Quantum-embedding formulation of the GA/RISB equations

Introduction to DFT+GA/RISB Code

Comscope Summer School 2021

June 21–25, 2021

Phys. Rev. X **5**, *011008 (2015)*

Phys. Rev. Lett. ***118***, *126401 (2017)*

Introduction to **Hands-on Training DFT+GA/RISB Code**:

Yongxin Yao, Sangkook Choi, Andrey Kutepov, Nicola Lanatà and Gabriel Kotliar

Nicola Lanatà (Aarhus University) *(lanata@phys.au.dk)*

Why is it useful?

1. <u>Orders of magnitude less computationally demanding</u> than DMFT
   (note also recent combination with ML).

2. Variational (*T=0*).

3. Accuracy can be systematically improved
   (RISB formulation, recent extension g-GA)

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.

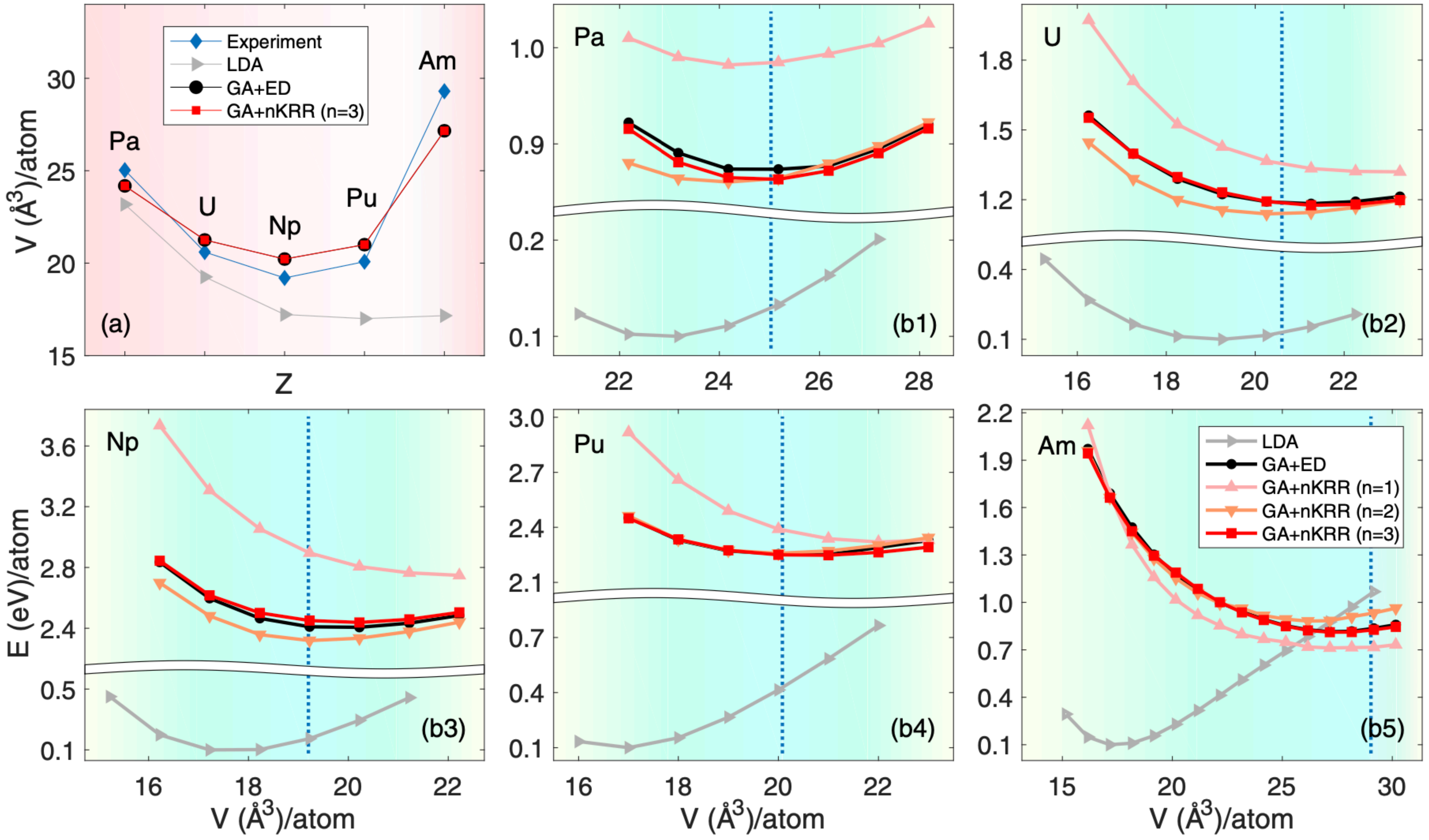
*(**Note:** recent extension may resolve these problems…)*

Why is computational speed important?

PHYSICAL REVIEW RESEARCH 3, 013101 (2021)

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

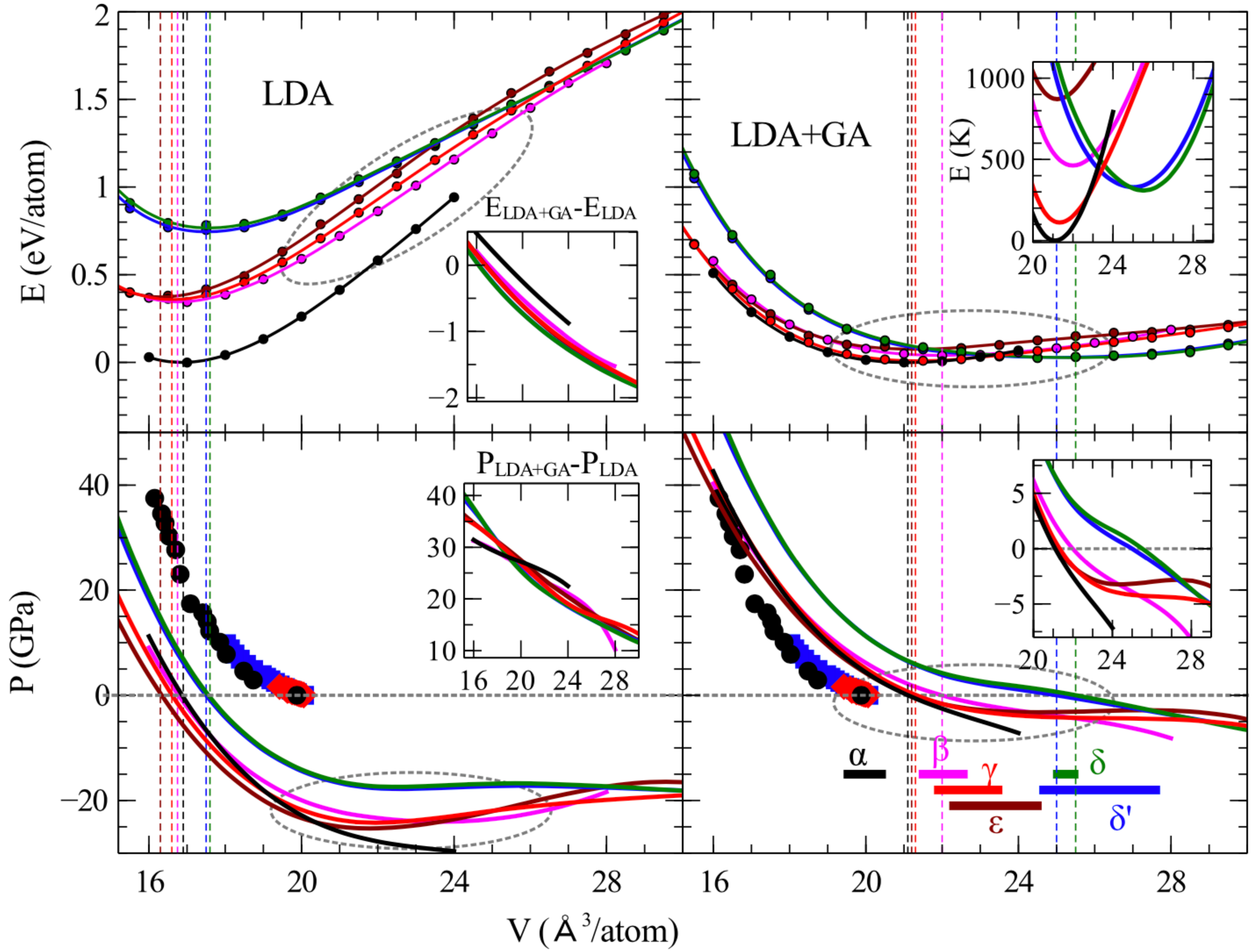
John Rogers,[1,2] Tsung-Han Lee,[3] Sahar Pakdel,[4] Wenhu Xu,[5] Vladimir Dobrosavljević,[2] Yong-Xin Yao,[6] Ove Christiansen,[7,*] and Nicola Lanatà[4,8,†]



PHYSICAL REVIEW X 5, 011008 (2015)

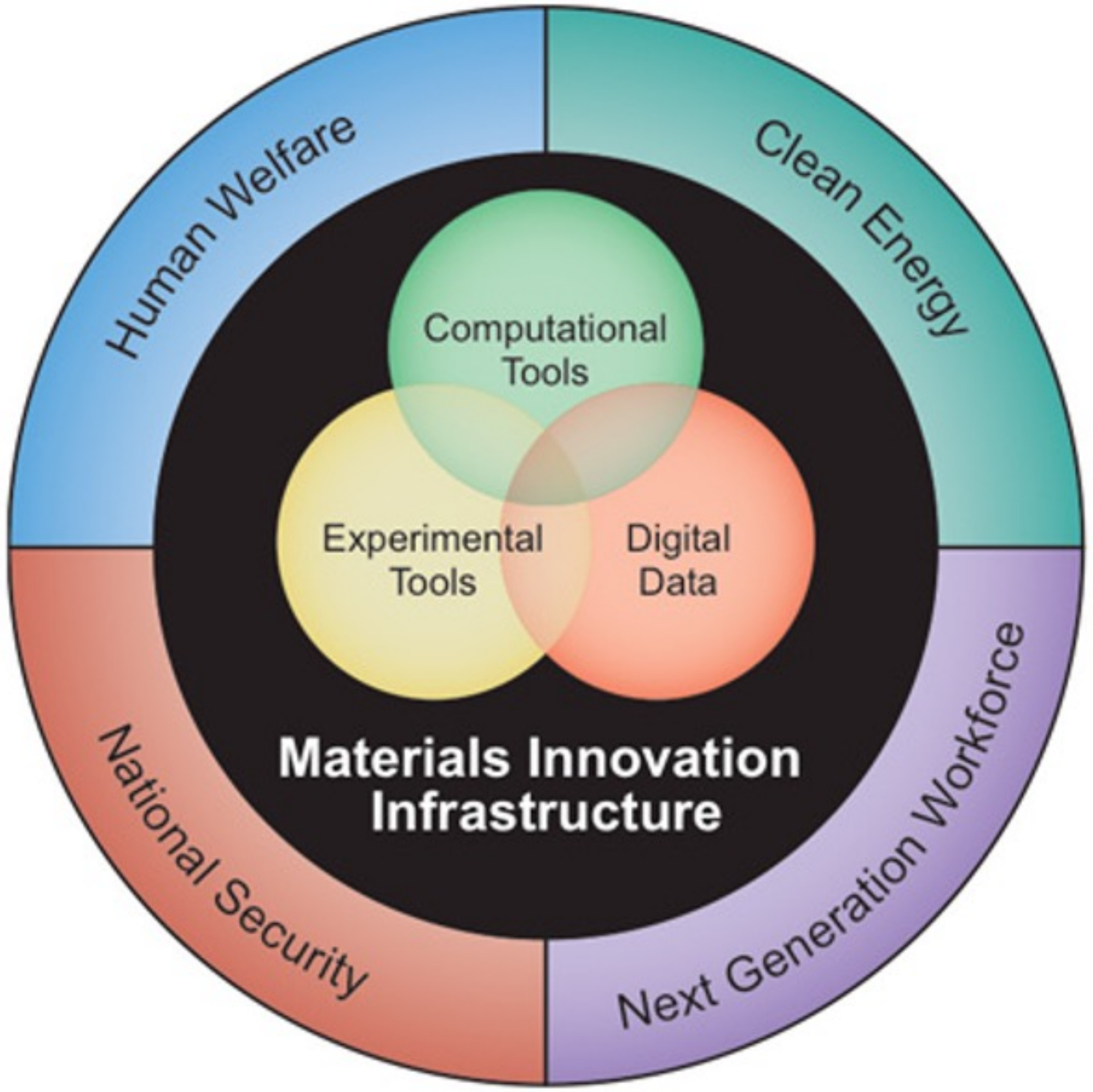
Phase Diagram and Electronic Structure of Praseodymium and Plutonium

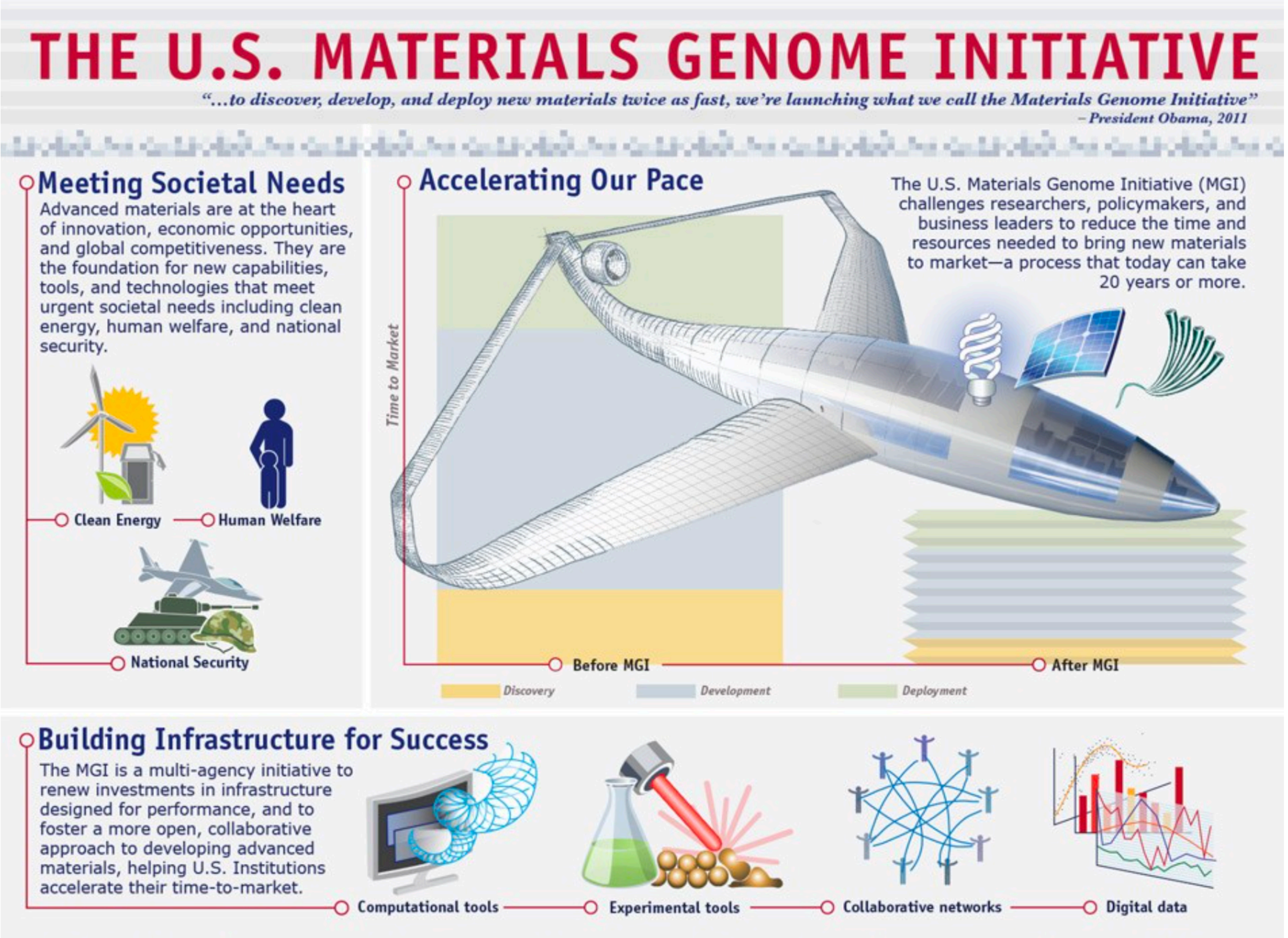
Nicola Lanatà,[1,*] Yongxin Yao,[2,†] Cai-Zhuang Wang,[2] Kai-Ming Ho,[2] and Gabriel Kotliar[1]



Why is computational speed important?

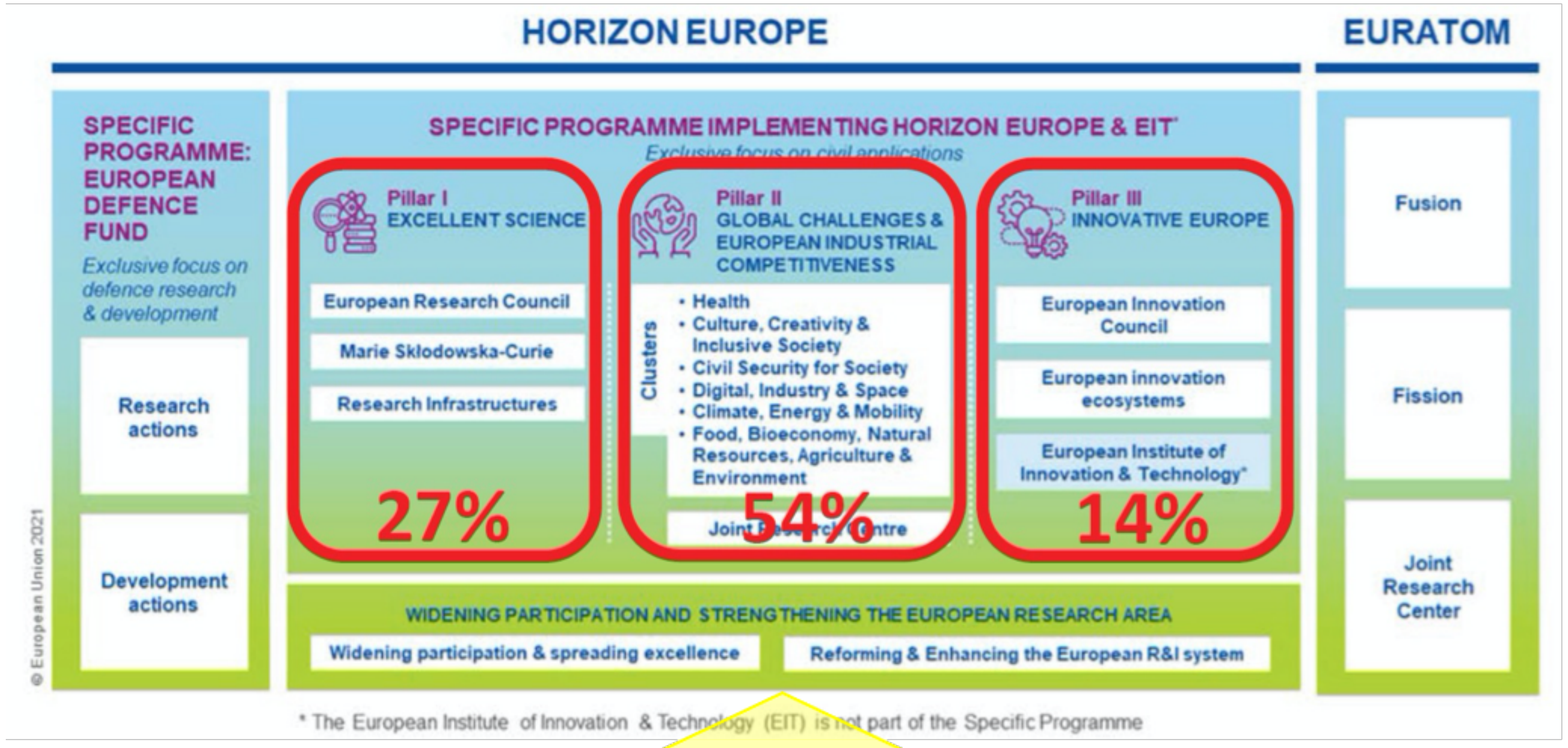
Materials are useful for society !

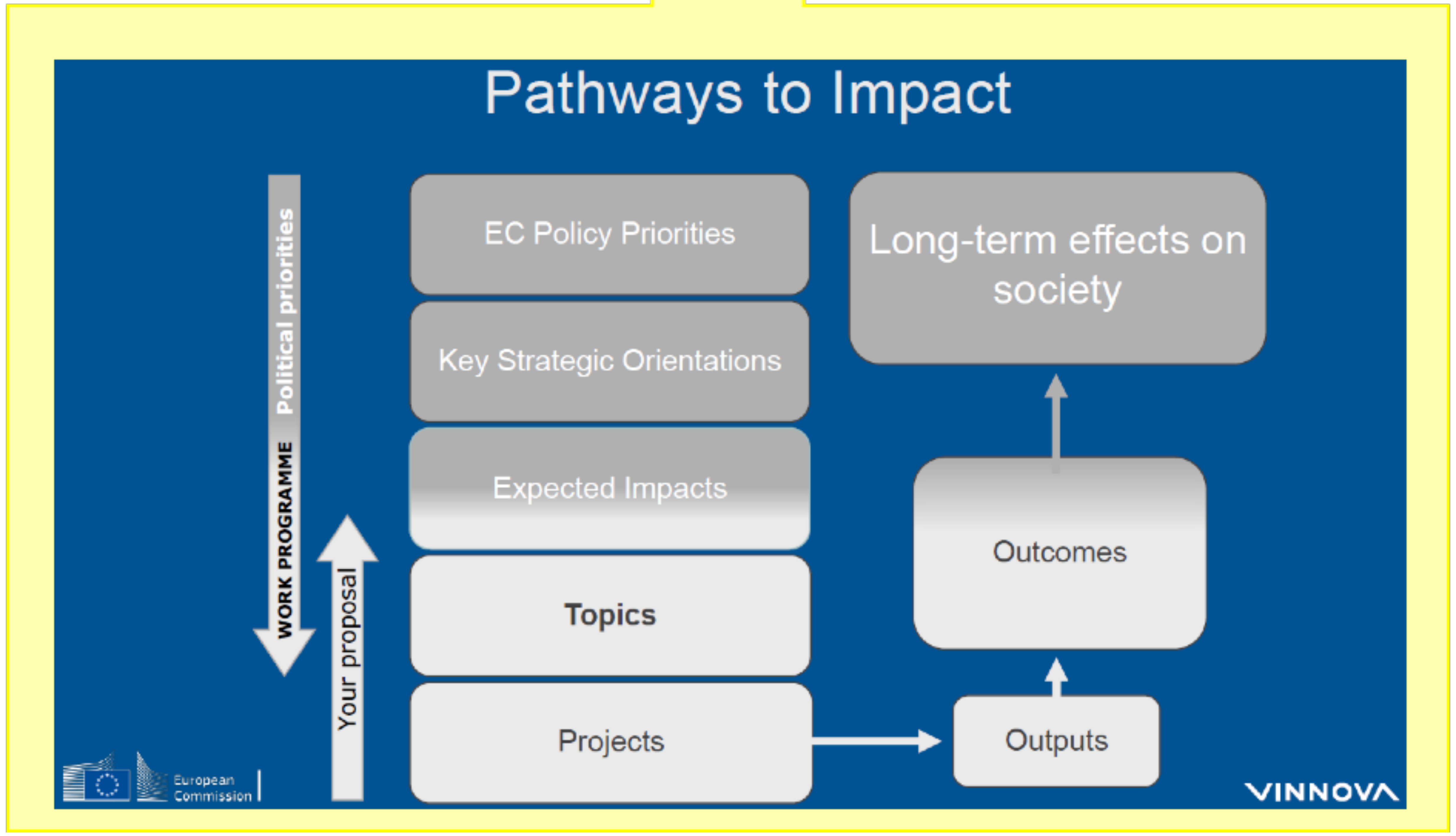




Why is computational speed important?

Increase of scientific programs prioritising research that can benefit society





Outline

A. GA method (multi-orbital models): QE formulation.
B. DFT+GA algorithmic structure.
C. Spectral properties.
D. Recent formalism extensions.

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)

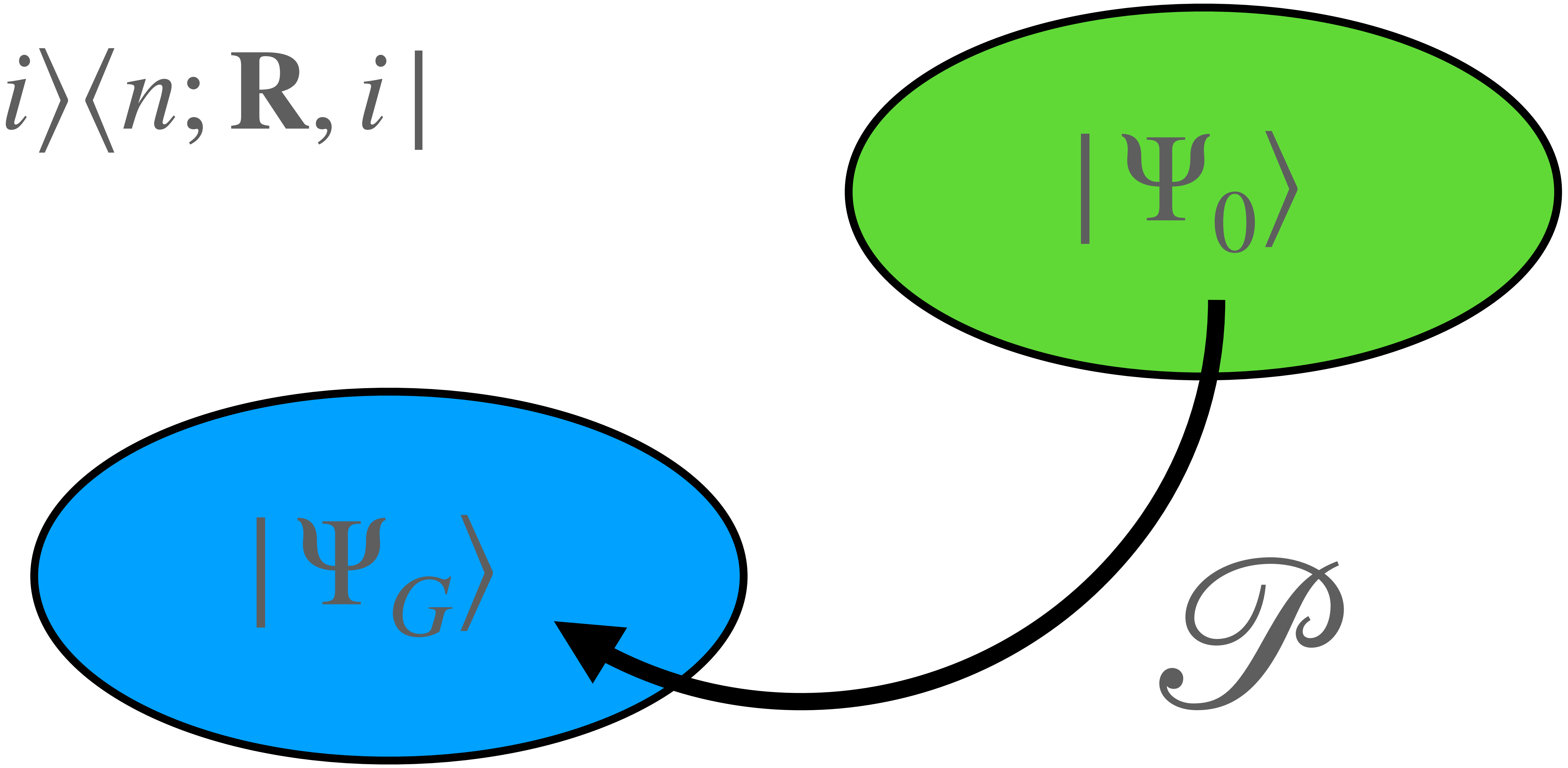
$i = 2$: Second subset of correlated modes (e.g. *f* orbitals of atom 1 in unit cell)

…

The GA variational wave function:

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

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



The GA variational wave function:

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

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

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

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

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

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

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

Phase Diagram and Electronic Structure of Praseodymium and Plutonium

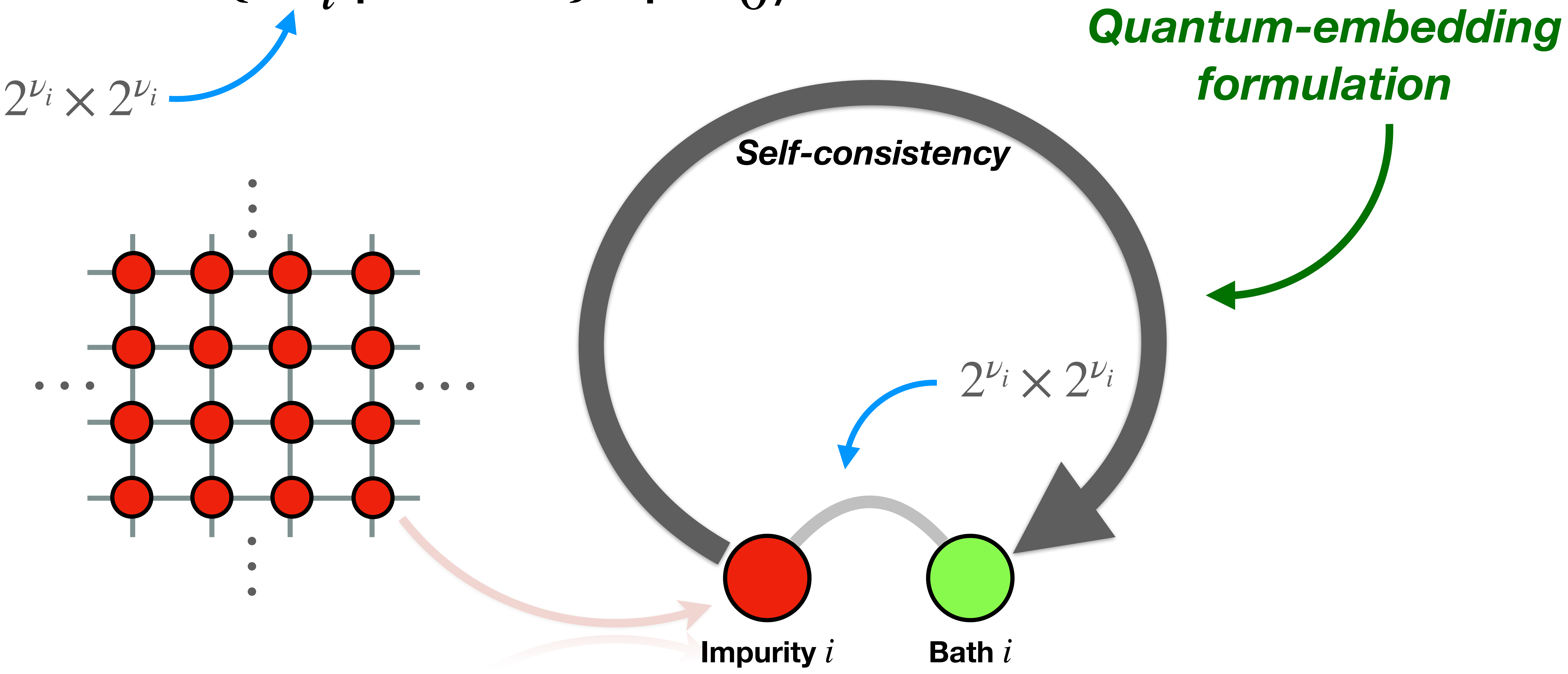
Nicola Lanatà,[1,*] Yongxin Yao,[2,†] Cai-Zhuang Wang,[2] Kai-Ming Ho,[2] and Gabriel Kotliar[1]

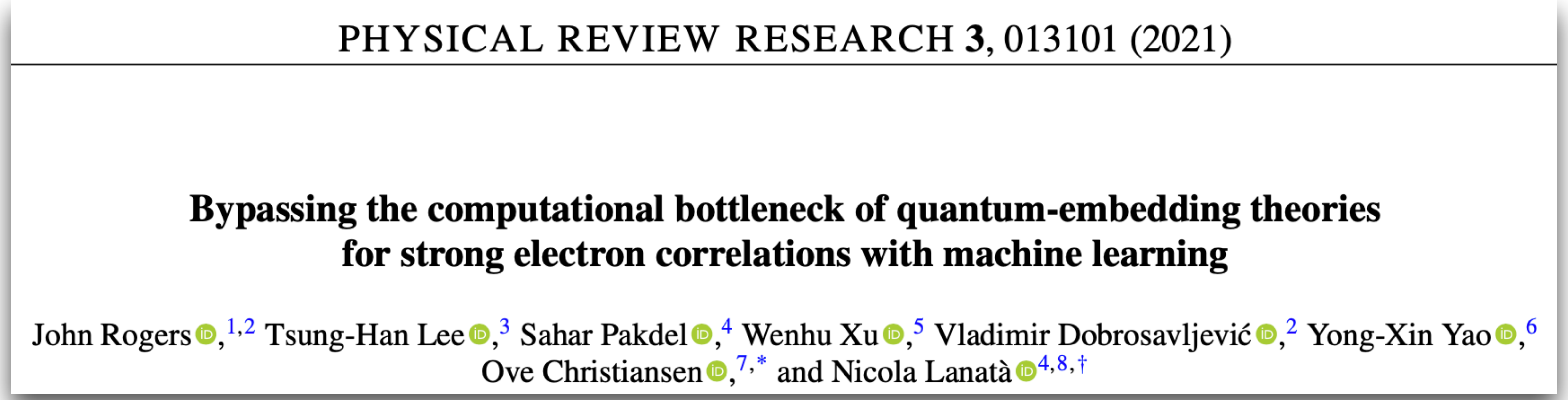
PRL **118,** 126401 (2017) PHYSICAL REVIEW LETTERS week ending 24 MARCH 2017

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]

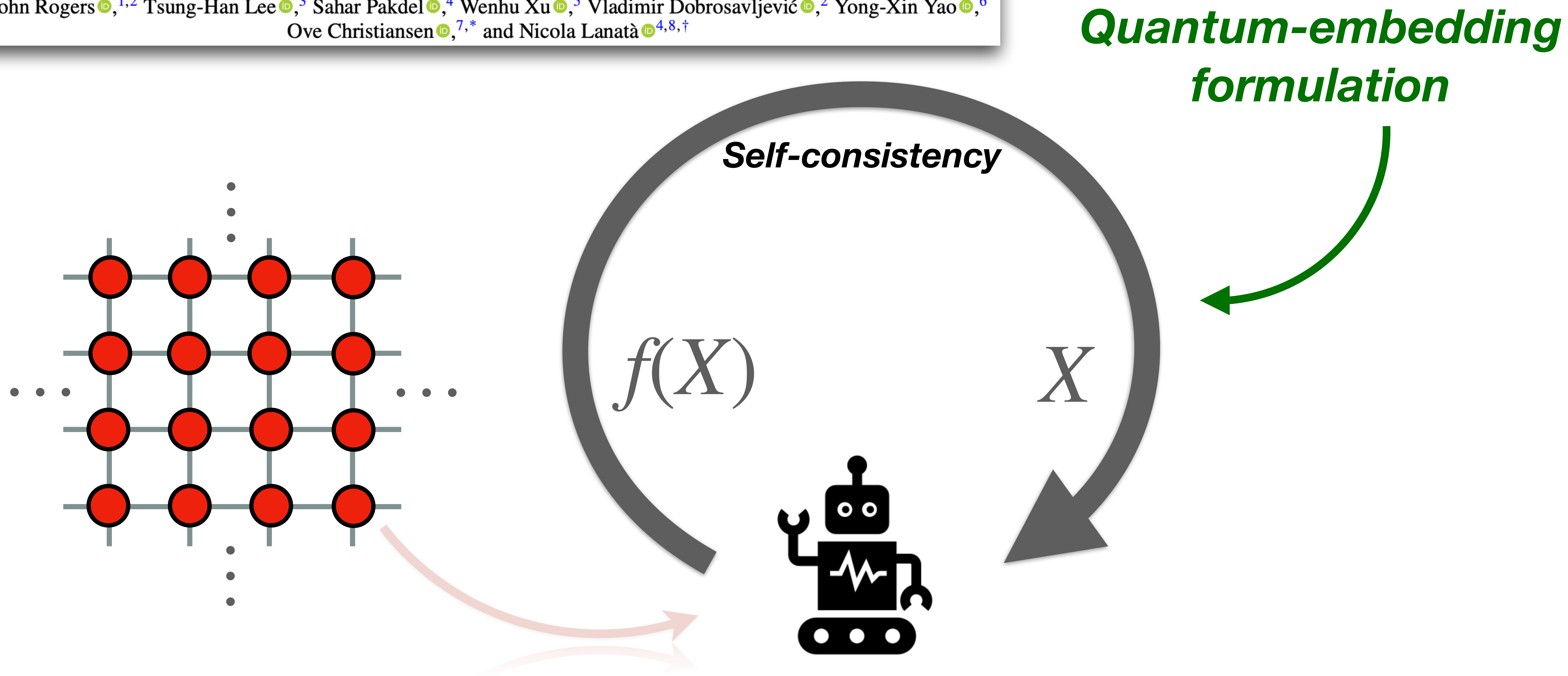
Our goal is to minimize $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ w.r.t. $\{\Lambda_i \,|\, i \geq 1\}, |\Psi_0\rangle$.




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,†]



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:

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

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

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:

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

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

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:

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

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

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:

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

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

Key consequence:

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

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

Gutzwiller constraints:

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

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

Key consequence:

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

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

Gutzwiller constraints:

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

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

Key consequence:

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

Gutzwiller constraints:

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

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

Key consequence:

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

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.

The Hamiltonian:

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

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

$\mathbf{k}$: 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)

…

Local operators:

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

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

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)

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

(GA and G. constraints)

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

Local operators: (disconnected terms)

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

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

Local operators: (connected terms)

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

Local operators: (connected terms)

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

(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:

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

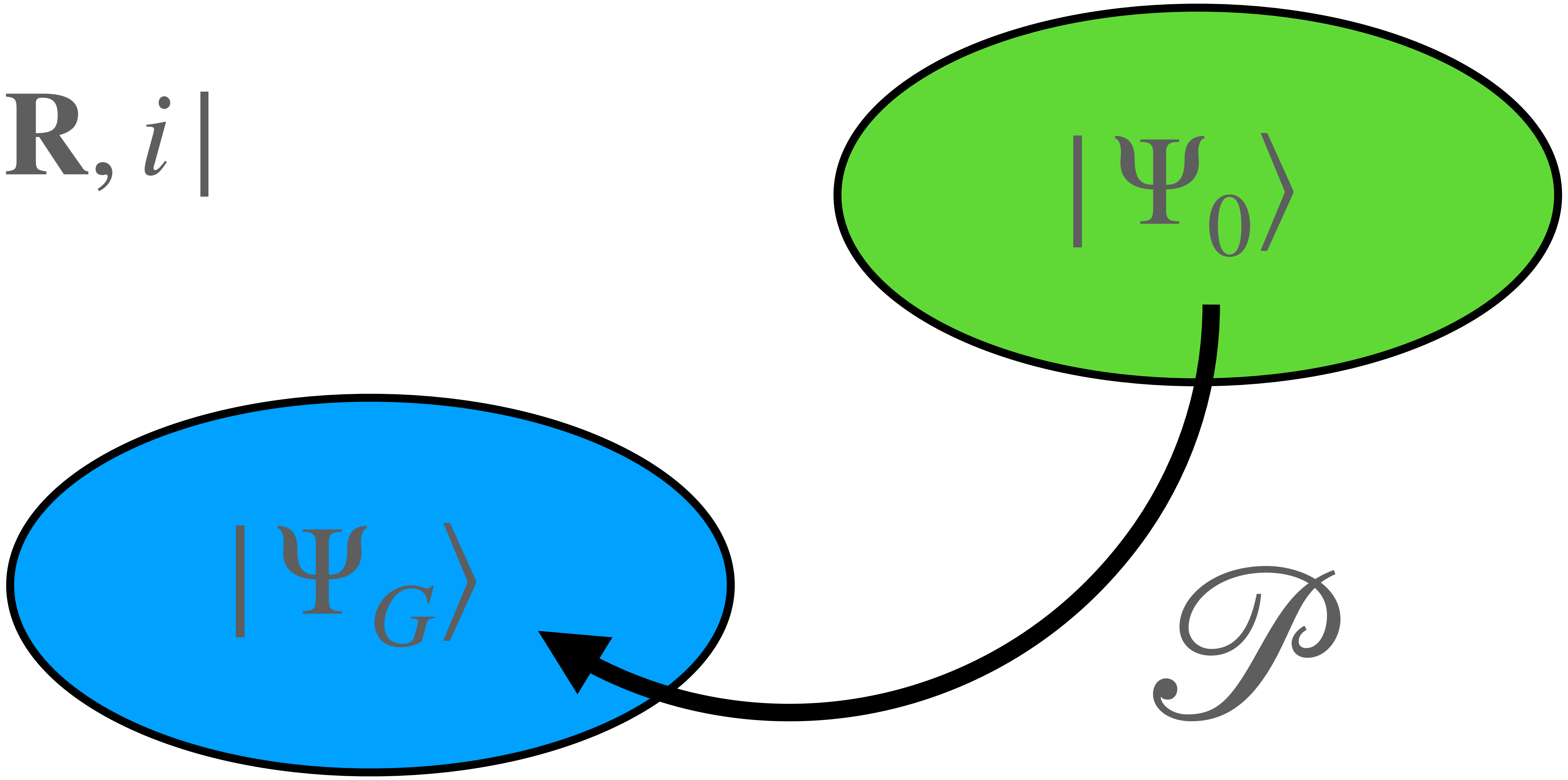
Non-local quadratic operators:

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

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

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

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



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

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

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

Necessary steps:

1. Definition of approximations (GA and G. constraints).
2. Evaluation of $\langle \Psi_G | \hat{H} | \Psi_G \rangle$ in terms of $\{\Lambda_{i\geq 1}\}, |\Psi_0\rangle$.
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: $$\langle \Psi_0 | \mathscr{P}^\dagger_{\mathbf{R}i} c^\dagger_{\mathbf{R}i\alpha} \mathscr{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle = \sum_{a'} \left[\mathscr{R}_i \right]_{a'\alpha} \langle \Psi_0 | f^\dagger_{\mathbf{R}ia'} f_{\mathbf{R}ia} | \Psi_0 \rangle$$

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

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

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

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

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

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

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

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

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

Where:

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

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

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

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

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

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

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

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

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

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:

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

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

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

Necessary steps:

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

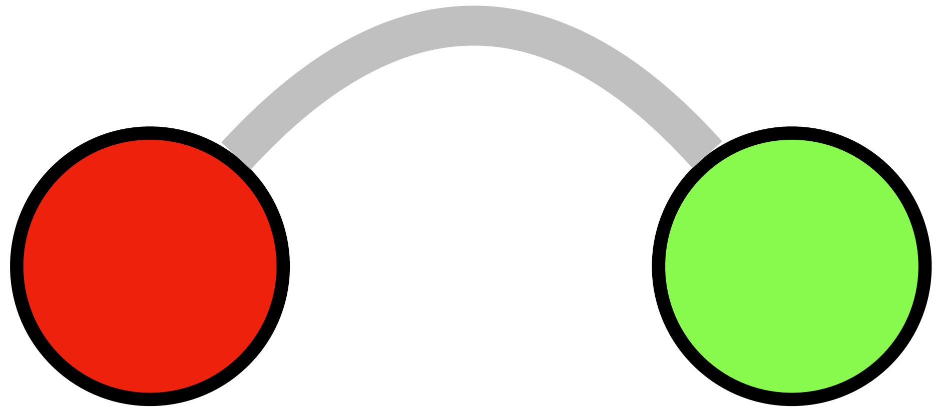
Quantum-embedding formulation

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

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

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

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



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

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

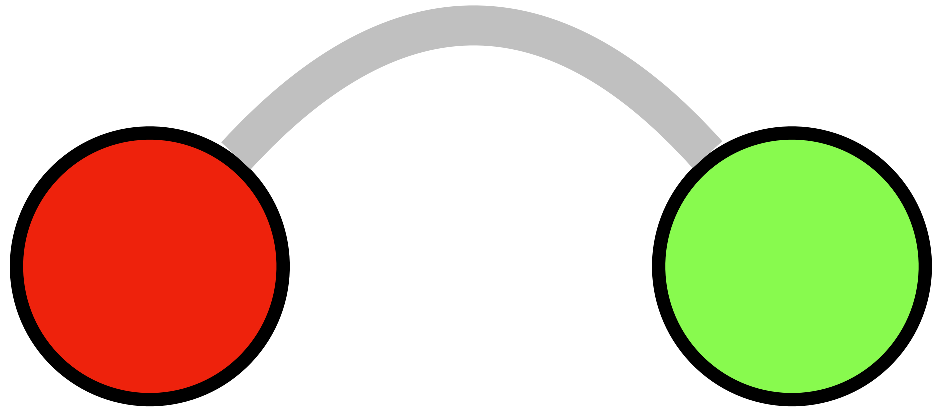
Quantum-embedding formulation

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

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

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

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



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

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

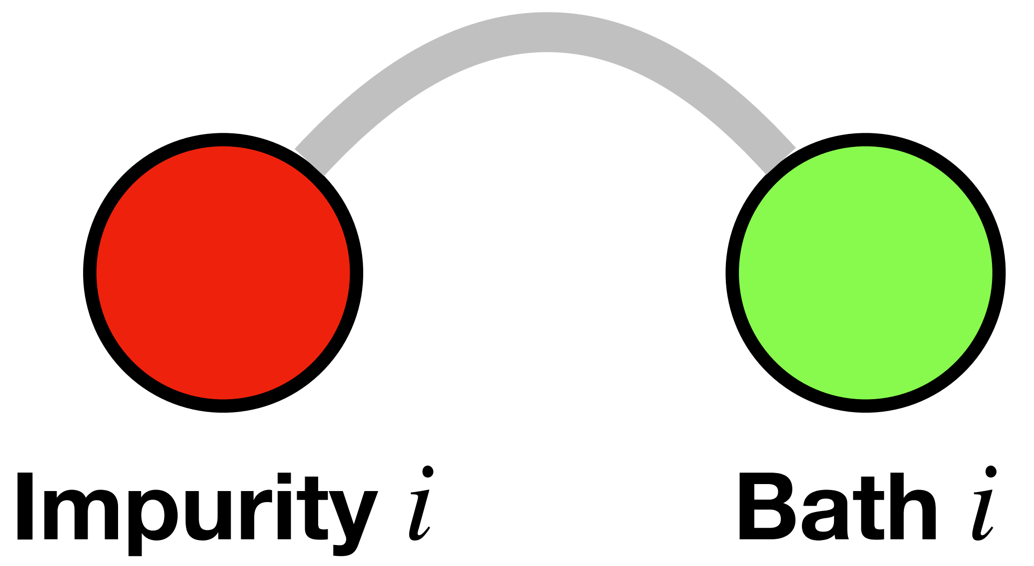
Quantum-embedding formulation

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

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

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

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



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

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

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

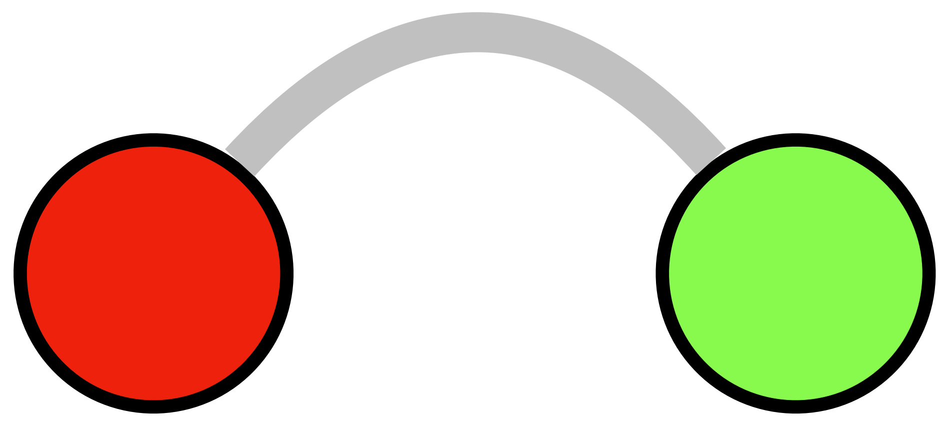
Quantum-embedding formulation

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

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

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

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



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

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

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

Variational energy:

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

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

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

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

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

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:

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

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

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

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

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

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

Variational energy:

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

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

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

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

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

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

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

Lagrange function:

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

$$+ \sum_{i \geq 1} \langle \Phi_i | \hat{H}_i^{emb}[\mathscr{D}_i, \lambda_i^c] | \Phi_i \rangle + E_i^c(1 - \langle \Phi_i | \Phi_i \rangle)$$

$$- \sum_{i \geq 1} \left[\sum_{ab} \left([\lambda_i]_{ab} + [\lambda_i^c]_{ab} \right) [\Delta_i]_{ab} + \sum_{ca\alpha} \left([\mathscr{D}_i]_{a\alpha} [\mathscr{R}_{c\alpha} [\Delta_i (1 - \Delta_i)]^{\frac{1}{2}}_{ca} + \text{c.c.} \right) \right]$$

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:

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

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

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

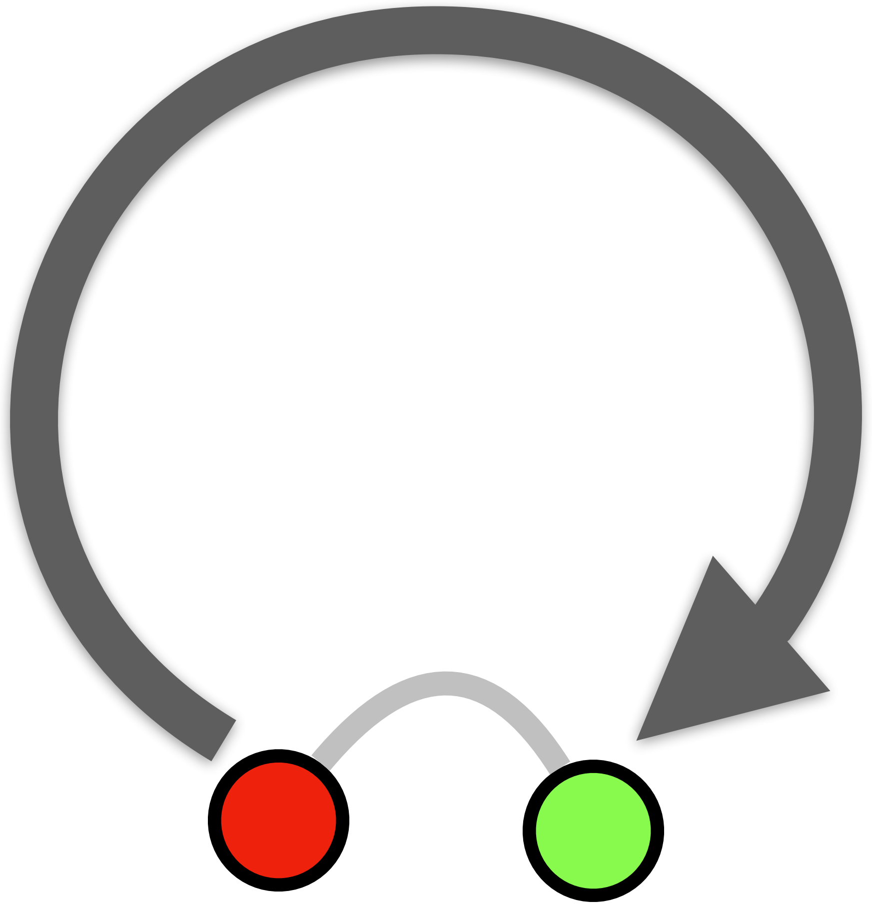
$$\hat{H}_i^{\mathrm{emb}}\left|\Phi_i\right\rangle = E_i^c\left|\Phi_i\right\rangle \longrightarrow \left|\Phi_i\right\rangle$$

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

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

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

Lagrange equations:



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

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

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

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

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

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

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. GA method (multi-orbital models): QE formulation.
B. DFT+GA algorithmic structure.
C. Spectral properties.
D. Recent formalism extensions.

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:

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

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

Kohn-Sham scheme:

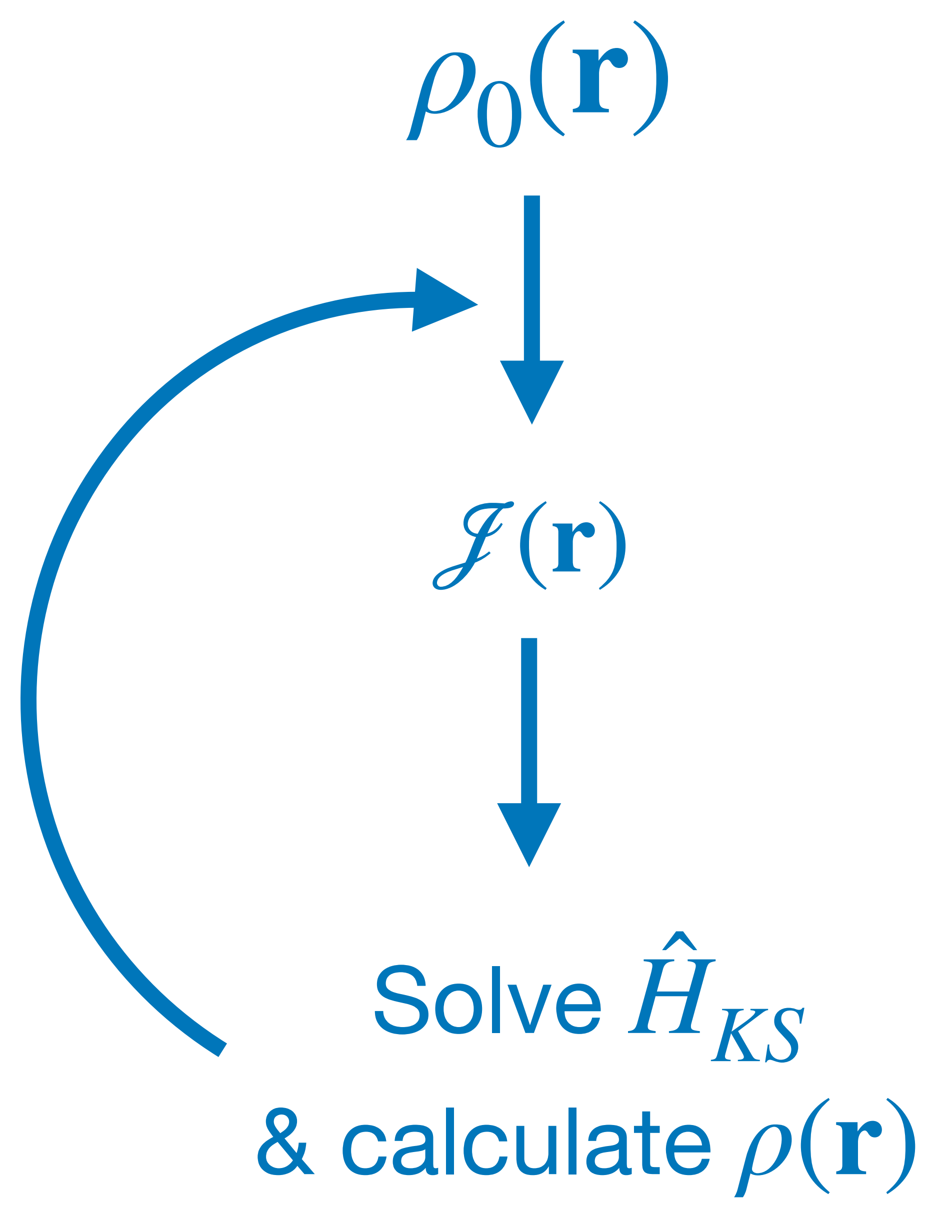
$$\begin{cases} \mathscr{E}[\rho] = T_{KS}[\rho] + E_{HXC}[\rho] + \displaystyle\int \mathbf{dr}\, V(\mathbf{r})\, \rho(\mathbf{r}) \\ T_{KS}[\rho] = \min\limits_{\Psi_0 \to \rho} \langle \Psi_0 | \hat{T} | \Psi_0 \rangle \end{cases}$$

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

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

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

Kohn-Sham scheme:



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

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

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

Kohn-Sham-**Hubbard** scheme:

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

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

Projectors over "correlated" degrees of freedom

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

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

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

Kohn-Sham-Hubbard scheme:

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

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

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

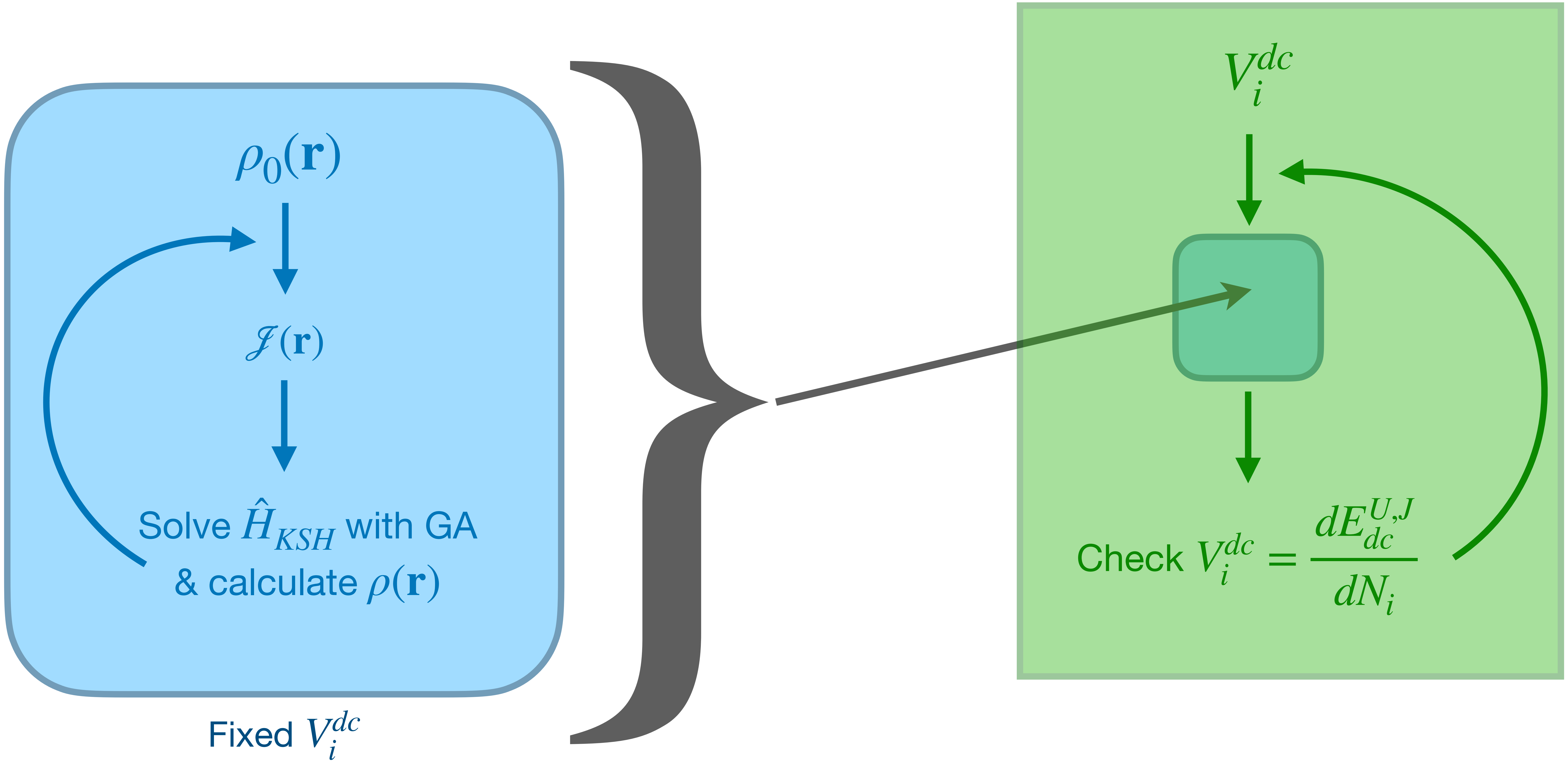
Enforcing definition of $\rho(\mathbf{r})$

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

Enforcing definition of N_i

Algorithmic structure:

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



Outline

A. GA method (multi-orbital models): QE formulation.
B. DFT+GA algorithmic structure.
C. Spectral properties.
D. Recent formalism extensions.

Spectral properties

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

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

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

Phys. Rev. B **67**, 075103 (2003)

Spectral properties

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

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

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

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

Spectral properties

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

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

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

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

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

Outline

A. GA method (multi-orbital models): QE formulation.
B. DFT+GA algorithmic structure.
C. Spectral properties.
D. 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]

arXiv:2106.05985 (2021)

Quantum-embedding description of the Anderson lattice model with the ghost Gutzwiller Approximation

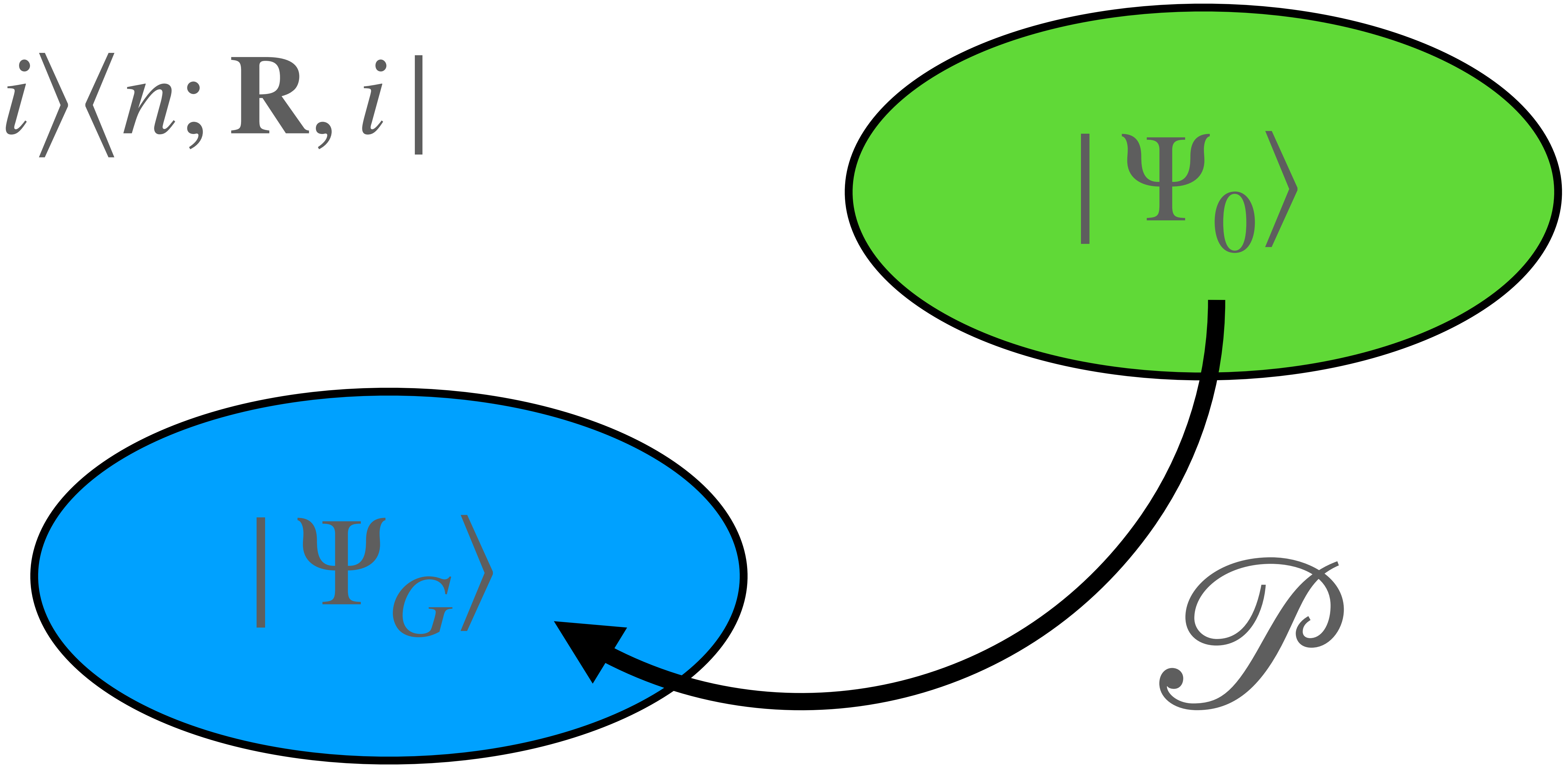
Marius S. Frank,[1] Tsung-Han Lee,[2] Gargee Bhattacharyya,[1] Pak Ki Henry Tsang,[3] Victor L. Quito,[4,3] Vladimir Dobrosavljević,[3] Ove Christiansen,[5] and Nicola Lanatà[1,6,*]

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

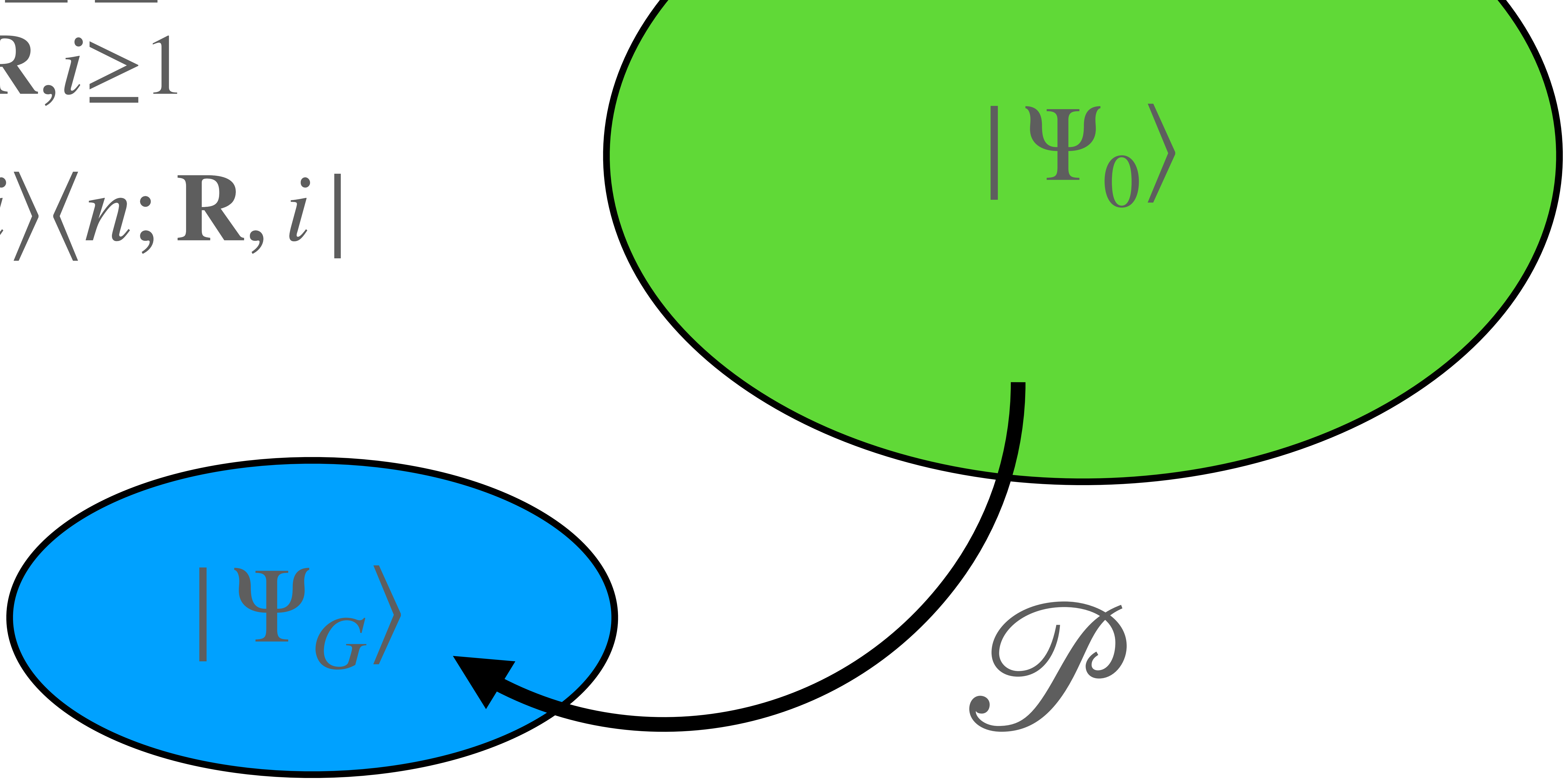


The g-GA variational wave function:

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

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

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

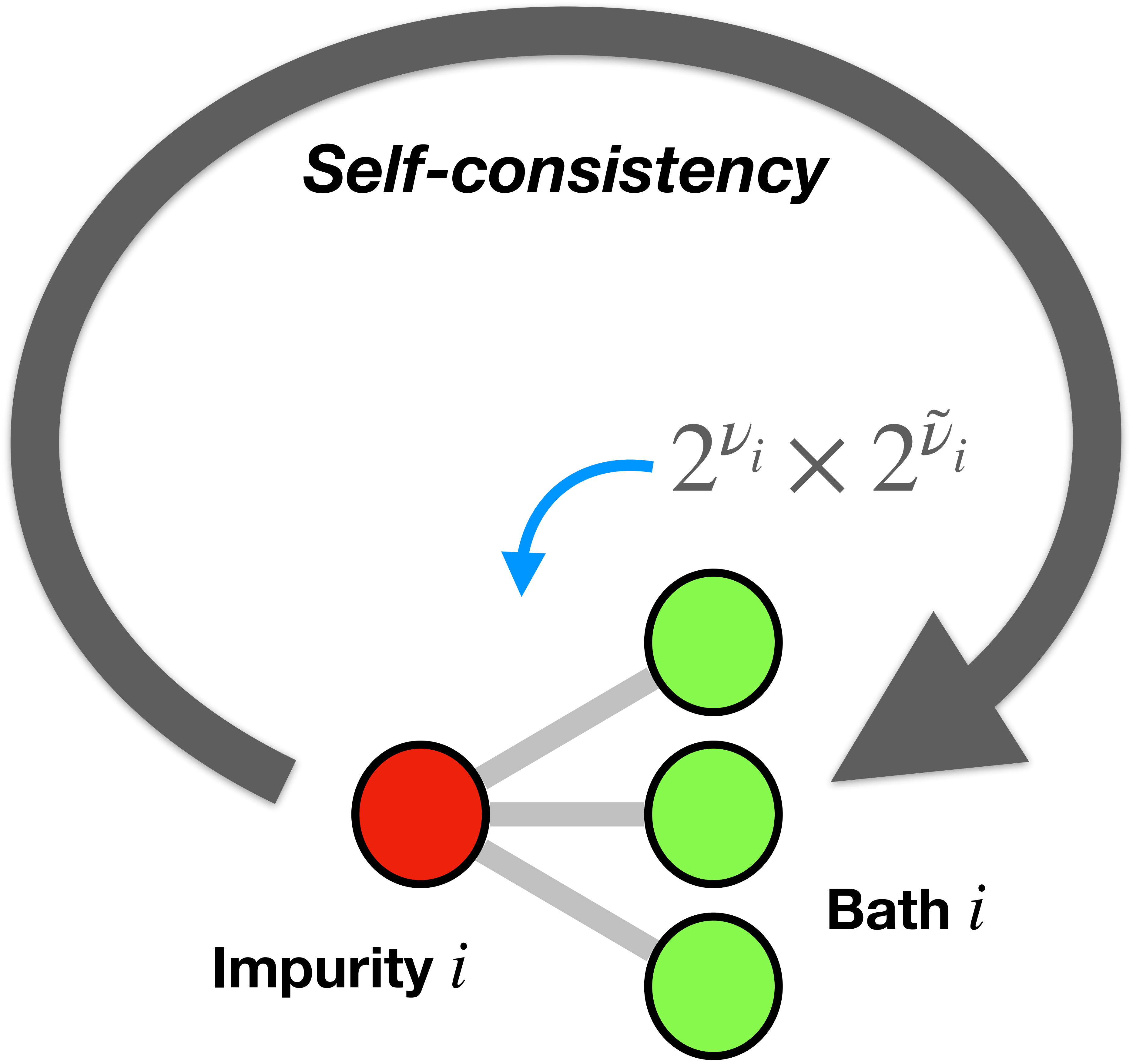


The g-GA variational wave function:

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

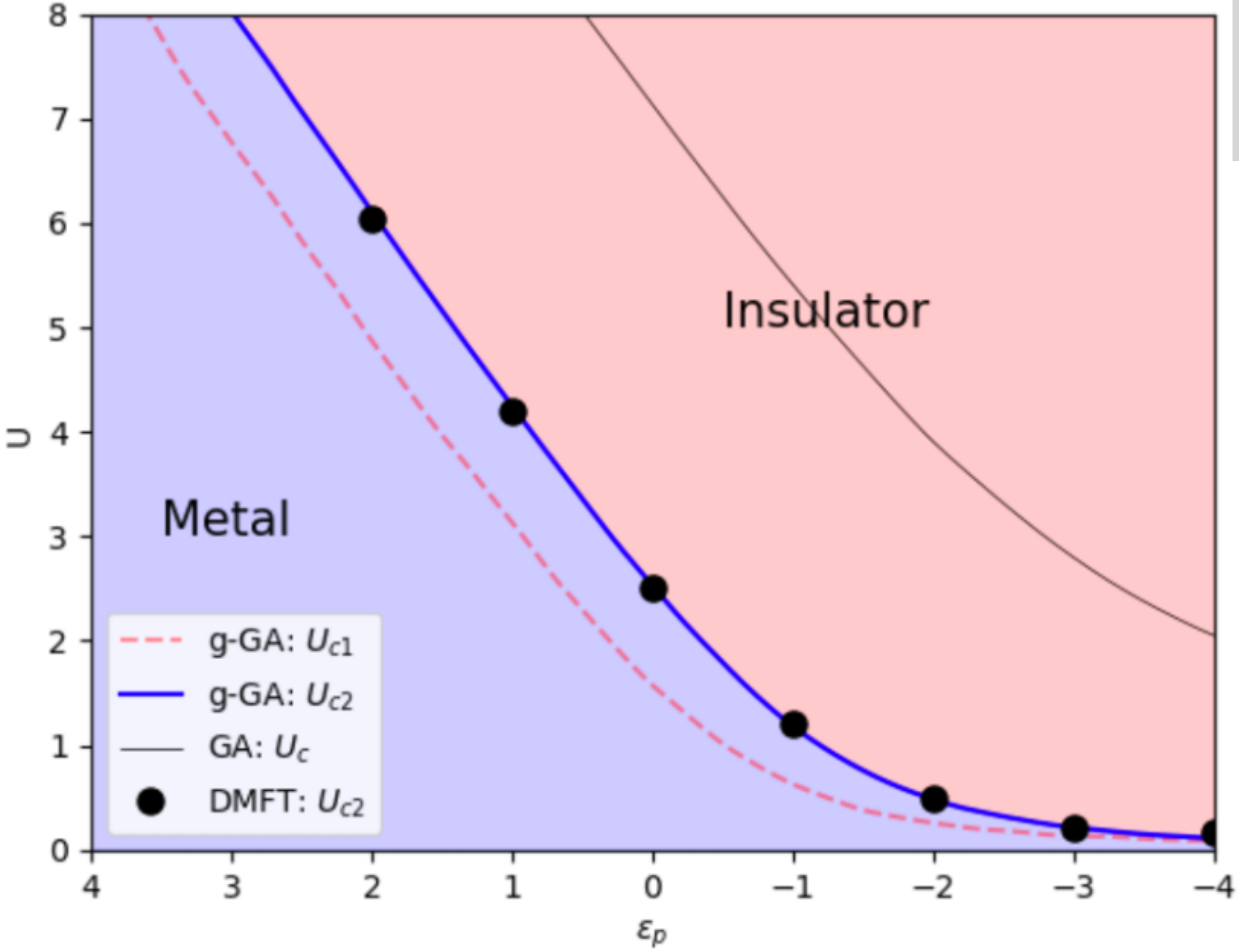
$$\mathcal{P}_{\mathbf{R}i} = \sum_{\Gamma n}[\Lambda_i]_{\Gamma n}|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i|$$

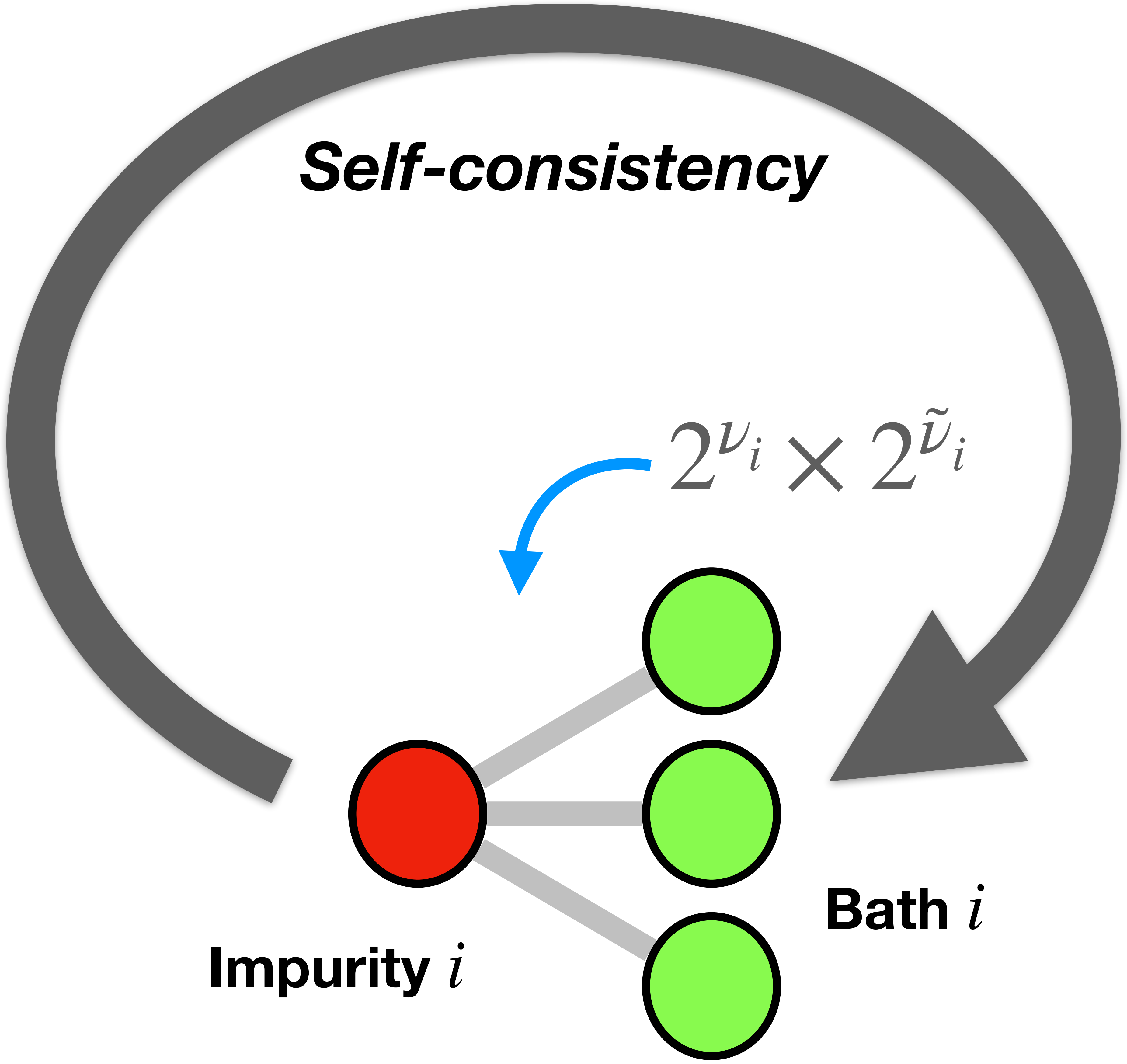
Rectangular matrix: $2^{\nu_i}\times 2^{\tilde{\nu}_i}$



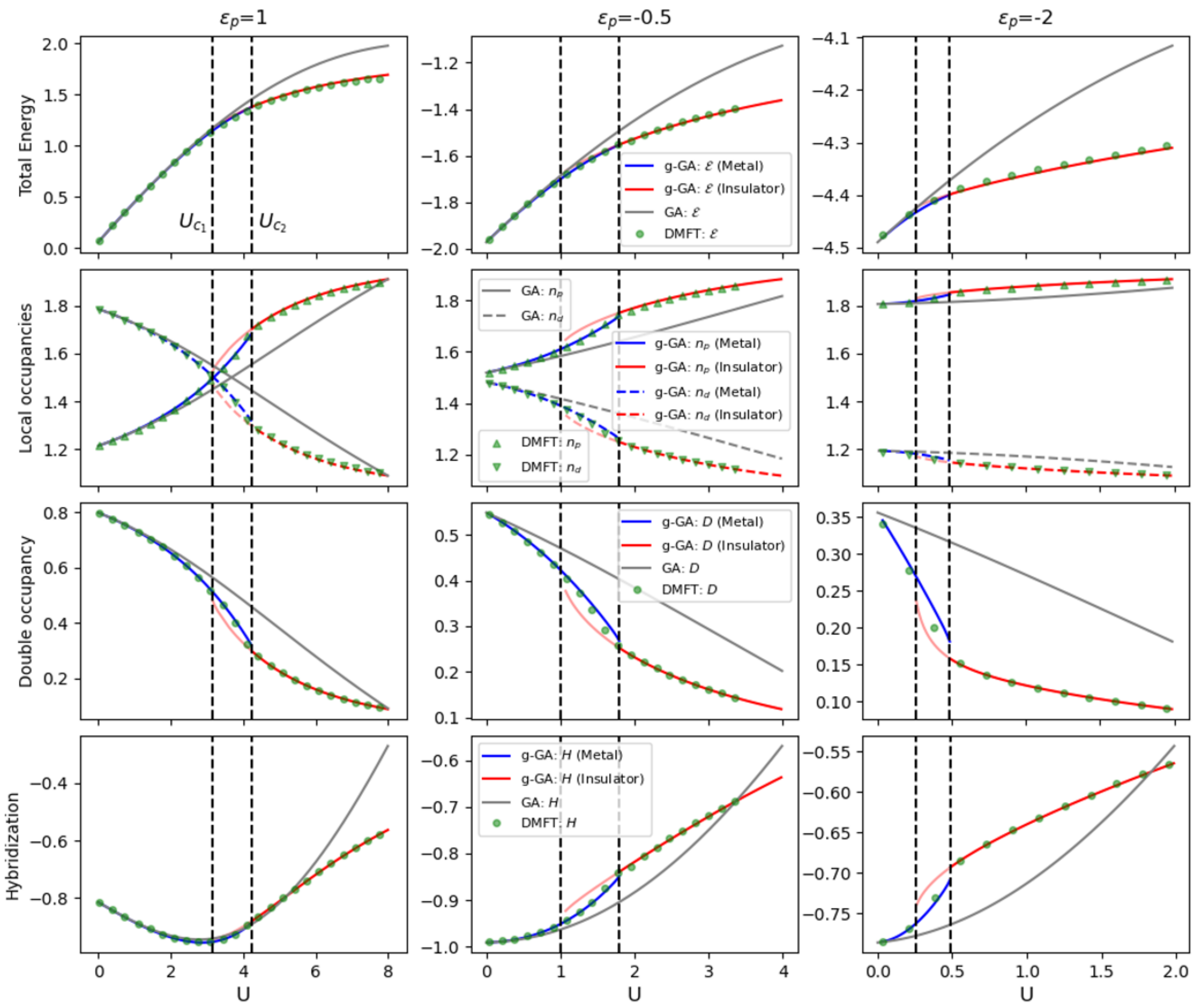
Benchmark calculations ALM:

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

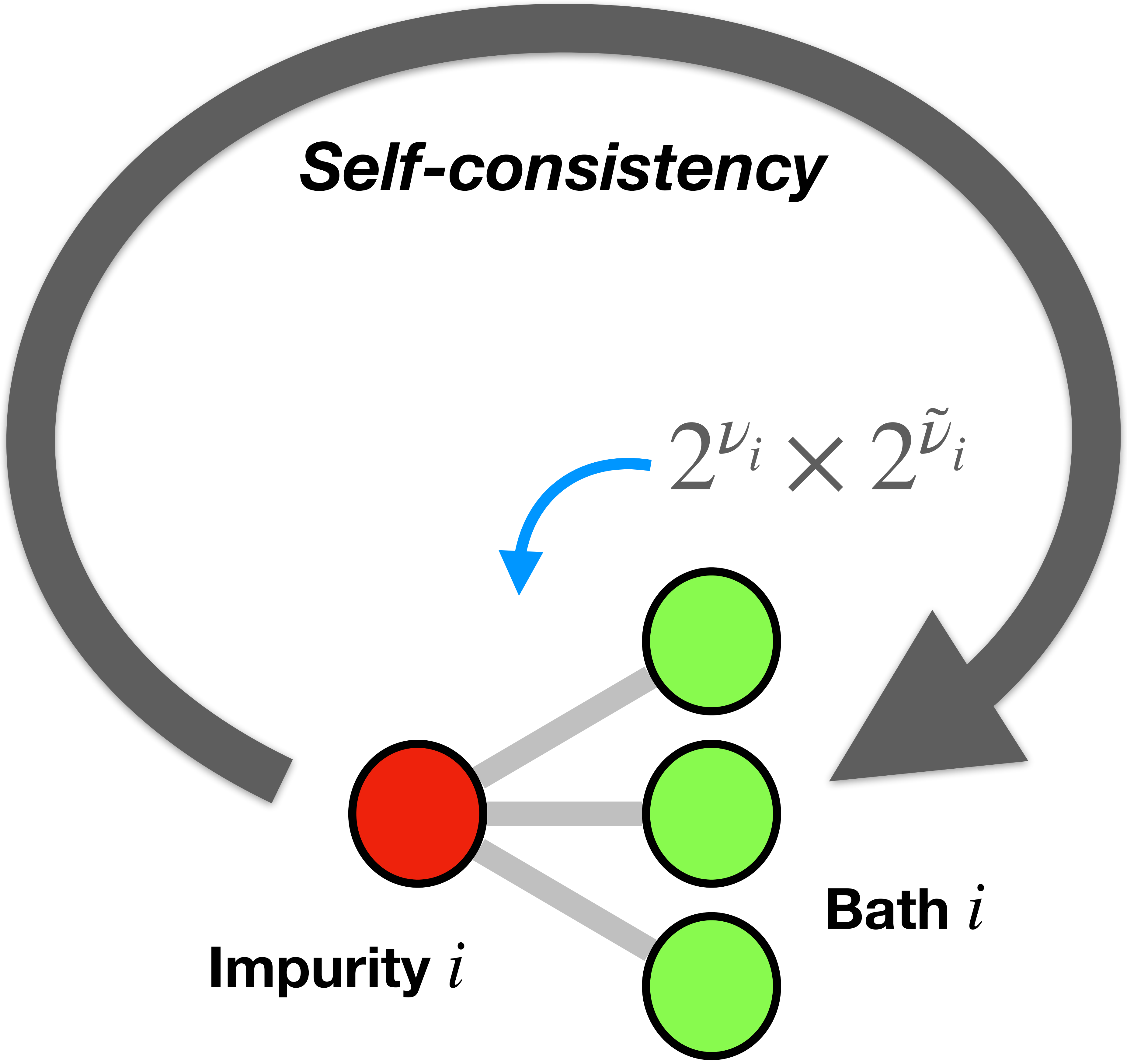




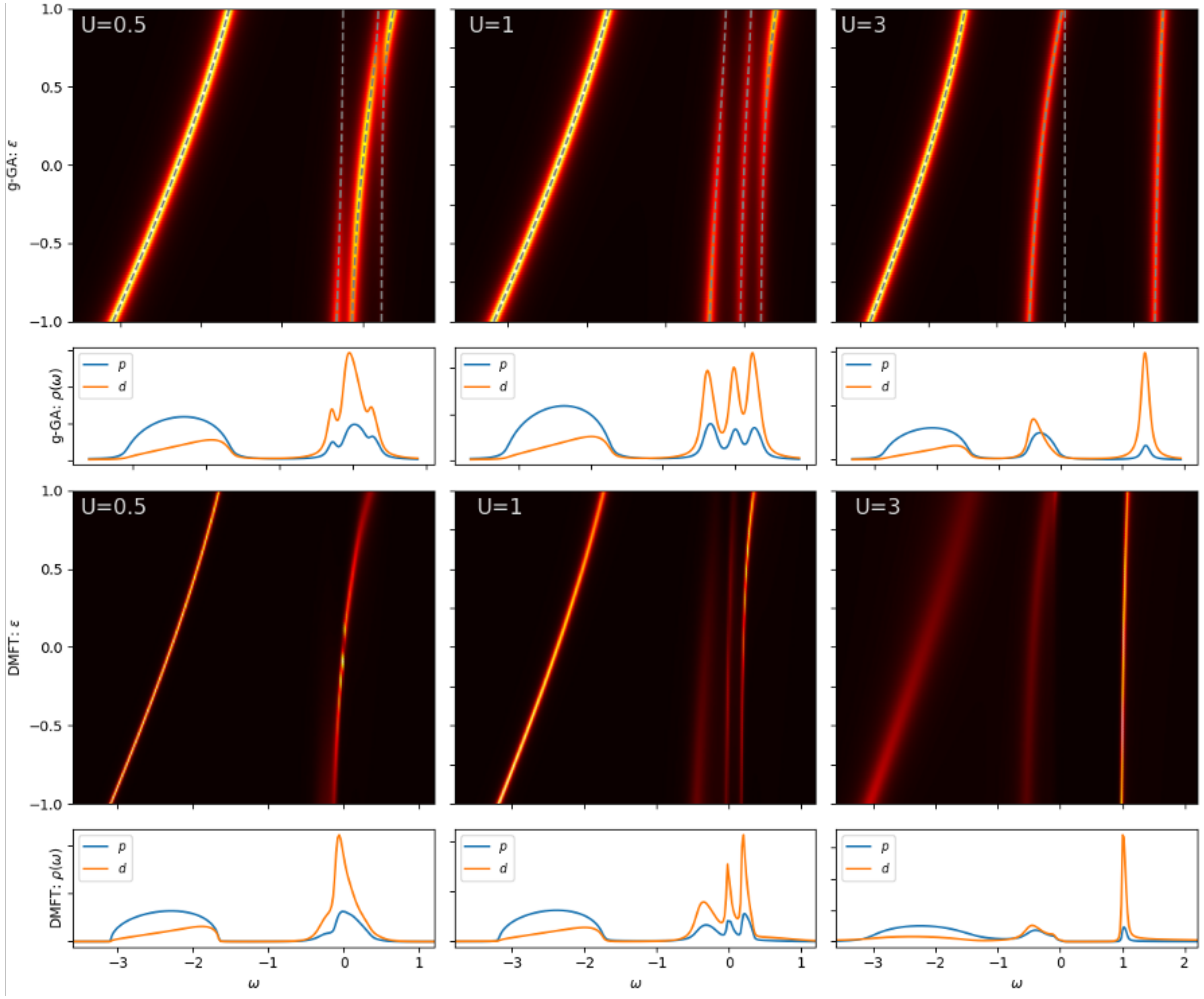
Benchmark calculations ALM:



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



Benchmark calculations ALM:



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

Analytical (approximate) expression for self-energy

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

THANK YOU FOR YOUR ATTENTION !!!