Quantum-embedding formulation of the GA/RISB equations

Introduction to DFT+GA/RISB

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COMPUTATIONAL
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MATERIALS
2022

Why is it useful?

1. Orders of magnitude less computationally demanding than DMFT *(note also recent combination with ML)*.

2. Variational (*T=0*).

3. Extensions to finite temperature & time-dependent problems.

Limitations

1. No accurate description of the Mott phase.

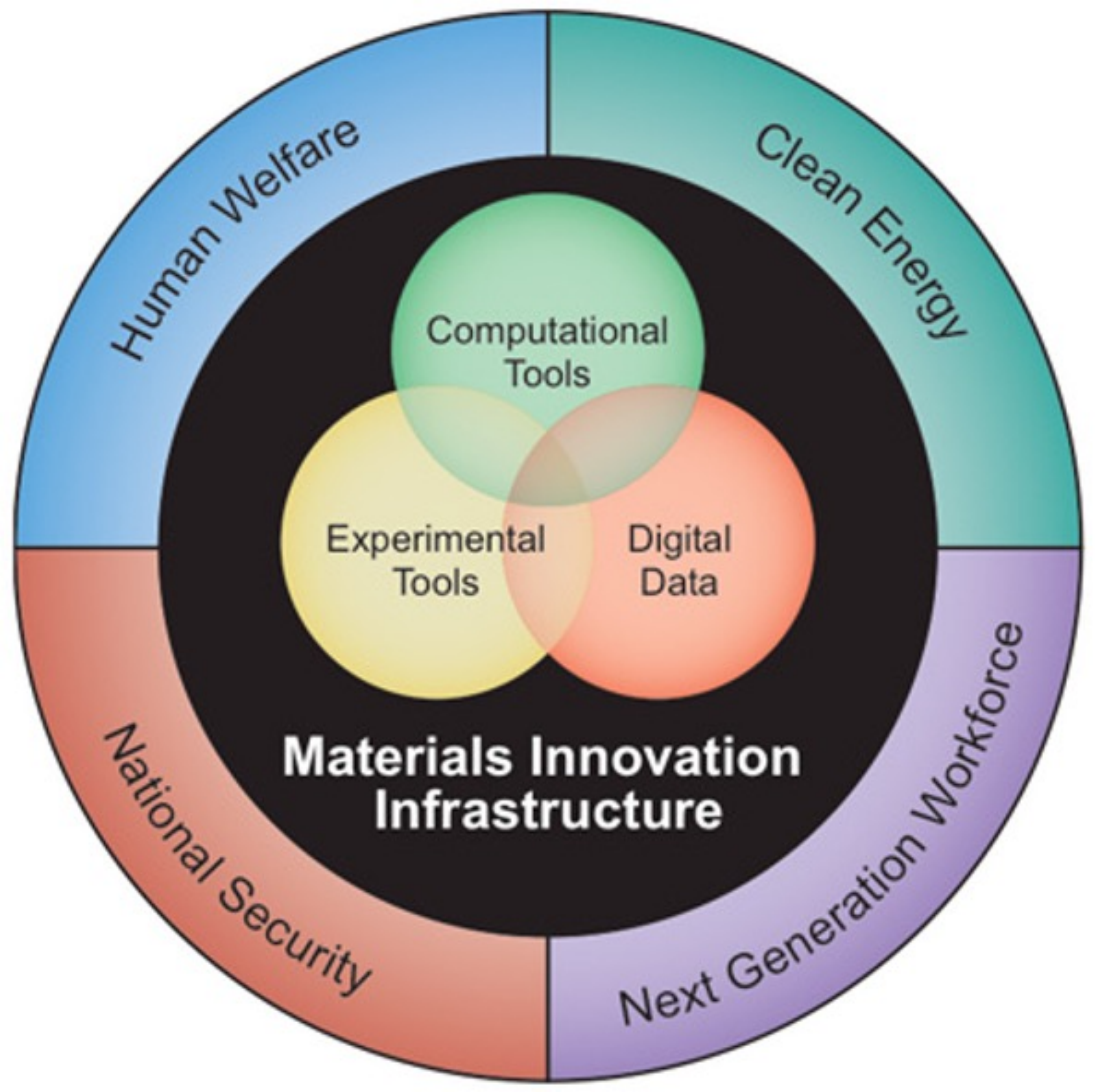
2. No access to high-energy excitations (Hubbard bands).

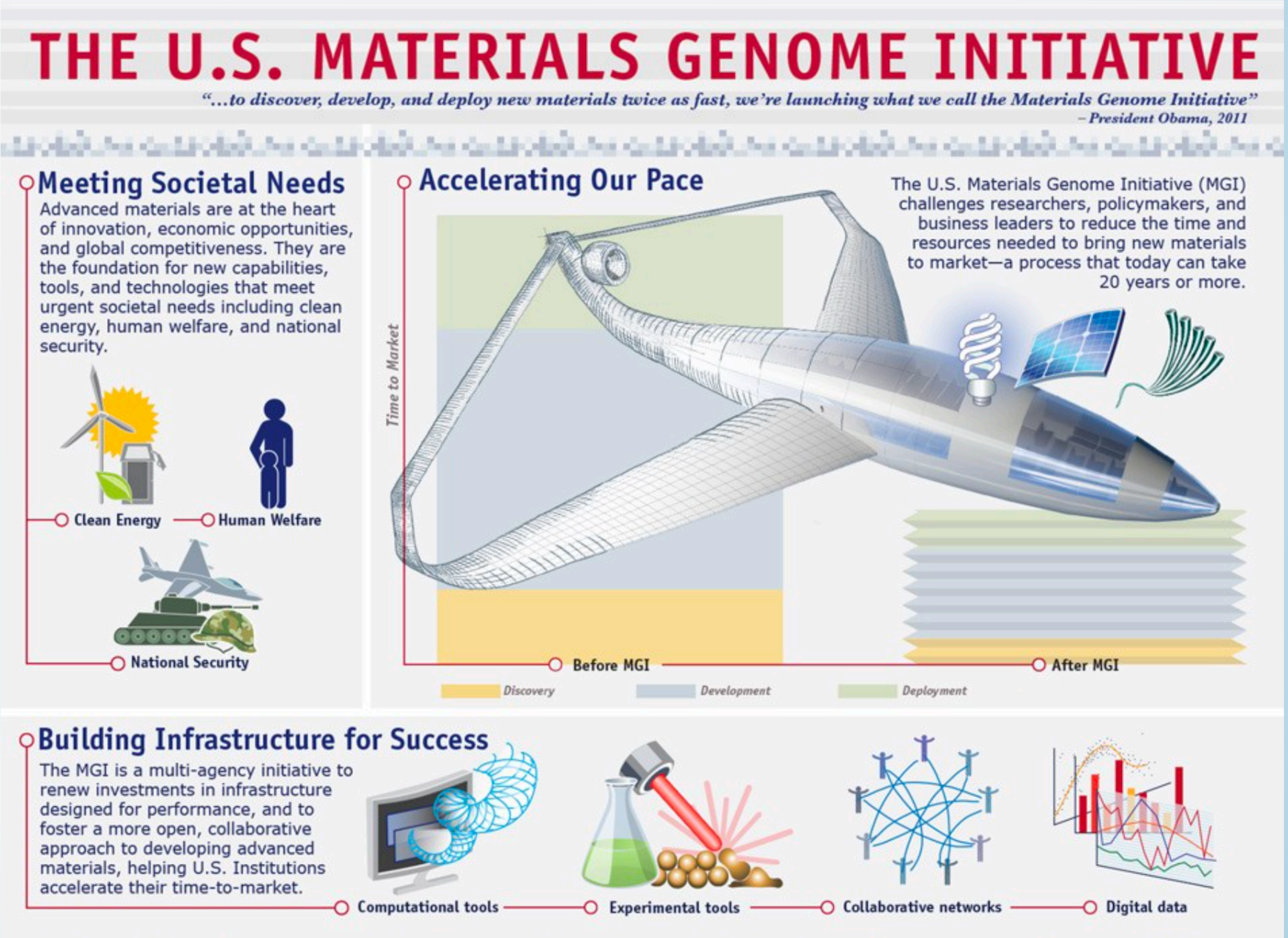
3. Mott metal-insulator transition-point can be overestimated.

*(**Note:** recent extension g-GA resolve these problems…)*

Why is computational speed important?

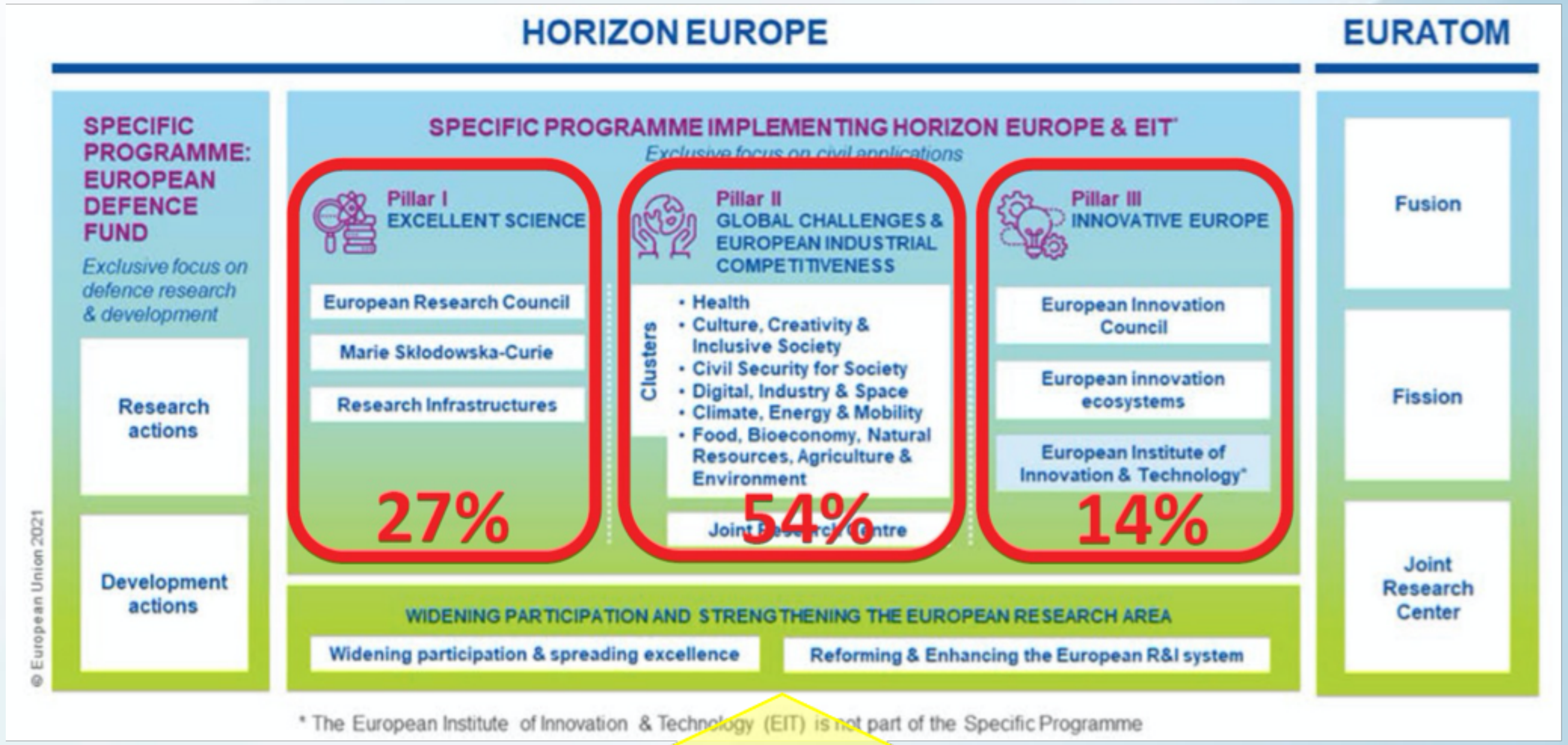
Exploring large chemical spaces

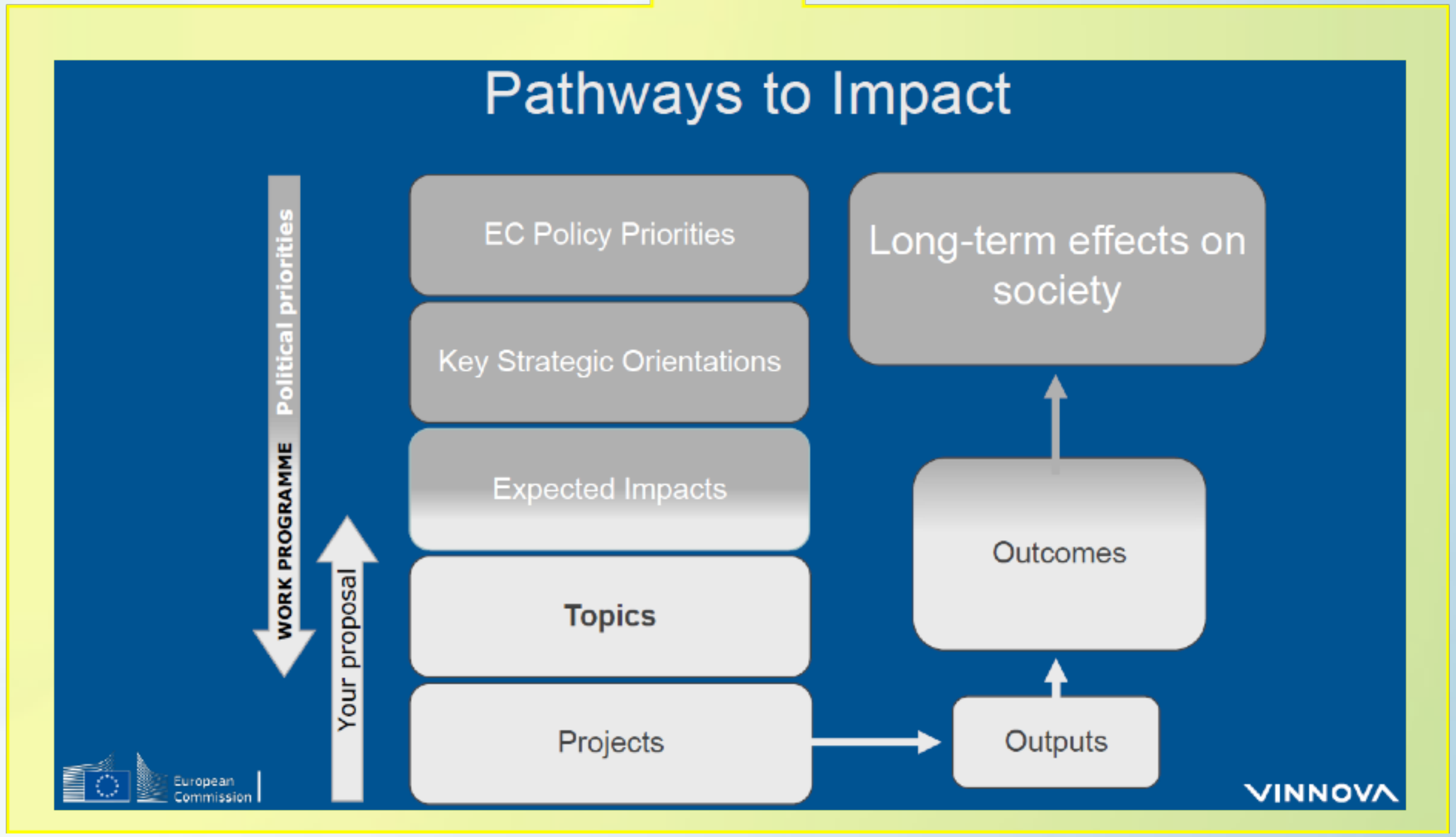




Why is computational speed important?

Increase of scientific programs prioritising research that can benefit society





Outline

A. Quantum Embedding (QE) methods.

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

C. DFT+GA algorithmic structure.

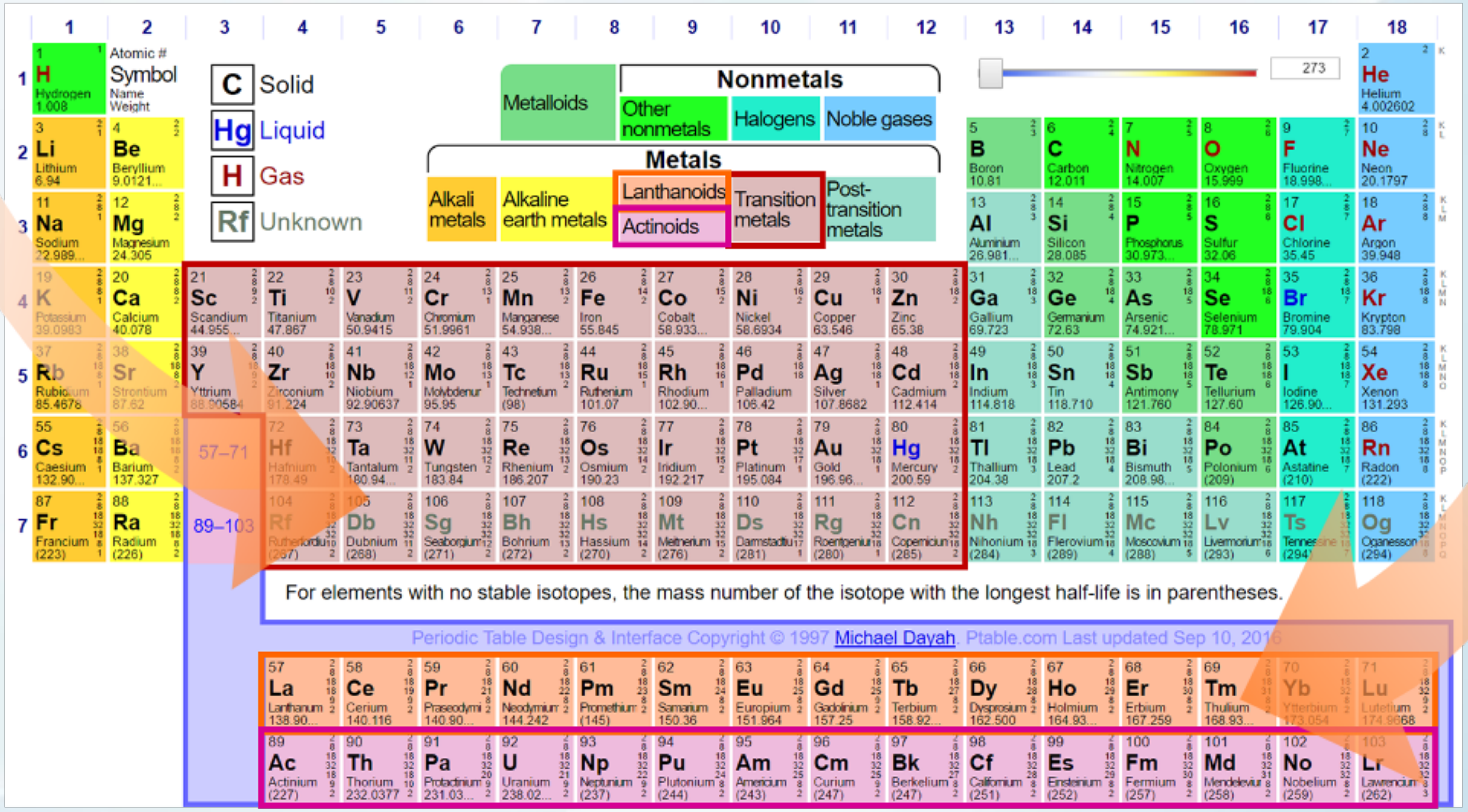
D. Spectral properties.

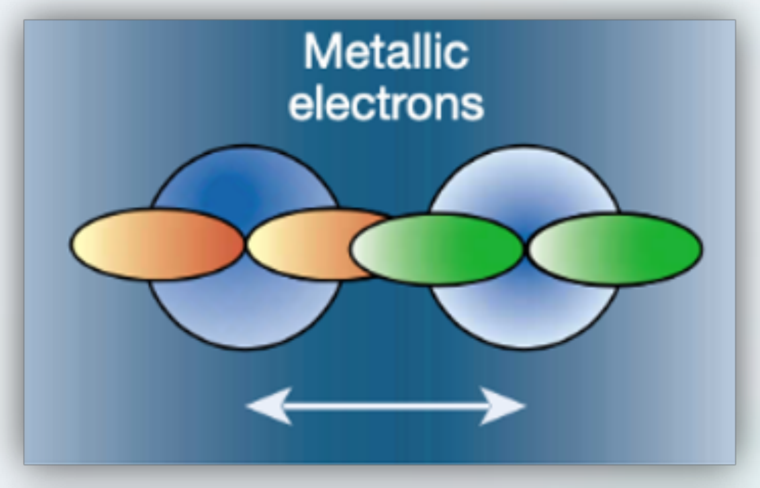
E. Examples of applications.

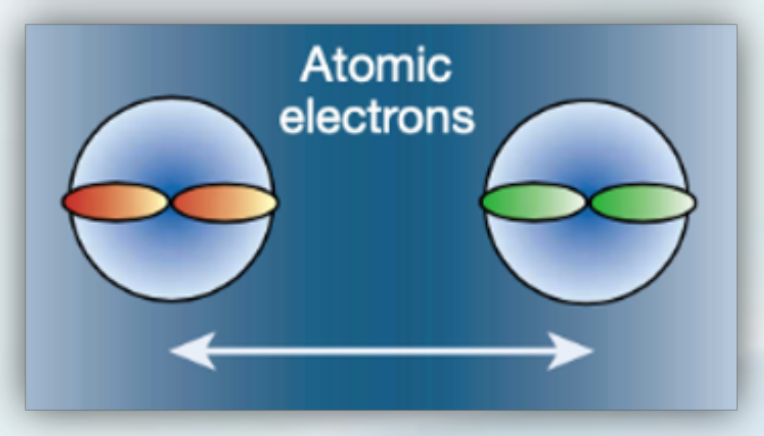
F. Recent formalism extensions (g-GA).

Strongly Correlated Materials

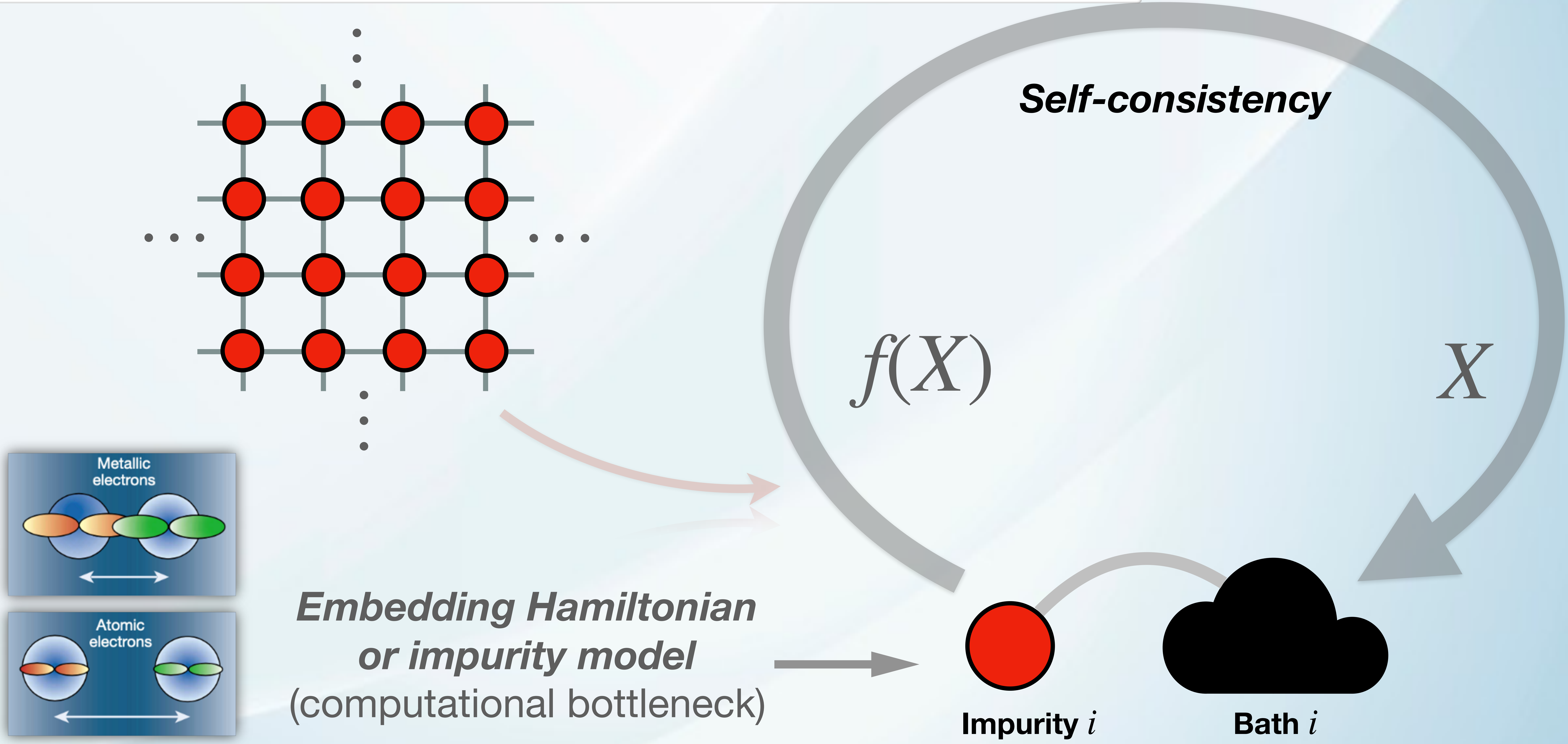
Systems with localized *d*- or *f*-electrons:
Single-particle picture not sufficient!







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



Embedding Hamiltonian or impurity model
(computational bottleneck)

Example: DMFT

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

Antoine Georges

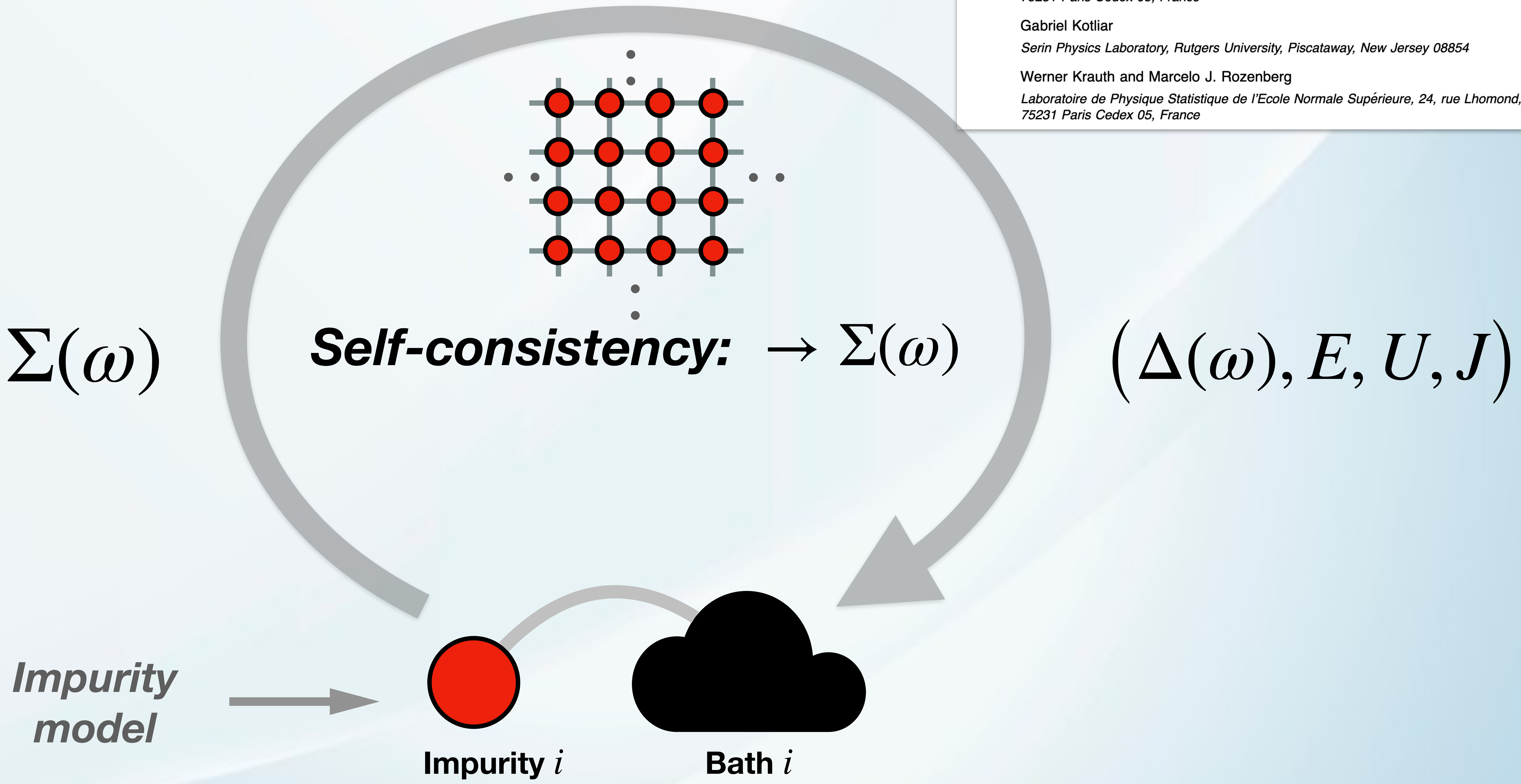
Laboratoire de Physique Théorique de l'Ecole Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France

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

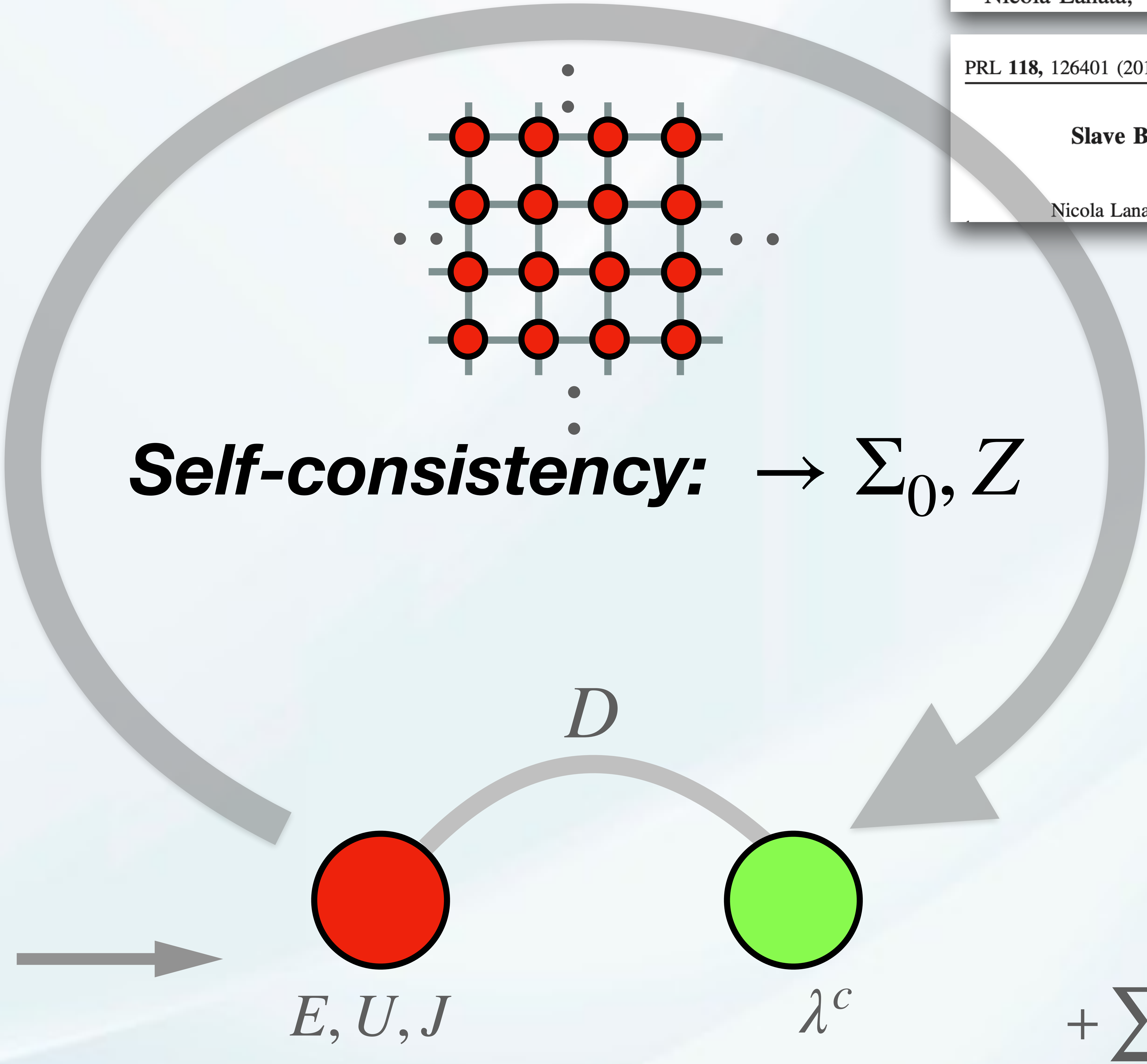
Nicola Lanatà,[1,*] Yongxin Yao,[2,†] Cai-Zhuang Wang,[2] Kai-Ming Ho,[2] and Gabriel Kotliar[1]

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]

$$\begin{bmatrix} \langle c^\dagger_\alpha c_\beta \rangle & \langle c^\dagger_\alpha f_a \rangle \\ \langle f^\dagger_a c_\alpha \rangle & \langle f^\dagger_a f_b \rangle \end{bmatrix}$$



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

Embedding Hamiltonian →

$$\hat{H}_{emb} = \hat{H}_{int}(U,J) + \sum_{\alpha\beta} E_{\alpha\beta}\, c^\dagger_\alpha c_\beta + \sum_{a\alpha} \left(D_{a\alpha}\, c^\dagger_\alpha f_a + H.c. \right) + \sum_a \lambda^c_{aa}\, f_a f^\dagger_a$$

g-GA/g-RISB (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

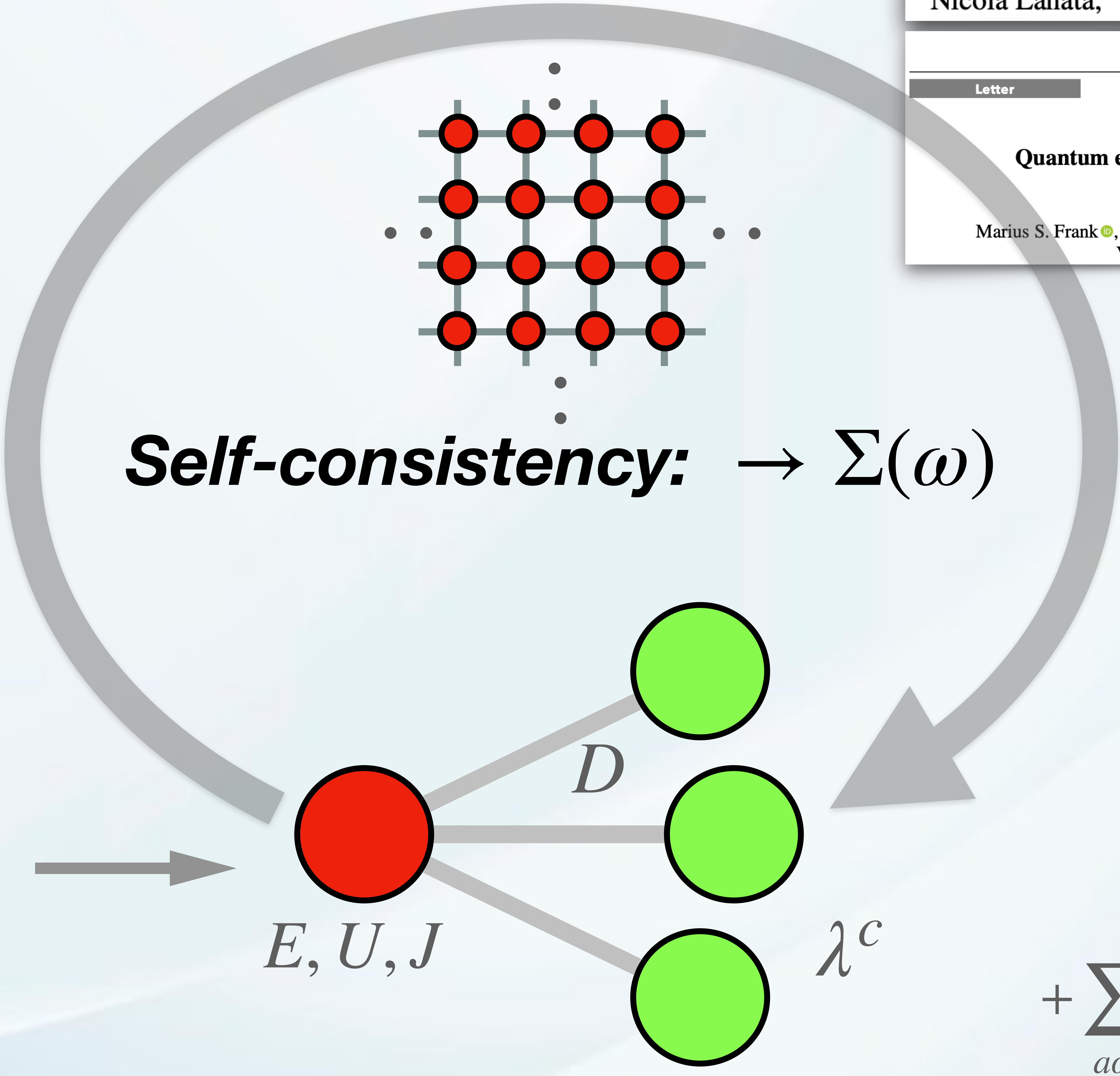
Quantum embedding description of the Anderson lattice model with the ghost Gutzwiller approximation

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,*]

$$\begin{bmatrix} \langle c^\dagger_\alpha c_\beta \rangle & \langle c^\dagger_\alpha f_a \rangle \\ \langle f^\dagger_a c_\alpha \rangle & \langle f^\dagger_a f_b \rangle \end{bmatrix}$$

Self-consistency: $\rightarrow \Sigma(\omega)$

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



Embedding Hamiltonian

$$\hat{H}_{emb} = \hat{H}_{int}(U,J) + \sum_{\alpha\beta} E_{\alpha\beta} c^\dagger_\alpha c_\beta + \sum_{a\alpha} \left(D_{a\alpha} c^\dagger_\alpha f_a + H.c. \right) + \sum_a \lambda^c_{aa} f_a f^\dagger_a$$

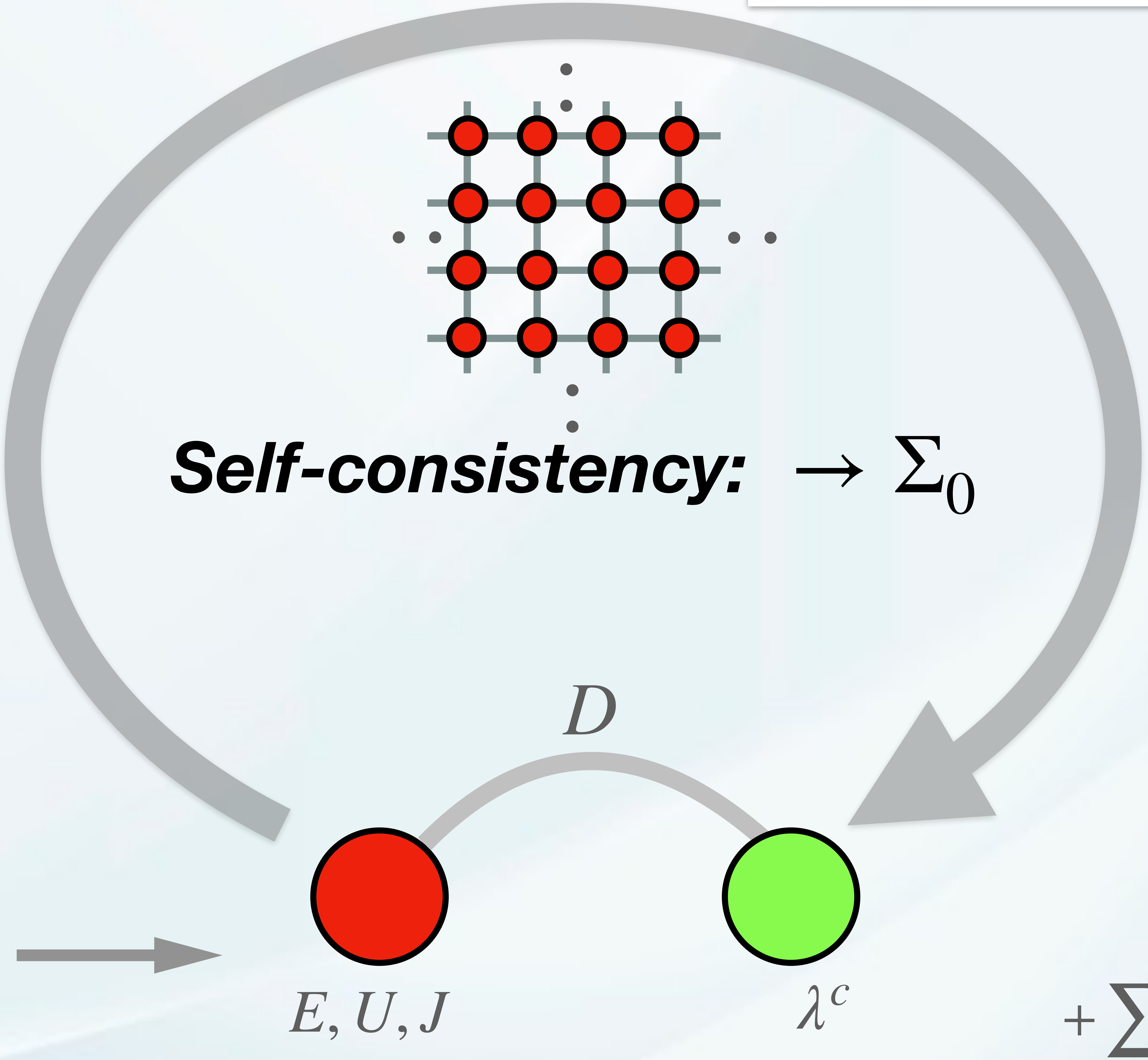
Example: DMET

PRL **109**, 186404 (2012) PHYSICAL REVIEW LETTERS week ending 2 NOVEMBER 2012

Density Matrix Embedding: A Simple Alternative to Dynamical Mean-Field Theory

Gerald Knizia and Garnet Kin-Lic Chan

$$\begin{bmatrix} \langle c_\alpha^\dagger c_\beta \rangle & \langle c_\alpha^\dagger f_a \rangle \\ \langle f_a^\dagger c_\alpha \rangle & \langle f_a^\dagger f_b \rangle \end{bmatrix}$$



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

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$$\hat{H}_{emb} = \hat{H}_{int}(U, J) + \sum_{\alpha\beta} E_{\alpha\beta}\, c_\alpha^\dagger c_\beta + \sum_{a\alpha} \left(D_{a\alpha}\, c_\alpha^\dagger f_a + H.c.\right) + \sum_a \lambda_{aa}^c\, f_a f_a^\dagger$$

GA/RISB (connection with DMET)

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

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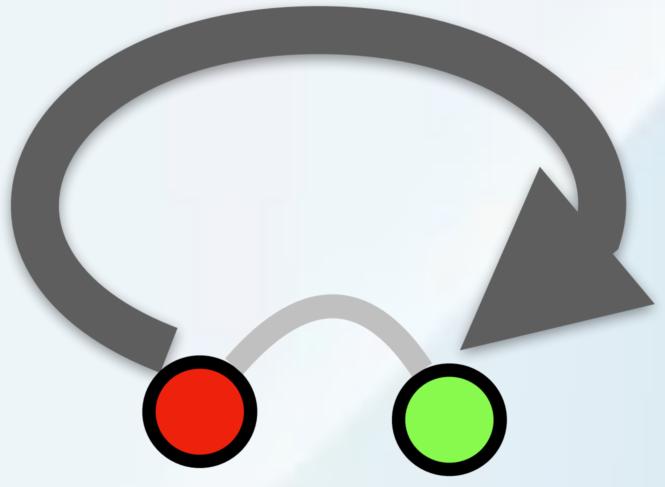
Formulation of GA/RISB as QE theory



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

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

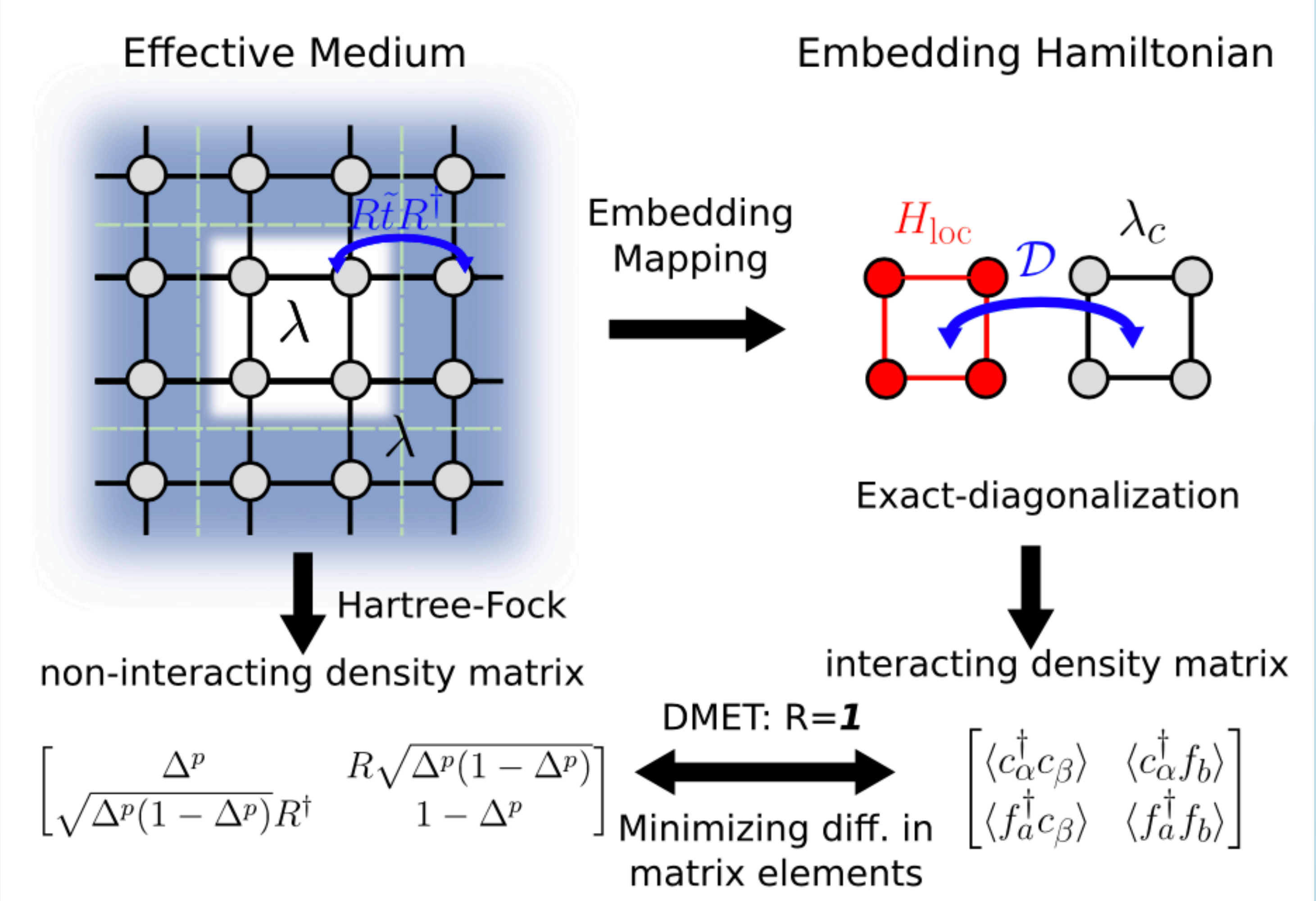
Thomas Ayral,[1] Tsung-Han Lee,[1] and Gabriel Kotliar[1,2]

PHYSICAL REVIEW B **99**, 115129 (2019)

Rotationally invariant slave-boson and density matrix embedding theory: Unified framework and comparative study on the one-dimensional and two-dimensional Hubbard model

Tsung-Han Lee,[1,*] Thomas Ayral,[1,2] Yong-Xin Yao,[3] Nicola Lanata,[4] and Gabriel Kotliar[1,5]

Comparison between GA/RISB & DMET QE equations & performance



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The Hamiltonian:

$$\hat{H} = \sum_{\mathbf{k}} \sum_{i,j\geq 0} \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} t^{\alpha\beta}_{\mathbf{k},ij}\, c^\dagger_{\mathbf{k}i\alpha} c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}} \sum_{i\geq 1} \hat{H}^{loc}_{\mathbf{R}i}$$

$\mathbf{k}$: Crystal momentum

$\mathbf{R}$: Unit cell

i: Projector information:

$i = 0$: Uncorrelated modes

$i = 1$: First subset of correlated modes (e.g. *d* orbitals of atom 1 in unit cell)

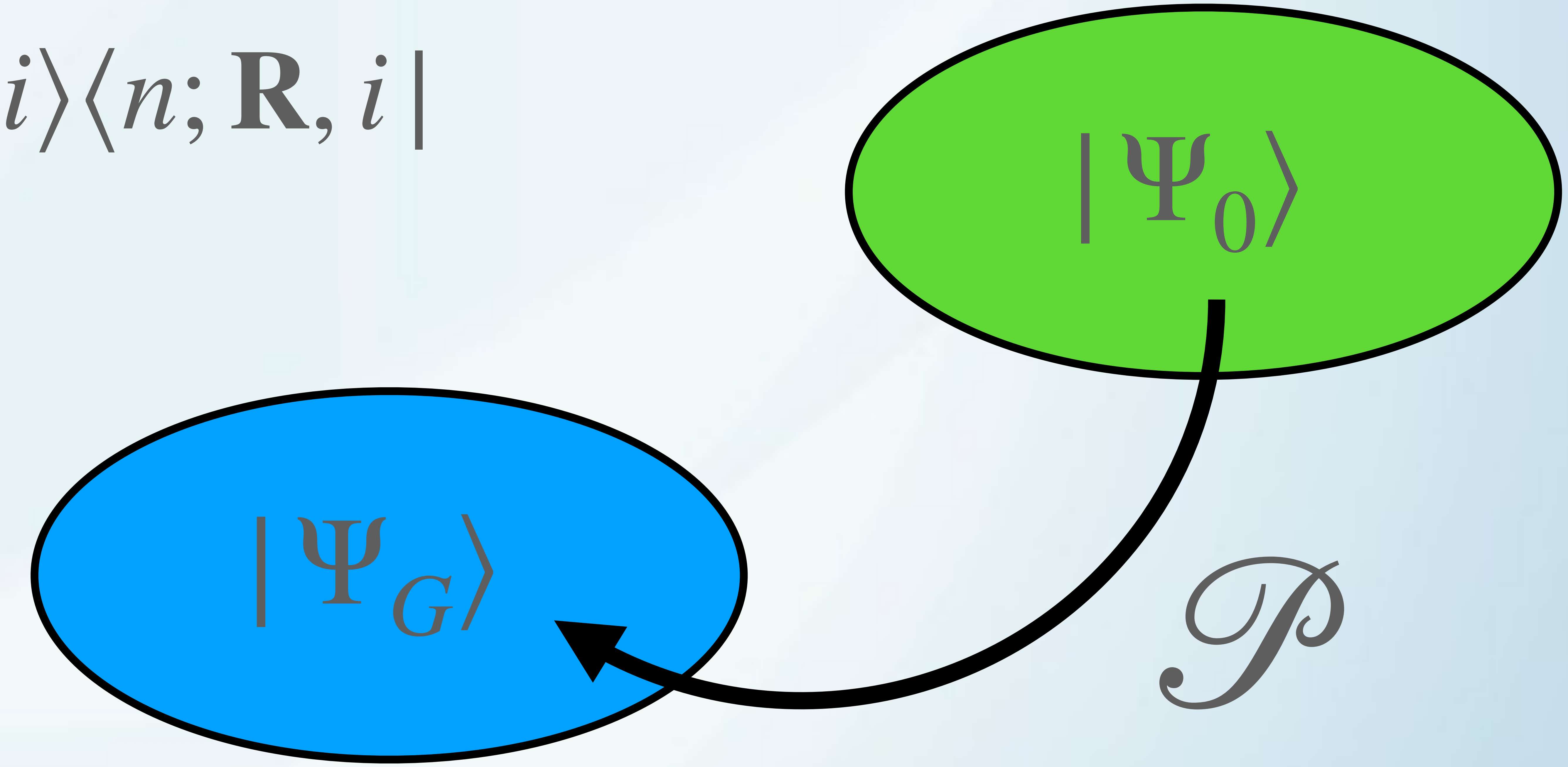
$i = 2$: Second subset of correlated modes (e.g. *f* orbitals of atom 1 in unit cell)

…

The GA variational wave function:

$$|\Psi_G\rangle = \mathscr{P}\,|\Psi_0\rangle = \prod_{\mathbf{R},i\geq 1} \mathscr{P}_{\mathbf{R}i}\,|\Psi_0\rangle$$

$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma n} [\Lambda_i]_{\Gamma n}\,|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i\,|$$



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$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma n} [\Lambda_i]_{\Gamma n} |\Gamma; \mathbf{R}, i\rangle\langle n; \mathbf{R}, i|$$

$$|\Gamma; \mathbf{R}, i\rangle = \left[c^\dagger_{\mathbf{R}i1}\right]^{q_1(\Gamma)} \ldots \left[c^\dagger_{\mathbf{R}i\nu_i}\right]^{q_{\nu_i}(\Gamma)} |0\rangle$$

$$|n; \mathbf{R}, i\rangle = \left[f^\dagger_{\mathbf{R}i1}\right]^{q_1(n)} \ldots \left[f^\dagger_{\mathbf{R}i\nu_i}\right]^{q_{\nu_i}(n)} |0\rangle$$

Our goal is to minimize $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ w.r.t. $\{\Lambda_i \,|\, i \geq 1\}, |\Psi_0\rangle$.

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

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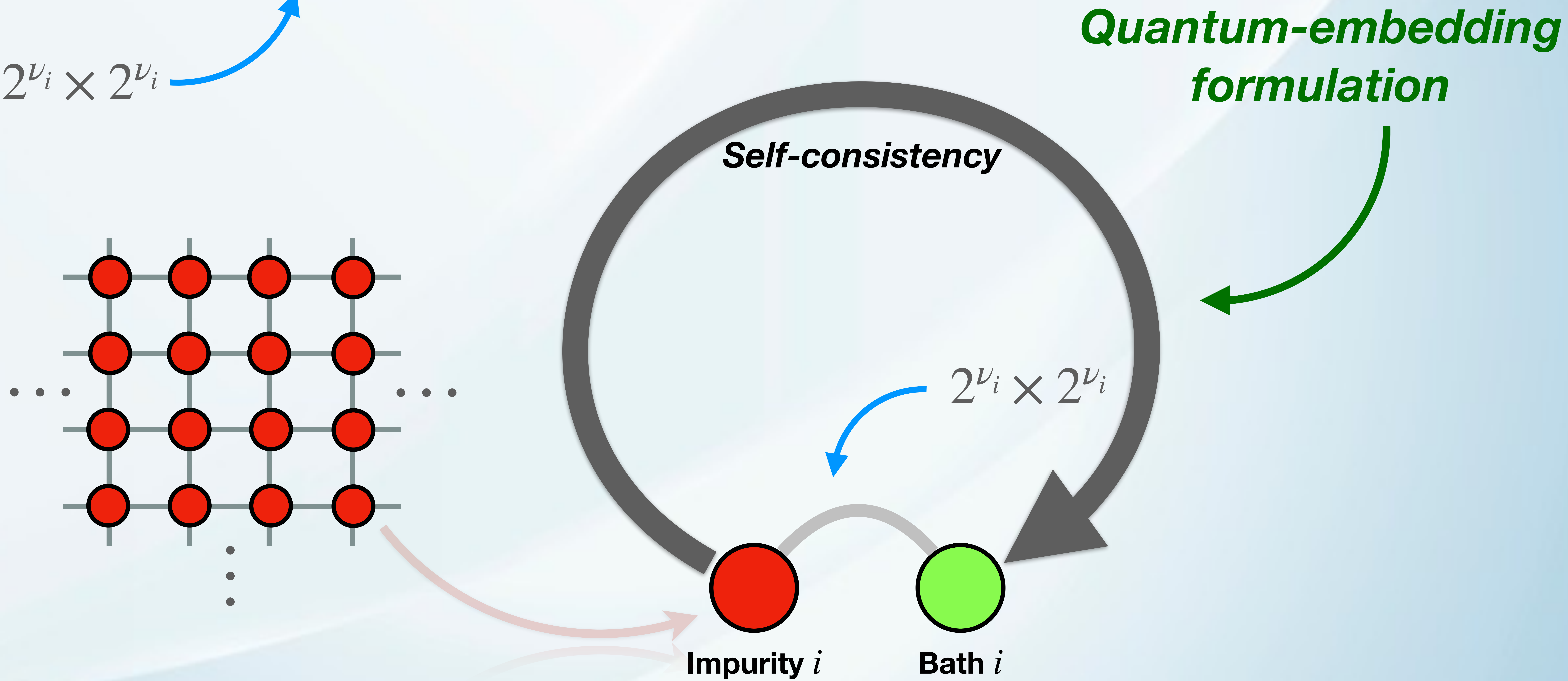

Necessary steps:

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

Gutzwiller approximation:

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

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:

$$\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle = \langle\Psi_0|\Psi_0\rangle = 1$$

$$\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}\, f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib}|\Psi_0\rangle = \langle\Psi_0|f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib}|\Psi_0\rangle \qquad \forall\, a,b \in \{1,..,\nu_i\}$$

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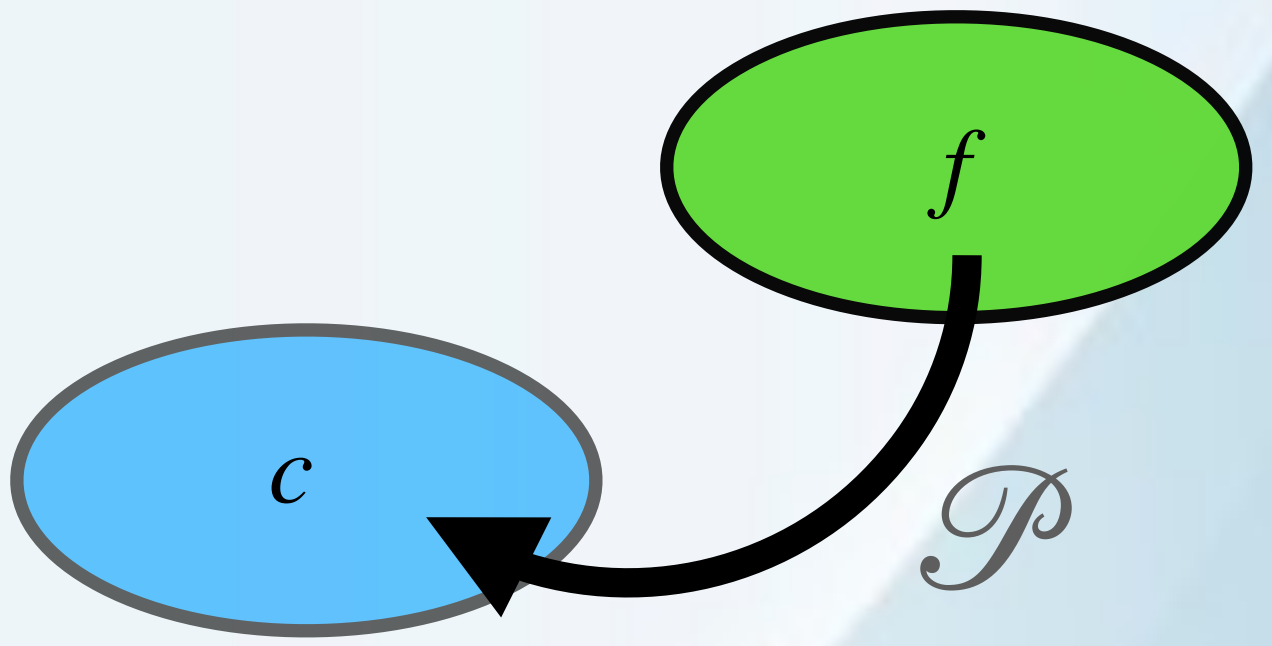
Wick's theorem: $\langle\Psi_0|c^\dagger_a c^\dagger_b c_c c_d|\Psi_0\rangle = \langle\Psi_0|c^\dagger_a c_d|\Psi_0\rangle\langle\Psi_0|c^\dagger_b c_c|\Psi_0\rangle - \langle\Psi_0|c^\dagger_a c_c|\Psi_0\rangle\langle\Psi_0|c^\dagger_b c_d|\Psi_0\rangle$

Gutzwiller constraints:



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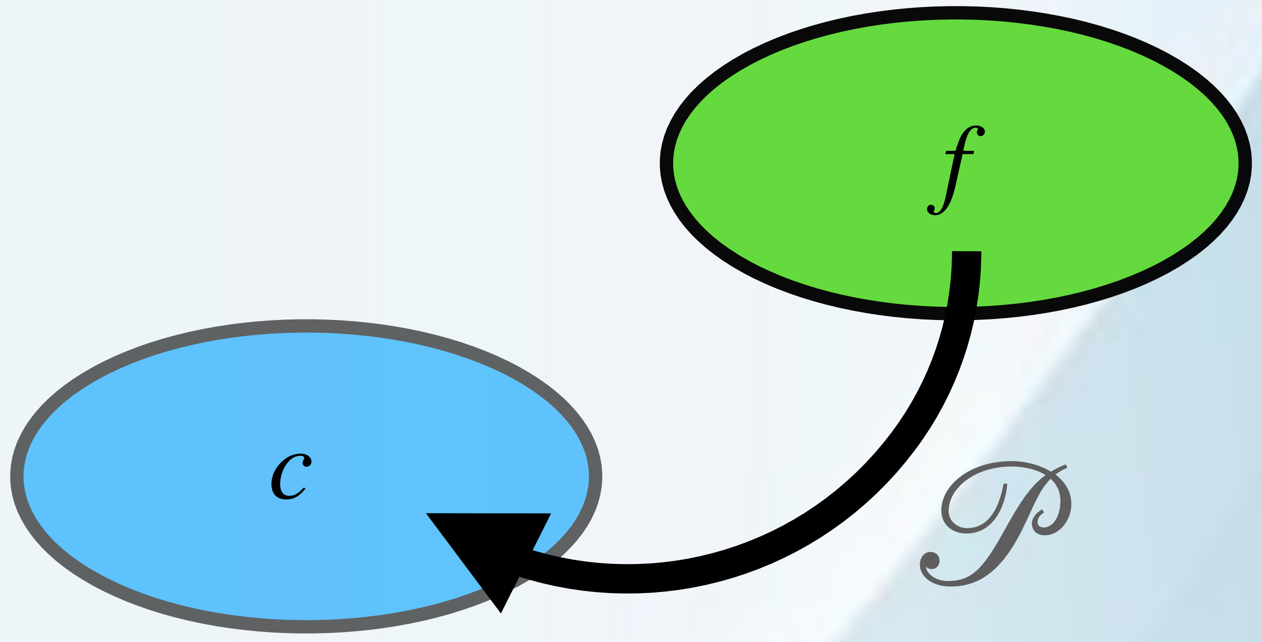
Key consequence:

$$\langle\Psi_0|\,\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}\,f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle = \langle\Psi_0|\,\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}\,|\Psi_0\rangle\langle\Psi_0|\,f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle$$
$$+\langle\Psi_0|\left[\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}\right]f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle_{2-legs}$$

Gutzwiller constraints:



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Key consequence:

$$\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}\, f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib}|\Psi_0\rangle = \cancel{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle}\langle\Psi_0|f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib}|\Psi_0\rangle$$

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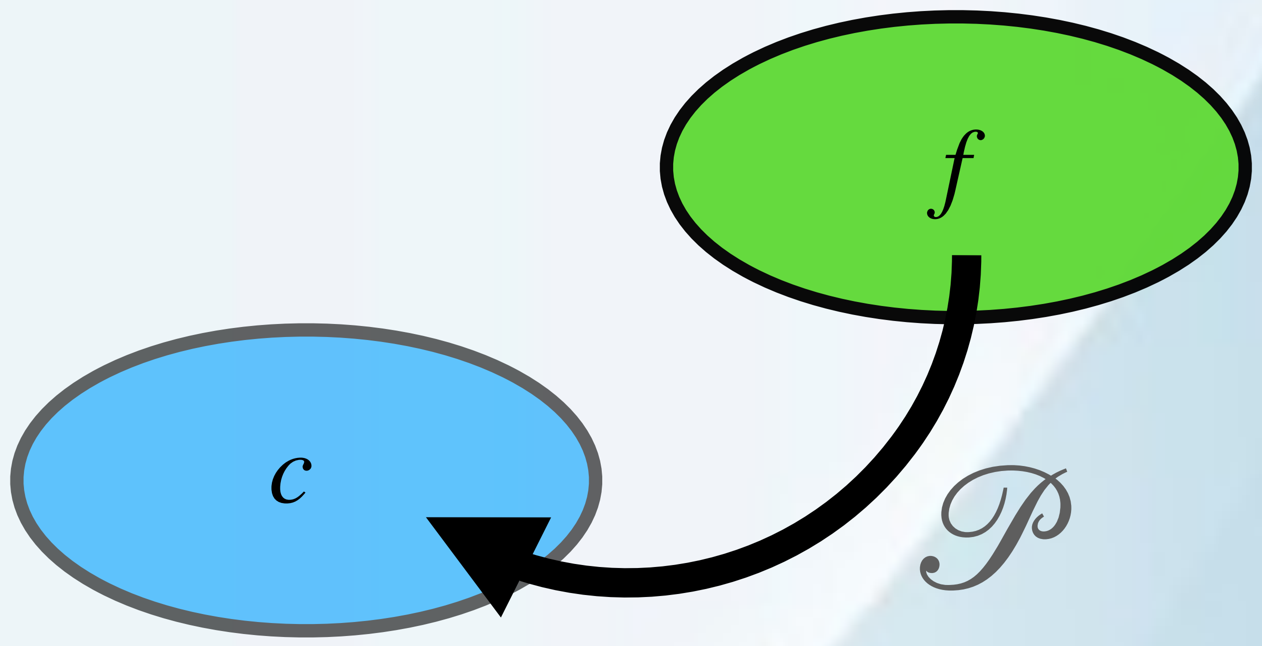

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Key consequence:

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$$+ \langle \Psi_0 | \left[\mathscr{P}^\dagger_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} \right] f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle_{2-legs}$$

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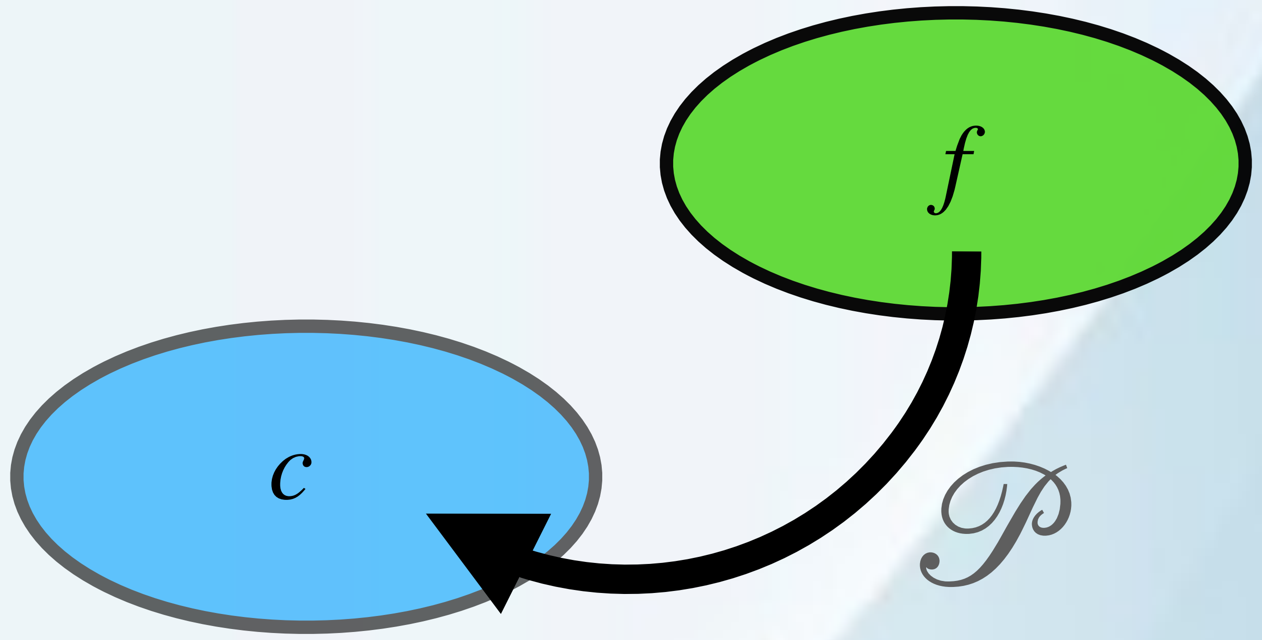

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$$\boxed{\langle \Psi_0 | \left[\mathscr{P}^\dagger_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} \right] f^\dagger_{\mathbf{R}'ja} f_{\mathbf{R}'jb} | \Psi_0 \rangle_{2-legs} = 0 \qquad \forall\, a, b}$$

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The Hamiltonian:

$$\sum_{\mathbf{k}} t^{\alpha\beta}_{\mathbf{k},ii} = 0 \quad \forall\, i \geq 1$$

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$\mathbf{k}$: Crystal momentum

$\mathbf{R}$: Unit cell

i: Projector information:

$i = 0$: Uncorrelated modes

$i = 1$: First subset of correlated modes (e.g. *d* orbitals of atom 1 in unit cell)

$i = 2$: Second subset of correlated modes (e.g. *f* orbitals of atom 1 in unit cell)

…

Local operators:

$$\langle \Psi_G | \hat{\mathscr{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] | \Psi_G \rangle = \langle \Psi_0 | \mathscr{P}^\dagger \hat{\mathscr{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] \mathscr{P} \; | \Psi_0 \rangle$$

$$= \langle \Psi_0 | \left[\prod_{(\mathbf{R}',i') \neq (\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'} \mathscr{P}_{\mathbf{R}'i'} \right] \mathscr{P}^\dagger_{\mathbf{R}i} \hat{\mathscr{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle$$

Local operators: (disconnected terms)

$$\langle\Psi_0|\left[\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'}\mathscr{P}_{\mathbf{R}'i'}\right]\mathscr{P}^\dagger_{\mathbf{R}i}\hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle$$

$$= \langle\Psi_0|\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'}\mathscr{P}_{\mathbf{R}'i'}|\Psi_0\rangle \times \langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle$$

Local operators: (disconnected terms)

$$\langle\Psi_0|\left[\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'}\mathscr{P}_{\mathbf{R}'i'}\right]\mathscr{P}^\dagger_{\mathbf{R}i}\hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle$$

(GA and G. constraints)

$$= \cancel{\langle\Psi_0|\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'}\mathscr{P}_{\mathbf{R}'i'}|\Psi_0\rangle} \times \langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle$$

Local operators: (disconnected terms)

$$\langle \Psi_0 | \left[\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^{\dagger}_{\mathbf{R}'i'} \mathscr{P}_{\mathbf{R}'i'} \right] \mathscr{P}^{\dagger}_{\mathbf{R}i} \hat{\mathscr{O}}\left[c^{\dagger}_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle$$

$$\boxed{= \langle \Psi_0 | \mathscr{P}^{\dagger}_{\mathbf{R}i} \hat{\mathscr{O}}\left[c^{\dagger}_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle}$$

Local operators: (connected terms)

$$\langle \Psi_0 | \left[\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'} \mathscr{P}_{\mathbf{R}'i'} \right] \mathscr{P}^\dagger_{\mathbf{R}i} \hat{\mathcal{O}}[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}] \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle$$

Local operators: (connected terms)

$$\xcancel{\langle\Psi_0|\left[\prod_{(\mathbf{R}',i')\neq(\mathbf{R},i)} \mathscr{P}^\dagger_{\mathbf{R}'i'}\mathscr{P}_{\mathbf{R}'i'}\right]\mathscr{P}^\dagger_{\mathbf{R}i}\,\hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle}$$

(GA and G. constraints)

Local operators:

$$\langle \Psi_G | \hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] | \Psi_G \rangle = \boxed{\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \hat{\mathcal{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right] \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle}$$

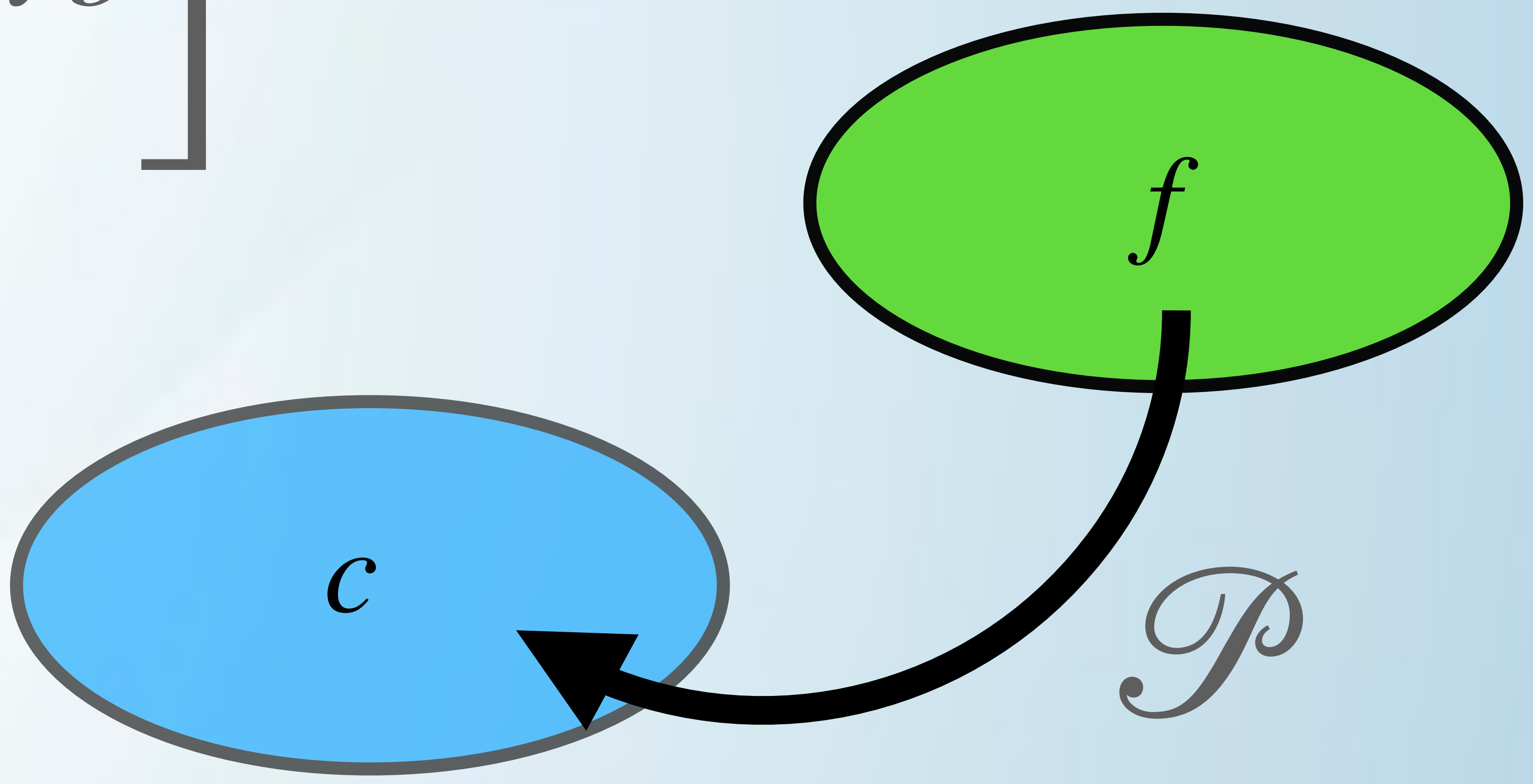
Non-local 1-body operators, i.e., $(\mathbf{R}, i) \neq (\mathbf{R}', i')$:

$$\langle \Psi_G | c^\dagger_{\mathbf{R}i\alpha} c_{\mathbf{R}'i'\beta} | \Psi_G \rangle = \boxed{\langle \Psi_0 | \left[\mathcal{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathcal{P}_{\mathbf{R}i}\right] \left[\mathcal{P}^\dagger_{\mathbf{R}'i'} c_{\mathbf{R}'i'\beta} \mathcal{P}_{\mathbf{R}'i'}\right] | \Psi_0 \rangle}$$

Non-local quadratic operators:

$$\langle \Psi_G | c^\dagger_{\mathbf{R}i\alpha} c_{\mathbf{R}'i'\beta} | \Psi_G \rangle = \langle \Psi_0 | \left[\mathscr{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathscr{P}_{\mathbf{R}i} \right] \left[\mathscr{P}^\dagger_{\mathbf{R}'i'} c_{\mathbf{R}'i'\beta} \mathscr{P}_{\mathbf{R}'i'} \right] | \Psi_0 \rangle$$

$$= \langle \Psi_0 | \left[\sum_a [\mathscr{R}_i]_{a\alpha} f^\dagger_{\mathbf{R}ia} \right] \left[\sum_b [\mathscr{R}_i]^\dagger_{\beta b} f_{\mathbf{R}'i'b} \right] | \Psi_0 \rangle$$



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

$$\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathscr{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle = \sum_{a'} [\mathscr{R}_i]_{a'\alpha} \langle \Psi_0 | f^\dagger_{\mathbf{R}ia'} f_{\mathbf{R}ia} | \Psi_0 \rangle$$

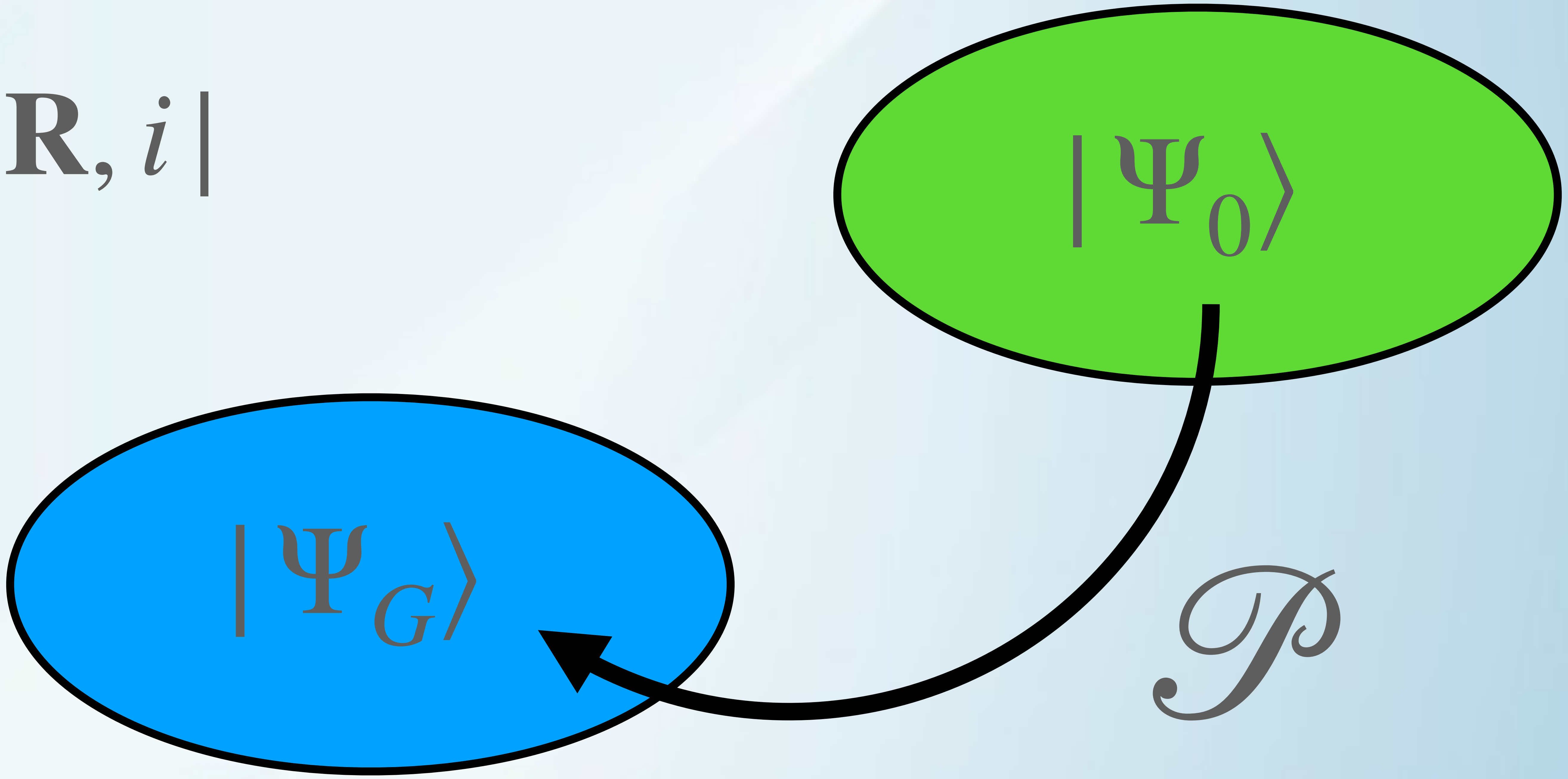
Non-local quadratic operators:

$$\mathscr{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathscr{P}_{\mathbf{R}i} \to \sum_a [\mathscr{R}_i]_{a\alpha} f^\dagger_{\mathbf{R}ia}$$

$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma,n} [\Lambda_i]_{\Gamma,n} \,|\,\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i\,|$$

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

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



Variational energy:

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

$$\mathscr{E} = \sum_{\mathbf{k}ij} \sum_{ab} \left[\mathscr{R}_i t_{\mathbf{k},ij} \mathscr{R}_j^{\dagger} \right]_{ab} \langle \Psi_0 | f_{\mathbf{k}ia}^{\dagger} f_{\mathbf{k}jb} | \Psi_0 \rangle + \sum_{\mathbf{R},i\geq 1} \langle \Psi_0 | \mathscr{P}_{\mathbf{R}i}^{\dagger} \hat{H}_{\mathbf{R}i}^{loc} \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle$$

Where: $\langle \Psi_0 | \mathscr{P}_{\mathbf{R}i}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} \mathscr{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle = \sum_{a'} [\mathscr{R}_i]_{a'\alpha} \langle \Psi_0 | f_{\mathbf{R}ia'}^{\dagger} f_{\mathbf{R}ia} | \Psi_0 \rangle$

$$\langle \Psi_0 | \mathscr{P}_{\mathbf{R}i}^{\dagger} \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Psi_0 | \mathscr{P}_{\mathbf{R}i}^{\dagger} \mathscr{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,\nu_i\}$$

Necessary steps:

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

Variational energy:

$$\mathscr{E} = \sum_{\mathbf{k}ij} \sum_{ab} \left[\mathscr{R}_i t_{\mathbf{k},ij} \mathscr{R}_j^\dagger \right]_{ab} \langle \Psi_0 | f^\dagger_{\mathbf{k}i\alpha} f_{\mathbf{k}j\beta} | \Psi_0 \rangle + \sum_{\mathbf{R},i\geq 1} \langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} \hat{H}^{loc}_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle$$

Where: $\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathscr{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle = \sum_{a'} [\mathscr{R}_i]_{a'\alpha} \langle \Psi_0 | f^\dagger_{\mathbf{R}ia'} f_{\mathbf{R}ia} | \Psi_0 \rangle$

$$\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,\nu_i\}$$

Variational energy:

$$\mathcal{E} = \sum_{\mathbf{k}ij} \sum_{ab} \left[\mathcal{R}_i t_{\mathbf{k},ij} \mathcal{R}_j^\dagger\right]_{ab} \langle \Psi_0 | f^\dagger_{\mathbf{k}i\alpha} f_{\mathbf{k}j\beta} | \Psi_0 \rangle + \sum_{\mathbf{R},i\geq 1} \boxed{\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \hat{H}^{loc}_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle}$$

Where: $\boxed{\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle} = \sum_{a'} [\mathcal{R}_i]_{a'\alpha} \boxed{\langle \Psi_0 | f^\dagger_{\mathbf{R}ia'} f_{\mathbf{R}ia} | \Psi_0 \rangle}$

$$\boxed{\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle} = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$\boxed{\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle} = \langle \Psi_0 | f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle \qquad \forall\, a, b \in \{1,..,\nu_i\}$$

$$\boxed{\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle} = Tr\left[P_i^0 \Lambda_i^\dagger \Lambda_i \right] = 1$$

$$\boxed{\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} \mathscr{P}_{\mathbf{R}i} f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle} = Tr\left[P_i^0 \Lambda_i^\dagger \Lambda_i F^\dagger_{ia} F_{ib} \right] = \langle \Psi_0 | f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle =: [\Delta_i]_{ab}$$

$$\boxed{\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} \hat{\mathscr{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha} \right] \mathscr{P}_{\mathbf{R}i} | \Psi_0 \rangle} = Tr\left[P_i^0 \Lambda_i^\dagger \hat{\mathscr{O}}\left[F^\dagger_{i\alpha}, F_{i\alpha} \right] \Lambda_i \right]$$

$$\boxed{\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathscr{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle} = Tr\left[P_i^0 \Lambda_i^\dagger F^\dagger_{i\alpha} \Lambda_i F_{ia} \right]$$

Where:

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

$$[F_{ia}]_{nn'} = \langle n; \mathbf{R}, i | f_{\mathbf{R}ia} | n'; \mathbf{R}, i \rangle$$

$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma n} [\Lambda_i]_{\Gamma n} | \Gamma; \mathbf{R}, i \rangle \langle n; \mathbf{R}, i |$$

$$| \Gamma; \mathbf{R}, i \rangle = \left[c^\dagger_{\mathbf{R}i1} \right]^{q_1(\Gamma)} \ldots \left[c^\dagger_{\mathbf{R}i\nu_i} \right]^{q_{\nu_i}(\Gamma)} | 0 \rangle$$

$$| n; \mathbf{R}, i \rangle = \left[f^\dagger_{\mathbf{R}i1} \right]^{q_1(n)} \ldots \left[f^\dagger_{\mathbf{R}i\nu_i} \right]^{q_{\nu_i}(n)} | 0 \rangle$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle} = Tr\left[P^0_i\Lambda^\dagger_i\Lambda_i\right] = 1$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}\,f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}|\Psi_0\rangle} = Tr\left[P^0_i\Lambda^\dagger_i\Lambda_i F^\dagger_{ia}F_{ib}\right] = \langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}|\Psi_0\rangle =: [\Delta_i]_{ab}$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\hat{\mathscr{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle} = Tr\left[P^0_i\Lambda^\dagger_i\hat{\mathscr{O}}\left[F^\dagger_{i\alpha}, F_{i\alpha}\right]\Lambda_i\right]$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}c^\dagger_{\mathbf{R}i\alpha}\mathscr{P}_{\mathbf{R}i}f_{\mathbf{R}ia}|\Psi_0\rangle} = Tr\left[P^0_i\Lambda^\dagger_i F^\dagger_{i\alpha}\Lambda_i F_{ia}\right]$$

Where:

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

$$[F_{ia}]_{nn'} = \langle n;\mathbf{R},i|f_{\mathbf{R}ia}|n';\mathbf{R},i\rangle$$

Matrix of SB amplitudes:

$$\phi_i = \Lambda_i\sqrt{P^0_i}$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle} = Tr\left[\phi_i^\dagger\phi_i\right] = 1$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\mathscr{P}_{\mathbf{R}i}f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}|\Psi_0\rangle} = Tr\left[\phi_i^\dagger\phi_i F^\dagger_{ia}F_{ib}\right] = \langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}|\Psi_0\rangle =: [\Delta_i]_{ab}$$

$$\boxed{\langle\Psi_0|\mathscr{P}^\dagger_{\mathbf{R}i}\hat{\mathscr{O}}\left[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}\right]\mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle} = Tr\left[\phi_i\,\phi_i^\dagger\hat{\mathscr{O}}\left[F^\dagger_{i\alpha}, F_{i\alpha}\right]\right]$$

$$Tr\left[\phi_i^\dagger F^\dagger_{i\alpha}\phi_i F_{ia}\right] = \sum_c \boxed{[\mathscr{R}_i]_{c\alpha}}\left[\Delta_i(1-\Delta_i)\right]^{\frac{1}{2}}_{ca}$$

Matrix of SB amplitudes:

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

Variational energy:

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

$$\mathscr{E} = \sum_{\mathbf{k}ij} \sum_{ab} \left[\mathscr{R}_i t_{\mathbf{k},ij} \mathscr{R}_j^{\dagger}\right]_{ab} \langle \Psi_0 | f_{\mathbf{k}ia}^{\dagger} f_{\mathbf{k}jb} | \Psi_0 \rangle + \sum_{\mathbf{R},i\geq 1} Tr\left[\phi_i \phi_i^{\dagger} \hat{H}_{\mathbf{R}i}^{loc}\left[F_{i\alpha}^{\dagger}, F_{i\alpha}\right]\right]$$

Where: $$Tr\left[\phi_i^{\dagger} F_{i\alpha}^{\dagger} \phi_i F_{ia}\right] = \sum_c \left[\mathscr{R}_i\right]_{c\alpha} \left[\Delta_i(1-\Delta_i)\right]_{ca}^{\frac{1}{2}}$$

$$Tr\left[\phi_i^{\dagger}\phi_i\right] = \langle \Psi_0 | \Psi_0 \rangle = 1$$

$$Tr\left[\phi_i^{\dagger}\phi_i F_{ia}^{\dagger} F_{ib}\right] = \langle \Psi_0 | f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} | \Psi_0 \rangle =: \left[\Delta_i\right]_{ab} \qquad \forall\, a,b \in \{1,\ldots,\nu_i\}$$

Necessary steps:

1. Definition of approximations (GA and G. constraints).
2. Evaluation of $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ in terms of $\{ \Lambda_{i \geq 1} \}, | \Psi_0 \rangle$.
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5. Lagrange formulation of the optimization problem.

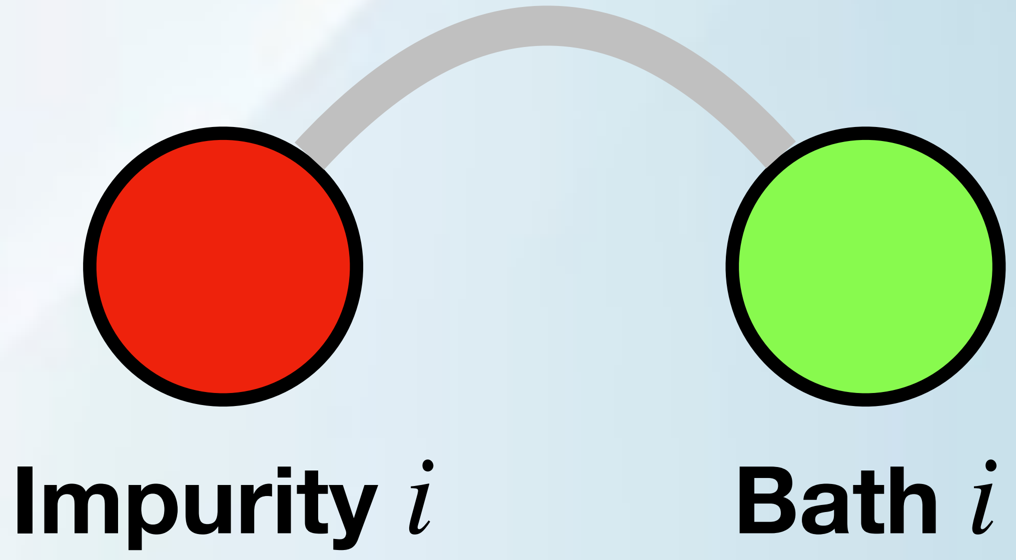
Quantum-embedding formulation

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

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

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

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



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

$$|n;i\rangle = [\hat{f}^{\dagger}_{i1}]^{q_1(n)} \dots [\hat{f}^{\dagger}_{i\nu_i}]^{q_{\nu_i}(n)}|0\rangle$$

Quantum-embedding formulation

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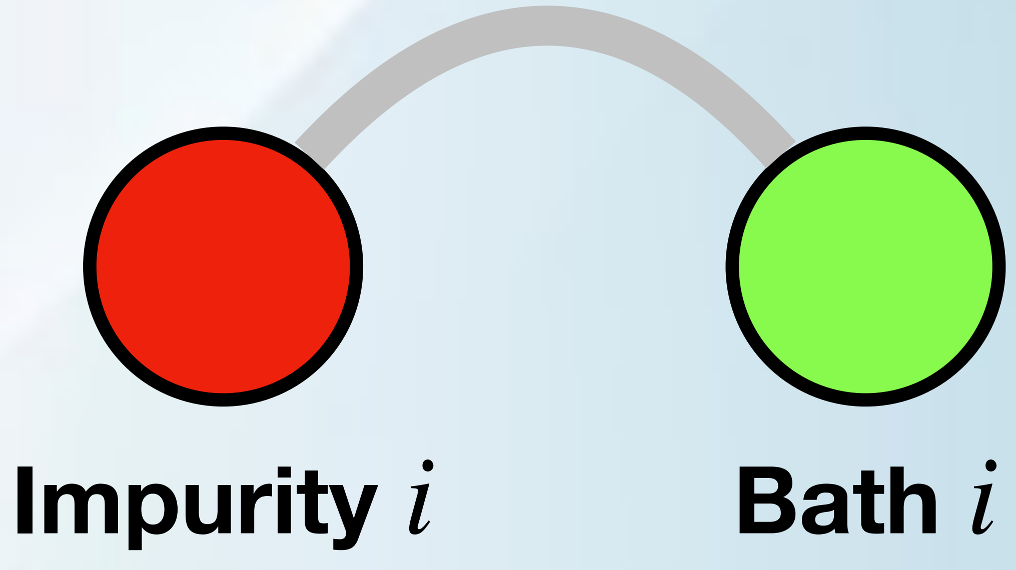

$$|\Gamma; i\rangle = [\hat{c}^\dagger_{i1}]^{q_1(\Gamma)} \dots [\hat{c}^\dagger_{i\nu_i}]^{q_{\nu_i}(\Gamma)} |0\rangle$$

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

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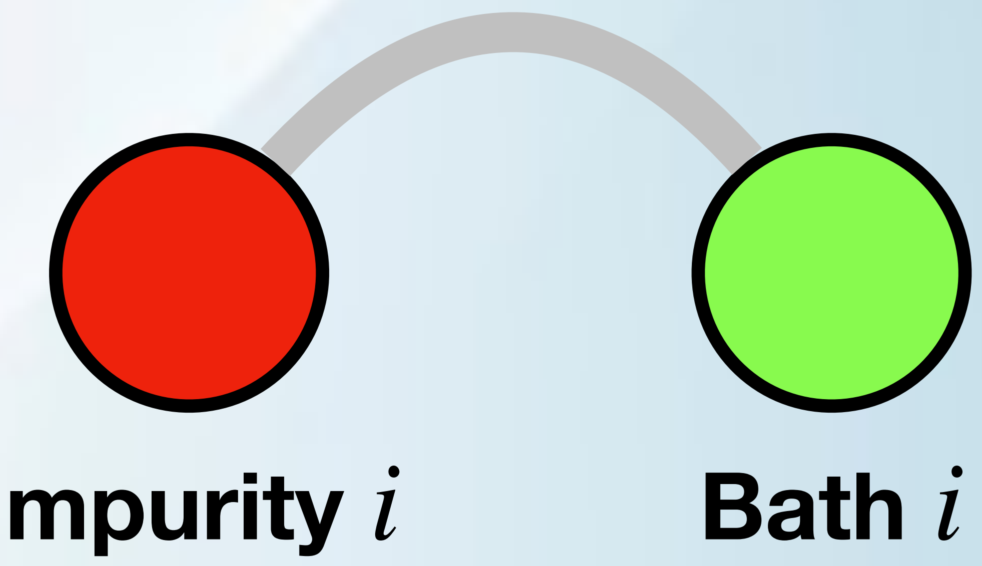
$$N(n) = \sum_{a=1}^{\nu_i} q_a(n)$$



$$\left[\mathscr{P}_{\mathbf{R}i}, \hat{N}_{\mathbf{R,i}}\right] = 0 \leftrightarrow \left[\sum_{\alpha=1}^{\nu_i} \hat{c}^\dagger_\alpha \hat{c}_\alpha + \sum_{a=1}^{\nu_i} \hat{f}^\dagger_a \hat{f}_a\right] |\Phi_i\rangle = \nu_i |\Phi_i\rangle$$

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

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

Quantum-embedding formulation

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

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

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

$$Tr\left[\phi_i \phi_i^\dagger \hat{\mathcal{O}}\left[F_{i\alpha}^\dagger, F_{i\alpha}\right]\right] = \langle \Phi_i | \hat{\mathcal{O}}\left[\hat{c}_{i\alpha}^\dagger, \hat{c}_{i\alpha}\right] | \Phi_i \rangle$$

$$Tr\left[\phi_i^\dagger F_{i\alpha}^\dagger \phi_i F_{ia}\right] = \langle \Phi_i | \hat{c}_{i\alpha}^\dagger \hat{f}_{ia} | \Phi_i \rangle$$

Variational energy:

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

$$\mathscr{E} = \sum_{\mathbf{k}ij} \sum_{ab} \left[\mathscr{R}_i t_{\mathbf{k},ij} \mathscr{R}_j^{\dagger} \right]_{ab} \langle \Psi_0 | f_{\mathbf{k}ia}^{\dagger} f_{\mathbf{k}jb} | \Psi_0 \rangle + \sum_{\mathbf{R},i\geq 1} \langle \Phi_i | \hat{H}_{\mathbf{R}i}^{loc} \left[\hat{c}_{i\alpha}^{\dagger}, \hat{c}_{i\alpha} \right] | \Phi_i \rangle$$

Where: $$\langle \Phi_i | \hat{c}_{i\alpha}^{\dagger} \hat{f}_{ia} | \Phi_i \rangle = \sum_c \left[\mathscr{R}_i \right]_{c\alpha} \left[\Delta_i (1 - \Delta_i) \right]_{ca}^{\frac{1}{2}}$$

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

$$\langle \Phi_i | \hat{f}_{ib} \hat{f}_{ia}^{\dagger} | \Phi_i \rangle = \langle \Psi_0 | f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} | \Psi_0 \rangle =: \left[\Delta_i \right]_{ab} \qquad \forall\, a, b \in \{1,..,\nu_i\}$$

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Variational energy:

$$\mathscr{E} = \sum_{\mathbf{k}ij} \sum_{ab} \left[\mathscr{R}_i t_{\mathbf{k},ij} \mathscr{R}_j^\dagger \right]_{ab} \langle \Psi_0 | f_{\mathbf{k}ia}^\dagger f_{\mathbf{k}jb} | \Psi_0 \rangle + \sum_{\mathbf{R},i\geq 1} \langle \Phi_i | \hat{H}^{loc}_{\mathbf{R}i} [\hat{c}_{i\alpha}^\dagger, \hat{c}_{i\alpha}] | \Phi_i \rangle$$

Where: $\langle \Phi_i | \hat{c}_{i\alpha}^\dagger \hat{f}_{ia} | \Phi_i \rangle =: \sum_c [\mathscr{R}_i]_{c\alpha} \left[\Delta_i (1 - \Delta_i) \right]^{\frac{1}{2}}_{ca}$

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

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

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

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

Variational energy:

$$\mathcal{E} = \sum_{\mathbf{k}ij}\sum_{ab}\left[\mathcal{R}_i t_{\mathbf{k},ij}\mathcal{R}_j^\dagger\right]_{ab}\langle\Psi_0|f^\dagger_{\mathbf{k}ia} f_{\mathbf{k}jb}|\Psi_0\rangle + \sum_{\mathbf{R},i\geq 1}\langle\Phi_i|\hat{H}^{loc}_{\mathbf{R}i}\left[\hat{c}^\dagger_{i\alpha},\hat{c}_{i\alpha}\right]|\Phi_i\rangle$$

Where: $\langle\Phi_i|\hat{c}^\dagger_{i\alpha}\hat{f}_{ia}|\Phi_i\rangle =: \sum_c [\mathcal{R}_i]_{c\alpha}\left[\Delta_i(1-\Delta_i)\right]^{\frac{1}{2}}_{ca}$

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

$\langle\Psi_0|\Psi_0\rangle = 1$ — E

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

$\langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}|\Psi_0\rangle =: [\Delta_i]_{ab}$ — $[\lambda_i]_{ab}$

$\langle\Phi_i|\hat{f}_{ib}\hat{f}^\dagger_{ia}|\Phi_i\rangle = [\Delta_i]_{ab}$ — $[\lambda_i^c]_{ab}$

Lagrange function:

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

Where:

$$\hat{H}_{qp}[\mathscr{R},\lambda] = \sum_{\mathbf{k},ij}\sum_{ab}\left[\mathscr{R}_i t_{\mathbf{k},ij}\mathscr{R}_j^\dagger\right]_{ab} f^\dagger_{\mathbf{k}ia}f_{\mathbf{k}jb} + \sum_{\mathbf{R}i}\sum_{ab}[\lambda_i]_{ab}f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}jb}$$

$$\hat{H}_i^{emb}[\mathscr{D}_i,\lambda_i^c] = \hat{H}^{loc}_{\mathbf{R}i}\left[\hat{c}^\dagger_{i\alpha},\hat{c}_{i\alpha}\right] + \sum_{a\alpha}\left([\mathscr{D}_i]_{a\alpha}\,\hat{c}^\dagger_{i\alpha}\hat{f}_{ia}+\text{H.c.}\right) + \sum_{ab}[\lambda_i^c]_{ab}\,\hat{f}_{ib}\hat{f}^\dagger_{ia}$$

Lagrange equations:

$$(\mathcal{R},\lambda) \longrightarrow \frac{1}{\mathcal{N}}\left[\sum_{\mathbf{k}} \Pi_i f\left(\mathcal{R} t_{\mathbf{k}} \mathcal{R}^\dagger + \lambda\right)\Pi_i\right]_{ba} = [\Delta_i]_{ab} \longrightarrow [\Delta_i]_{ab}$$

$$\frac{1}{\mathcal{N}}\left[\sum_{\mathbf{k}} \Pi_i t_{\mathbf{k}}\mathcal{R}^\dagger f\left(\mathcal{R} t_{\mathbf{k}}\mathcal{R}^\dagger+\lambda\right)\Pi_i\right]_{\alpha a} = \sum_{c,a=1}^{\nu_i}\sum_{\alpha=1}^{\nu_i}[\mathcal{D}_i]_{c\alpha}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}} \longrightarrow [\mathcal{D}_i]_{c\alpha}$$

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

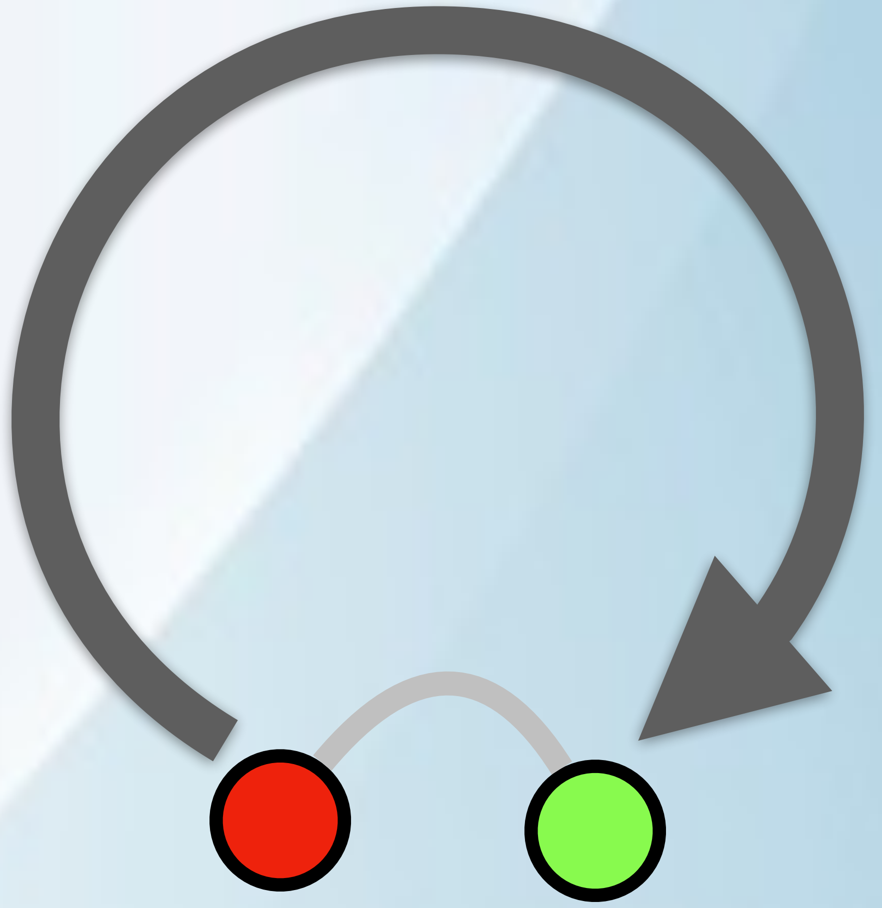
$$\hat{H}_i^{\mathrm{emb}}|\Phi_i\rangle = E_i^c|\Phi_i\rangle \longrightarrow |\Phi_i\rangle$$

$$\left[\mathcal{F}_i^{(1)}\right]_{\alpha a} = \langle\Phi_i|\hat{c}^\dagger_{i\alpha}\hat{f}_{ia}|\Phi_i\rangle - \sum_{c=1}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}[\mathcal{R}_i]_{c\alpha} \overset{!}{=} 0$$

$$\left[\mathcal{F}_i^{(2)}\right]_{ab} = \langle\Phi_i|\hat{f}_{ib}\hat{f}^\dagger_{ia}|\Phi_i\rangle - [\Delta_i]_{ab} \overset{!}{=} 0$$

$$\left\{\begin{aligned}\Delta_i &= \sum_{s=1}^{\nu_i^2}\left[d_i^0\right]_s{}^t\left[h_i\right]_s\\ \lambda_i &= \sum_{s=1}^{\nu_i^2}\left[l_i\right]_s\left[h_i\right]_s\\ \lambda_i^c &= \sum_{s=1}^{\nu_i^2}\left[l_i^c\right]_s\left[h_i\right]_s\end{aligned}\right.$$

Lagrange equations:



$$(\mathscr{R},\lambda) \longrightarrow \frac{1}{\mathcal{N}}\left[\sum_{\mathbf{k}} \Pi_i f\left(\mathscr{R} t_{\mathbf{k}} \mathscr{R}^\dagger + \lambda\right)\Pi_i\right]_{ba} = [\Delta_i]_{ab} \longrightarrow [\Delta_i]_{ab}$$

$$\frac{1}{\mathcal{N}}\left[\sum_{\mathbf{k}}\Pi_i t_{\mathbf{k}}\mathscr{R}^\dagger f\left(\mathscr{R}t_{\mathbf{k}}\mathscr{R}^\dagger+\lambda\right)\Pi_i\right]_{\alpha a} = \sum_{c,a=1}^{\nu_i}\sum_{\alpha=1}^{\nu_i}[\mathscr{D}_i]_{c\alpha}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}} \longrightarrow [\mathscr{D}_i]_{c\alpha}$$

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

$$\hat{H}_i^{\text{emb}}|\Phi_i\rangle = E_i^c|\Phi_i\rangle \longrightarrow |\Phi_i\rangle$$

$$\boxed{\begin{aligned}\left[\mathcal{F}_i^{(1)}\right]_{\alpha a} &= \langle\Phi_i|\hat{c}^\dagger_{i\alpha}\hat{f}_{ia}|\Phi_i\rangle - \sum_{c=1}\left[\Delta_i\left(1-\Delta_i\right)\right]^{\frac{1}{2}}[\mathscr{R}_i]_{c\alpha} \overset{!}{=} 0\\ \left[\mathcal{F}_i^{(2)}\right]_{ab} &= \langle\Phi_i|\hat{f}_{ib}\hat{f}^\dagger_{ia}|\Phi_i\rangle - [\Delta_i]_{ab} \overset{!}{=} 0\end{aligned}}$$

$$\left\{\begin{aligned}\Delta_i &= \sum_{s=1}^{\nu_i^2}\left[d_i^0\right]_s{}^t\left[h_i\right]_s\\ \lambda_i &= \sum_{s=1}^{\nu_i^2}\left[l_i\right]_s\left[h_i\right]_s\\ \lambda_i^c &= \sum_{s=1}^{\nu_i^2}\left[l_i^c\right]_s\left[h_i\right]_s\end{aligned}\right.$$

Necessary steps:

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

Outline

A. Quantum Embedding (QE) methods.

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

C. DFT+GA algorithmic structure.

D. Spectral properties.

E. Examples of applications.

F. Recent formalism extensions (g-GA).

DFT+GA: algorithmic structure

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]

Kohn-Sham scheme:

$$\begin{cases} \mathscr{E}[\rho] = T_{KS}[\rho] + E_{HXC}[\rho] + \int \mathbf{dr}\, V(\mathbf{r})\, \rho(\mathbf{r}) \\ T_{KS}[\rho] = \min\limits_{\Psi_0 \to \rho} \langle \Psi_0 | \hat{T} | \Psi_0 \rangle \end{cases}$$

$$\min_{\rho} \mathscr{E}[\rho] = \min_{\Psi_0} \left[\langle \Psi_0 | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\, \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle + E_{HXC}\big[\langle \Psi_0 | \hat{\rho} | \Psi_0 \rangle\big] \right]$$

Kohn-Sham scheme:

$$\begin{cases} \mathscr{E}[\rho] = T_{KS}[\rho] + E_{HXC}[\rho] + \displaystyle\int \mathbf{dr}\, V(\mathbf{r})\,\rho(\mathbf{r}) \\ T_{KS}[\rho] = \min\limits_{\Psi_0 \to \rho} \langle \Psi_0 | \hat{T} | \Psi_0 \rangle \end{cases}$$

$$\min_{\rho} \mathscr{E}[\rho] = \min_{\Psi_0} \left[\langle \Psi_0 | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\,\hat{\rho}(\mathbf{r}) | \Psi_0 \rangle + E_{HXC}\big[\langle \Psi_0 | \hat{\rho} | \Psi_0 \rangle\big] \right]$$

$$\mathcal{S}[\Psi_0, \rho(\mathbf{r}), \mathscr{J}(\mathbf{r})] = \langle \Psi_0 | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\,\hat{\rho}(\mathbf{r}) | \Psi_0 \rangle + E_{HXC}[\rho]$$

$$+ \int \mathbf{dr}\, \mathscr{J}(\mathbf{r}) \big(\langle \Psi_0 | \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle - \rho(\mathbf{r}) \big)$$

Enforcing definition of $\rho(\mathbf{r})$

Kohn-Sham scheme:

$$\begin{cases} \mathscr{E}[\rho] = T_{KS}[\rho] + E_{HXC}[\rho] + \displaystyle\int \mathbf{dr}\, V(\mathbf{r})\, \rho(\mathbf{r}) \\ T_{KS}[\rho] = \displaystyle\min_{\Psi_0 \rightarrow \rho} \langle \Psi_0 | \hat{T} | \Psi_0 \rangle \end{cases}$$

$\rho_0(\mathbf{r})$

$\downarrow$

$\mathscr{J}(\mathbf{r})$

$\downarrow$

Solve $\hat{H}_{KS}$

& calculate $\rho(\mathbf{r})$

$$\min_{\rho} \mathscr{E}[\rho] = \min_{\Psi_0} \left[\langle \Psi_0 | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\, \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle + E_{HXC}\big[\langle \Psi_0 | \hat{\rho} | \Psi_0 \rangle\big] \right]$$

$$\mathcal{S}[\Psi_0, \rho(\mathbf{r}), \mathscr{J}(\mathbf{r})] = \langle \Psi_0 | \underbrace{\boxed{\hat{T} + \int \mathbf{dr} \left(V(\mathbf{r}) + \mathscr{J}(\mathbf{r}) \right) \hat{\rho}(\mathbf{r})}}_{\hat{H}_{KS}} | \Psi_0 \rangle + E_{HXC}[\rho] - \int \mathbf{dr}\, \mathscr{J}(\mathbf{r}) \rho(\mathbf{r})$$

Kohn-Sham-Hubbard scheme:

$$+\sum_{i\geq 1} E_{dc}^{U_i,J_i}\left(\langle \Psi_G | \hat{N}_i | \Psi_G \rangle\right)$$

$$\begin{cases} \mathcal{E}[\rho] = T_{KSH}[\rho] + E_{HXC}[\rho] + \int \mathbf{dr}\, V(\mathbf{r})\, \rho(\mathbf{r}) \\ T_{KSH}[\rho] = \min\limits_{\Psi_G \to \rho} \langle \Psi_G | \hat{T} | \Psi_G \rangle \end{cases}$$

Projectors over "correlated" degrees of freedom

$$+\sum_{i\geq 1} \hat{H}_i^{U_i,J_i}$$

$$\min_{\rho} \mathcal{E}[\rho] = \min_{\Psi_G} \left[\langle \Psi_G | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\, \hat{\rho}(\mathbf{r}) + \sum_{i\geq 1} \hat{H}_i^{U_i,J_i} | \Psi_G \rangle + \right.$$

$$\left. + E_{HXC}\left[\langle \Psi_G | \hat{\rho} | \Psi_G \rangle\right] + E_{dc}^{U,J}\left(\langle \Psi_G | \hat{N}_i | \Psi_G \rangle\right) \right]$$

Kohn-Sham-**Hubbard** scheme:

$$\min_{\rho} \mathscr{E}[\rho] = \min_{\Psi_G} \Bigg[\langle \Psi_G | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\, \hat{\rho}(\mathbf{r}) + \sum_{i \geq 1} \hat{H}_i^{U_i, J_i} | \Psi_G \rangle + \\ + E_{HXC}\big[\langle \Psi_G | \hat{\rho} | \Psi_G \rangle\big] + \sum_{i \geq 1} E_{dc}^{U_i, J_i}\big(\langle \Psi_G | \hat{N}_i | \Psi_G \rangle\big) \Bigg]$$

$$+ \int \mathbf{dr}\, \mathscr{J}(\mathbf{r}) \big(\langle \Psi_G | \hat{\rho}(\mathbf{r}) | \Psi_G \rangle - \rho(\mathbf{r}) \big)$$

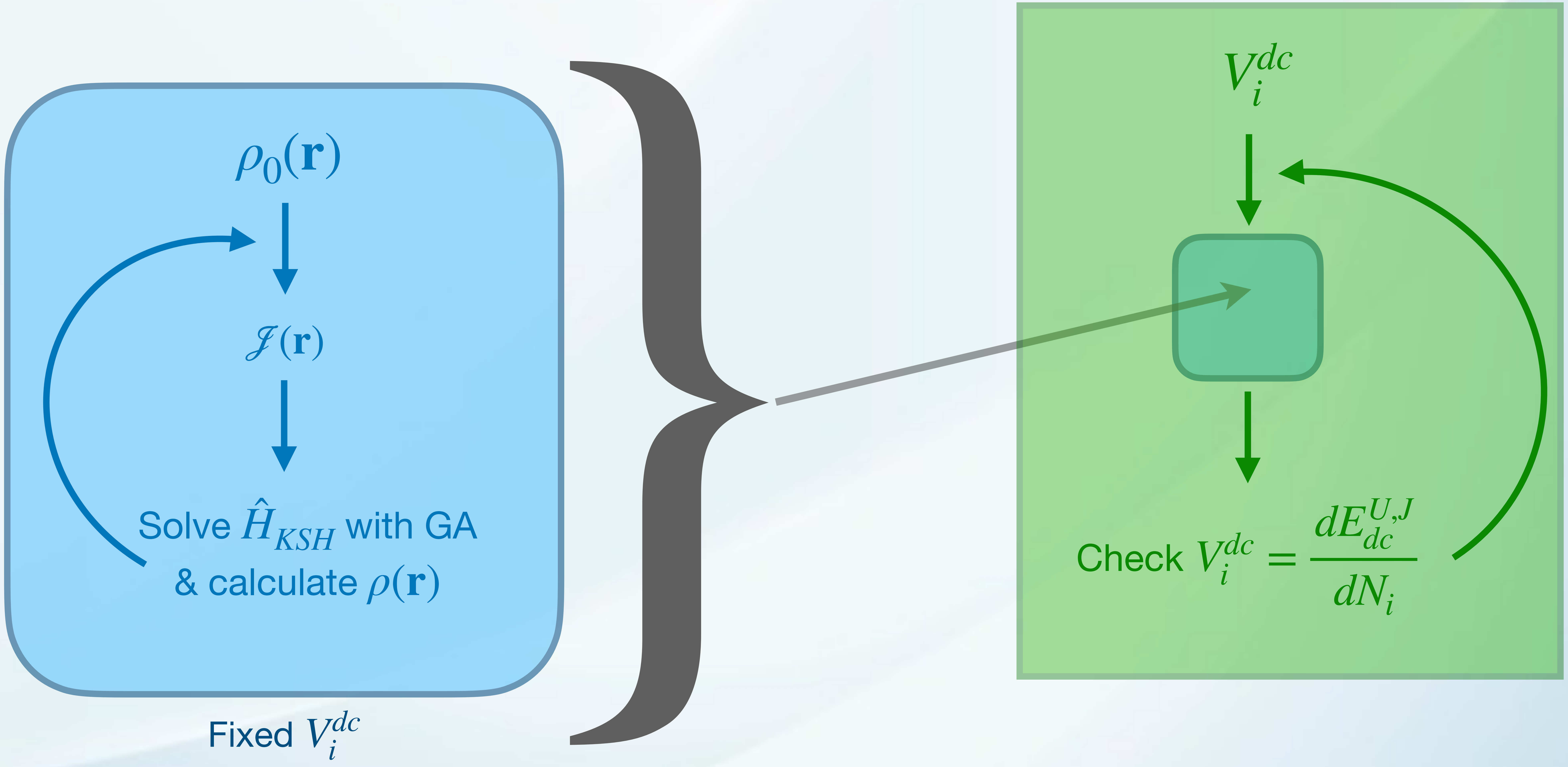
Enforcing definition of $\rho(\mathbf{r})$

$$+ \sum_{i \geq 1} V_i^{dc} \big(\langle \Psi_G | \hat{N}_i | \Psi_G \rangle - N_i \big)$$

Enforcing definition of N_i

Algorithmic structure:

$$\hat{H}_{KSH} = \hat{T} + \int \mathbf{dr}\left[V(\mathbf{r}) + \mathcal{J}(\mathbf{r})\right]\hat{\rho}(\mathbf{r}) + \sum_{i\geq 1}\left(\hat{H}_i^{U_i,J_i} + V_i^{dc}\hat{N}_i\right)$$



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F. Recent formalism extensions.

Spectral properties

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

Excited states: $$|\Psi_G^{\mathbf{k}n}\rangle = \mathscr{P}\,\xi^\dagger_{\mathbf{k}n}\,|\Psi_0\rangle$$

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

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

Landau-Gutzwiller quasiparticles

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Spectral properties

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

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

Spectral properties

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

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$$\Sigma(\omega) = \begin{pmatrix} [\mathbf{0}]_{\nu_0\times\nu_0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \Sigma_1(\omega) & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \dots & \dots & \Sigma_M(\omega) \end{pmatrix}$$

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

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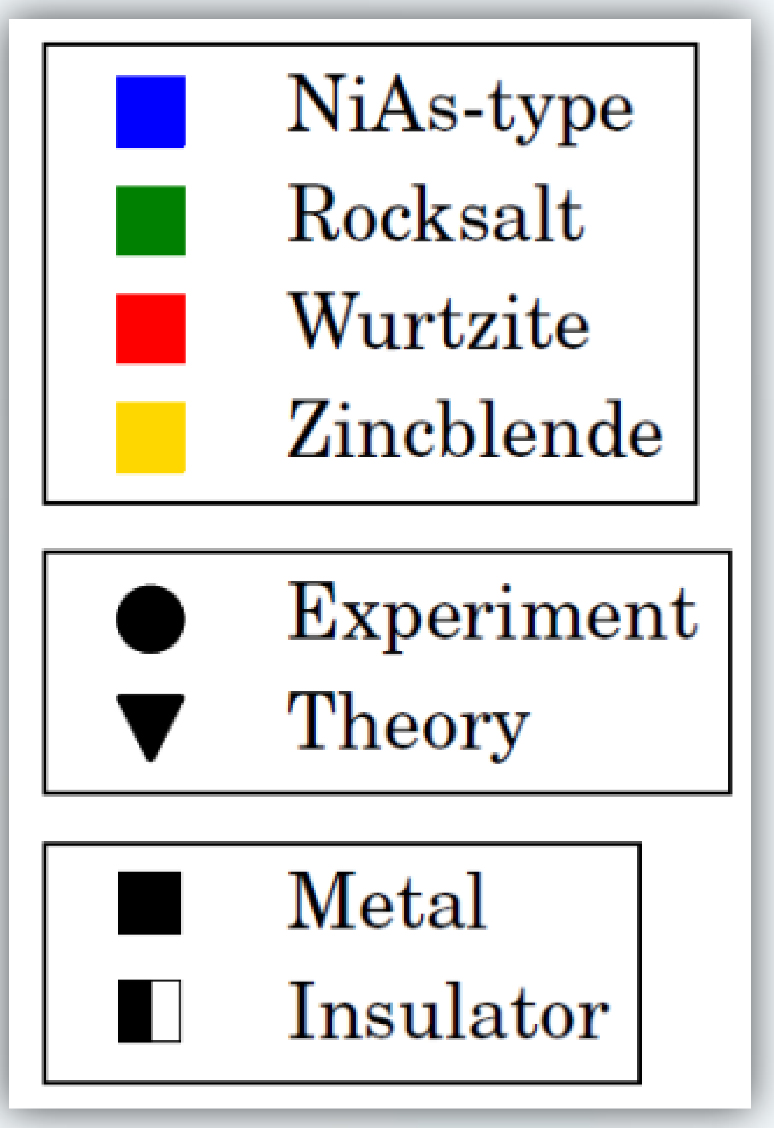
Example: *Structure, Density, Gap*
Theory vs Experiments

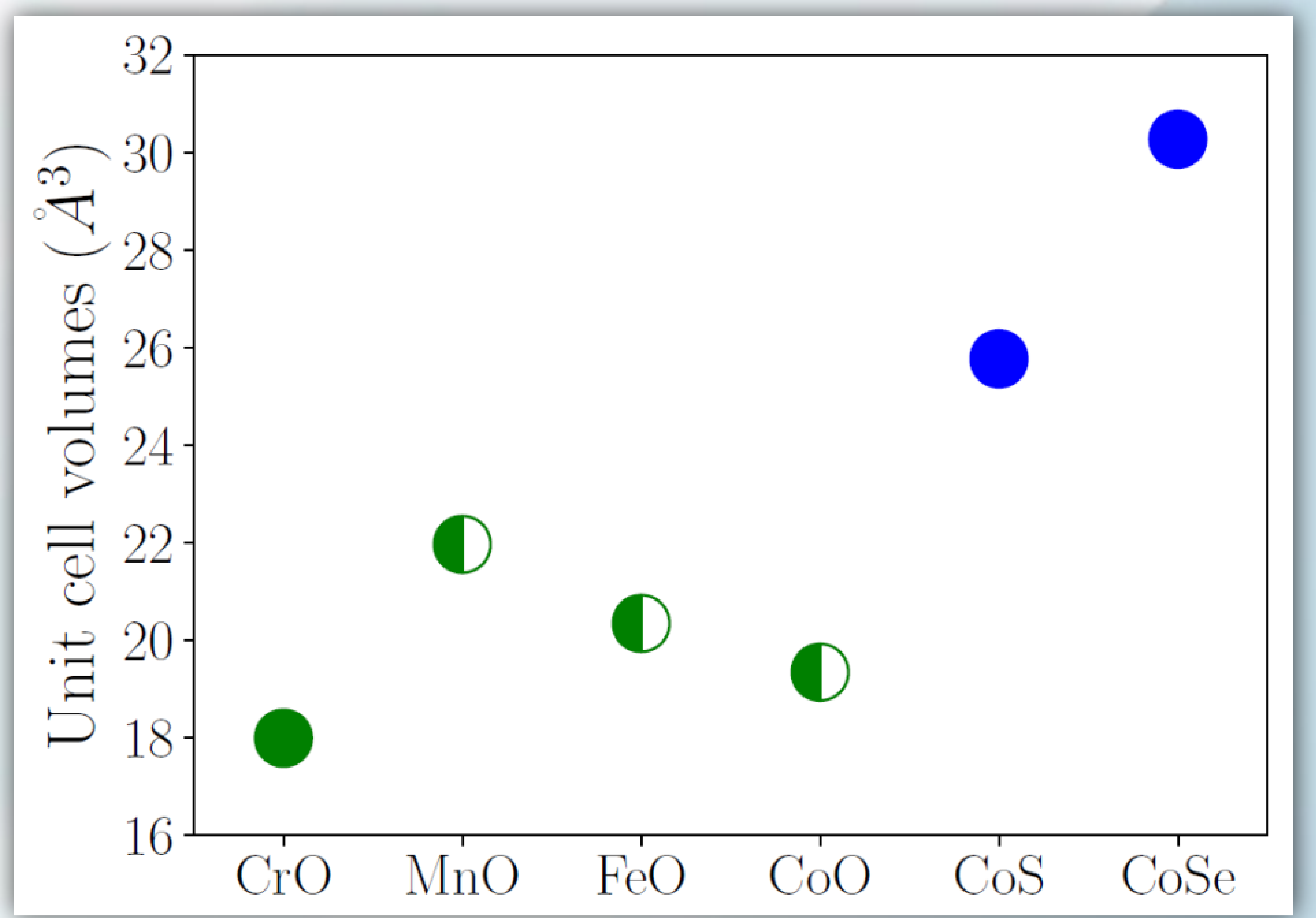
npj Computational Materials www.nature.com/npjcompumats

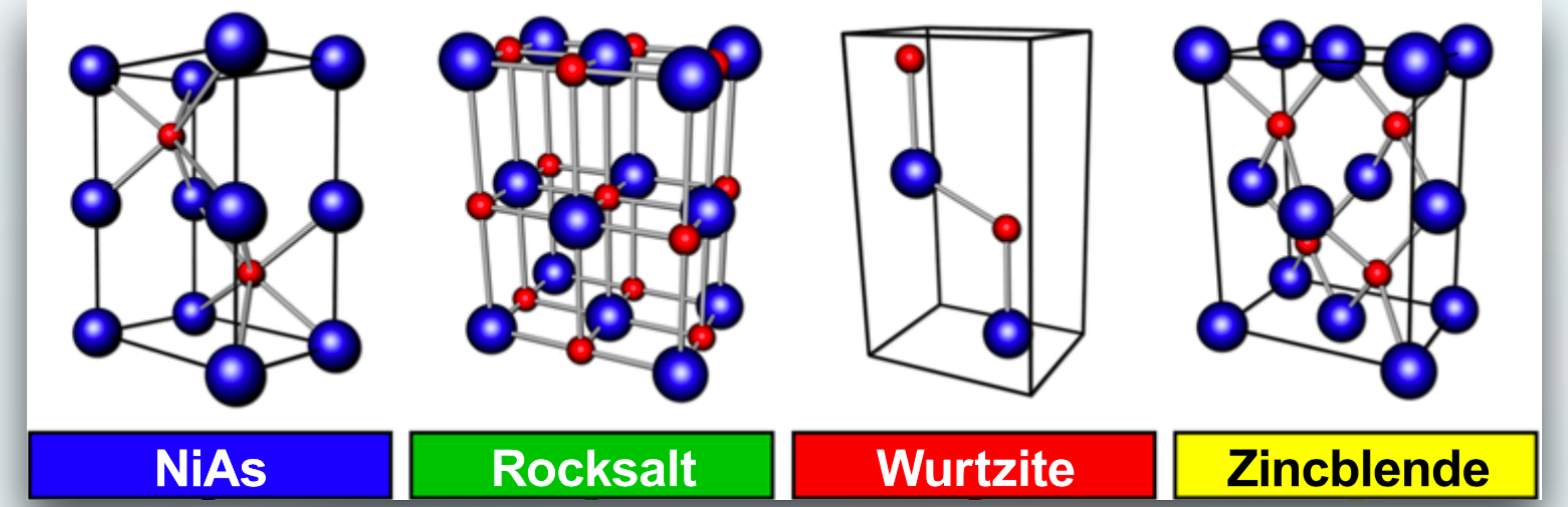
ARTICLE OPEN

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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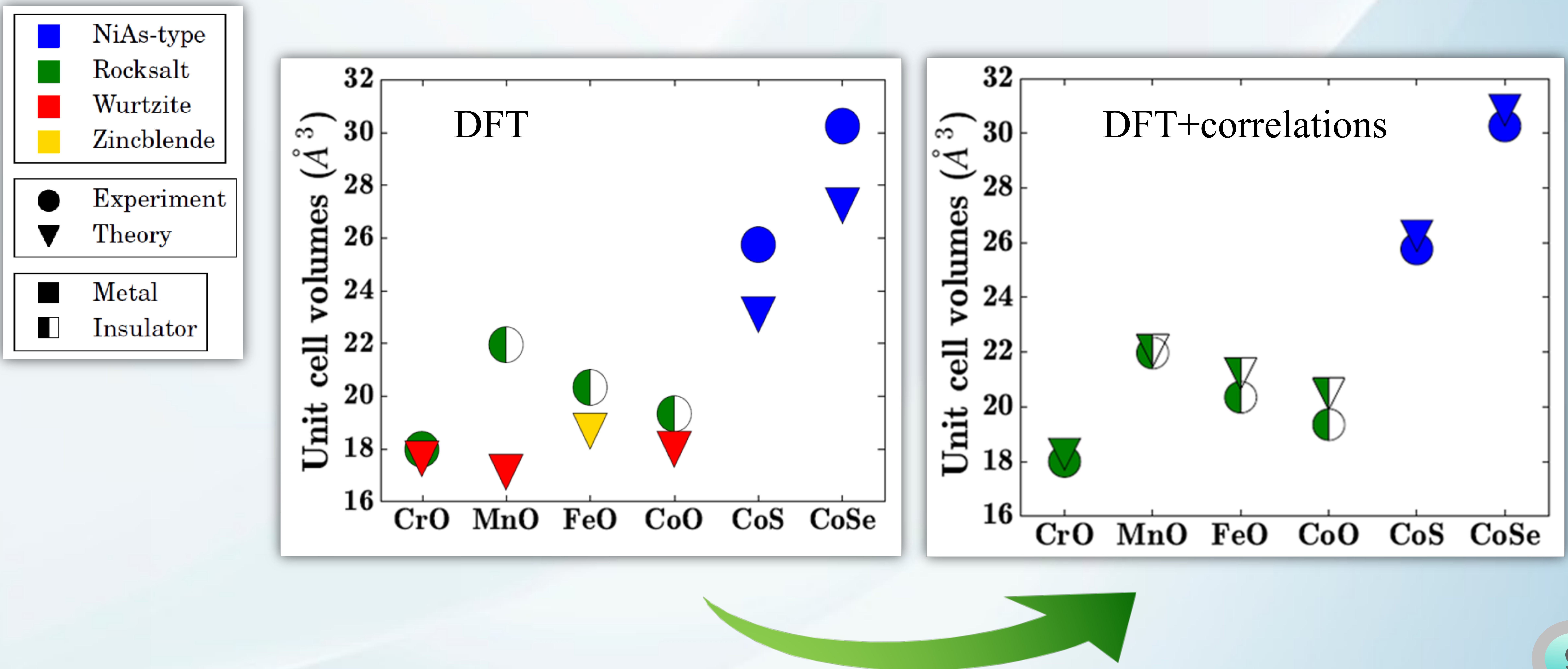
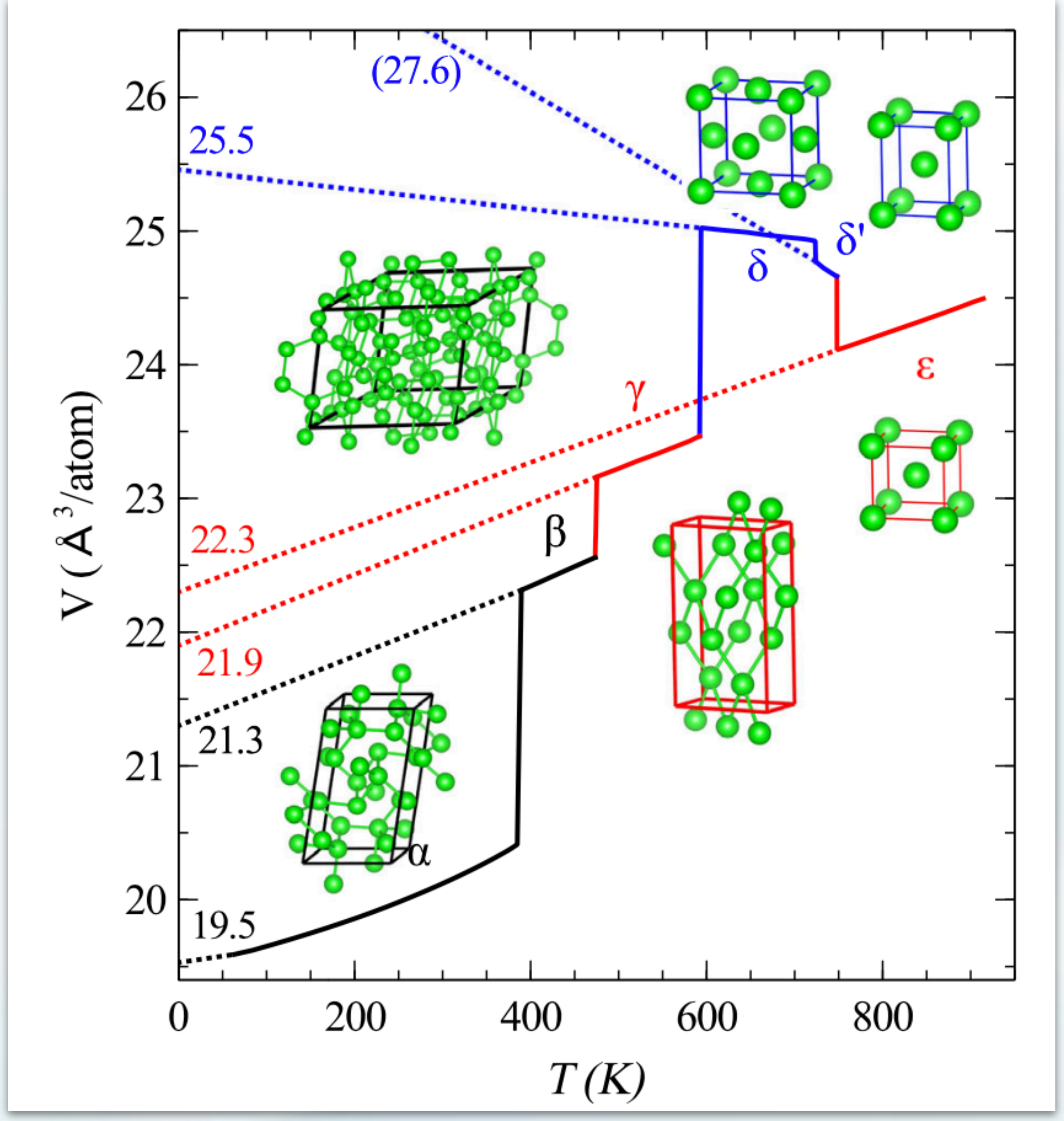


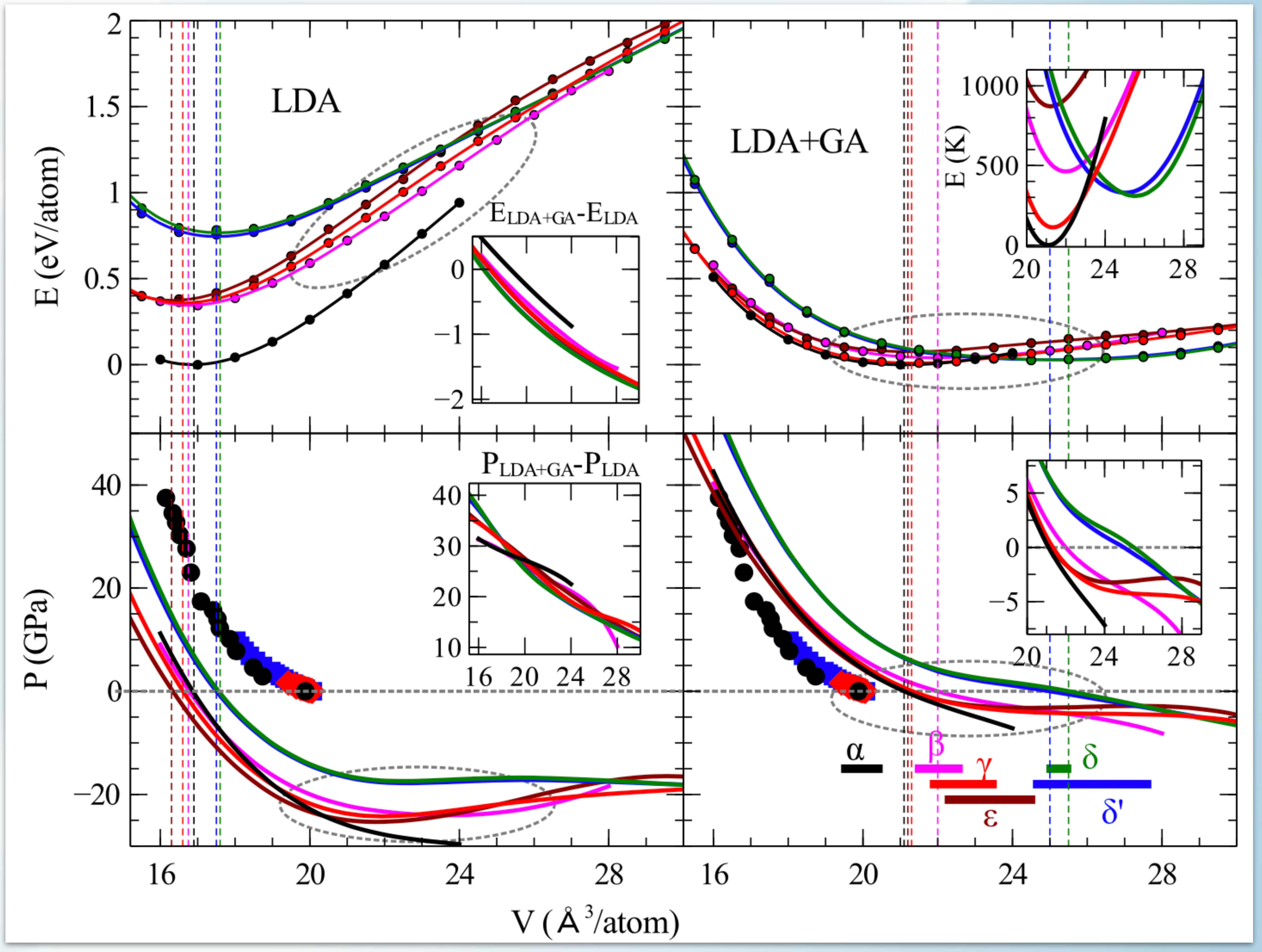
Example: phase diagram of Pu

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]





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F. Recent formalism extensions.

A more accurate extension: the g-GA method

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 **105**, 045111 (2022)

Operatorial formulation of the ghost rotationally invariant slave-boson theory

Nicola Lanatà[*]

PHYSICAL REVIEW MATERIALS **3**, 054605 (2019)

Exciton Mott transition revisited

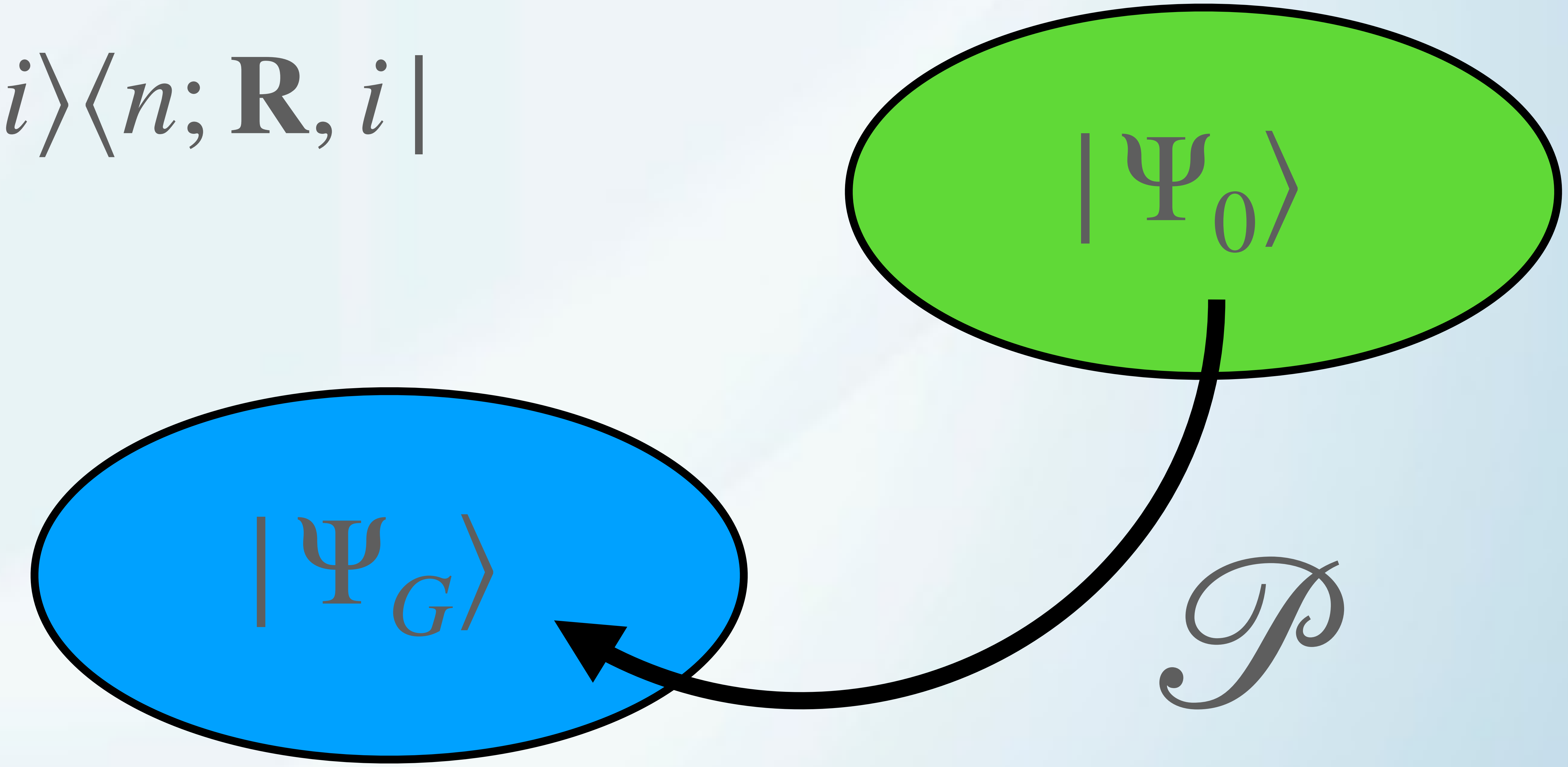
Daniele Guerci, Massimo Capone, and Michele Fabrizio

The GA variational wave function:

$$|\Psi_G\rangle = \mathscr{P}|\Psi_0\rangle = \prod_{\mathbf{R},i\geq 1} \mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle$$

$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma n} [\Lambda_i]_{\Gamma n} |\Gamma; \mathbf{R}, i\rangle\langle n; \mathbf{R}, i|$$

Square matrix: $2^{\nu_i} \times 2^{\nu_i}$



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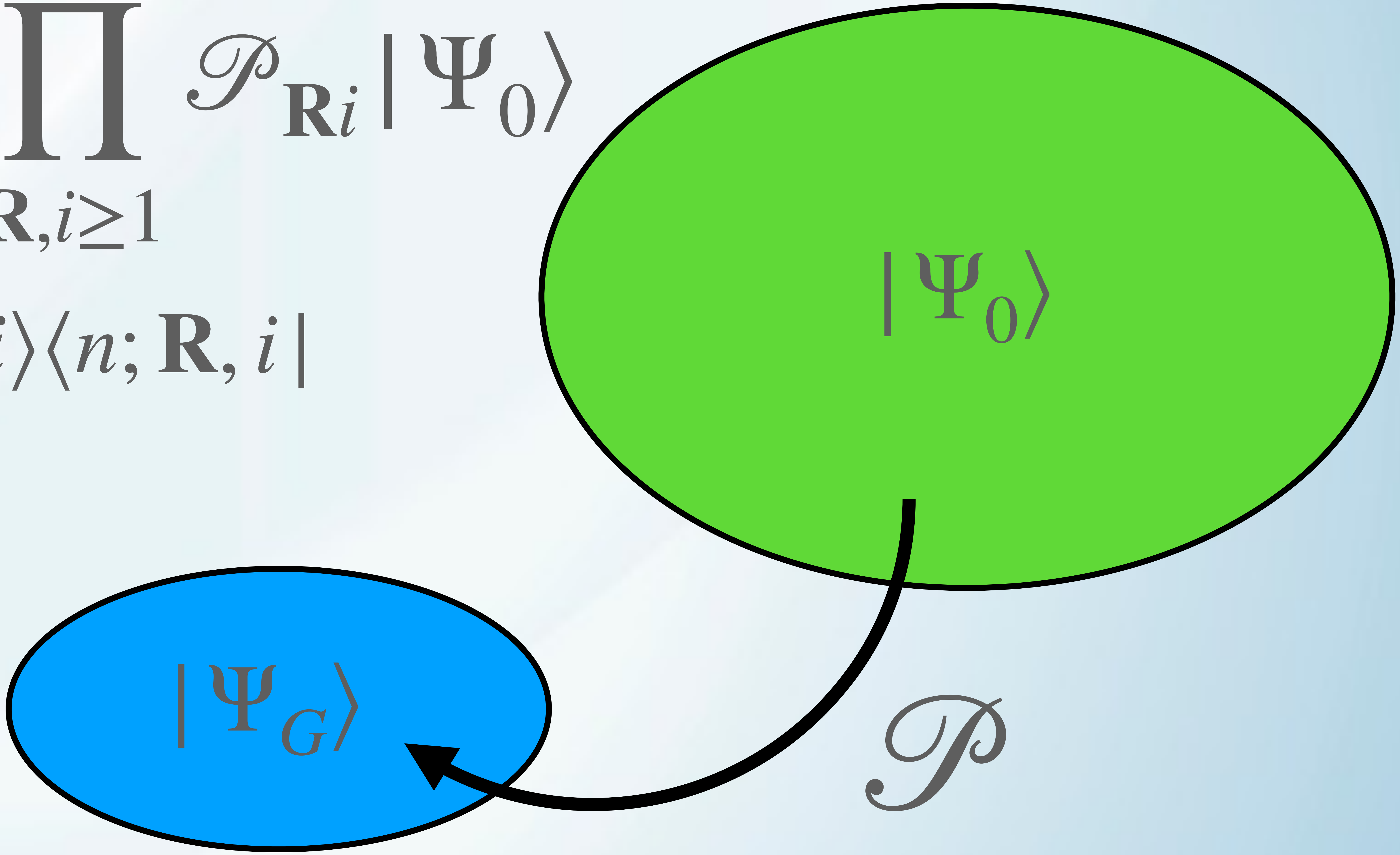
$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma n} [\Lambda_i]_{\Gamma n}\,|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i\,|$$

Rectangular matrix: $2^{\nu_i} \times 2^{\tilde{\nu}_i}$



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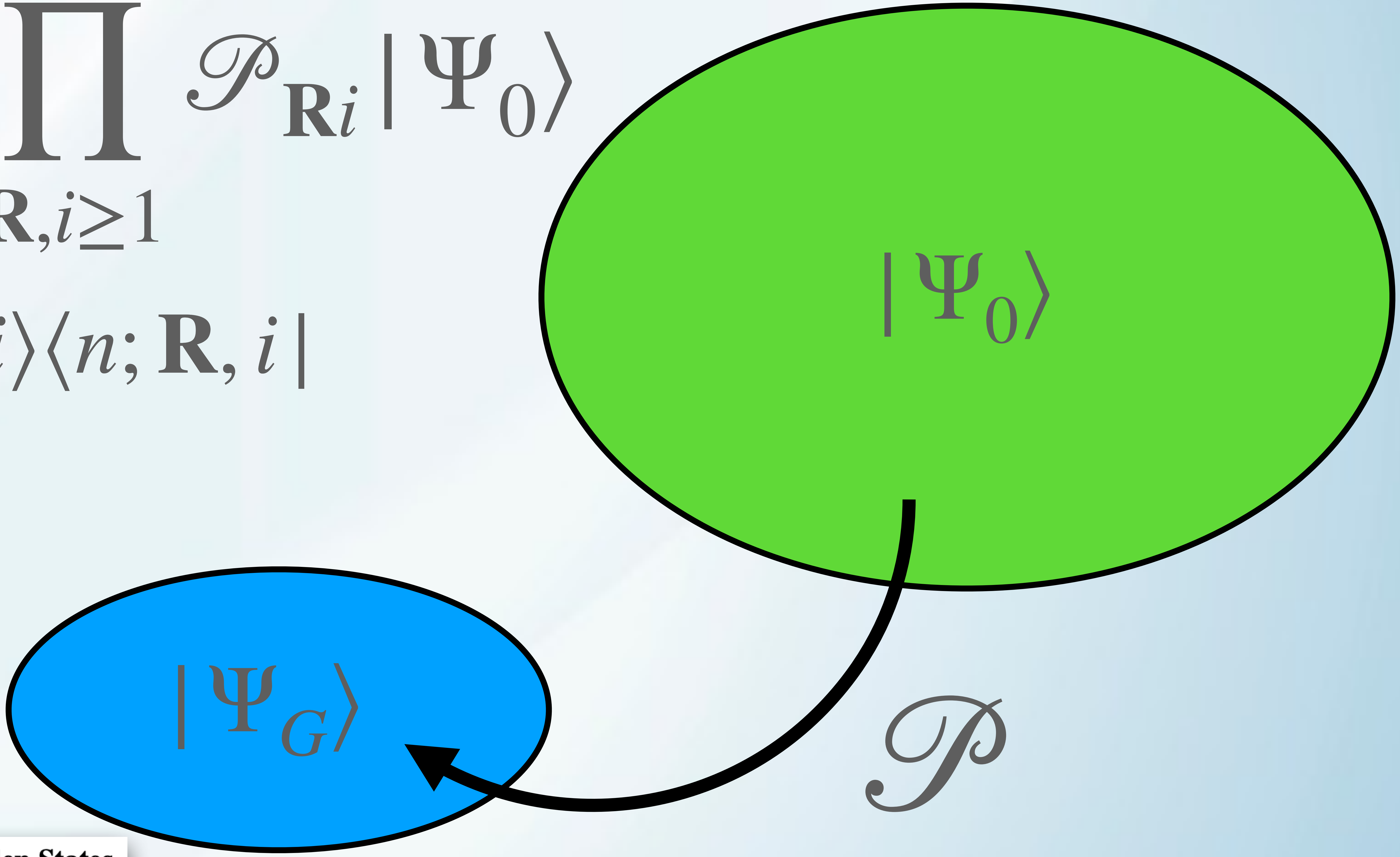
Rectangular matrix: $2^{\nu_i} \times 2^{\tilde{\nu}_i}$



Fermionic Wave Functions from Neural-Network Constrained Hidden States

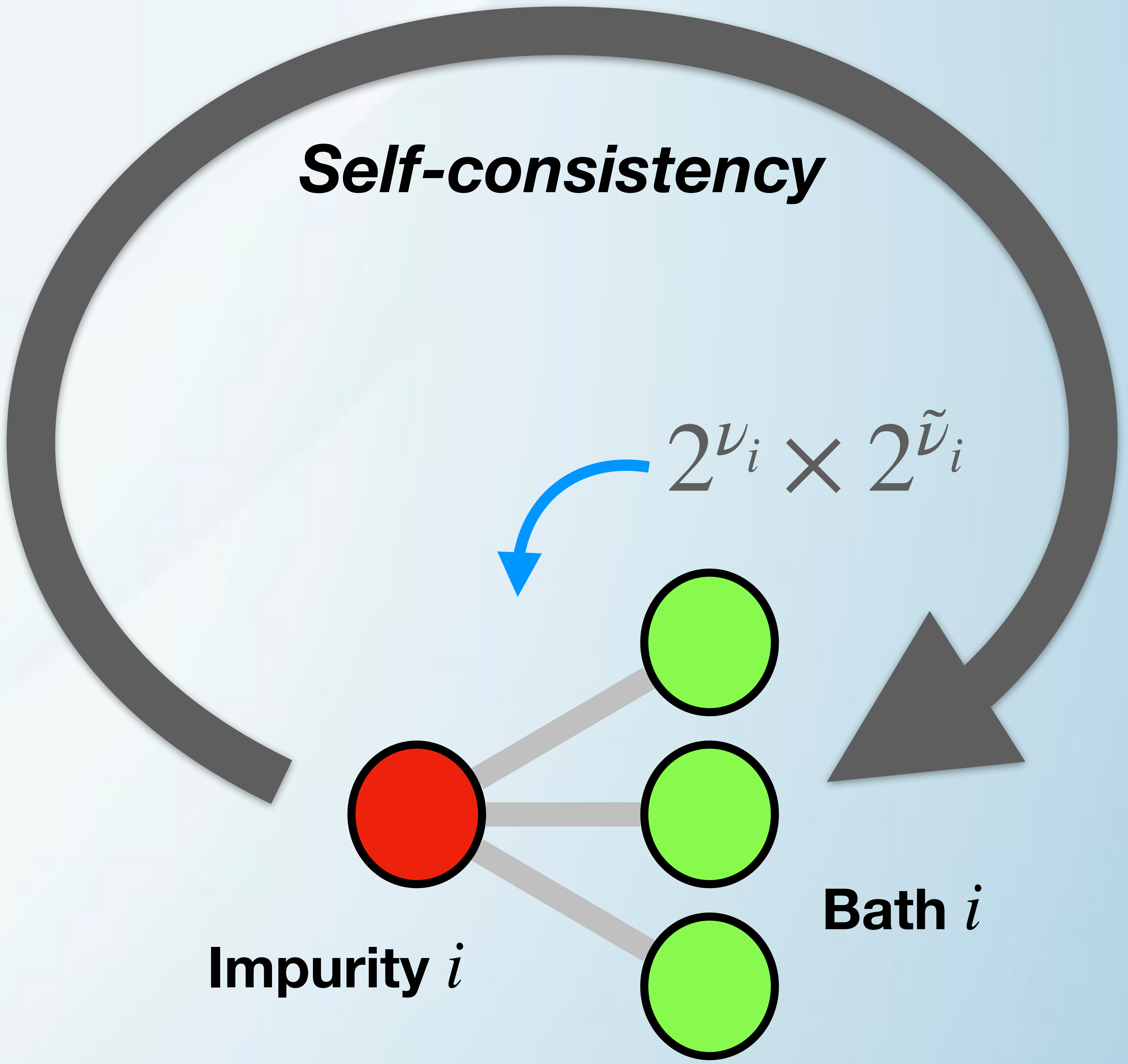
Javier Robledo Moreno,[1,2,*] Giuseppe Carleo,[3,†] Antoine Georges,[4,5,6,7,‡] and James Stokes[1,8,§]

The GA variational wave function:

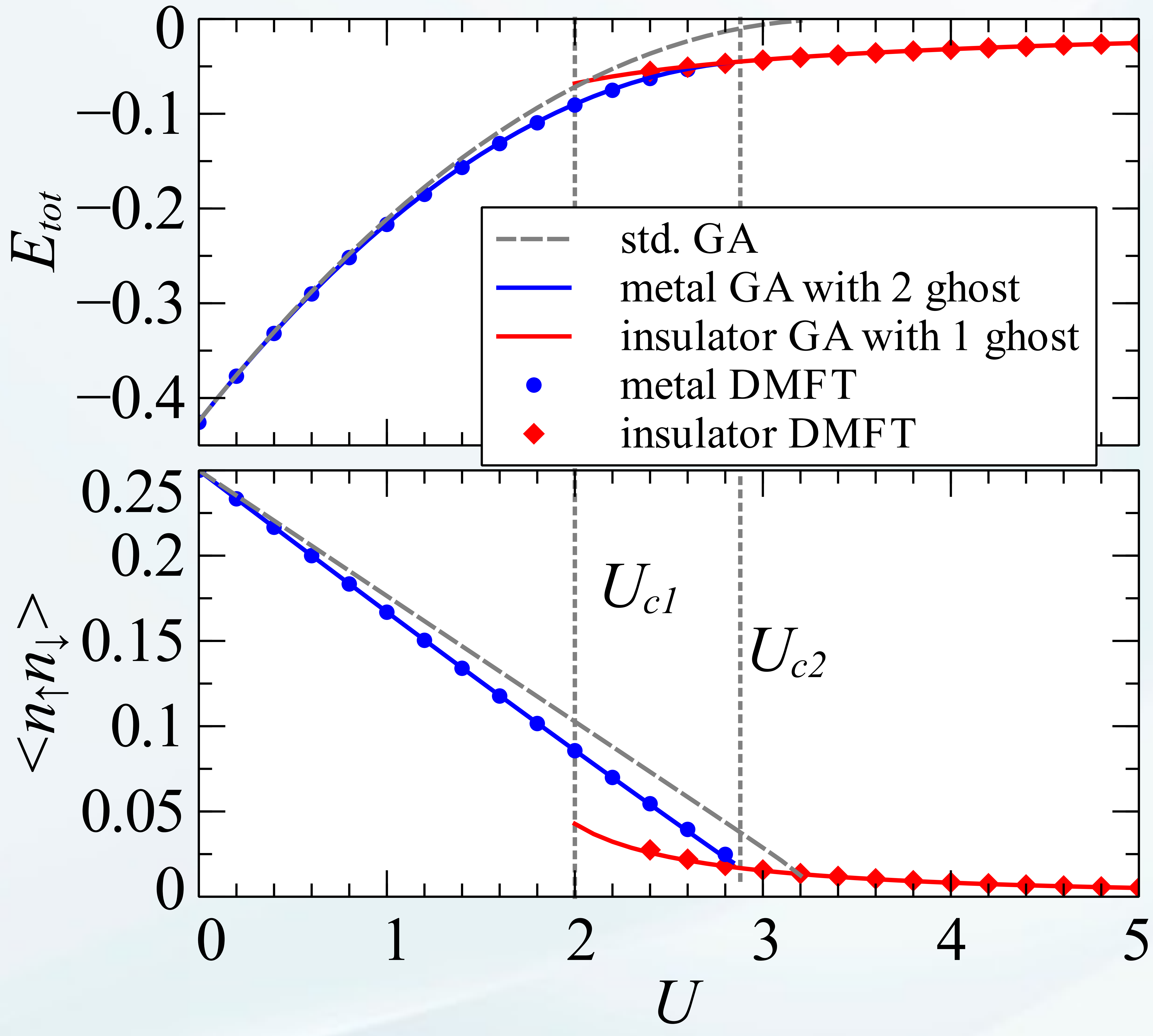
$$|\Psi_G\rangle = \mathscr{P}|\Psi_0\rangle = \prod_{\mathbf{R},i\geq 1} \mathscr{P}_{\mathbf{R}i}|\Psi_0\rangle$$

$$\mathscr{P}_{\mathbf{R}i} = \sum_{\Gamma n} [\Lambda_i]_{\Gamma n} |\Gamma; \mathbf{R}, i\rangle\langle n; \mathbf{R}, i|$$

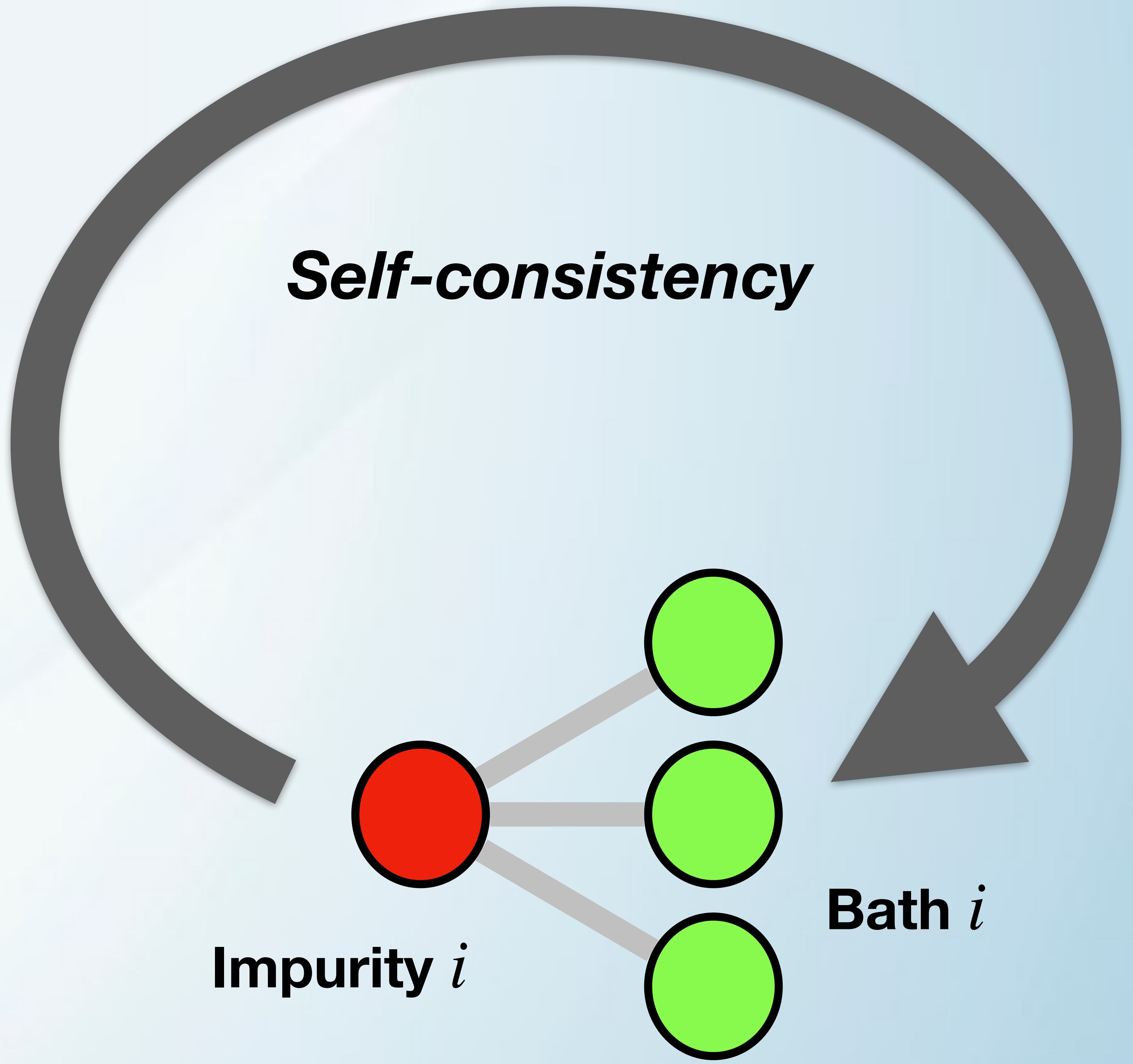
Rectangular matrix: $2^{\nu_i} \times 2^{\tilde{\nu}_i}$



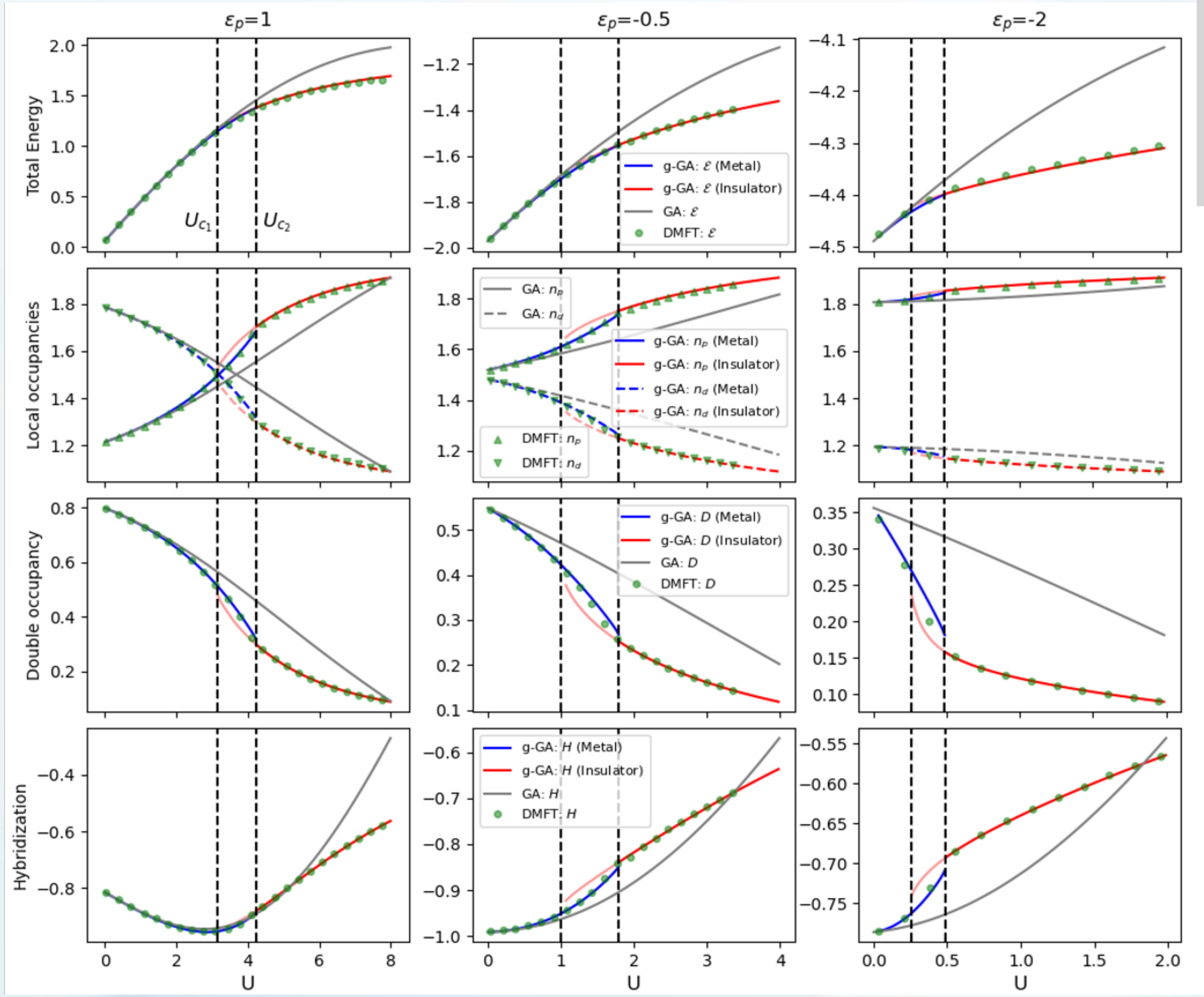
Benchmark calculations Hubbard model:



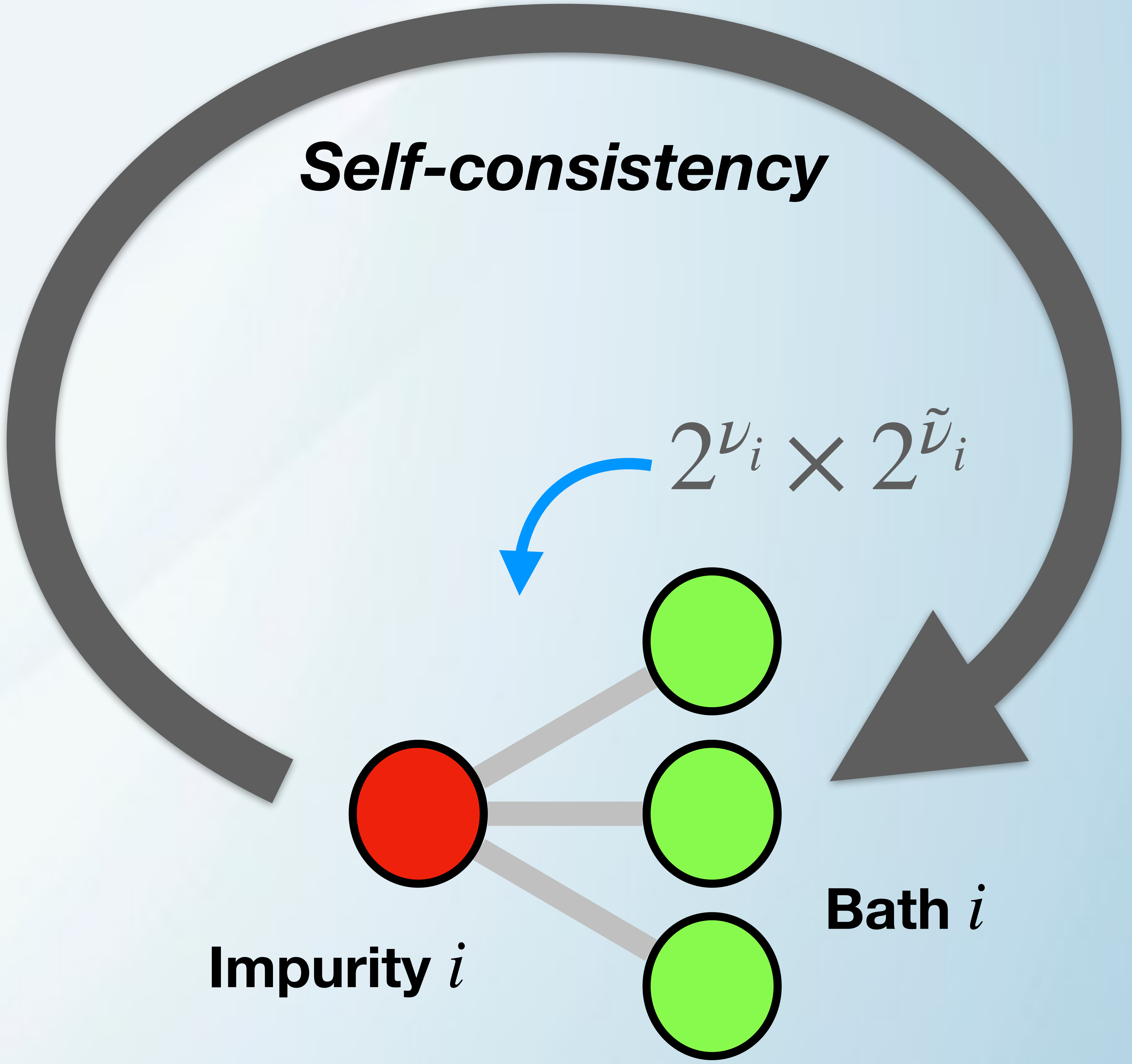
$$\hat{H} = \sum_{RR'} \sum_{\sigma} t_{RR'}\, c^\dagger_{R\sigma} c_{R'\sigma} + \sum_{R\sigma} U\, \hat{n}_{R\uparrow} \hat{n}_{R\downarrow}$$



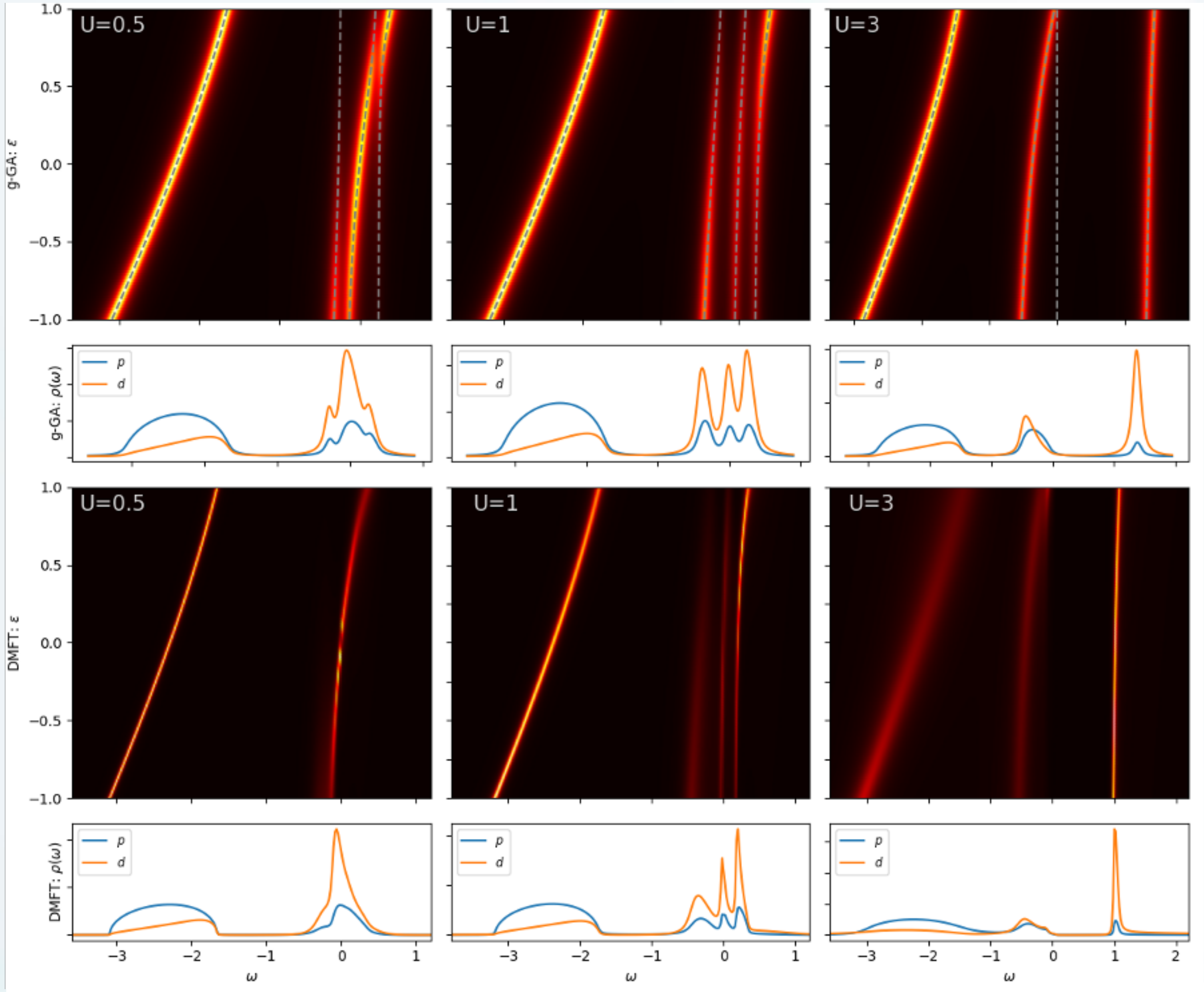
Benchmark calculations ALM:



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



Benchmark calculations ALM:



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

Analytical (approximate) expression for self-energy

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

Some useful references:

PHYSICAL REVIEW VOLUME 137, NUMBER 6A 15 MARCH 1965

Correlation of Electrons in a Narrow s Band

MARTIN C. GUTZWILLER

J. Phys.: Condens. Matter **9** (1997) 7343–7358. Printed in the UK PII: S0953-8984(97)83326-7

Gutzwiller-correlated wave functions for degenerate bands: exact results in infinite dimensions

J Bünemann†, F Gebhard‡ and W Weber†

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 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]

VOLUME 57, NUMBER 11 PHYSICAL REVIEW LETTERS 15 SEPTEMBER 1986

New Functional Integral Approach to Strongly Correlated Fermi Systems: The Gutzwiller Approximation as a Saddle Point

Gabriel Kotliar[(1)] and Andrei E. Ruckenstein[(2)]

PHYSICAL REVIEW B **76**, 155102 (2007)

Rotationally invariant slave-boson formalism and momentum dependence of the quasiparticle weight

Frank Lechermann,[1,2,*] Antoine Georges,[2] Gabriel Kotliar,[2,3] and Olivier Parcollet[4]

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 **76**, 193104 (2007)

Equivalence of Gutzwiller and slave-boson mean-field theories for multiband Hubbard models

J. Bünemann and F. Gebhard

PHYSICAL REVIEW B **78**, 155127 (2008)

Fermi-surface evolution across the magnetic phase transition in the Kondo lattice model

Nicola Lanatà,[1] Paolo Barone,[1] and Michele Fabrizio[1,2]

Some useful references:

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 MATERIALS **3**, 054605 (2019)

Exciton Mott transition revisited

Daniele Guerci, Massimo Capone, and Michele Fabrizio

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

Operatorial formulation of the ghost rotationally invariant slave-boson theory

Nicola Lanatà[*]

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 RESEARCH **3**, 013101 (2021)

Bypassing the computational bottleneck of quantum-embedding theories for strong electron correlations with machine learning

John Rogers,[1,2] Tsung-Han Lee,[3] Sahar Pakdel,[4] Wenhu Xu,[5] Vladimir Dobrosavljević,[2] Yong-Xin Yao,[6] Ove Christiansen,[7,*] and Nicola Lanatà[4,8,†]

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 B **86**, 115310 (2012)

Time-dependent and steady-state Gutzwiller approach for nonequilibrium transport in nanostructures

Nicola Lanatà[1] and Hugo U. R. Strand[2]

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **92**, 081108(R) (2015)

Finite-temperature Gutzwiller approximation from the time-dependent variational principle

Nicola Lanatà,[*] Xiaoyu Deng, and Gabriel Kotliar

THANK YOU FOR YOUR ATTENTION !!!

PHYSICAL REVIEW B **90**, 155136 (2014)

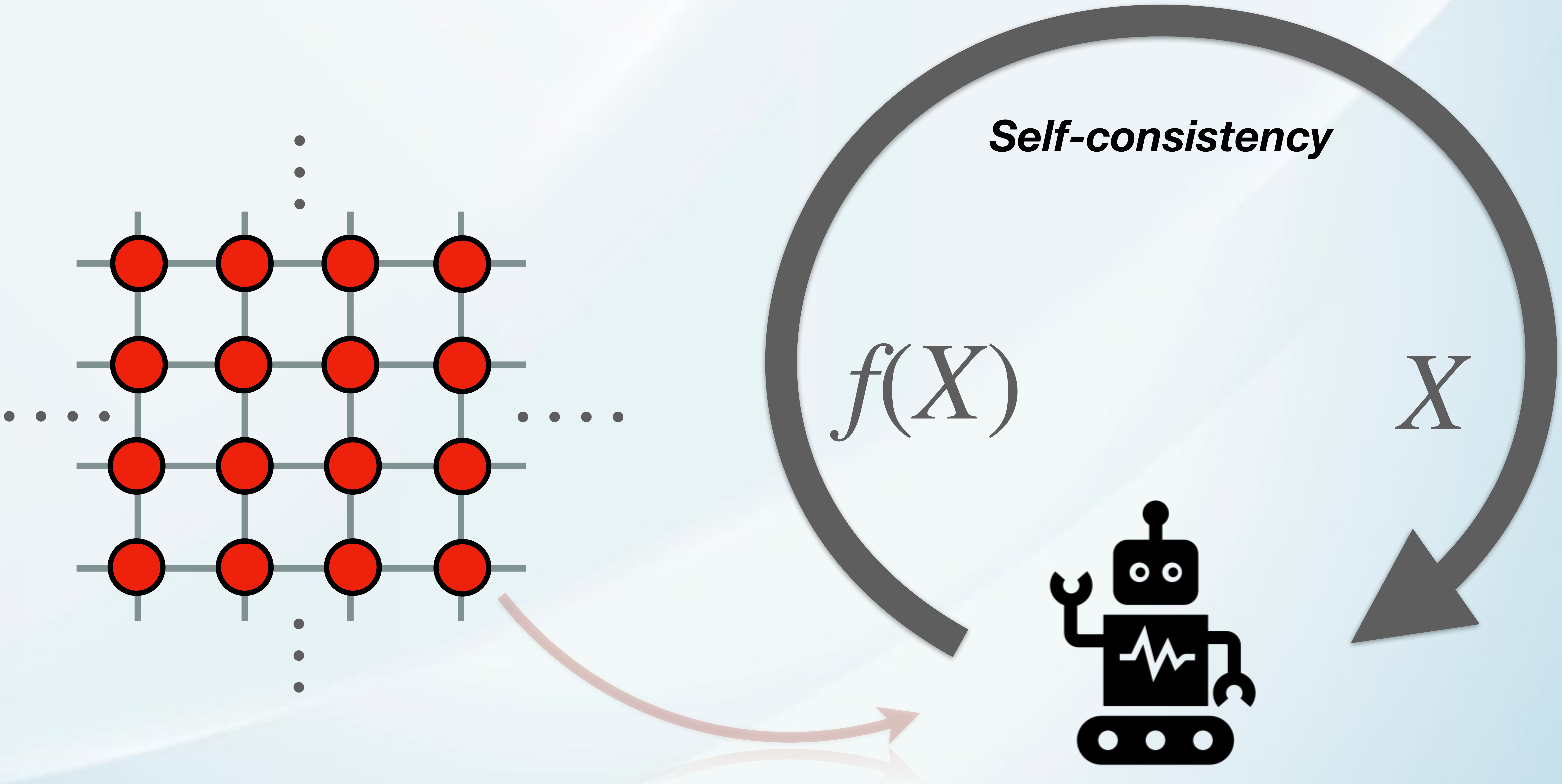
Machine learning for many-body physics: The case of the Anderson impurity model

Louis-François Arsenault,[1,*] Alejandro Lopez-Bezanilla,[2] O. Anatole von Lilienfeld,[3,4] and Andrew J. Millis[1]

PHYSICAL REVIEW RESEARCH **3**, 013101 (2021)

Bypassing the computational bottleneck of quantum-embedding theories for strong electron correlations with machine learning

John Rogers,[1,2] Tsung-Han Lee,[3] Sahar Pakdel,[4] Wenhu Xu,[5] Vladimir Dobrosavljević,[2] Yong-Xin Yao,[6] Ove Christiansen,[7,*] and Nicola Lanatà[4,8,†]



First exploratory benchmark: DFT+GA

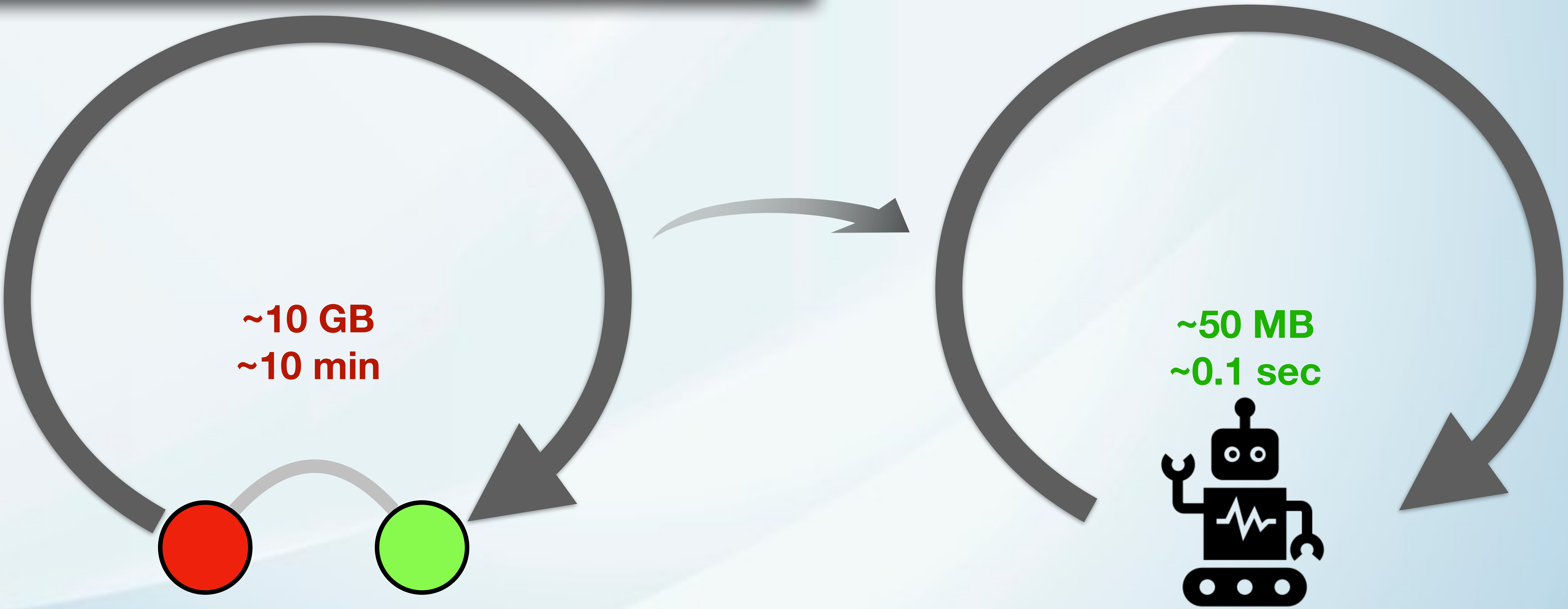
PHYSICAL REVIEW RESEARCH **3**, 013101 (2021)

Bypassing the computational bottleneck of quantum-embedding theories for strong electron correlations with machine learning

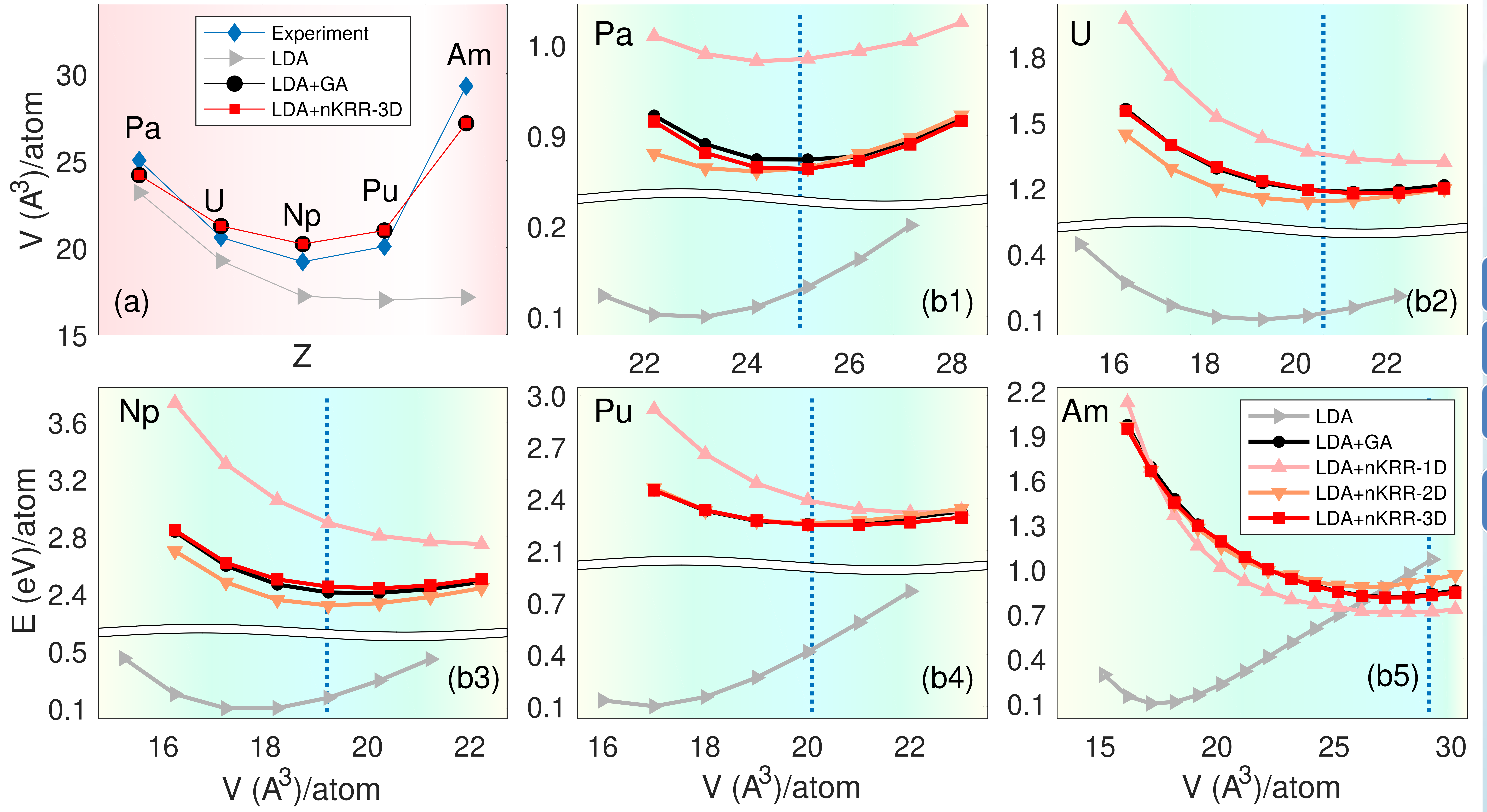
John Rogers,[1,2] Tsung-Han Lee,[3] Sahar Pakdel,[4] Wenhu Xu,[5] Vladimir Dobrosavljević,[2] Yong-Xin Yao,[6] Ove Christiansen,[7,*] and Nicola Lanatà[4,8,†]

Study of series of actinide systems.

Simplifications from prior knowledge imbued within the regression problem



First exploratory benchmark: DFT+GA actinide systems



$n = 1$: 65

$n = 2$: 1626

$n = 3$: 19346

$n = 5$: 1410031

Benchmark calculations ALM:

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