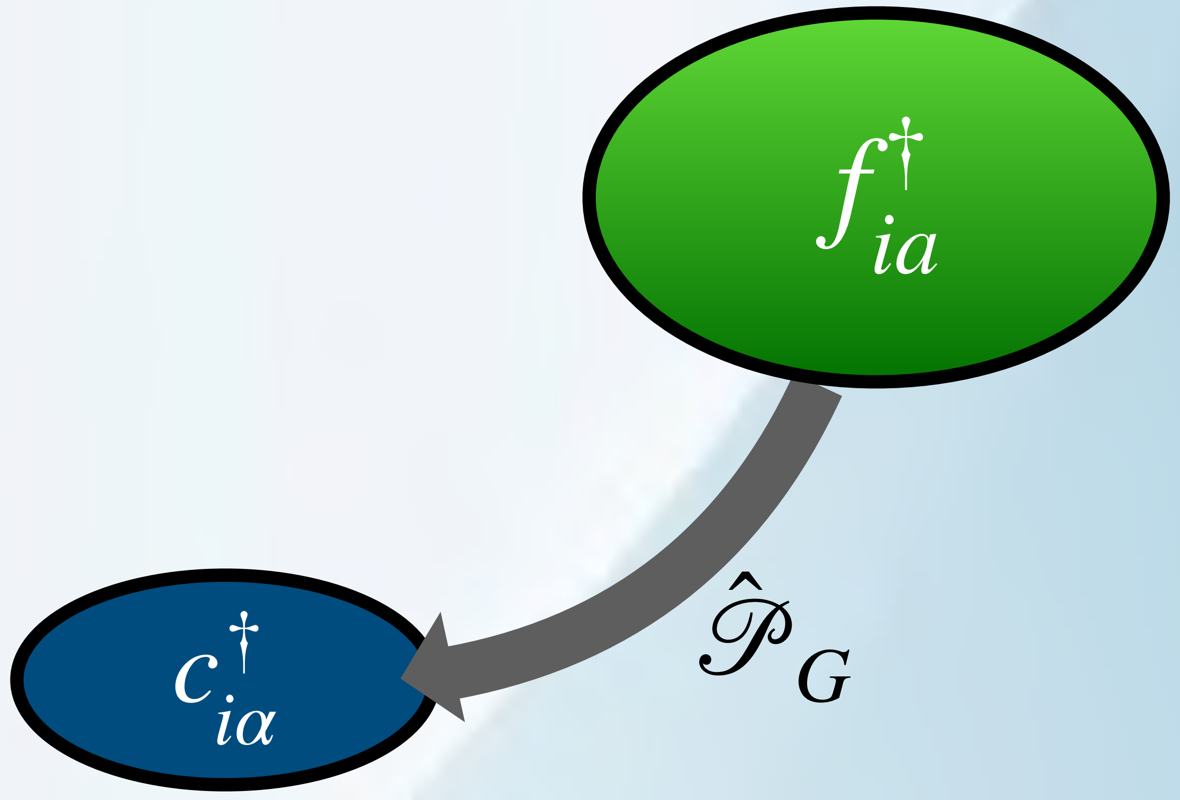
Gutzwiller approximation:

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

Gutzwiller constraints:

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

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



Key consequence:

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i \, f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \cancel{\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle} \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle$$

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

Gutzwiller constraints:

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

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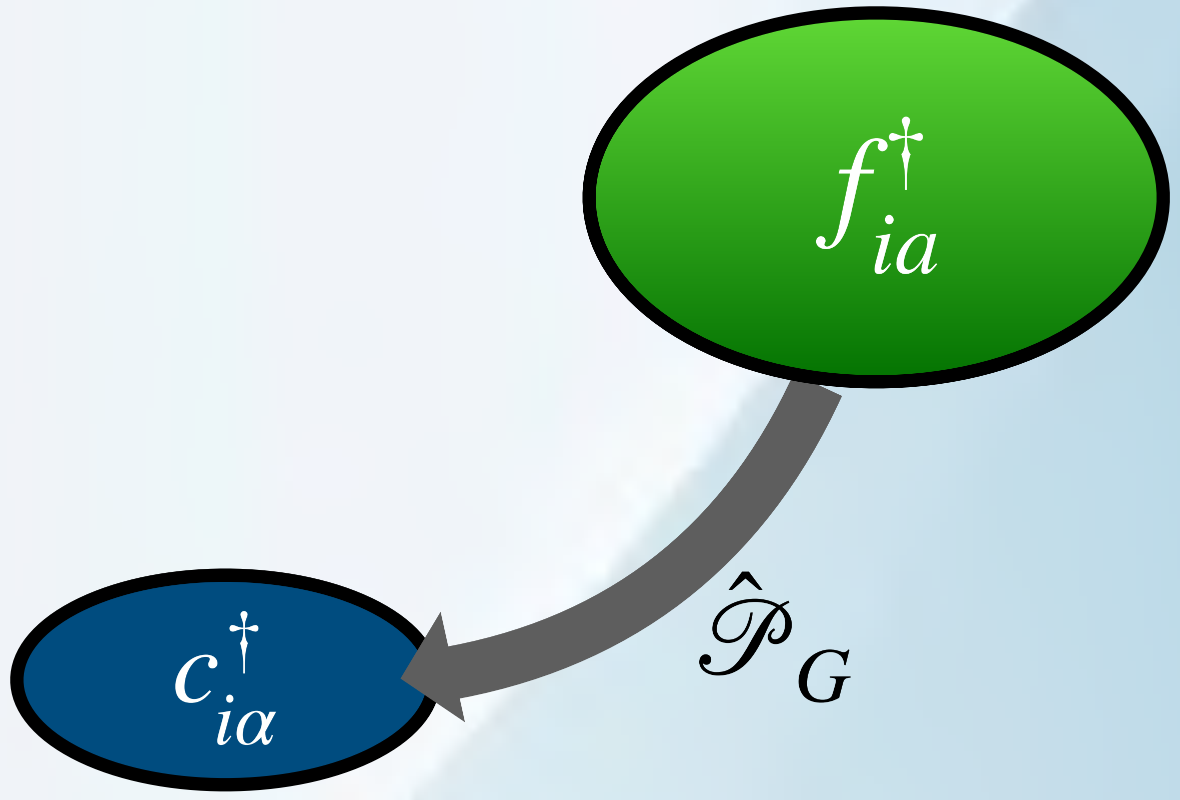
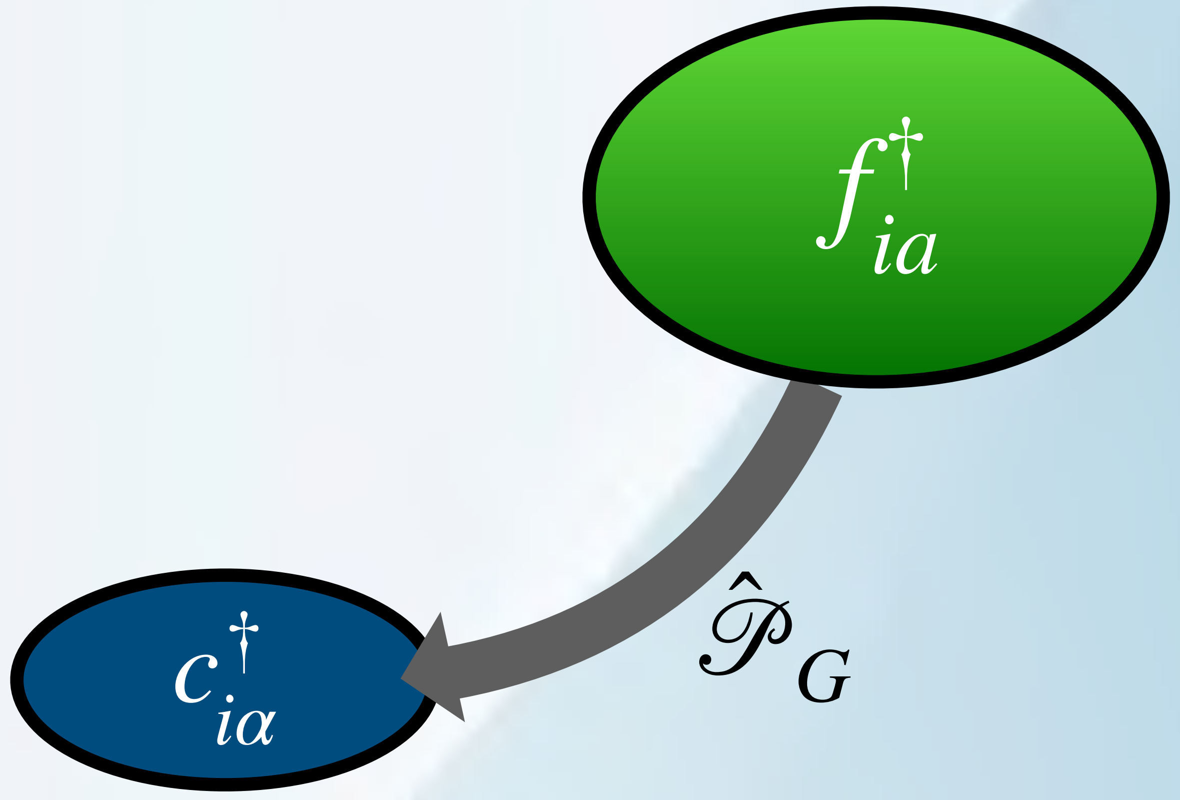


Key consequence:

$$\cancel{\langle \Psi_0 | \hat{\mathscr{P}}_i^\dagger \hat{\mathscr{P}}_i \, f_{ia}^\dagger f_{ib} | \Psi_0 \rangle} = \cancel{\langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle}$$

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

Gutzwiller constraints:



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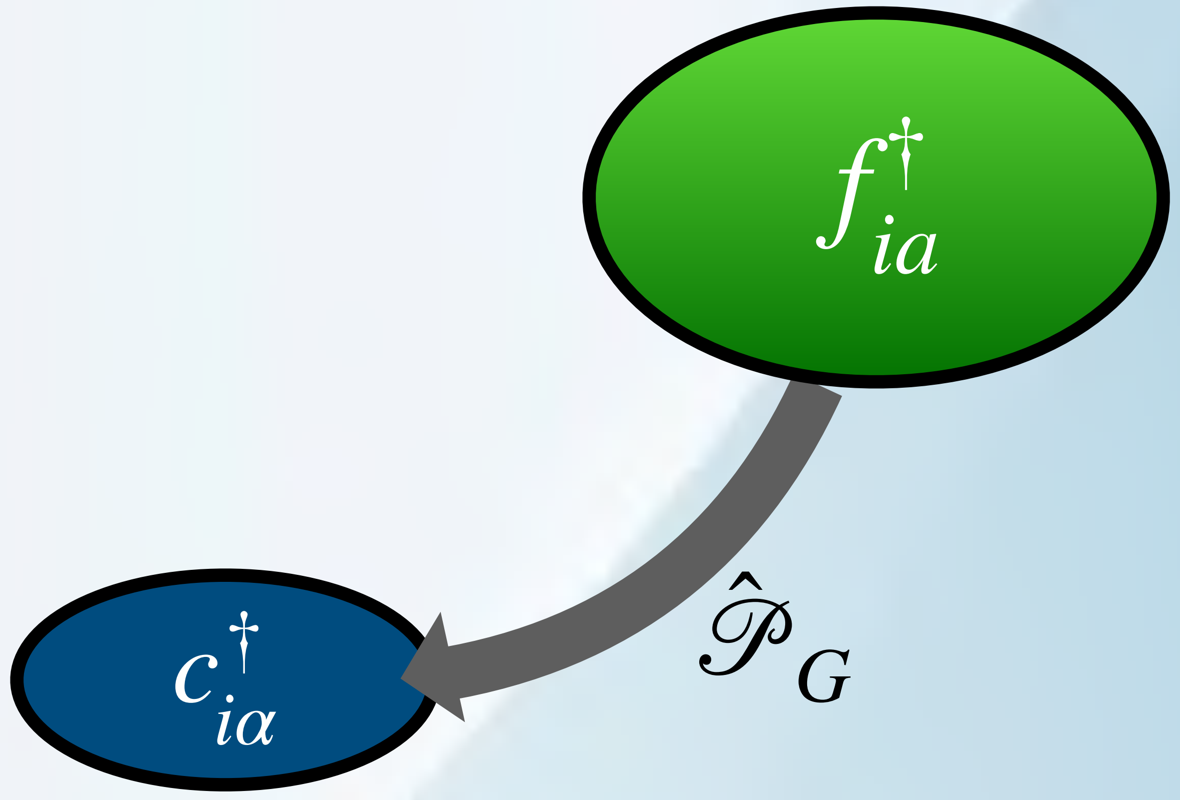
Key consequence:

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

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: *(If* $[\Delta_i]_{ab} := \langle \Psi_0 | f^\dagger_{ia} f_{ib} | \Psi_0 \rangle$ *such that* $\Delta_i(1-\Delta_i)$ *non degenerate)*

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

Necessary steps:

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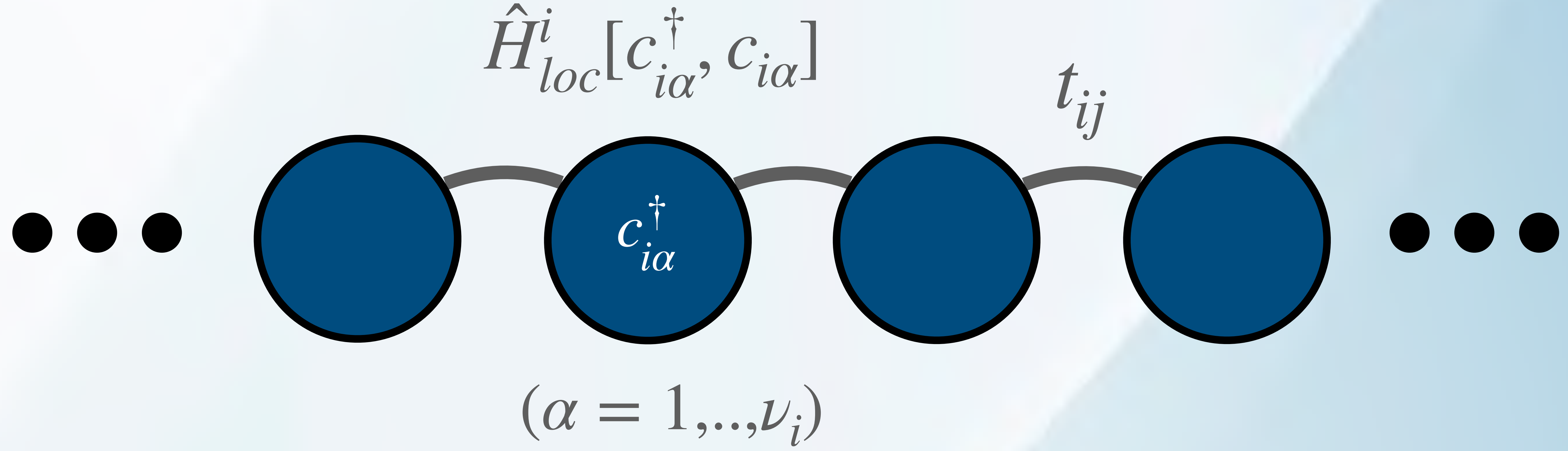
The Hamiltonian:



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

- 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:

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

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

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

Local operators: (disconnected terms)

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

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

(G. constraints)

Local operators: (disconnected terms)

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

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

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

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)

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

(G. Approximation)

(Exact in limit of ∞ dimension)

Local operators:

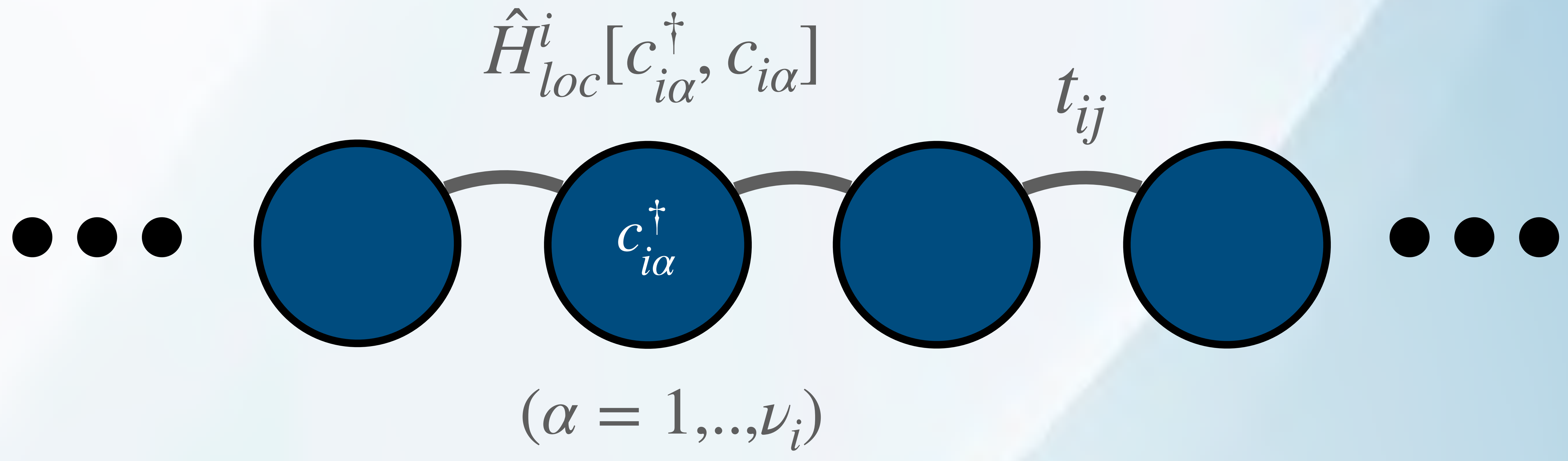
$$\langle \Psi_G | \hat{H}^i_{loc} | \Psi_G \rangle = \langle \Psi_0 | \left(\hat{\mathscr{P}}^\dagger_k \hat{\mathscr{P}}_k \right) \left(\prod_{k' \neq i,k} \hat{\mathscr{P}}^\dagger_{k'} \hat{\mathscr{P}}_{k'} \right) \left(\hat{\mathscr{P}}^\dagger_i \hat{H}^i_{loc} \hat{\mathscr{P}}_i \right) |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

(GA and G. constraints)

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

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

The Hamiltonian:



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

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- $\hat{H}^i_{loc}[c^\dagger_{i\alpha}, c_{i\alpha}]$: 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)

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

Local operators:

$$\langle \Psi_G | \hat{H}^i_{loc} | \Psi_G \rangle \approx \boxed{\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{H}^i_{loc} \hat{\mathcal{P}}_i | \Psi_0 \rangle}$$

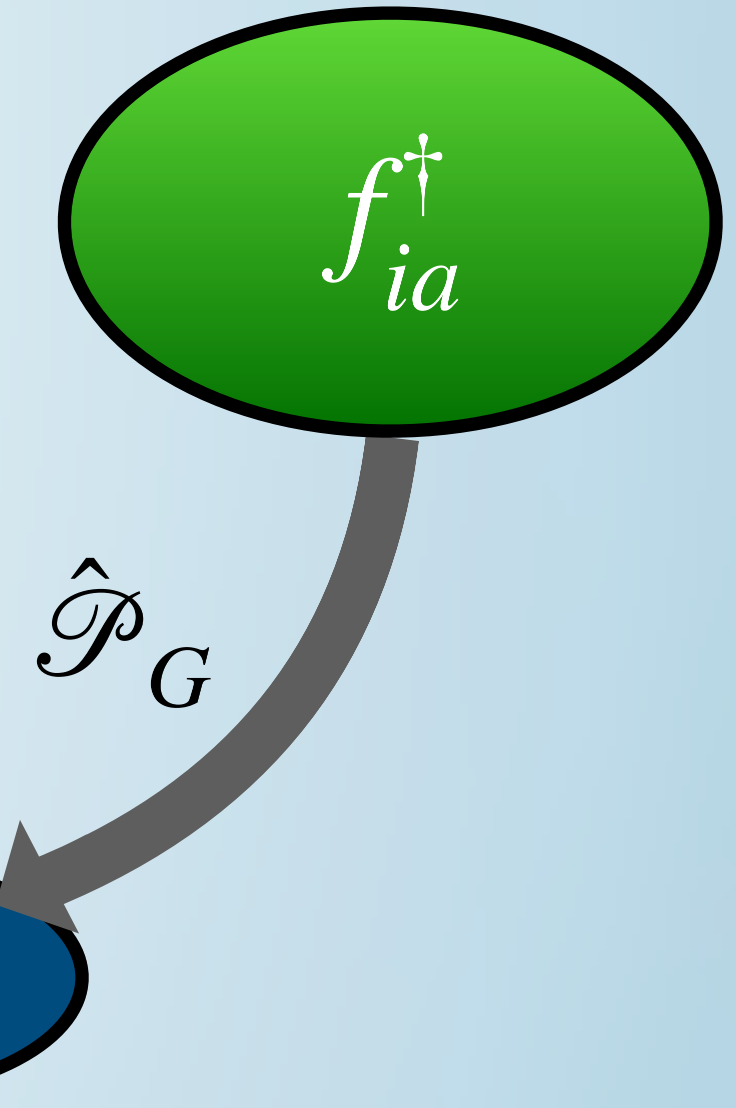
Non-local 1-body operators, i.e., $i \neq j$:

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

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

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

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



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

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

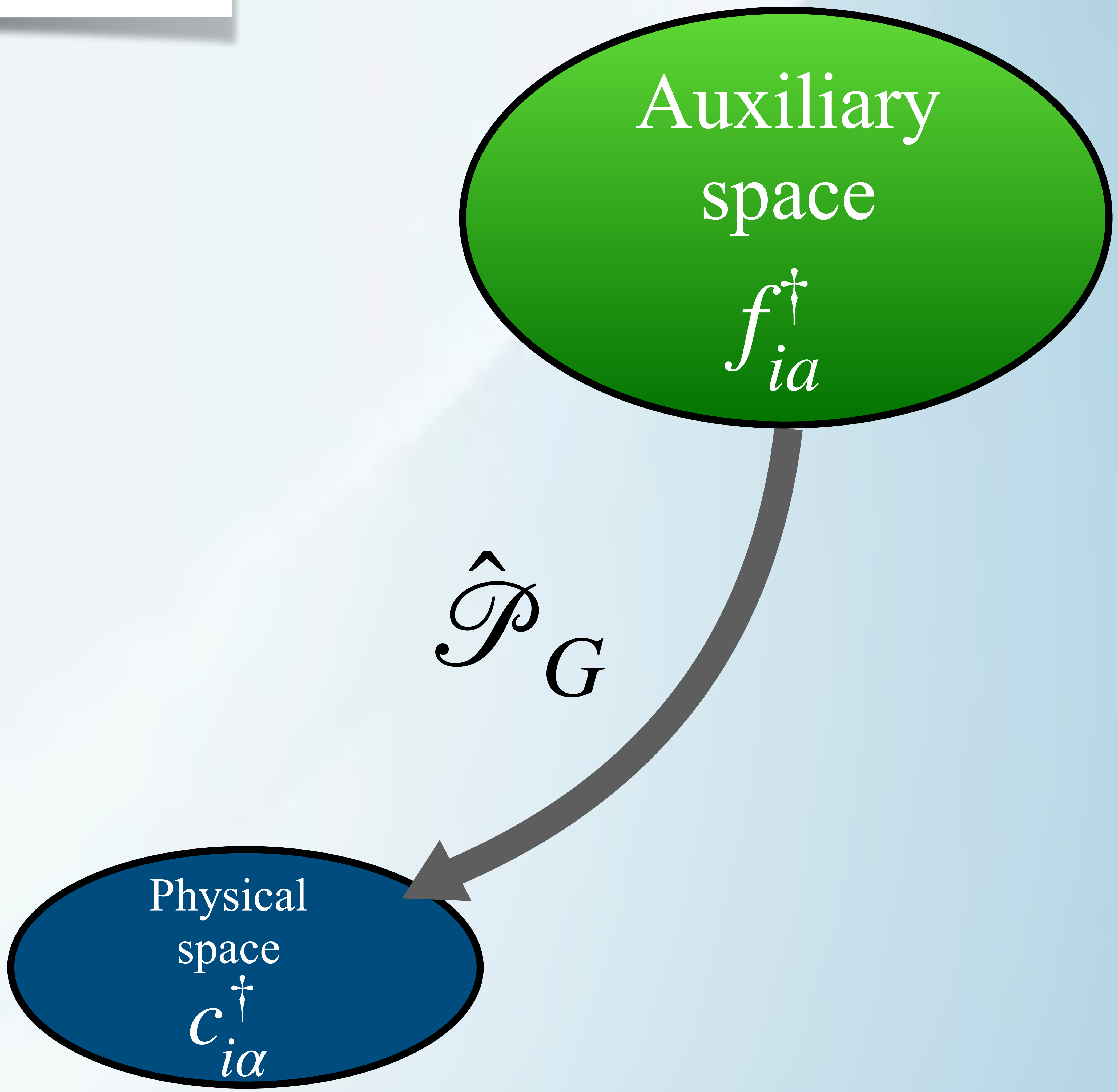
Non-local quadratic operators:

$$\hat{\mathscr{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathscr{P}}_i \to \sum_a [\mathscr{R}_i]_{a\alpha} f_{ia}^\dagger$$

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

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

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



Variational energy:

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

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

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

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

Necessary steps:

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

Variational energy:

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

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

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

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

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

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

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

Where:

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

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

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

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

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

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

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

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

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

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

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

Matrix of SB amplitudes:

$$\phi_i = \hat{\Lambda}_i\sqrt{P_i^0}$$

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

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

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

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

Matrix of SB amplitudes:

$$\phi_i = \hat{\Lambda}_i\sqrt{P_i^0}$$

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

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

Variational energy:

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

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

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

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

Necessary steps:

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

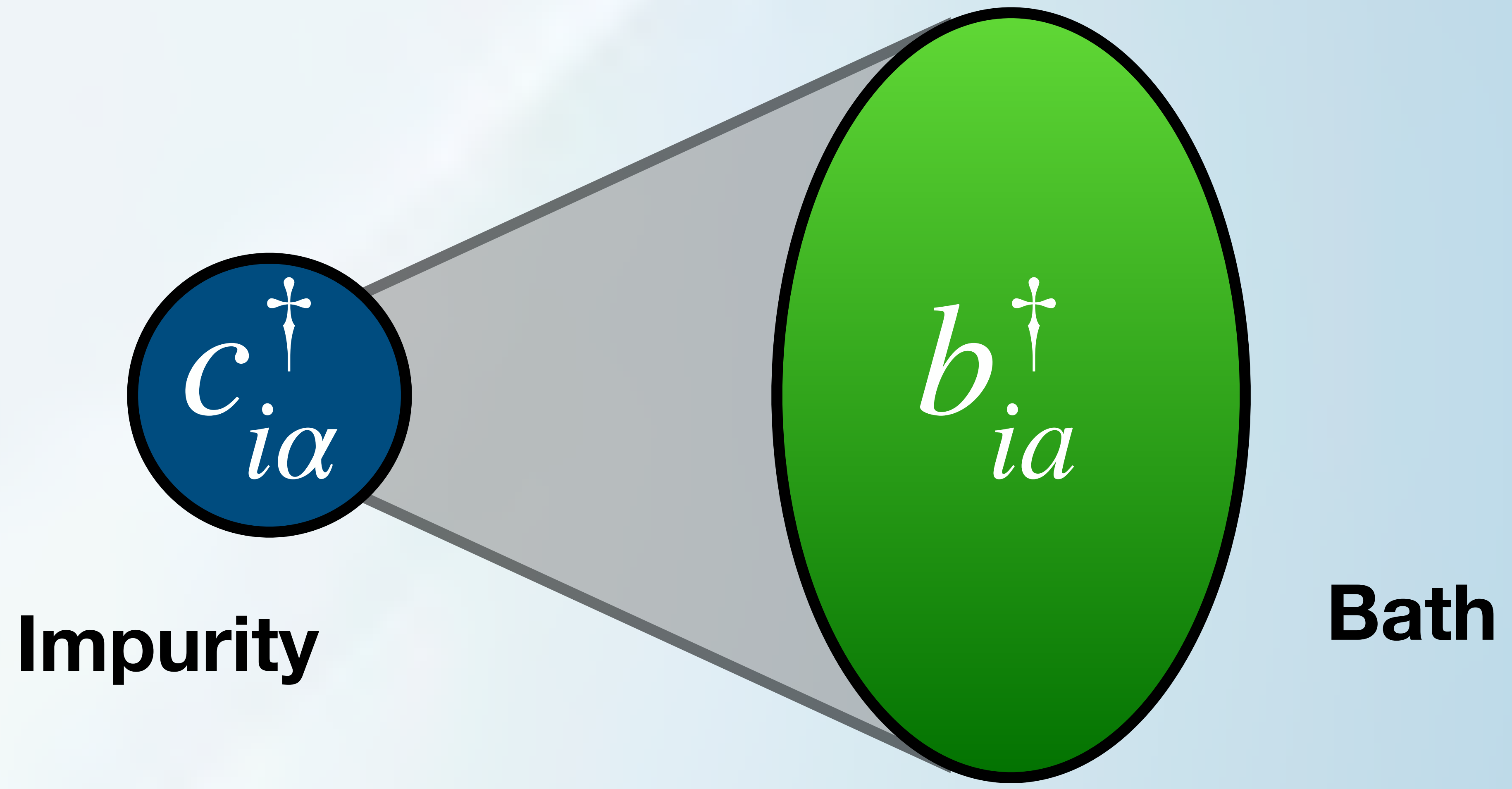
Quantum-embedding formulation

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

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

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

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



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

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

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

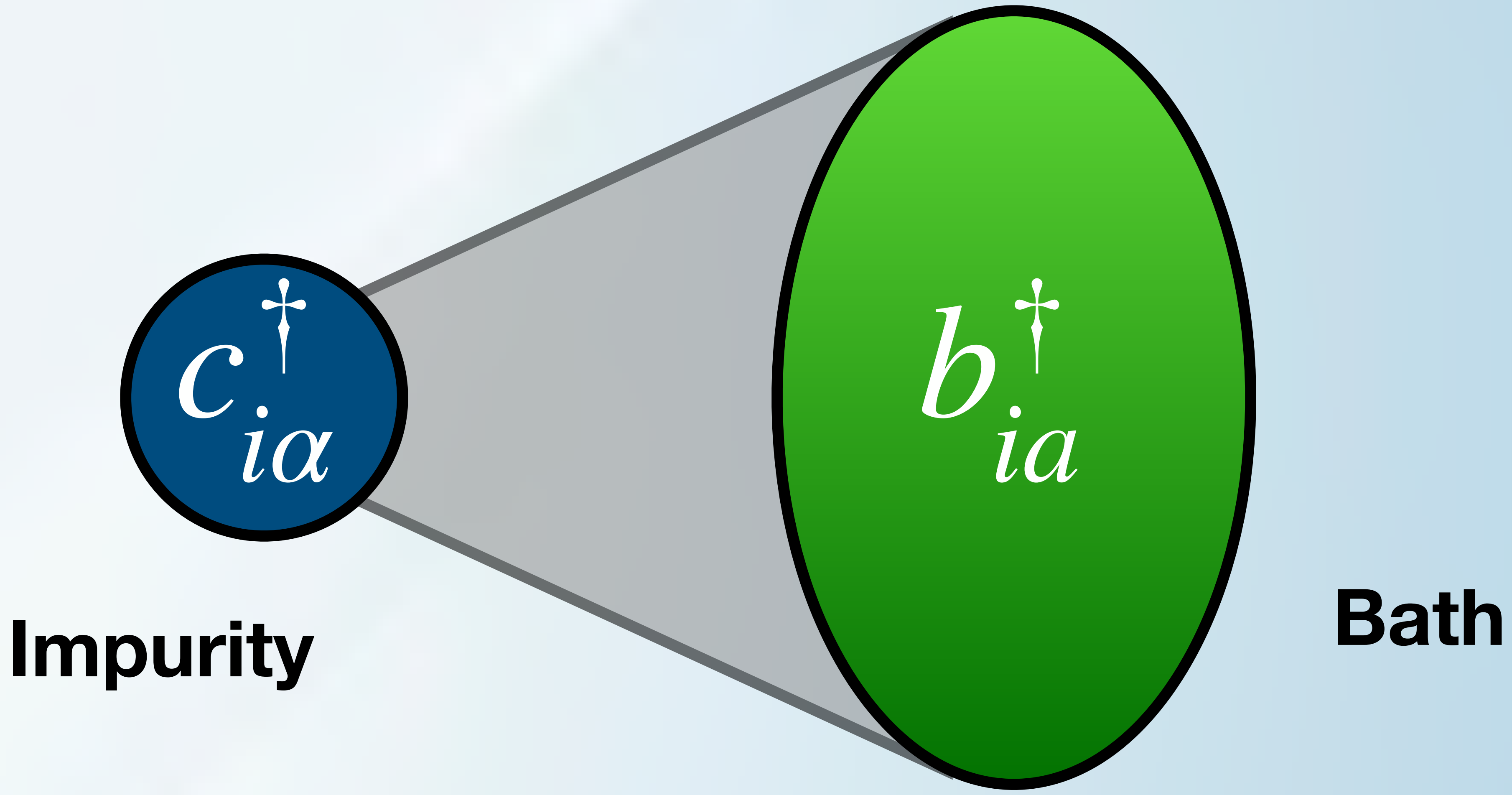
$$|n; i\rangle = [b^\dagger_{i1}]^{q_1(n)} \dots [b^\dagger_{iB\nu_i}]^{q_{B\nu_i}(n)} |0\rangle$$

Quantum-embedding formulation

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

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

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



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

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

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

Variational energy:

$$\hat{H} = \sum_{\mathbf{k}} \sum_{ij} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} t_{\mathbf{k},ij}^{\alpha\beta} c_{\mathbf{k}i\alpha}^\dagger c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}} \sum_{i\geq 1} \hat{H}_{\mathbf{R}i}^{loc}$$

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

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

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

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

Necessary steps:

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

Variational energy:

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

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

$[\mathcal{D}_i]_{a\alpha}$

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

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

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

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

Lagrange function:

$$\mathscr{L} = \langle \Psi_0 | \hat{H}_{qp}[\mathscr{R}, \Lambda] | \Psi_0 \rangle + E \left(1 - \langle \Psi_0 | \Psi_0 \rangle \right)$$

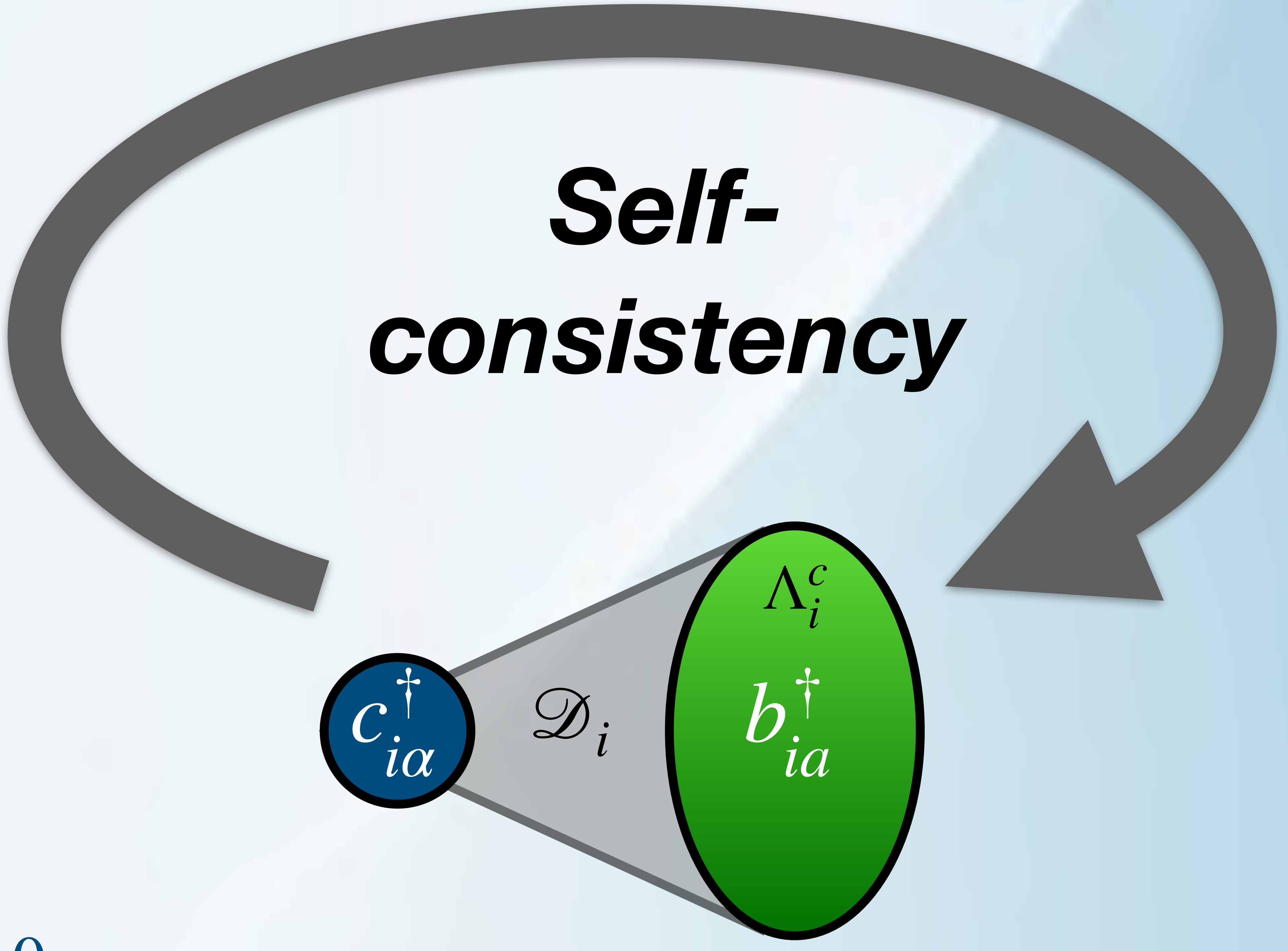
$$+ \sum_{i=1}^{\mathscr{N}} \left[\langle \Phi_i | \hat{H}_i^{emb}[\mathscr{D}_i, \Lambda_i^c] | \Phi_i \rangle + E_i^c \left(\mathbf{1} - \langle \Phi_i | \Phi_i \rangle \right) \right]$$

$$- \sum_{i=1}^{\mathscr{N}} \left[\sum_{a,b=1}^{B\nu_i} \left([\Lambda_i]_{ab} + [\Lambda_i^c]_{ab} \right) [\Delta_i]_{ab} + \sum_{c,a=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \left([\mathscr{D}_i]_{a\alpha} [\mathscr{R}_i]_{c\alpha} [\Delta_i(\mathbf{1} - \Delta_i)]_{ca}^{\frac{1}{2}} + \text{c.c.} \right) \right]$$

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

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

Lagrange equations:



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

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

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

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

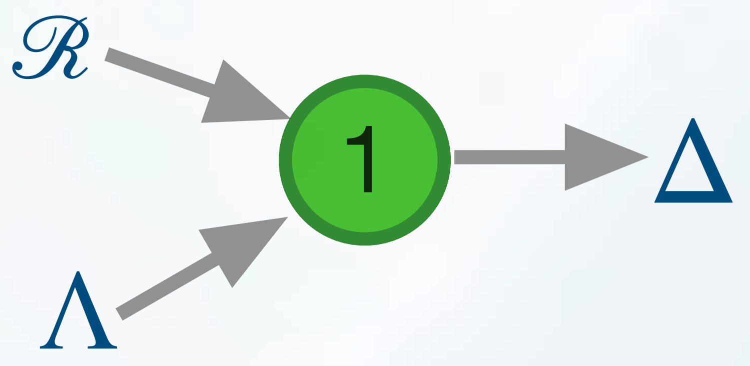
$$\left\langle\Phi_i\right| c_{i\alpha}^{\dagger} b_{ia} \left|\Phi_i\right\rangle - \sum_{c=1} \left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}} \left[\mathcal{R}_i\right]_{c\alpha} = 0$$

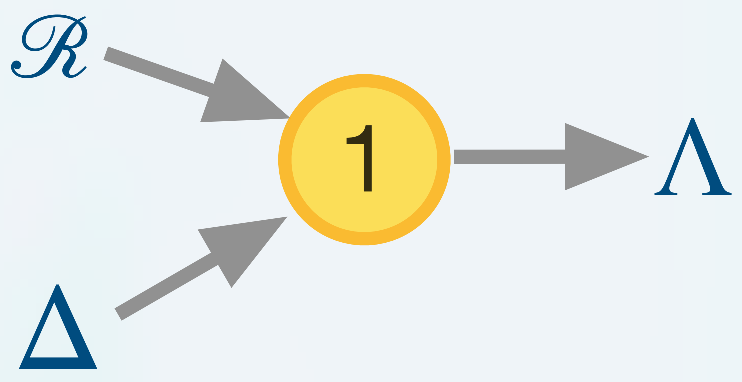
$$\left\langle\Phi_i\right| b_{ib} b_{ia}^{\dagger} \left|\Phi_i\right\rangle - \left[\Delta_i\right]_{ab} = 0$$

$$\begin{cases} \Delta_i = \sum_{s=1}^{(B\nu_i)^2} \left[d_i^0\right]_s {}^t \left[h_i\right]_s \\ \Lambda_i = \sum_{s=1}^{(B\nu_i)^2} \left[l_i\right]_s \left[h_i\right]_s \\ \Lambda_i^c = \sum_{s=1}^{(B\nu_i)^2} \left[l_i^c\right]_s \left[h_i\right]_s \end{cases}$$

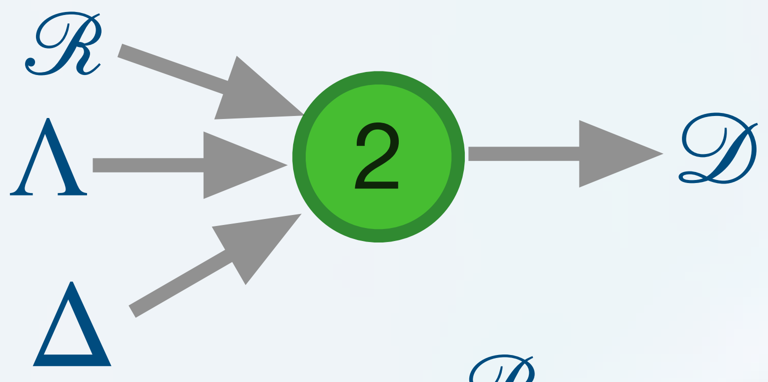
Lagrange equations:

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

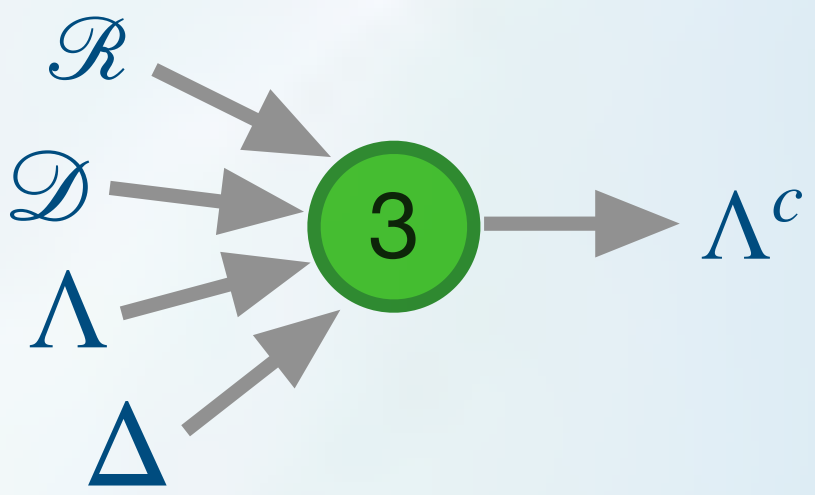


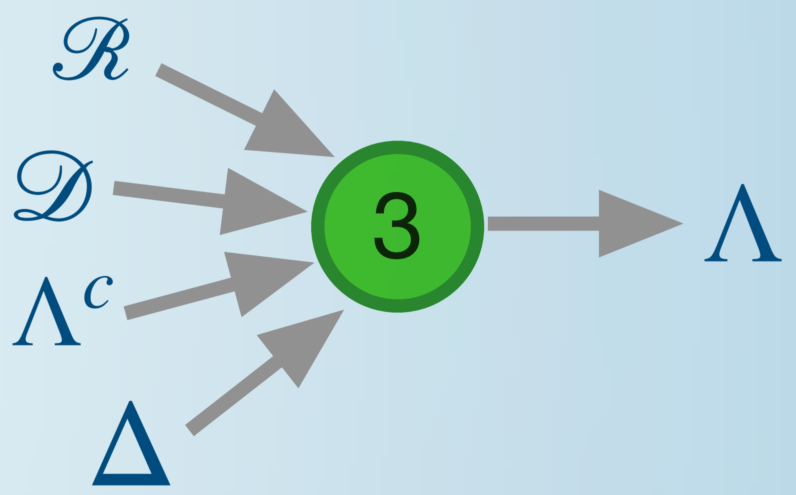


$$\left[\Pi_i t\mathscr{R}^\dagger f\left(\mathscr{R}t\mathscr{R}^\dagger+\Lambda\right)\Pi_i\right]_{\alpha a} = \sum_{c,a=1}^{B\nu_i}\sum_{\alpha=1}^{\nu_i}\left[\mathscr{D}_i\right]_{c\alpha}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}$$



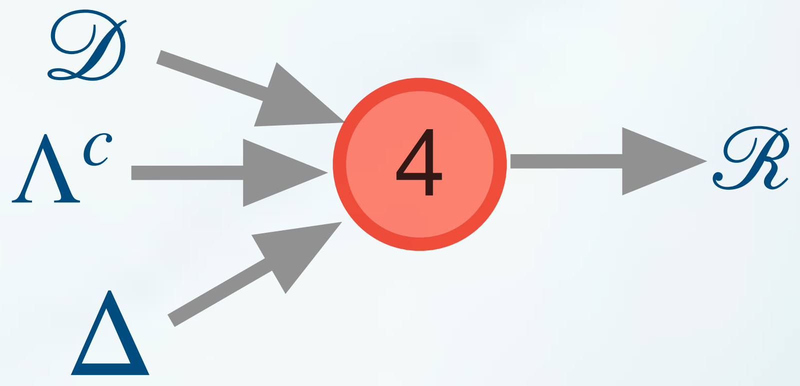
$$\sum_{c,b=1}^{B\nu_i}\sum_{\alpha=1}^{\nu_i}\frac{\partial}{\partial\left[d_i^0\right]_s}\left(\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}_{cb}\left[\mathscr{D}_i\right]_{b\alpha}\left[\mathscr{R}_i\right]_{c\alpha}+\mathrm{c.c.}\right)+\left[l_i+l_i^c\right]_s=0$$



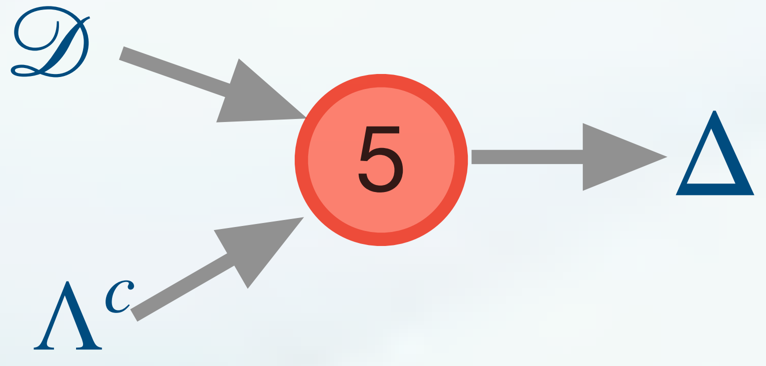


$$\hat{H}^i_{emb}[\mathscr{D}_i,\Lambda_i^c]\,|\,\Phi_i\rangle = E_i^c\,|\,\Phi_i\rangle \quad\longrightarrow\quad |\,\Phi_i\rangle$$

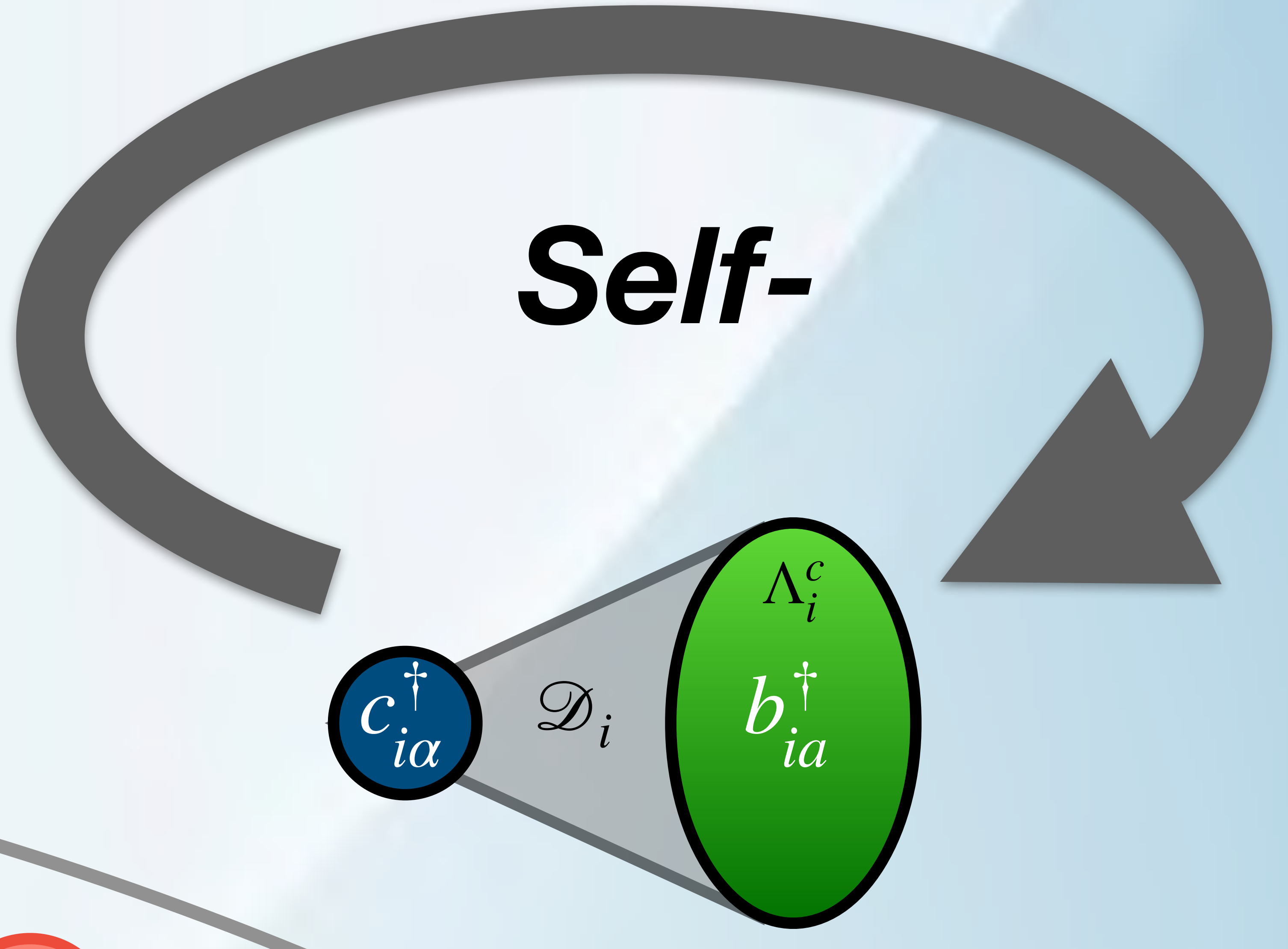
$$\langle\Phi_i\,|\,c^\dagger_{i\alpha}b_{ia}\,|\,\Phi_i\rangle - \sum_{c=1}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}\left[\mathscr{R}_i\right]_{c\alpha}=0$$

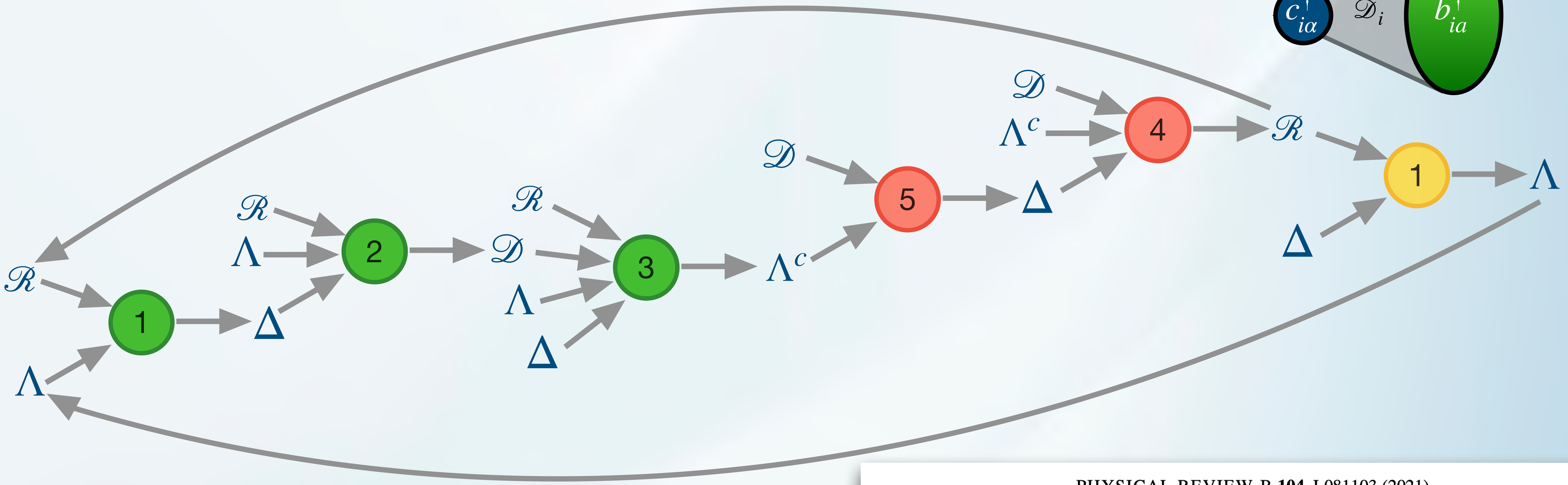


$$\langle\Phi_i\,|\,b_{ib}b^\dagger_{ia}\,|\,\Phi_i\rangle-\left[\Delta_i\right]_{ab}=0$$



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:

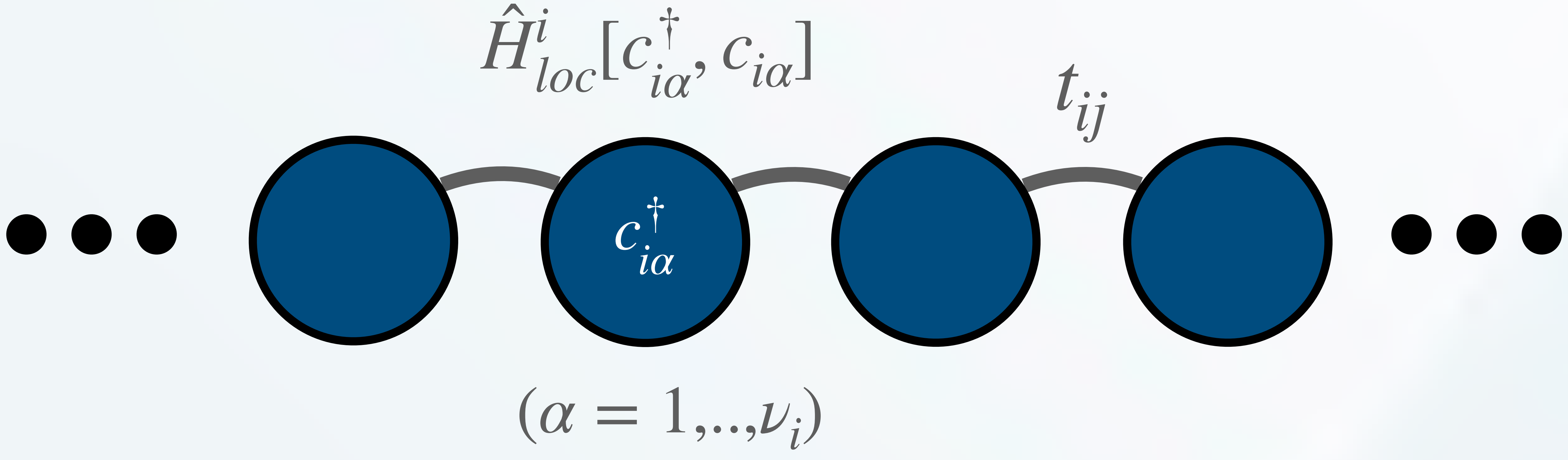
PHYSICAL REVIEW B **96**, 235139 (2017)

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]

Summary steps done

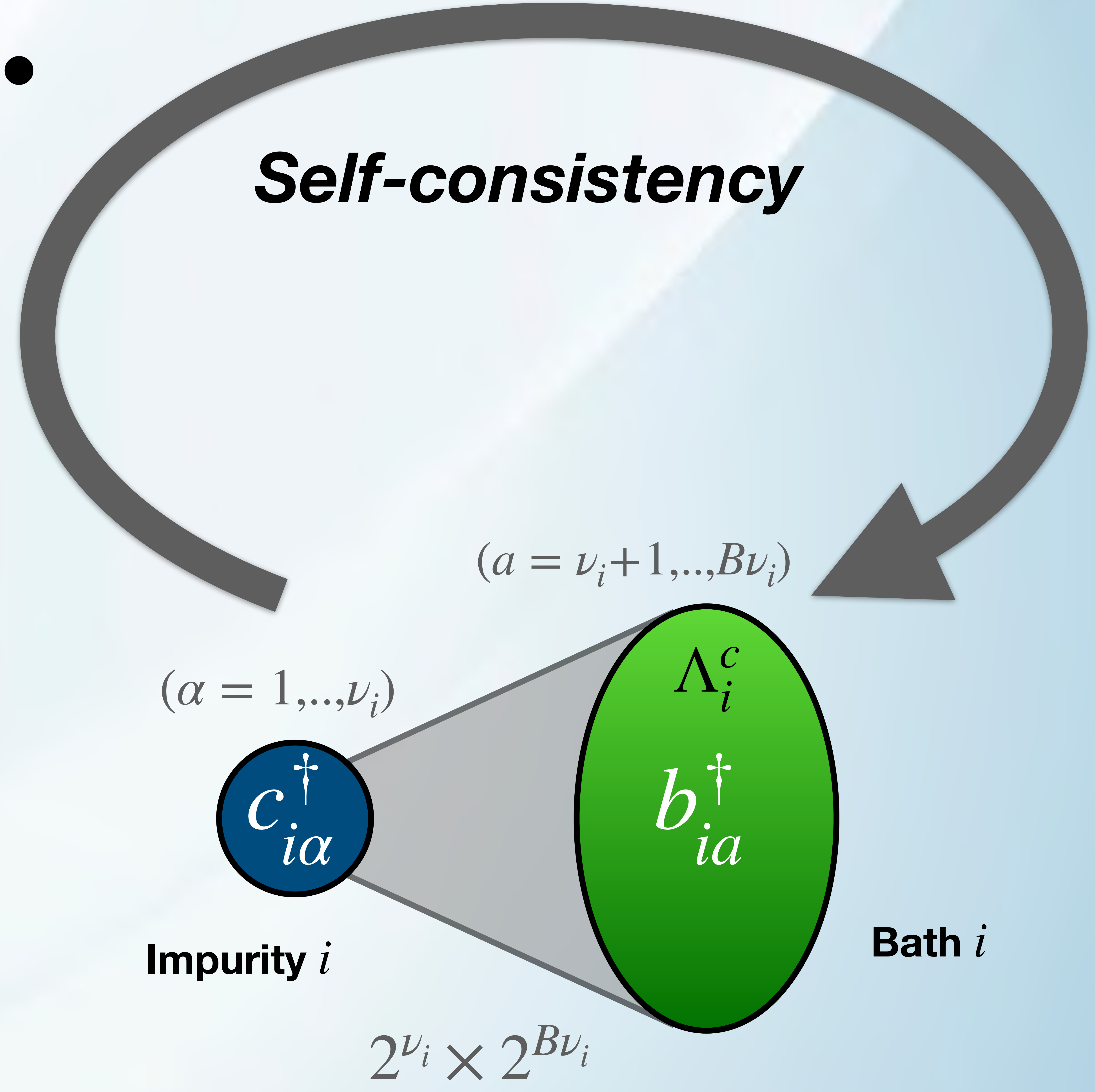
1. Definition of approximations (GA and G. constraints).
2. Evaluation of $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ in terms of $\{\hat{\Lambda}_i\}, | \Psi_0 \rangle$.
3. Definition of slave-boson (SB) amplitudes.
4. Mapping from SB amplitudes to embedding states.
5. Lagrange formulation of the optimization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



Quantum-embedding formulation

$$[\hat{\Lambda}_i]_{\Gamma n} \longleftrightarrow |\Phi_i\rangle$$

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



Outline

A. Quantum Embedding (QE) methods.

B. gGA method (multi-orbital models): *QE formulation*.

Supplementary topics:

- Spectral properties

- Examples of applications.

- Recent formalism extensions and open problems.

Spectral properties

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

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

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

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)

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

Spectral properties

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

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$$\Sigma_i(\omega) = t_{loc} - \omega\frac{\mathbf{1} - \mathscr{R}_i^\dagger\mathscr{R}_i}{\mathscr{R}_i^\dagger\mathscr{R}_i} + \left[\mathscr{R}_i\right]^{-1}\Lambda_i\left[\mathscr{R}_i^\dagger\right]^{-1}$$

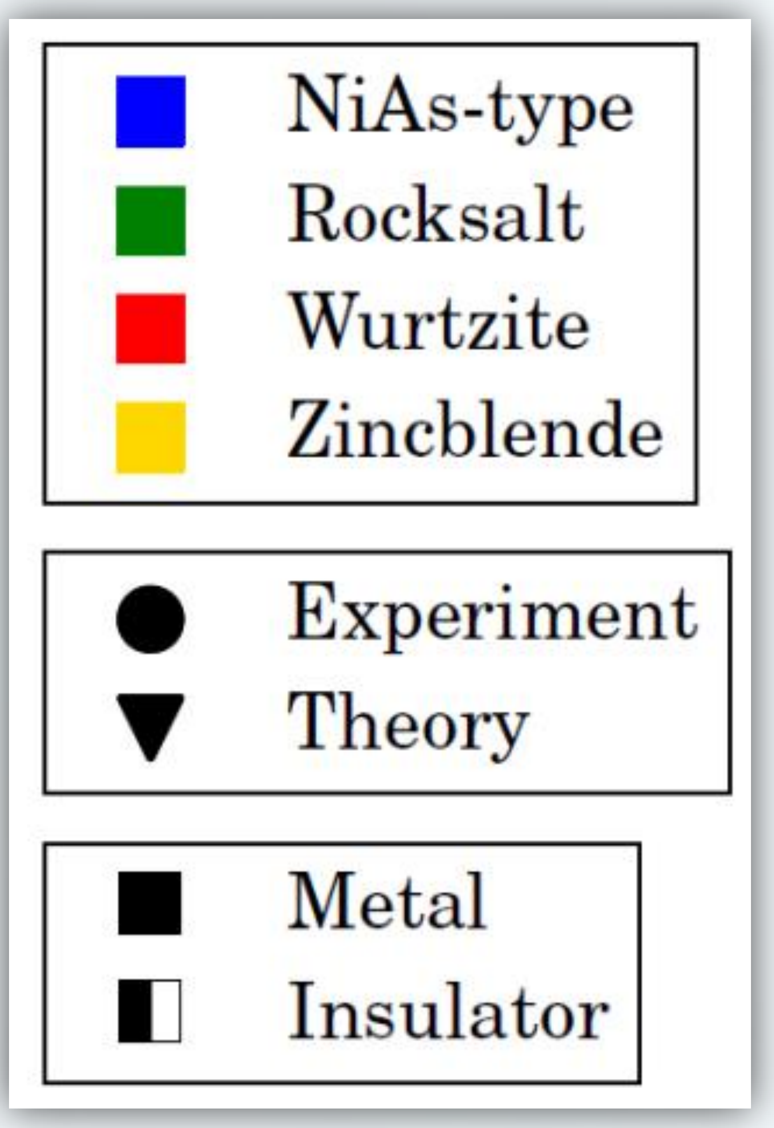
Example: *Structure, Density, Gap*
Theory vs Experiments

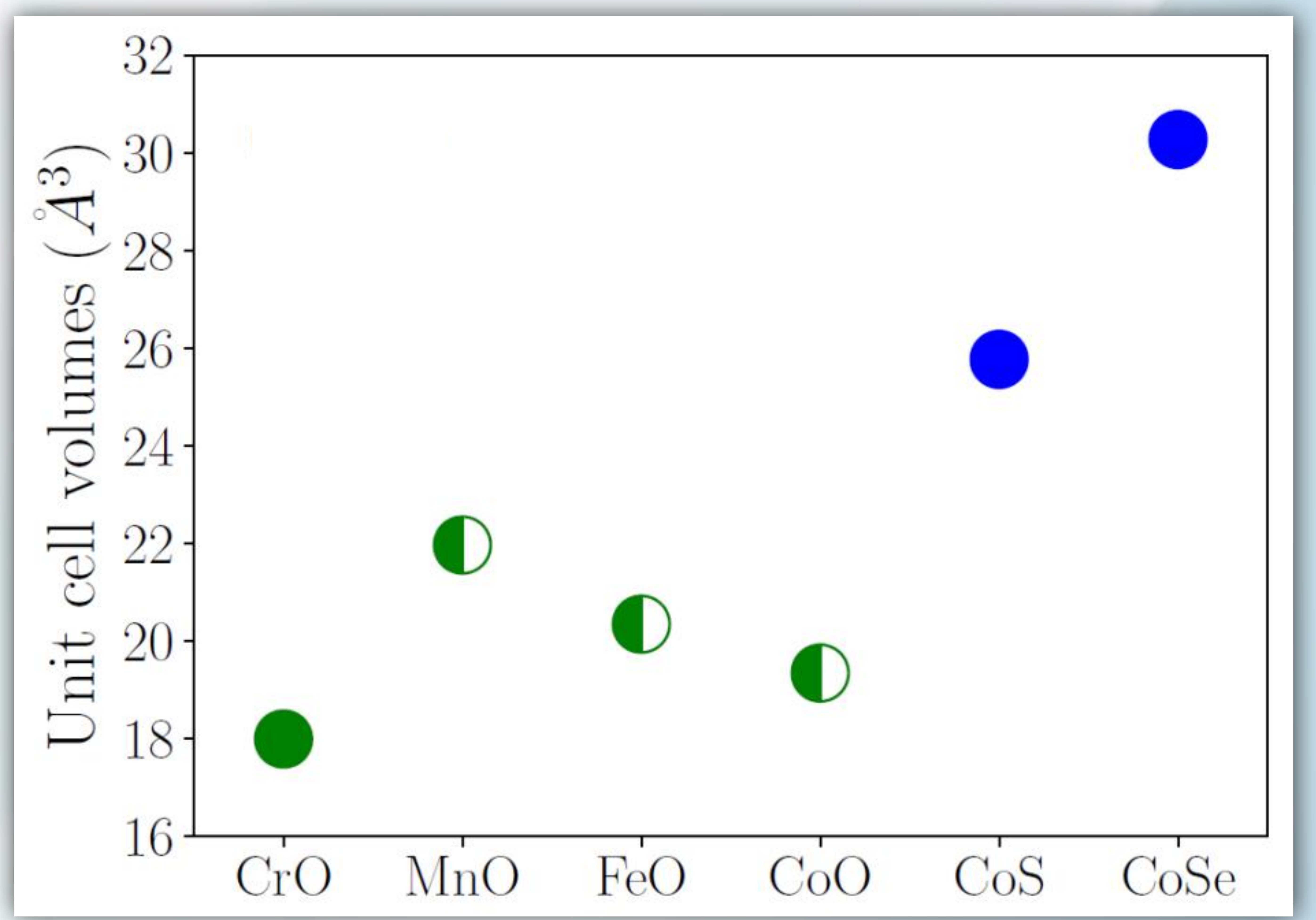
npj Computational Materials www.nature.com/npjcompumats

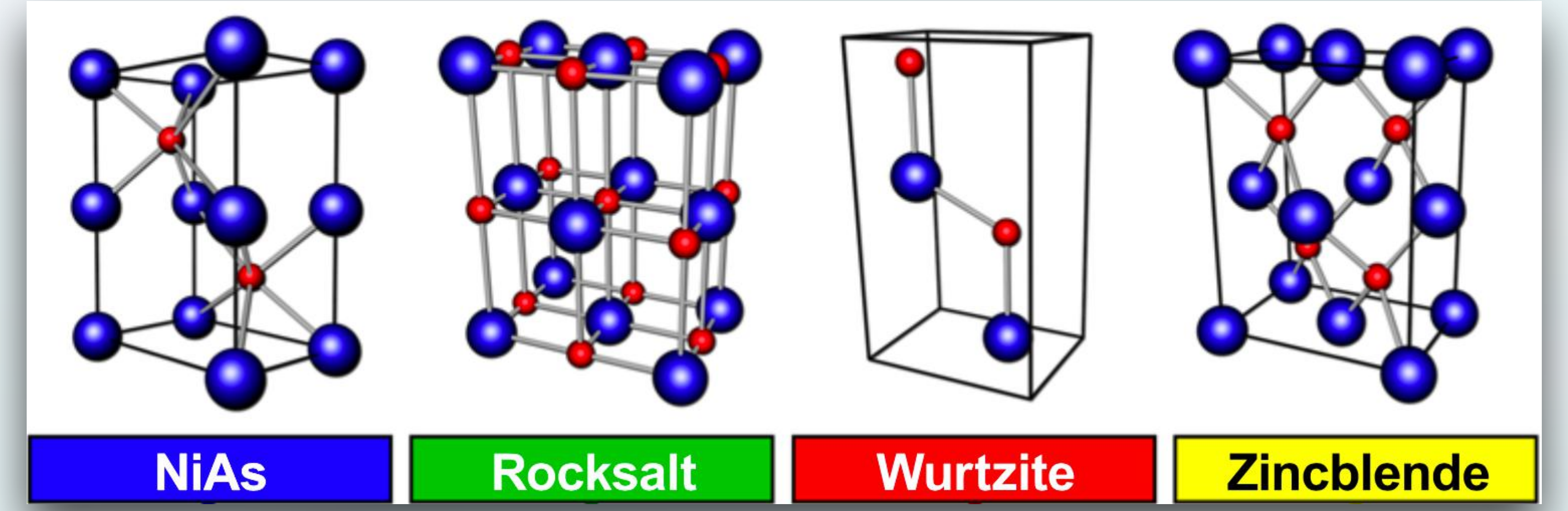
ARTICLE OPEN

Connection between Mott physics and crystal structure in a series of transition metal binary compounds

Nicola Lanatà[1], Tsung-Han Lee[2,3], Yong-Xin Yao[4], Vladan Stevanović[5] and Vladimir Dobrosavljević[2]







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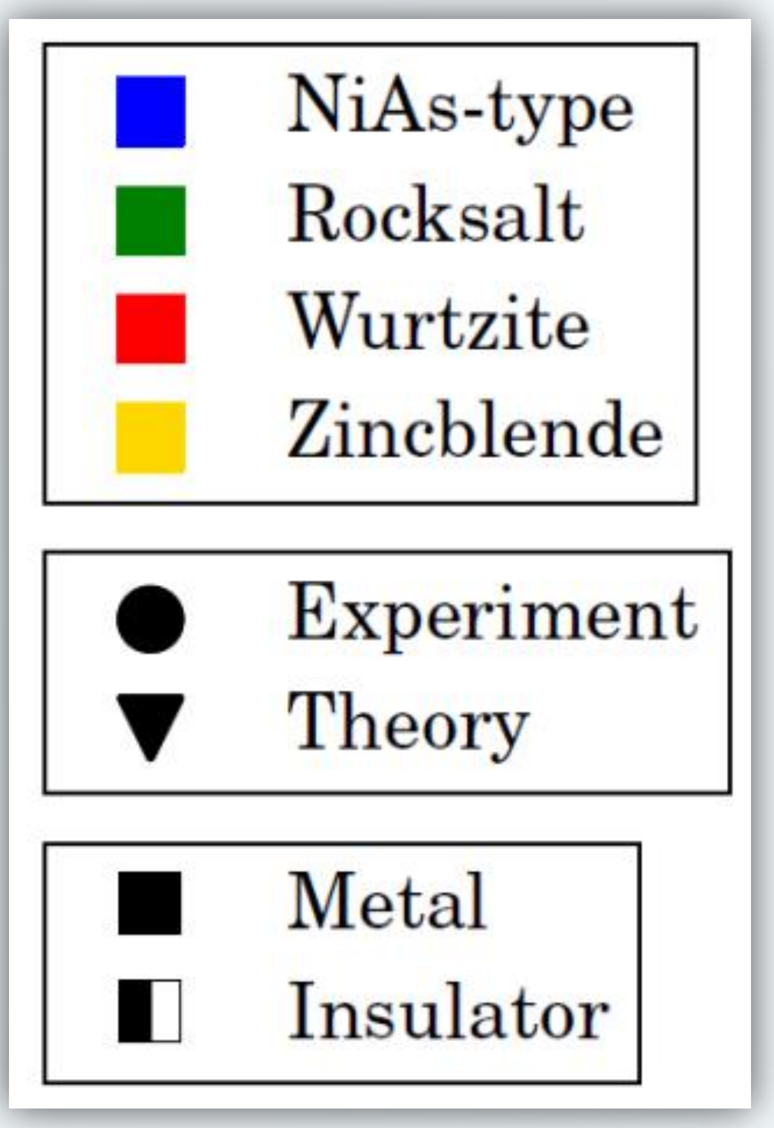
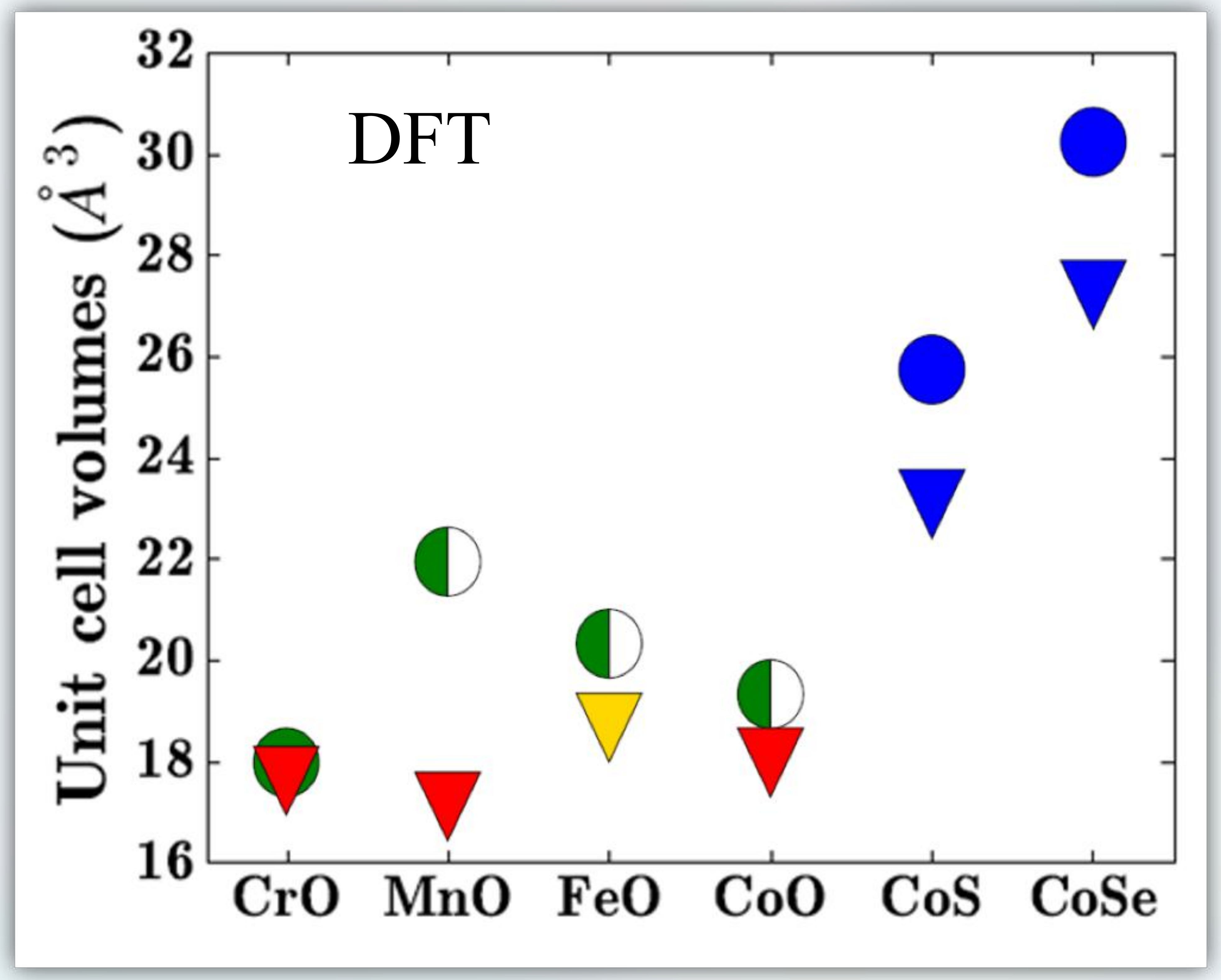
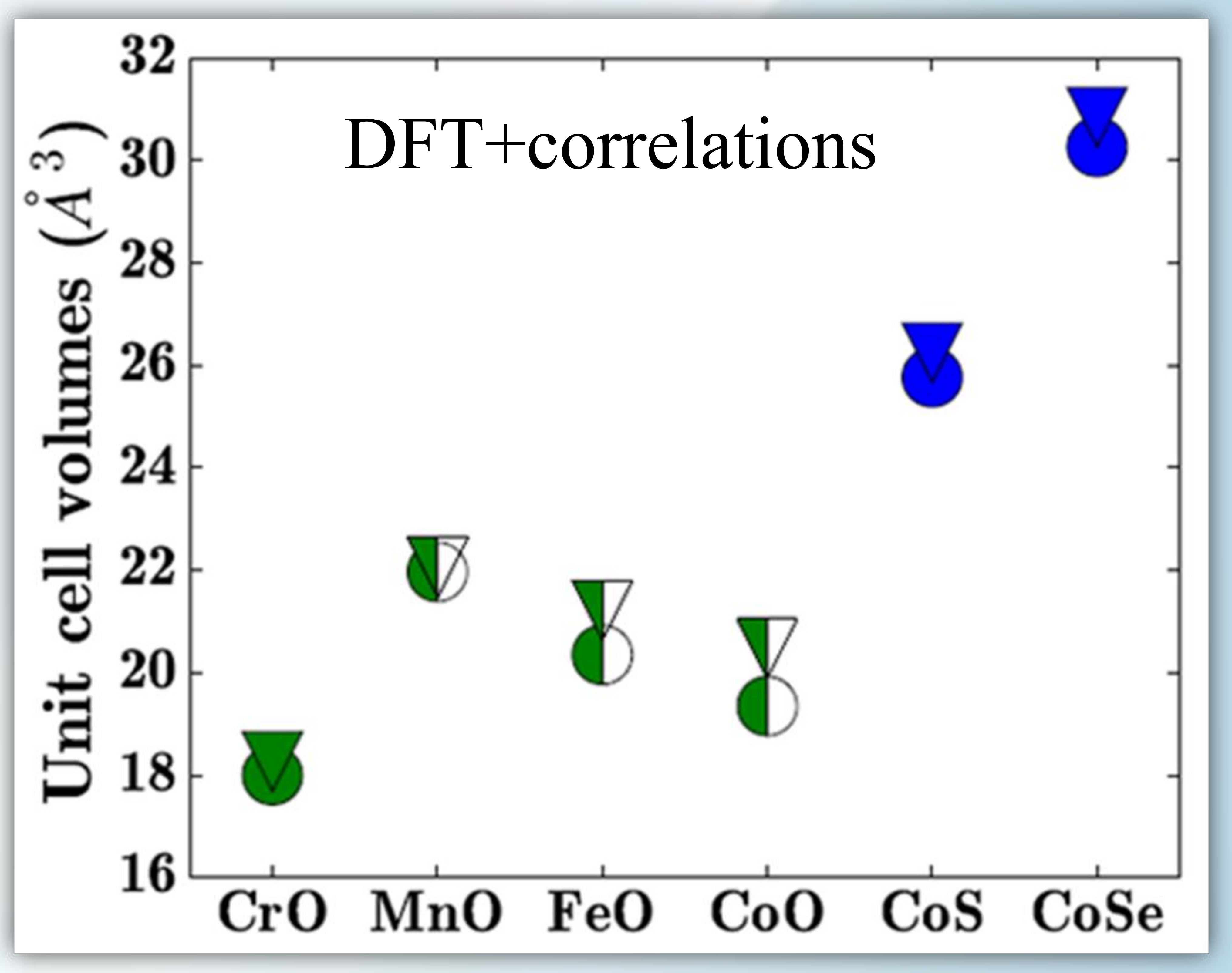




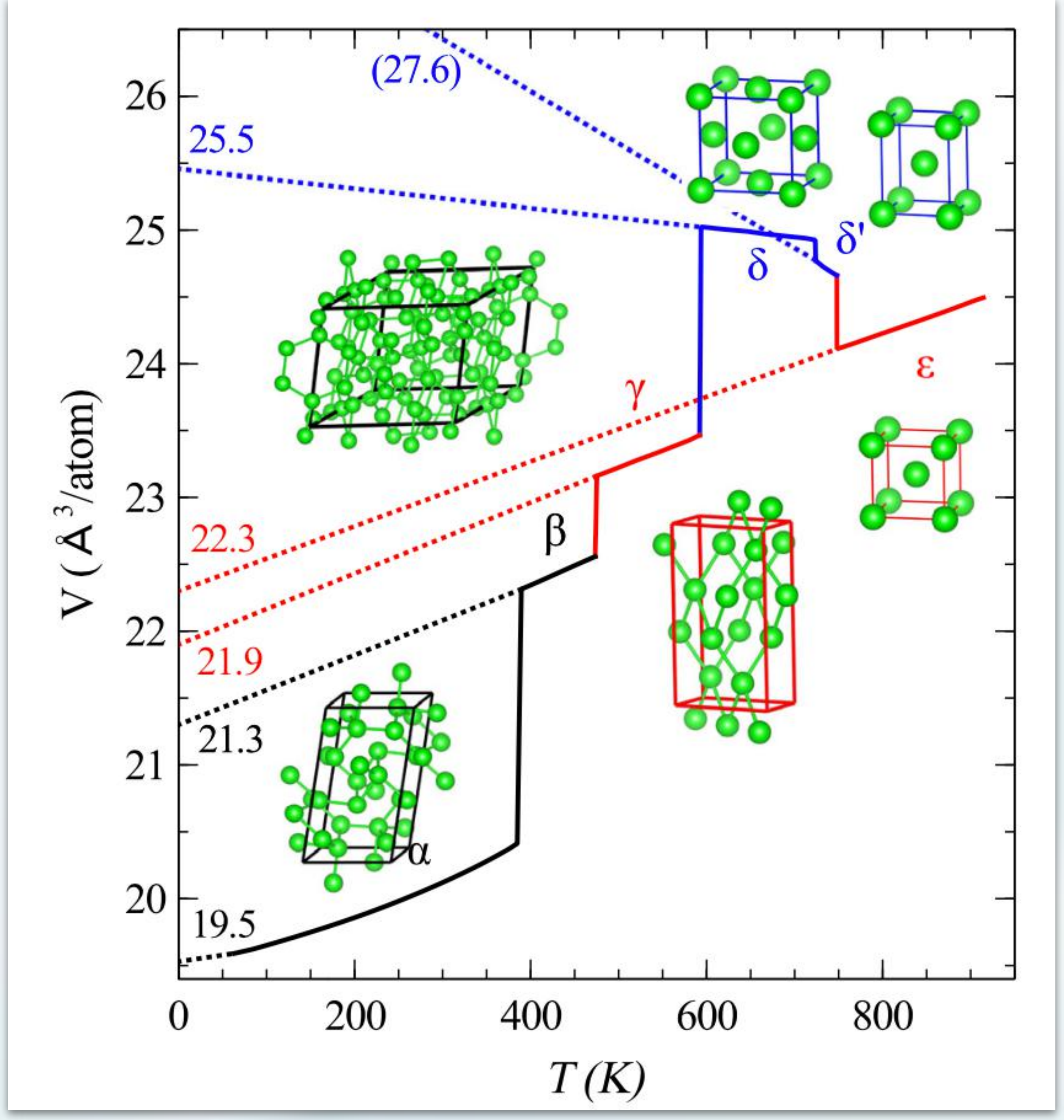


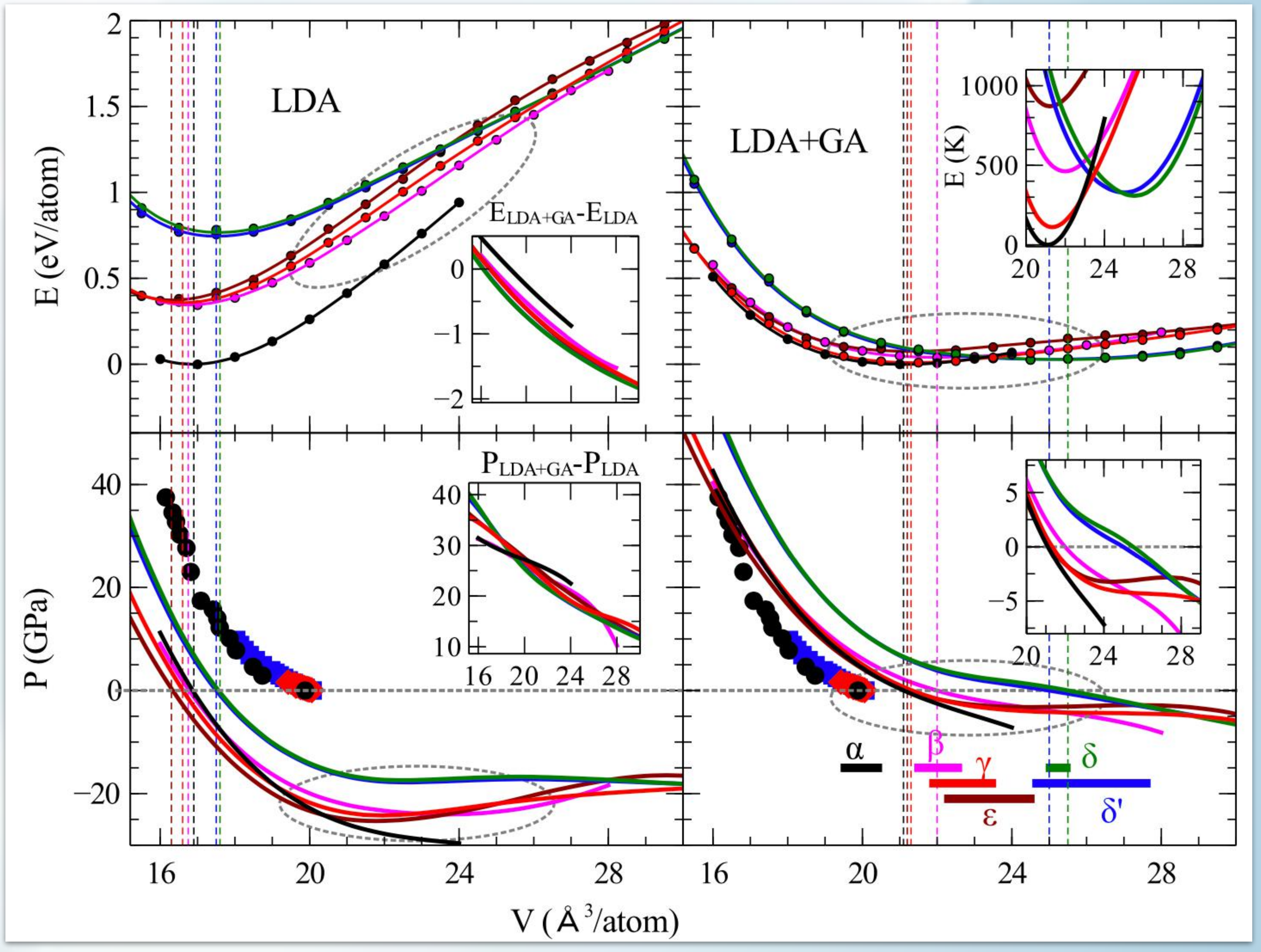
Example: phase diagram of Pu

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

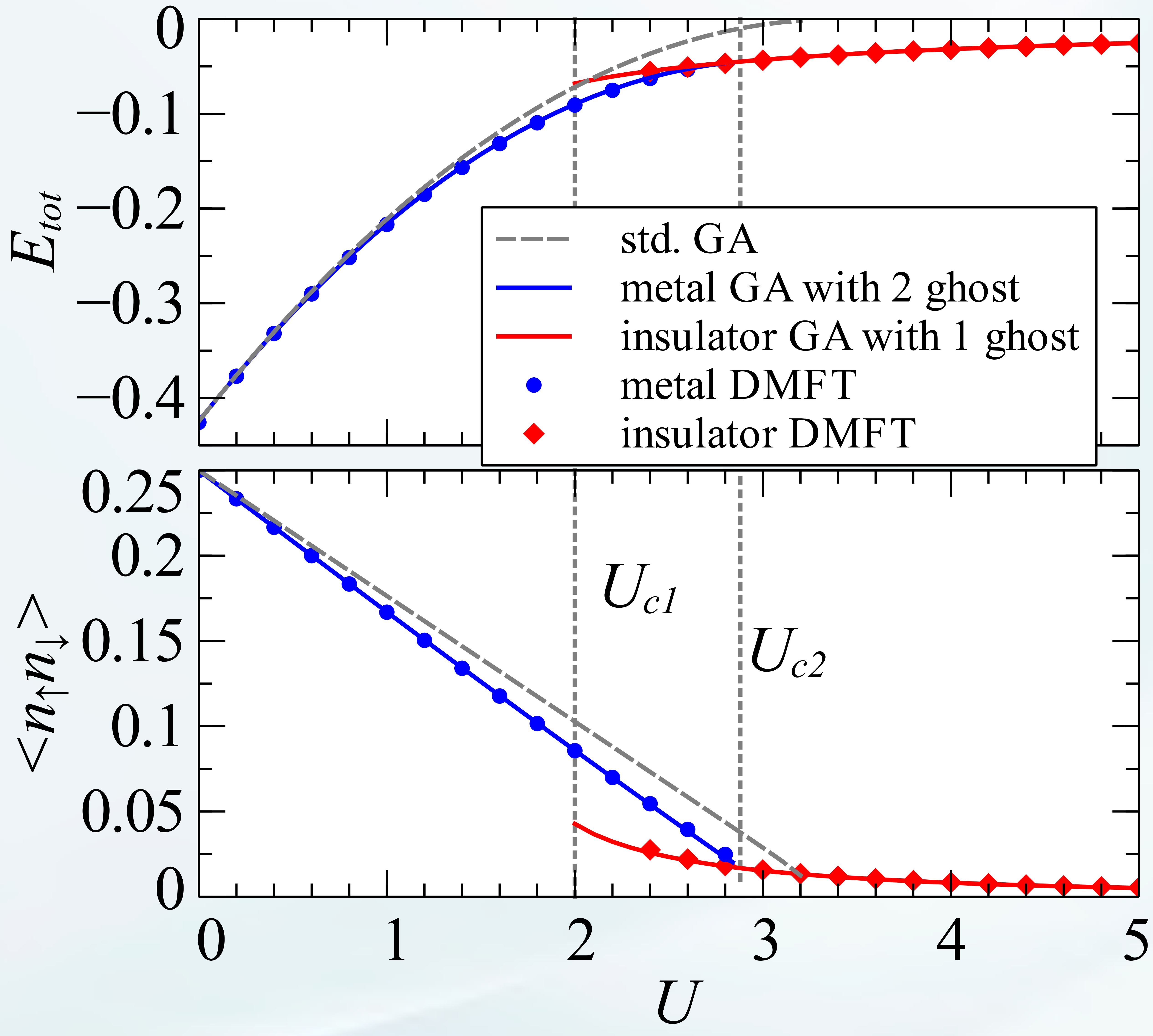
Phase Diagram and Electronic Structure of Praseodymium and Plutonium

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

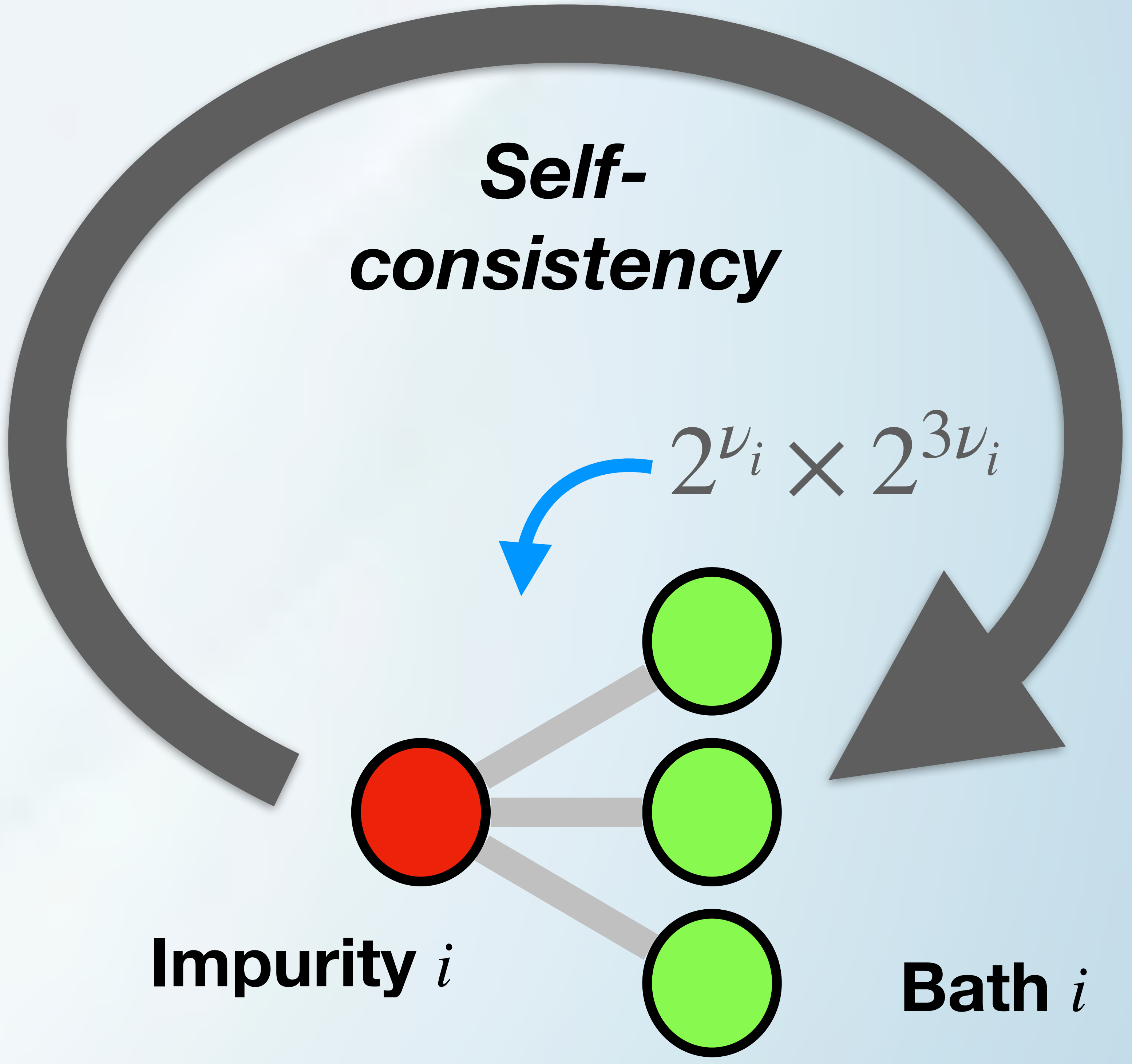




Benchmark calculations Hubbard model:



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



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]

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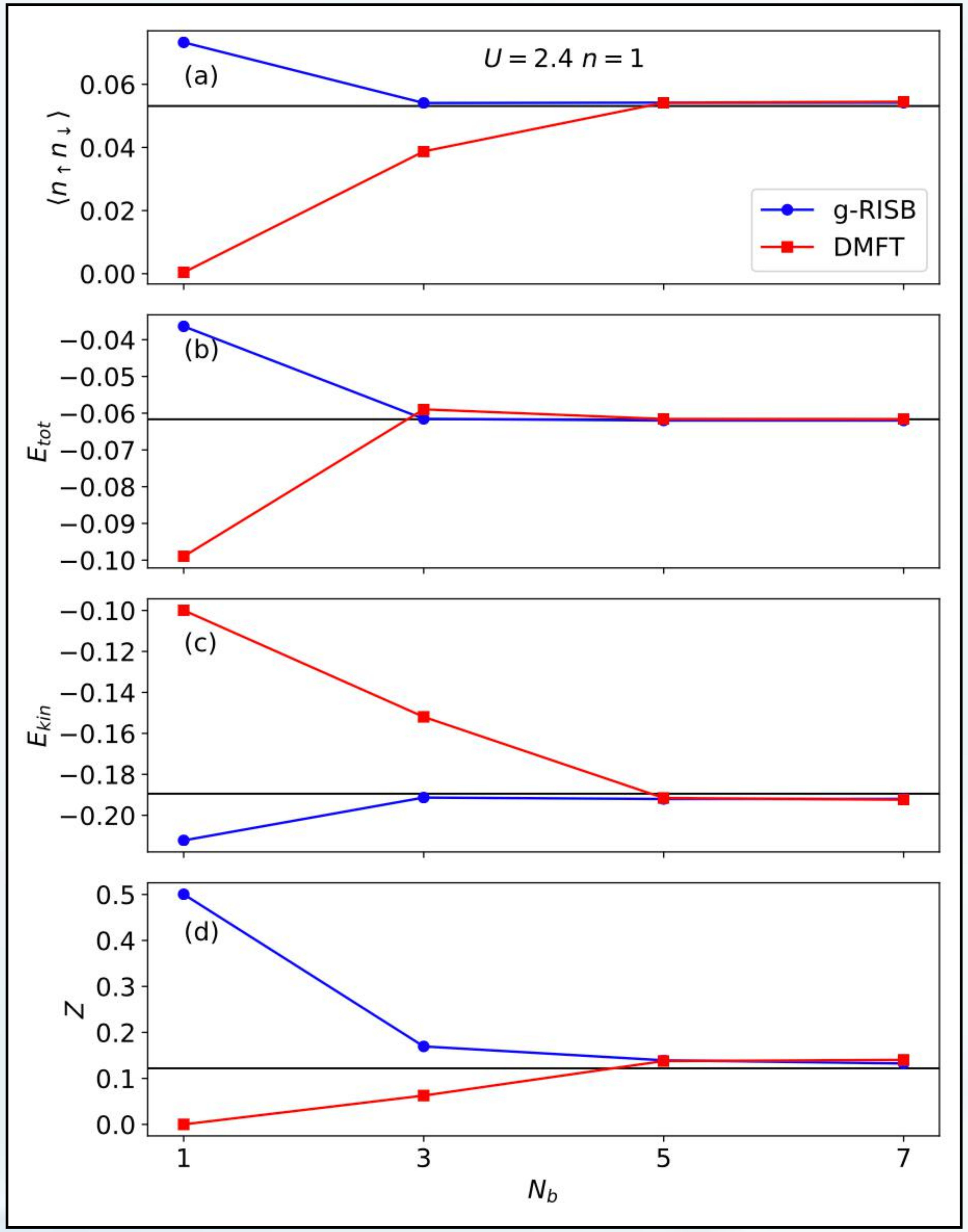
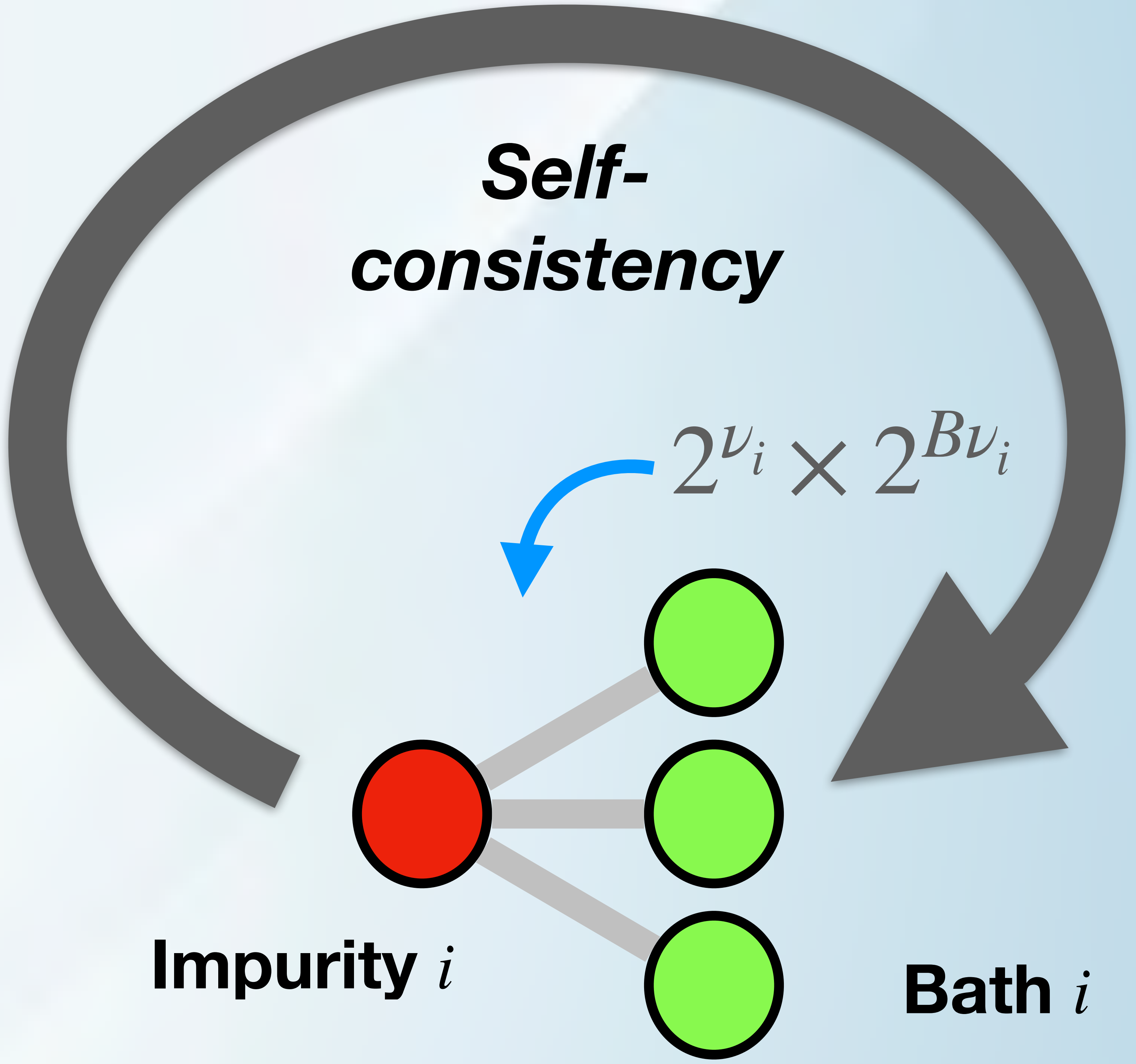




PHYSICAL REVIEW B **107**, L121104 (2023)

Letter

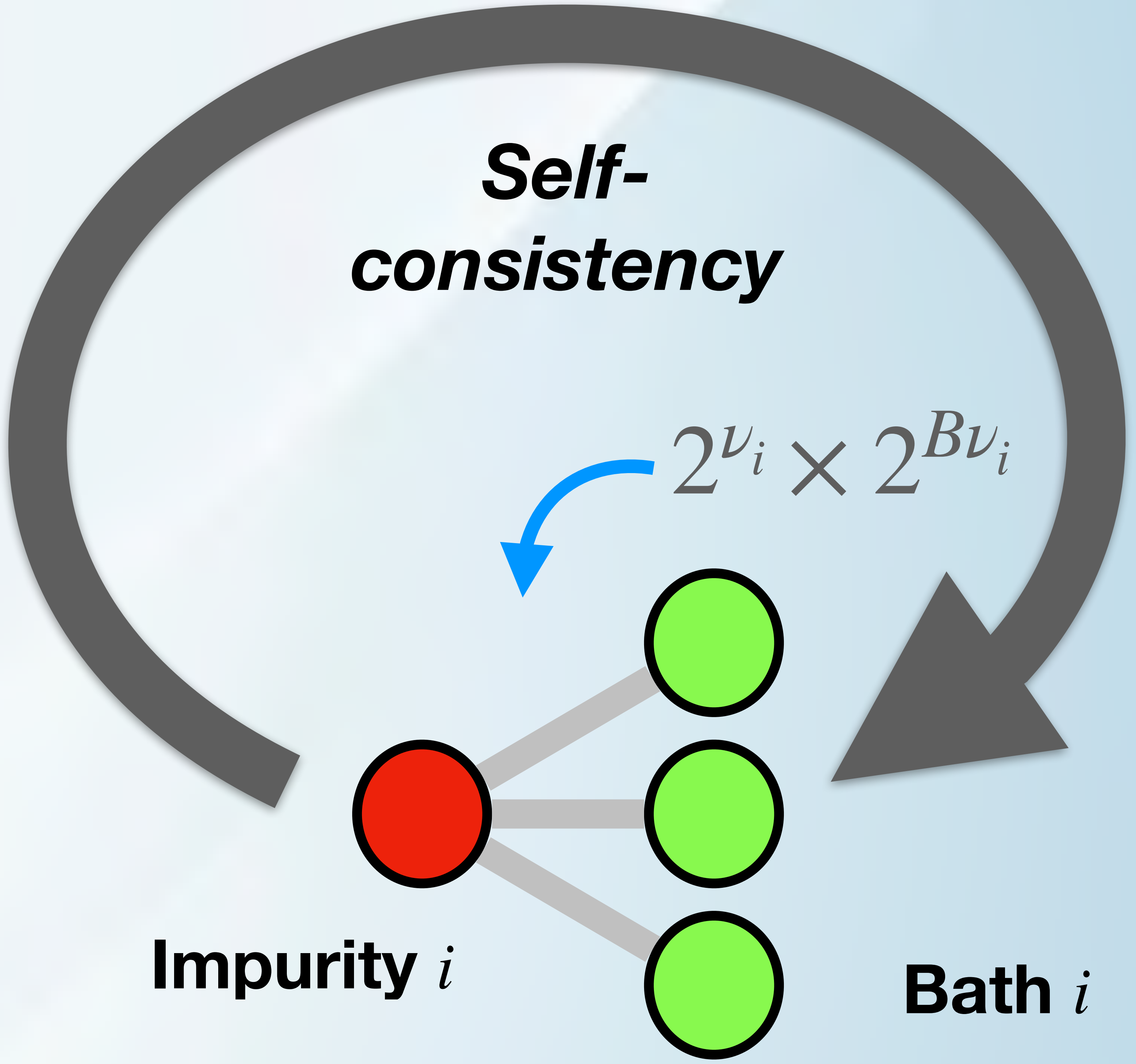
Accuracy of ghost rotationally invariant slave-boson and dynamical mean field theory as a function of the impurity-model bath size

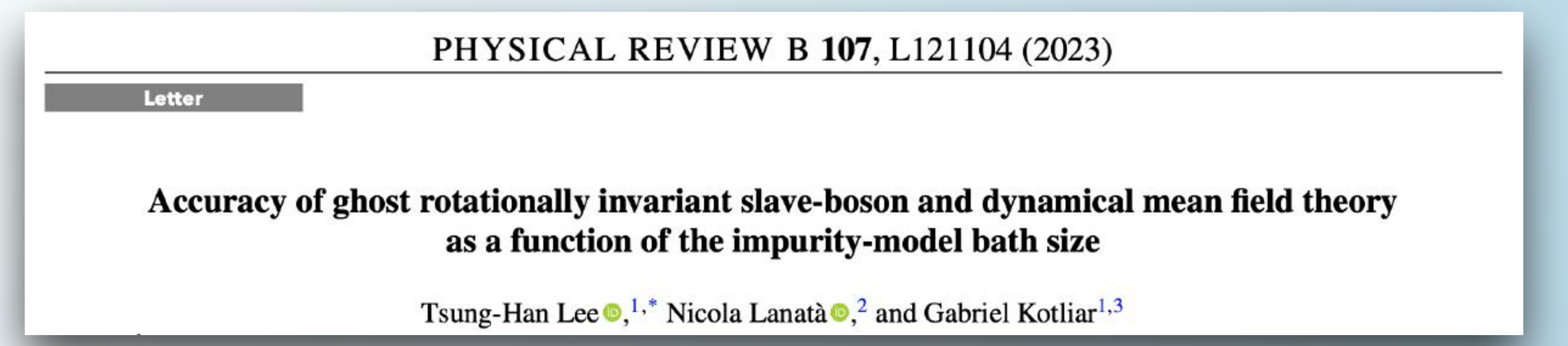
Tsung-Han Lee[1,*] Nicola Lanatà[2] and Gabriel Kotliar[1,3]

Benchmark calculations Hubbard model:

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




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

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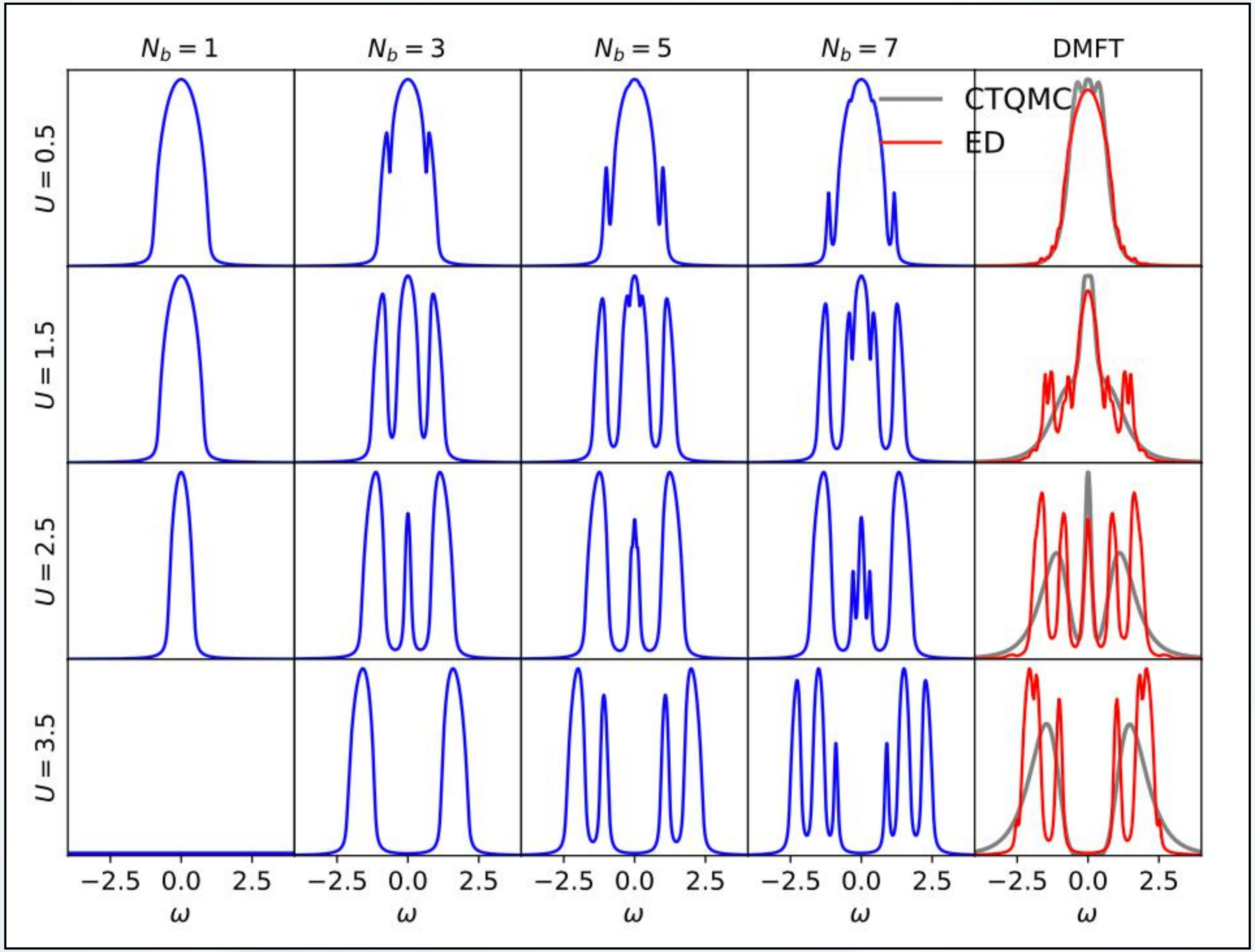

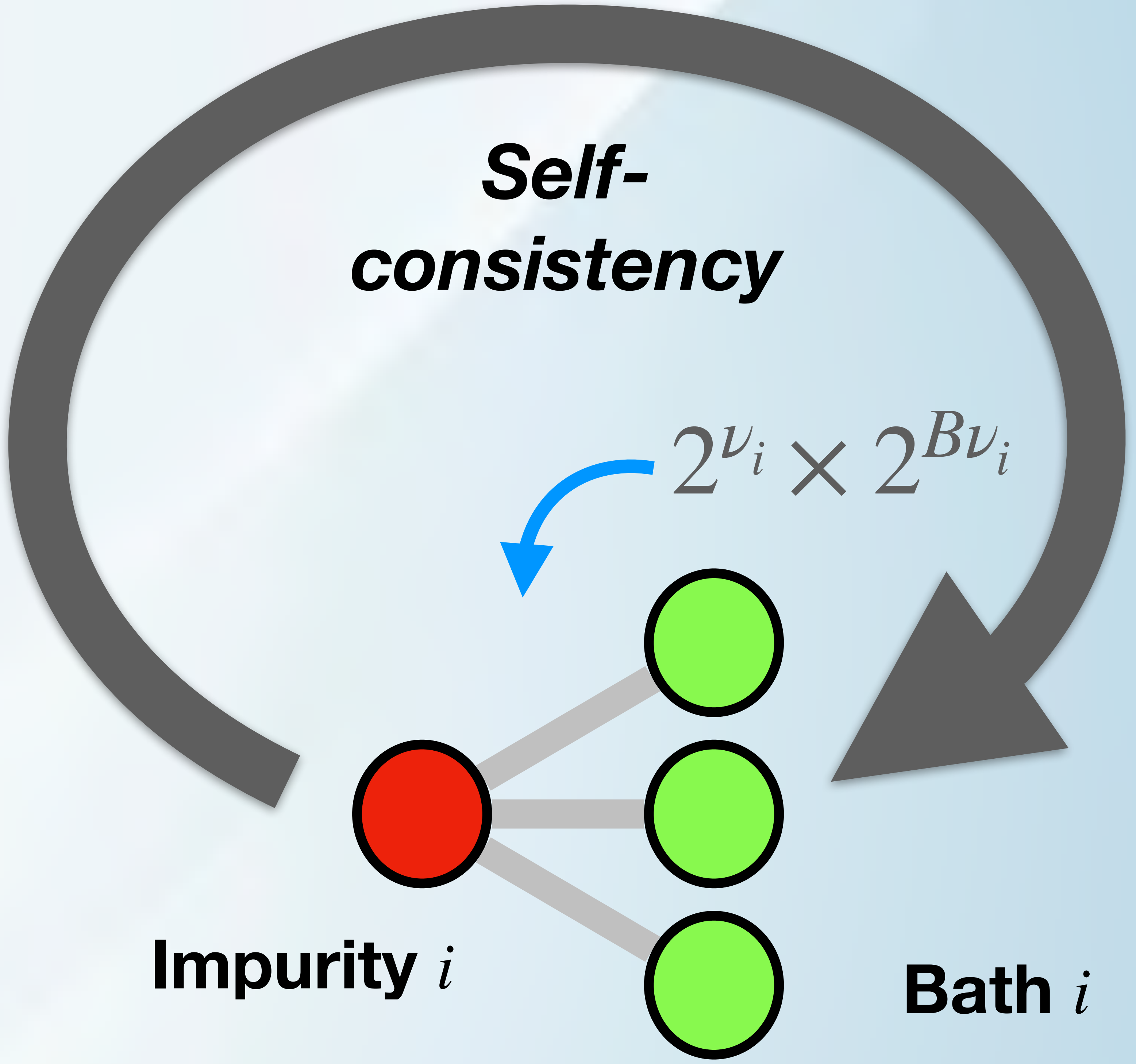

PHYSICAL REVIEW B **107**, L121104 (2023)

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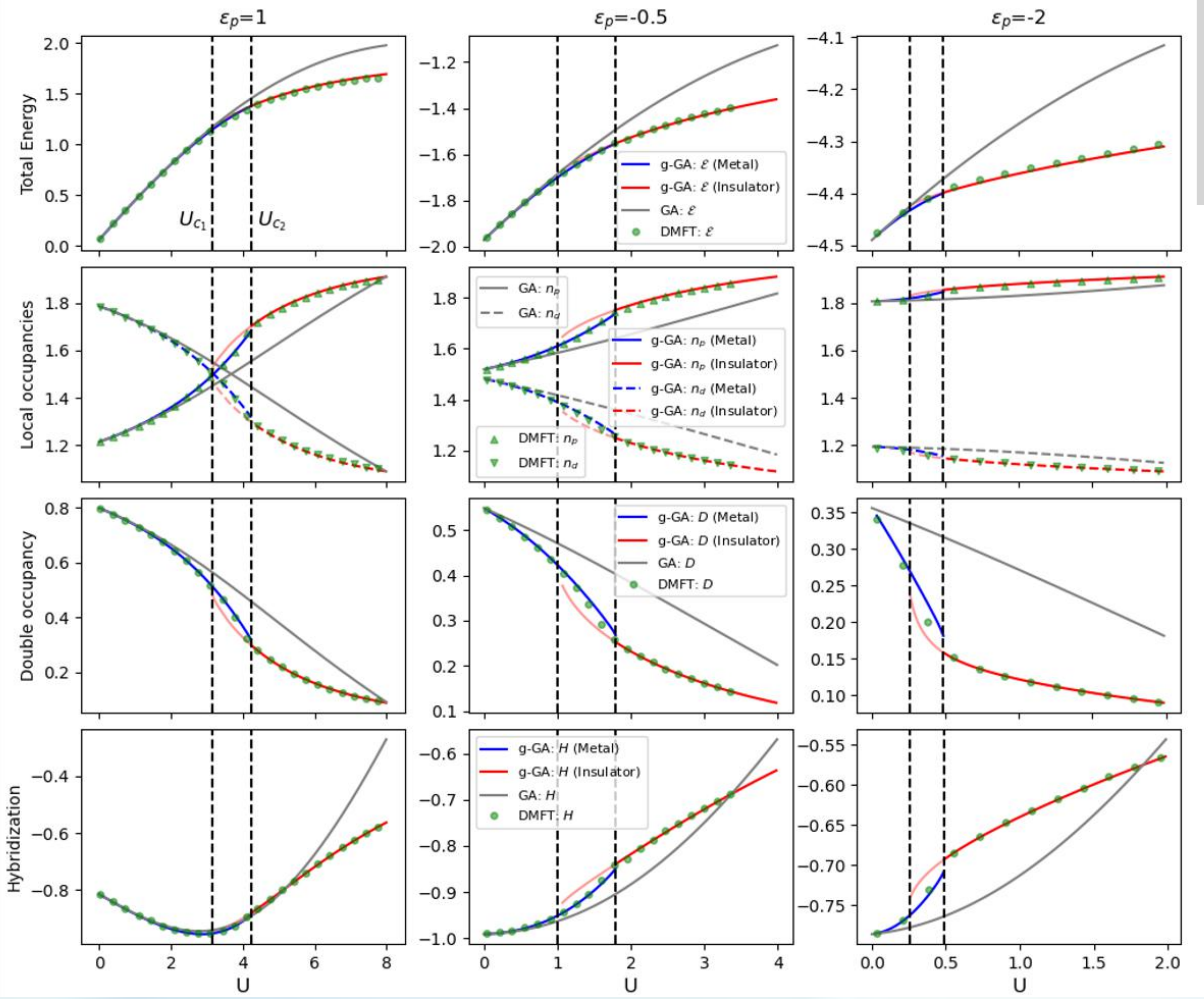
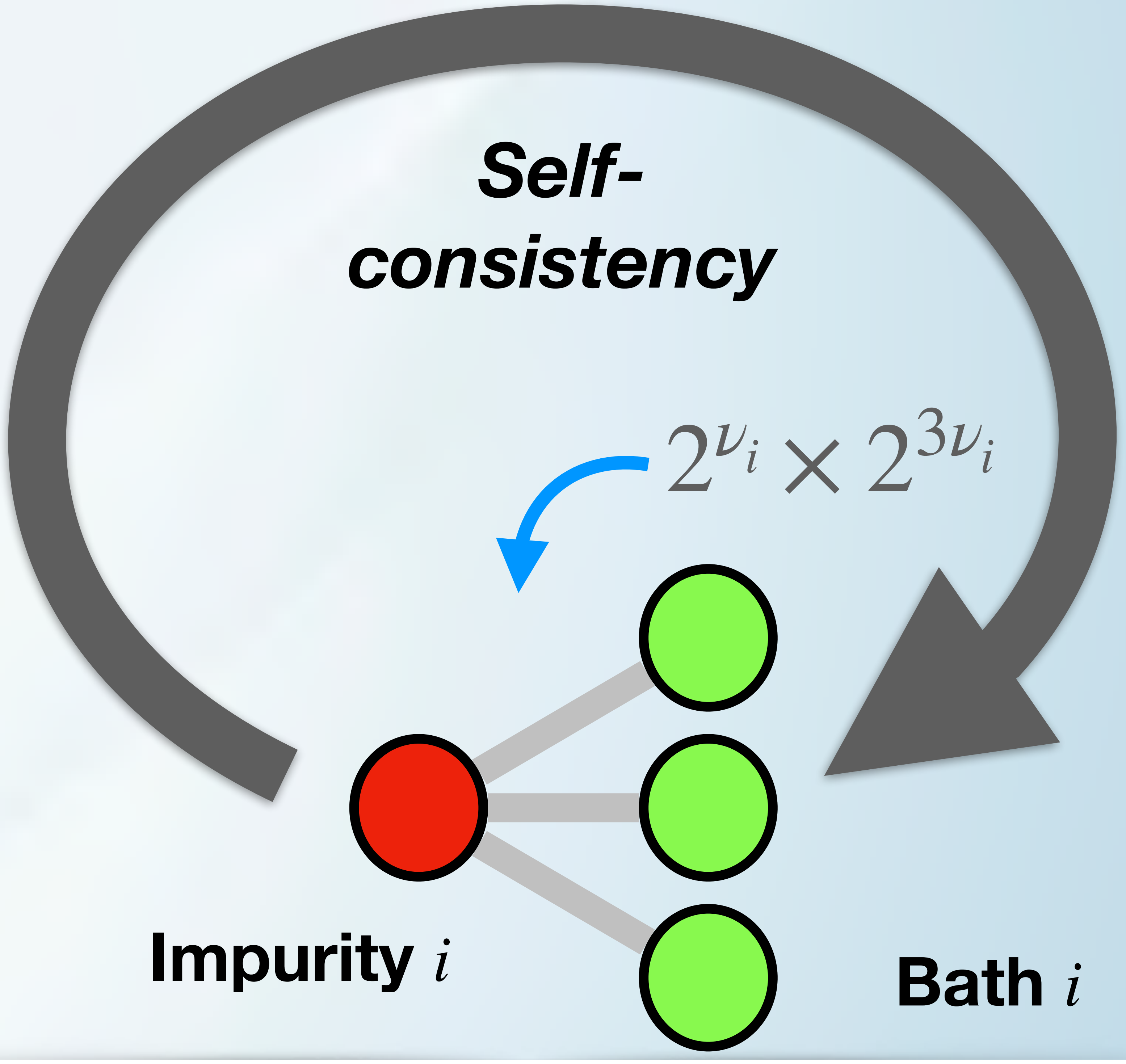
Benchmark calculations ALM:



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



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,*]

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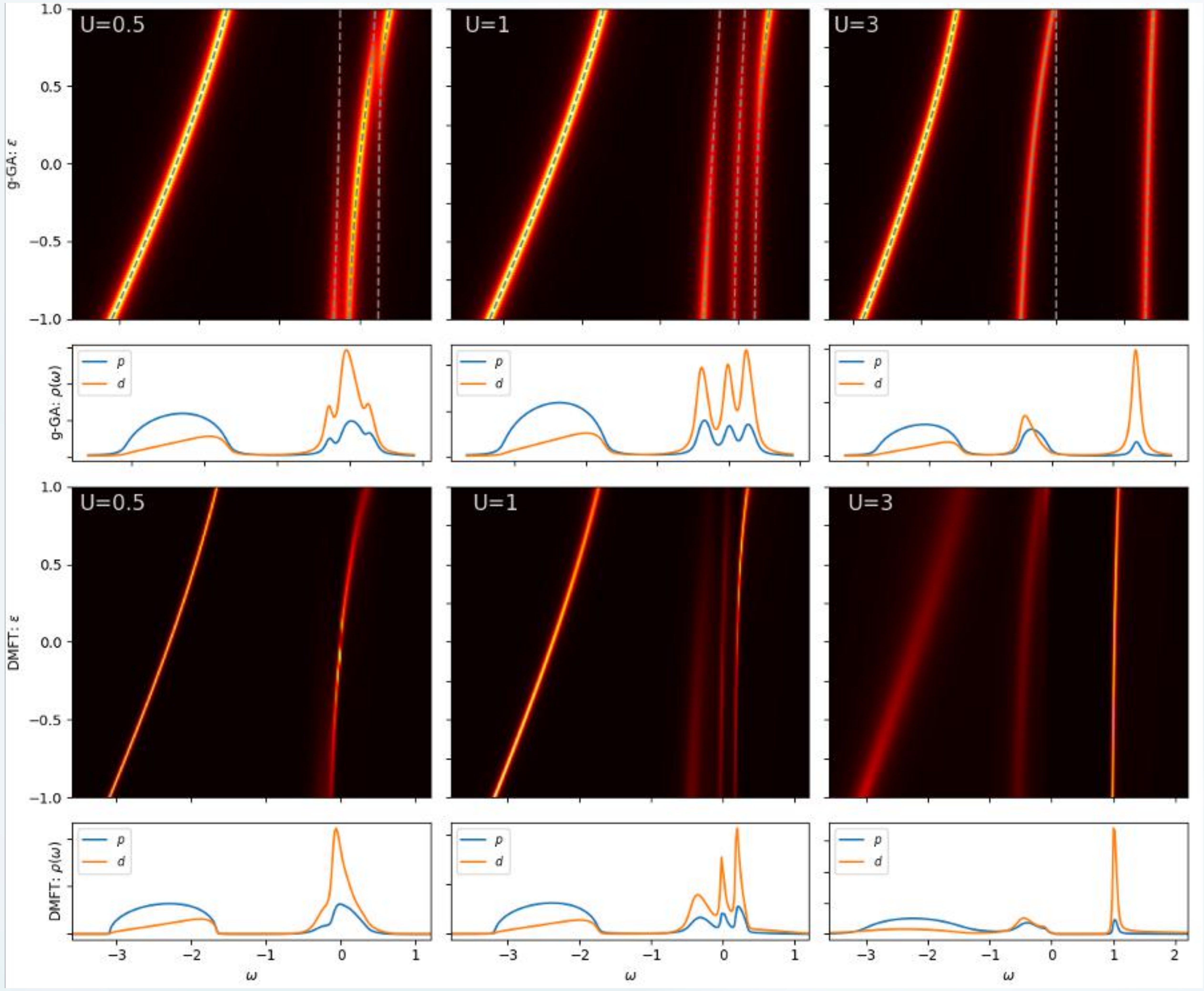

$$\hat{H} = \sum_{ij}\sum_{\sigma}\left(t_{ij} + \delta_{ij}\epsilon_p\right) p^\dagger_{i\sigma} p_{j\sigma} + \sum_i \frac{U}{2}\left(\hat{n}_{di} - 1\right)^2 + V\sum_{i\sigma}\left(p^\dagger_{i\sigma} d_{i\sigma} + \mathrm{H.c.}\right) - \mu \sum_i \hat{N}_i$$

Analytical (approximate) expression for self-energy

$$\Sigma^{\text{g-GA}}_{dd}(\omega) = \mu + \frac{U}{2} + \frac{l_1}{r_1^2} - \omega\frac{1-r_1^2}{r_1^2} + \frac{(\omega - l_1)^2}{r_1^4}\Big[(\omega - l_3)r_2^2 + (\omega - l_2)r_3^2\Big]\Bigg[(\omega - l_2)(\omega - l_3) + \frac{\omega - l_1}{r_1^2}\left(r_2^2(\omega - l_3) + r_3^2(\omega - l_2)\right)\Bigg]^{-1}$$

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,*]

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

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

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

$$[i\partial_t - \hat{H}_{\mathrm{emb}}]|\Phi\rangle = 0,$$

$$i\partial_t n_{ab}(\omega) = \omega\sum_{c=1}^{\mathcal{B}}[\mathcal{R}_b\mathcal{R}_c^\dagger n_{ac}(\omega) - \mathcal{R}_c\mathcal{R}_a^\dagger n_{cb}(\omega)],$$

$$\int_{-D}^{D} d\omega\,\rho(\omega)\,\omega[\mathcal{R}^{\dagger\,t} n(\omega)]_{1a} = \sum_{c,a=1}^{\mathcal{B}}\mathcal{D}_c[\Delta(1-\Delta)]^{\frac{1}{2}}_{ac},$$

$$\sum_{c,b=1}^{\mathcal{B}}\frac{\partial}{\partial d_s}([\Delta(1-\Delta)]^{\frac{1}{2}}_{cb}\mathcal{D}_b\mathcal{R}_c + \mathrm{c.c.}) + l_s^c = 0,$$

$$\langle\Phi|\hat{c}^\dagger_\sigma \hat{f}_{a\sigma}|\Phi\rangle - \sum_{c=1}^{\mathcal{B}}[\Delta(1-\Delta)]^{\frac{1}{2}}_{ca}\mathcal{R}_c = 0,$$

$$\langle\Phi|\hat{f}_{b\sigma}\hat{f}^\dagger_{a\sigma}|\Phi\rangle - \Delta_{ab} = 0,$$

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