

# Quantum-embedding formulation of the GA/RISB equations

**Introduction to DFT+GA/RISB**

June 16, 2022

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INTERNATIONAL  
**SUMMER**  
**SCHOOL** on  
COMPUTATIONAL  
QUANTUM  
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.

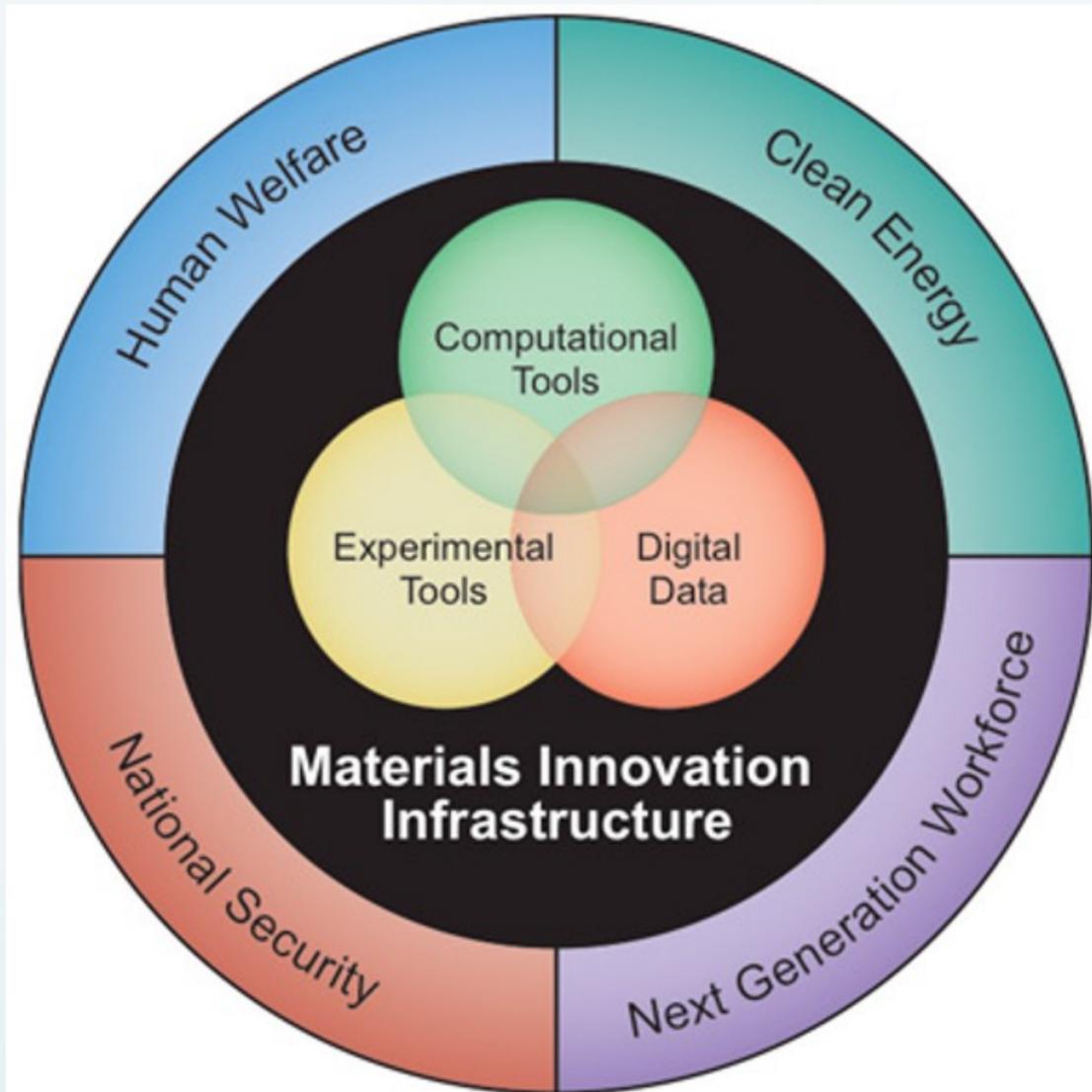
# Limitations

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*



## THE U.S. MATERIALS GENOME INITIATIVE

*"...to discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative"*  
— President Obama, 2011

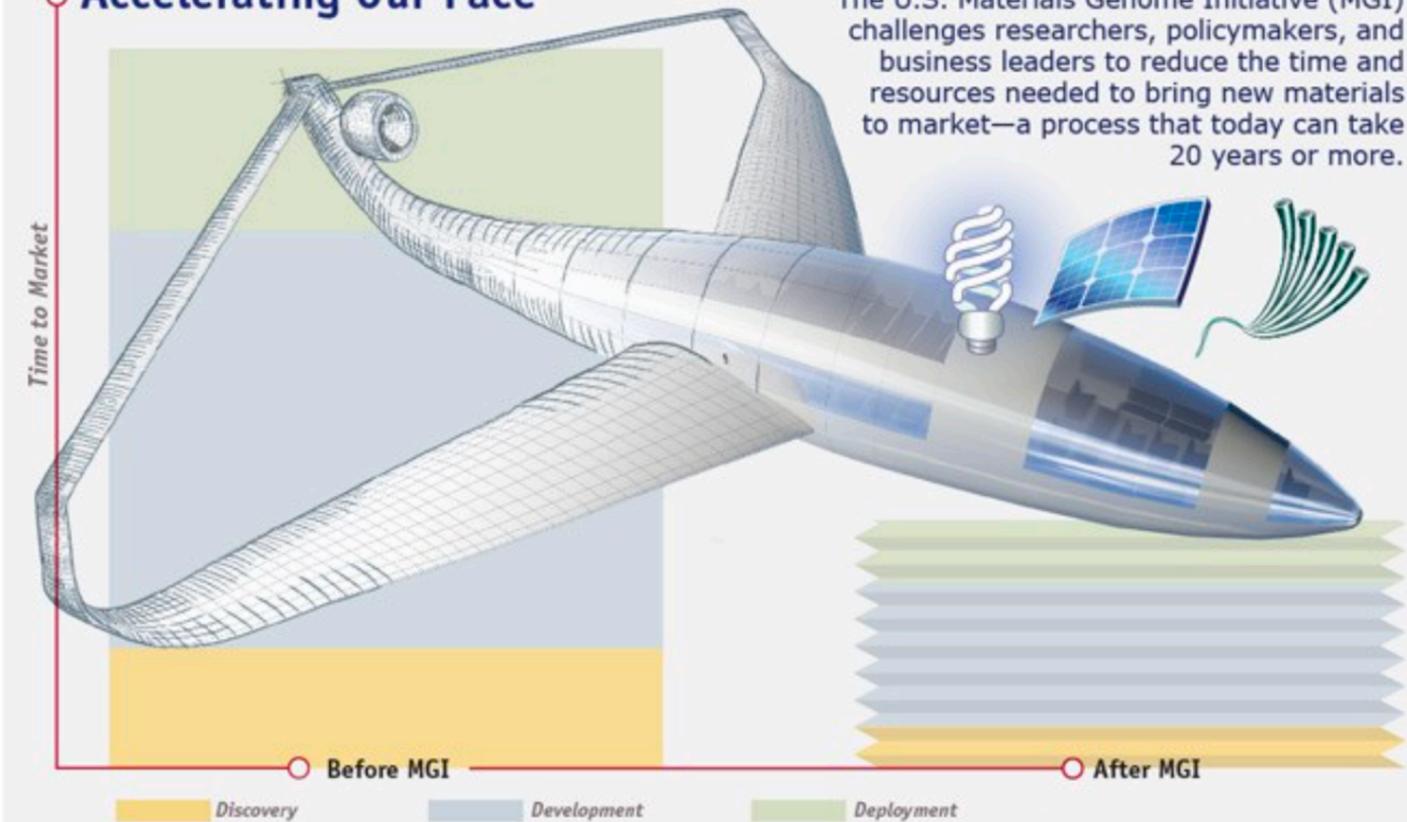
### Meeting Societal Needs

Advanced materials are at the heart of innovation, economic opportunities, and global competitiveness. They are the foundation for new capabilities, tools, and technologies that meet urgent societal needs including clean energy, human welfare, and national security.



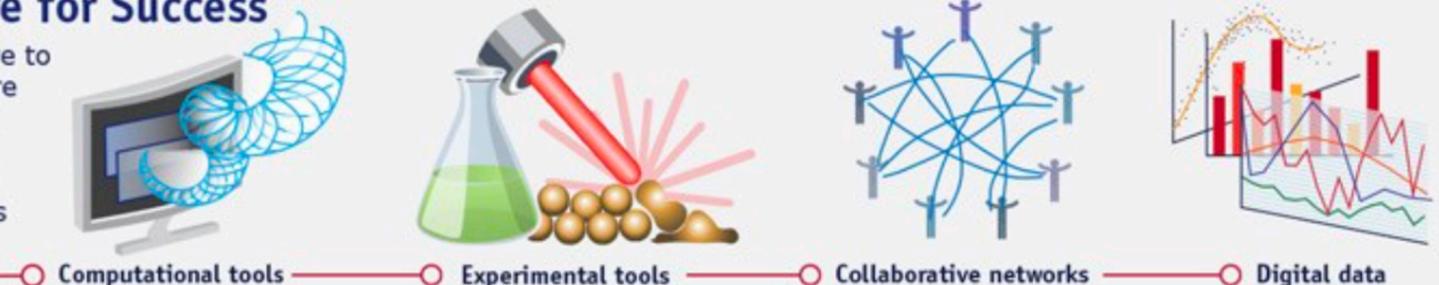
### Accelerating Our Pace

The U.S. Materials Genome Initiative (MGI) challenges researchers, policymakers, and business leaders to reduce the time and resources needed to bring new materials to market—a process that today can take 20 years or more.

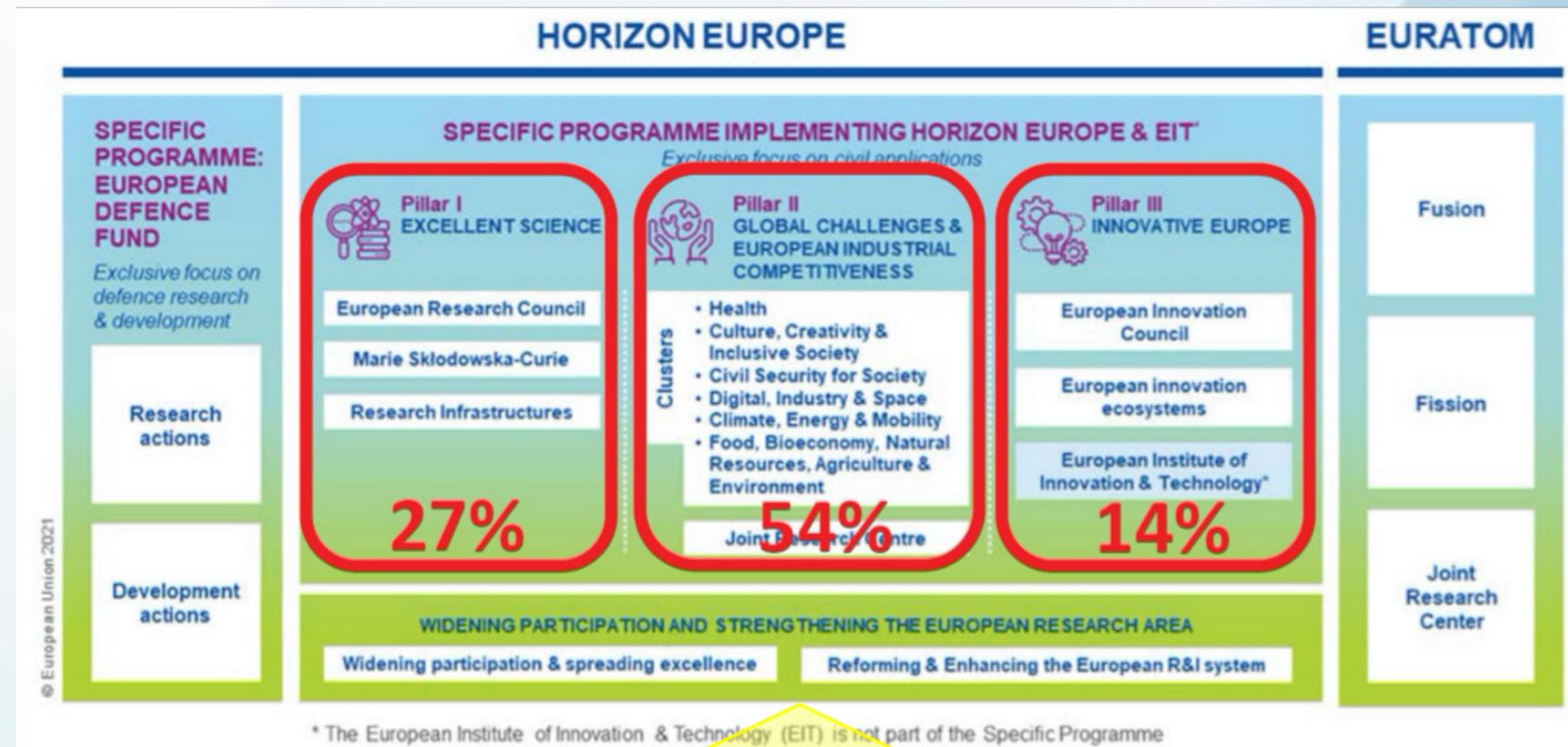


### Building Infrastructure for Success

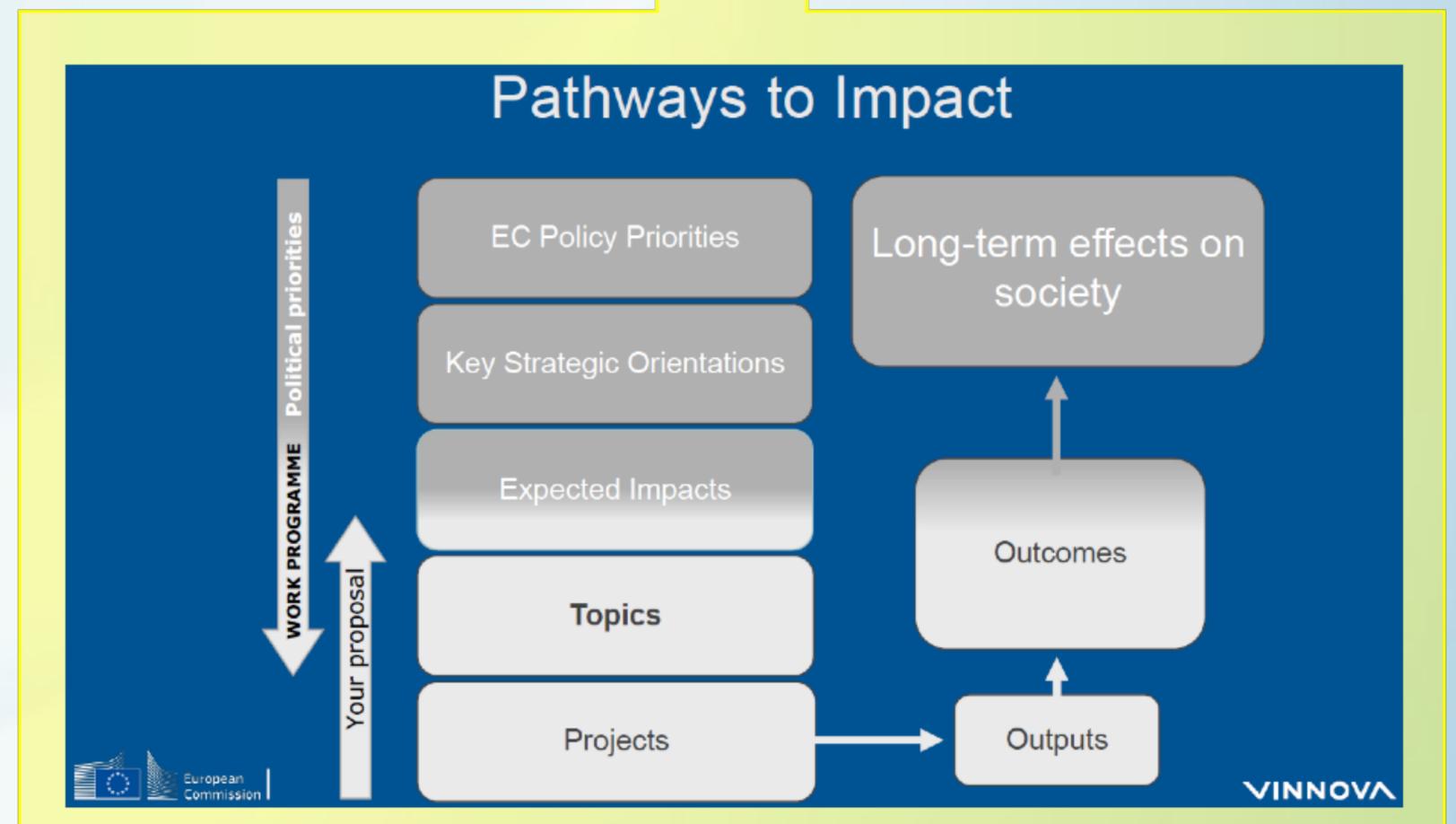
The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.



# 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

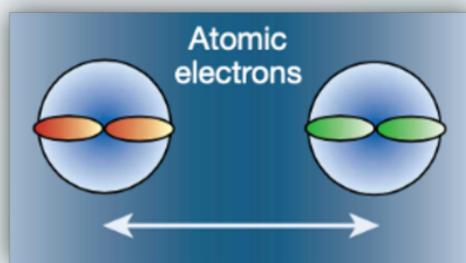
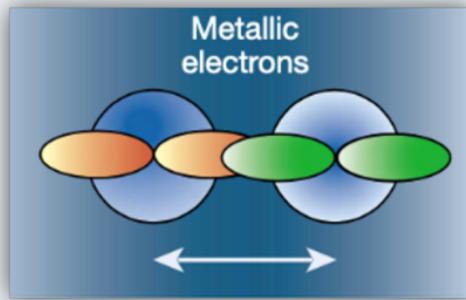
Systems with localized *d*- or *f*-electrons:  
*Single-particle picture not sufficient!*

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 <b>H</b> Hydrogen 1.008	2 <b>He</b> Helium 4.002602	<div style="display: flex; justify-content: space-between;"> <div style="width: 20%;"> <p><b>C</b> Solid</p> <p><b>Hg</b> Liquid</p> <p><b>H</b> Gas</p> <p><b>Rf</b> Unknown</p> </div> <div style="width: 40%; text-align: center;"> <p><b>Metals</b></p> <p>Alkali metals   Alkaline earth metals   Lanthanoids   Actinoids   Transition metals   Post-transition metals</p> </div> <div style="width: 20%; text-align: center;"> <p><b>Nonmetals</b></p> <p>Other nonmetals   Halogens   Noble gases</p> </div> </div>															
3 <b>Li</b> Lithium 6.94	4 <b>Be</b> Beryllium 9.012182	21 <b>Sc</b> Scandium 44.955912	22 <b>Ti</b> Titanium 47.867	23 <b>V</b> Vanadium 50.9415	24 <b>Cr</b> Chromium 51.9961	25 <b>Mn</b> Manganese 54.938044	26 <b>Fe</b> Iron 55.845	27 <b>Co</b> Cobalt 58.933195	28 <b>Ni</b> Nickel 58.6934	29 <b>Cu</b> Copper 63.546	30 <b>Zn</b> Zinc 65.38	31 <b>Ga</b> Gallium 69.723	32 <b>Ge</b> Germanium 72.63	33 <b>As</b> Arsenic 74.9216	34 <b>Se</b> Selenium 78.9718	35 <b>Br</b> Bromine 79.904	36 <b>Kr</b> Krypton 83.798
11 <b>Na</b> Sodium 22.989769	12 <b>Mg</b> Magnesium 24.305	39 <b>Y</b> Yttrium 88.90584	40 <b>Zr</b> Zirconium 91.224	41 <b>Nb</b> Niobium 92.90637	42 <b>Mo</b> Molybdenum 95.95	43 <b>Tc</b> Technetium (98)	44 <b>Ru</b> Ruthenium 101.07	45 <b>Rh</b> Rhodium 102.9055	46 <b>Pd</b> Palladium 106.42	47 <b>Ag</b> Silver 107.8682	48 <b>Cd</b> Cadmium 112.414	49 <b>In</b> Indium 114.818	50 <b>Sn</b> Tin 118.710	51 <b>Sb</b> Antimony 121.760	52 <b>Te</b> Tellurium 127.60	53 <b>I</b> Iodine 126.90545	54 <b>Xe</b> Xenon 131.293
19 <b>K</b> Potassium 39.0983	20 <b>Ca</b> Calcium 40.078	57-71	72 <b>Hf</b> Hafnium 178.49	73 <b>Ta</b> Tantalum 180.94788	74 <b>W</b> Tungsten 183.84	75 <b>Re</b> Rhenium 186.207	76 <b>Os</b> Osmium 190.23	77 <b>Ir</b> Iridium 192.222	78 <b>Pt</b> Platinum 195.084	79 <b>Au</b> Gold 196.966569	80 <b>Hg</b> Mercury 200.59	81 <b>Tl</b> Thallium 204.38	82 <b>Pb</b> Lead 207.2	83 <b>Bi</b> Bismuth 208.9804	84 <b>Po</b> Polonium (209)	85 <b>At</b> Astatine (210)	86 <b>Rn</b> Radon (222)
37 <b>Rb</b> Rubidium 85.4678	38 <b>Sr</b> Strontium 87.62	89-103	104 <b>Rf</b> Rutherfordium (261)	105 <b>Db</b> Dubnium (268)	106 <b>Sg</b> Seaborgium (271)	107 <b>Bh</b> Bohrium (272)	108 <b>Hs</b> Hassium (270)	109 <b>Mt</b> Meitnerium (276)	110 <b>Ds</b> Darmstadtium (281)	111 <b>Rg</b> Roentgenium (280)	112 <b>Cn</b> Copernicium (285)	113 <b>Nh</b> Nihonium (284)	114 <b>Fl</b> Flerovium (289)	115 <b>Mc</b> Moscovium (288)	116 <b>Lv</b> Livermorium (293)	117 <b>Ts</b> Tennessine (294)	118 <b>Og</b> Oganesson (294)
55 <b>Cs</b> Caesium 132.90545	56 <b>Ba</b> Barium 137.327																
87 <b>Fr</b> Francium (223)	88 <b>Ra</b> Radium (226)																

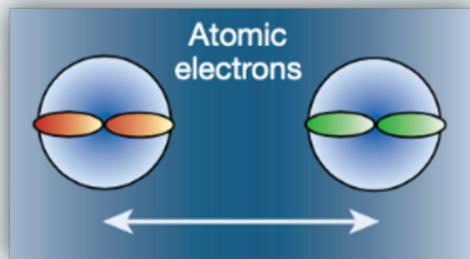
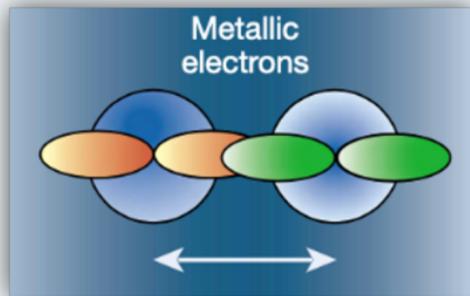
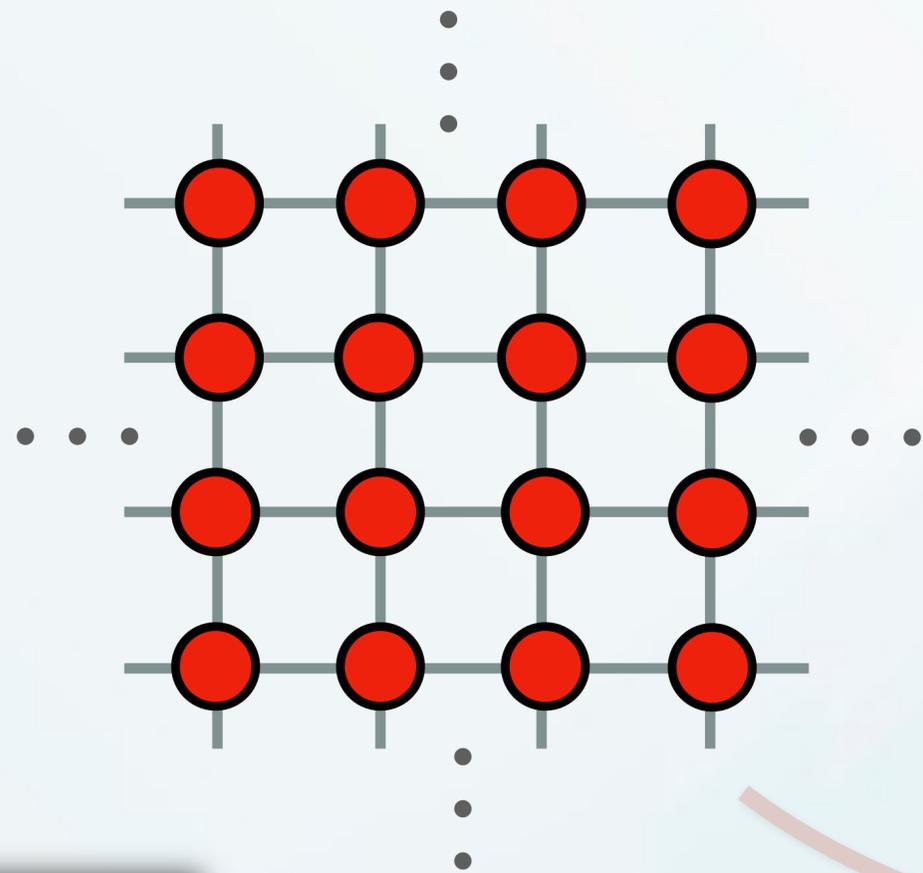
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

Periodic Table Design & Interface Copyright © 1997 Michael Dayah. Ptable.com Last updated Sep 10, 2016

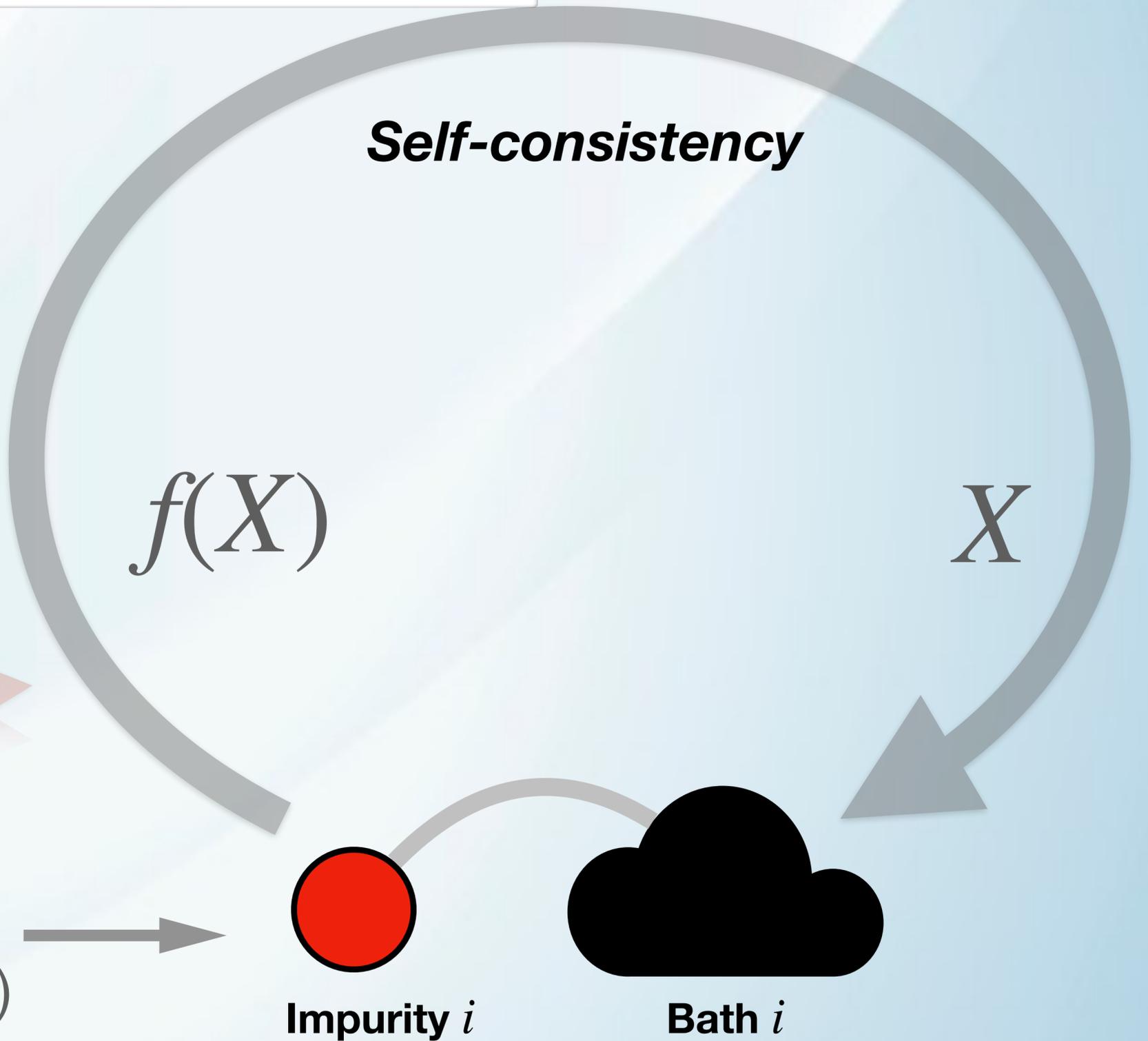
57 <b>La</b> Lanthanum 138.90547	58 <b>Ce</b> Cerium 140.116	59 <b>Pr</b> Praseodymium 140.90766	60 <b>Nd</b> Neodymium 144.242	61 <b>Pm</b> Promethium (145)	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.964	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.92535	66 <b>Dy</b> Dysprosium 162.500	67 <b>Ho</b> Holmium 164.93033	68 <b>Er</b> Erbium 167.259	69 <b>Tm</b> Thulium 168.93486	70 <b>Yb</b> Ytterbium 173.054	71 <b>Lu</b> Lutetium 174.96686
89 <b>Ac</b> Actinium (227)	90 <b>Th</b> Thorium 232.03772	91 <b>Pa</b> Protactinium 231.036888	92 <b>U</b> Uranium 238.02891	93 <b>Np</b> Neptunium (237)	94 <b>Pu</b> Plutonium (244)	95 <b>Am</b> Americium (243)	96 <b>Cm</b> Curium (247)	97 <b>Bk</b> Berkelium (247)	98 <b>Cf</b> Californium (251)	99 <b>Es</b> Einsteinium (252)	100 <b>Fm</b> Fermium (257)	101 <b>Md</b> Mendelevium (258)	102 <b>No</b> Nobelium (259)	103 <b>Lr</b> Lawrencium (262)



# 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

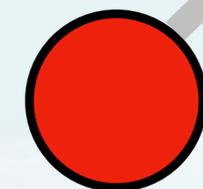
*Laboratoire de Physique Statistique de l'Ecole Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France*

$\Sigma(\omega)$

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

$(\Delta(\omega), E, U, J)$

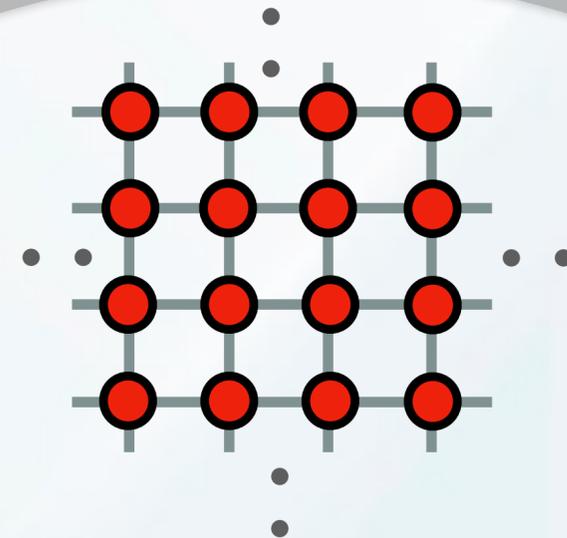
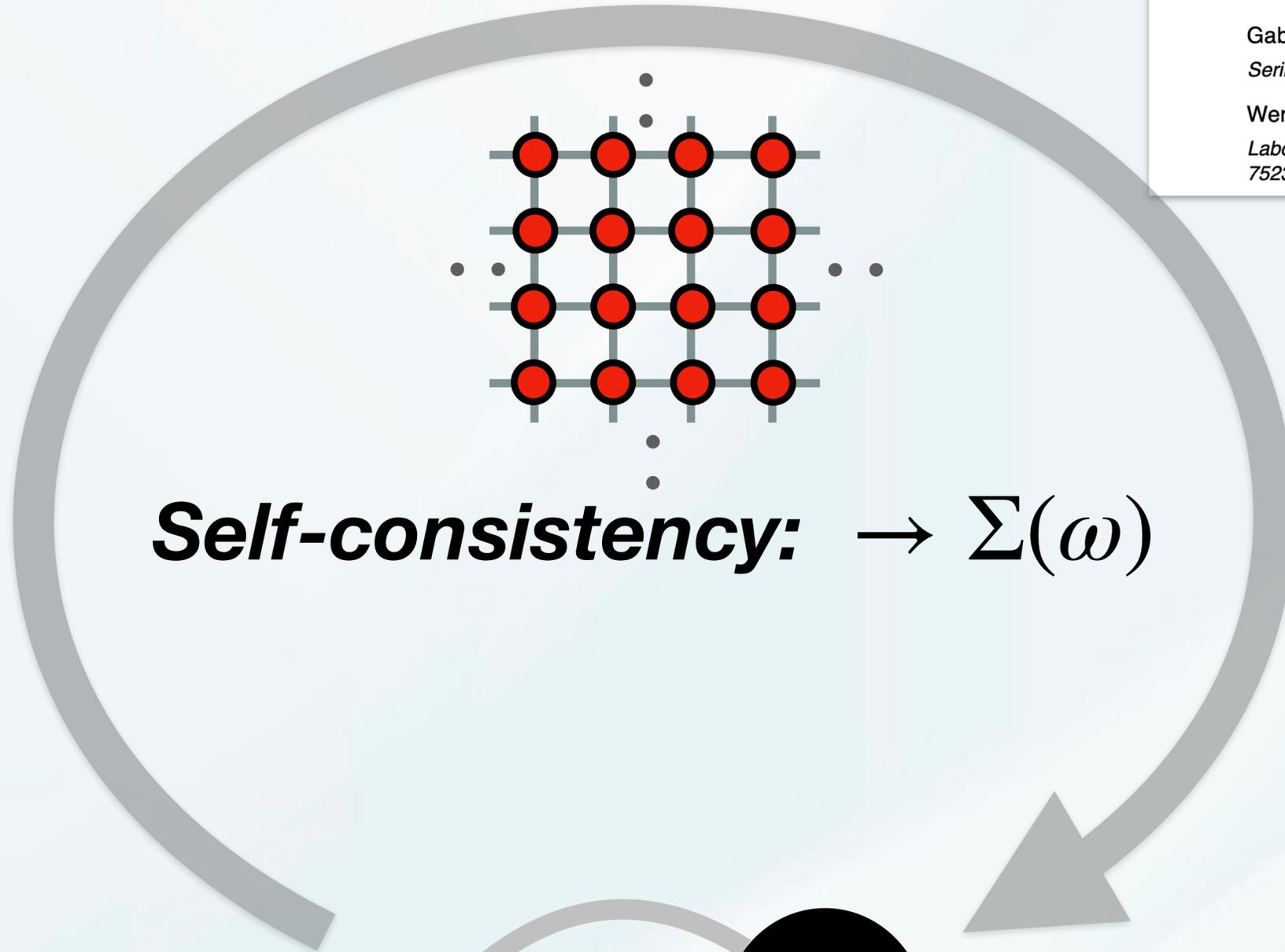
*Impurity model*



**Impurity  $i$**



**Bath  $i$**



# GA/RISB (QE formulation)

PHYSICAL REVIEW X 5, 011008 (2015)

Phase Diagram and Electronic Structure of Praseodymium and Plutonium

Nicola Lanatà,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Cai-Zhuang Wang,<sup>2</sup> Kai-Ming Ho,<sup>2</sup> and Gabriel Kotliar<sup>1</sup>

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<sub>2</sub>

Nicola Lanatà,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Xiaoyu Deng,<sup>3</sup> Vladimir Dobrosavljević,<sup>1</sup> and Gabriel Kotliar<sup>3,4</sup>

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

**Self-consistency:**  $\rightarrow \Sigma_0, Z$   $(D, \lambda^c, E, U, J)$

**Embedding  
Hamiltonian**



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

# g-GA/g-RISB (QE formulation)

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

## Emergent Bloch excitations in Mott matter

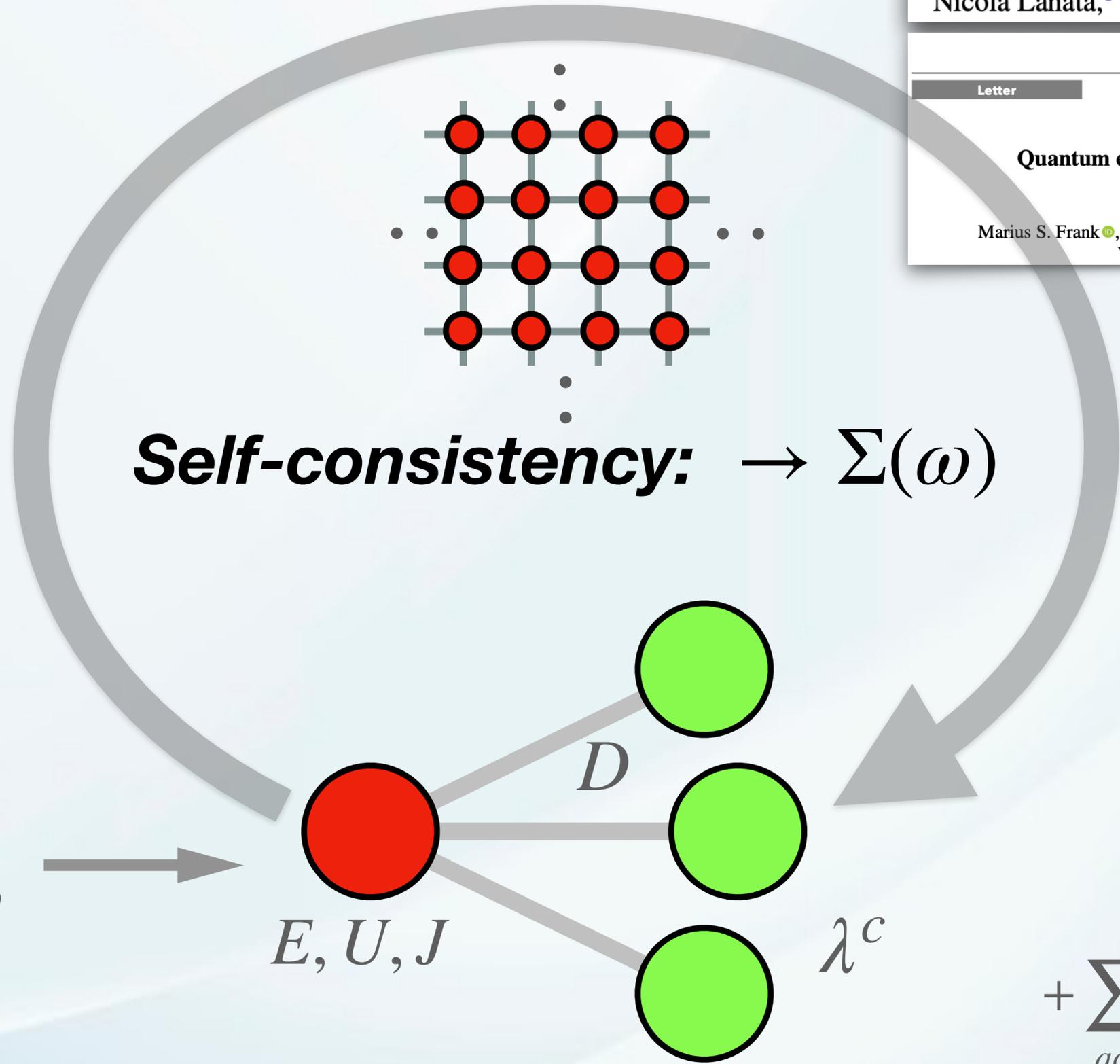
Nicola Lanatà,<sup>1</sup> Tsung-Han Lee,<sup>1</sup> Yong-Xin Yao,<sup>2</sup> and Vladimir Dobrosavljević<sup>1</sup>

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

Letter

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

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



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

**Self-consistency:**  $\rightarrow \Sigma(\omega)$   $(D, \lambda^c, E, U, J)$

Embedding Hamiltonian

$E, U, J$

$D$

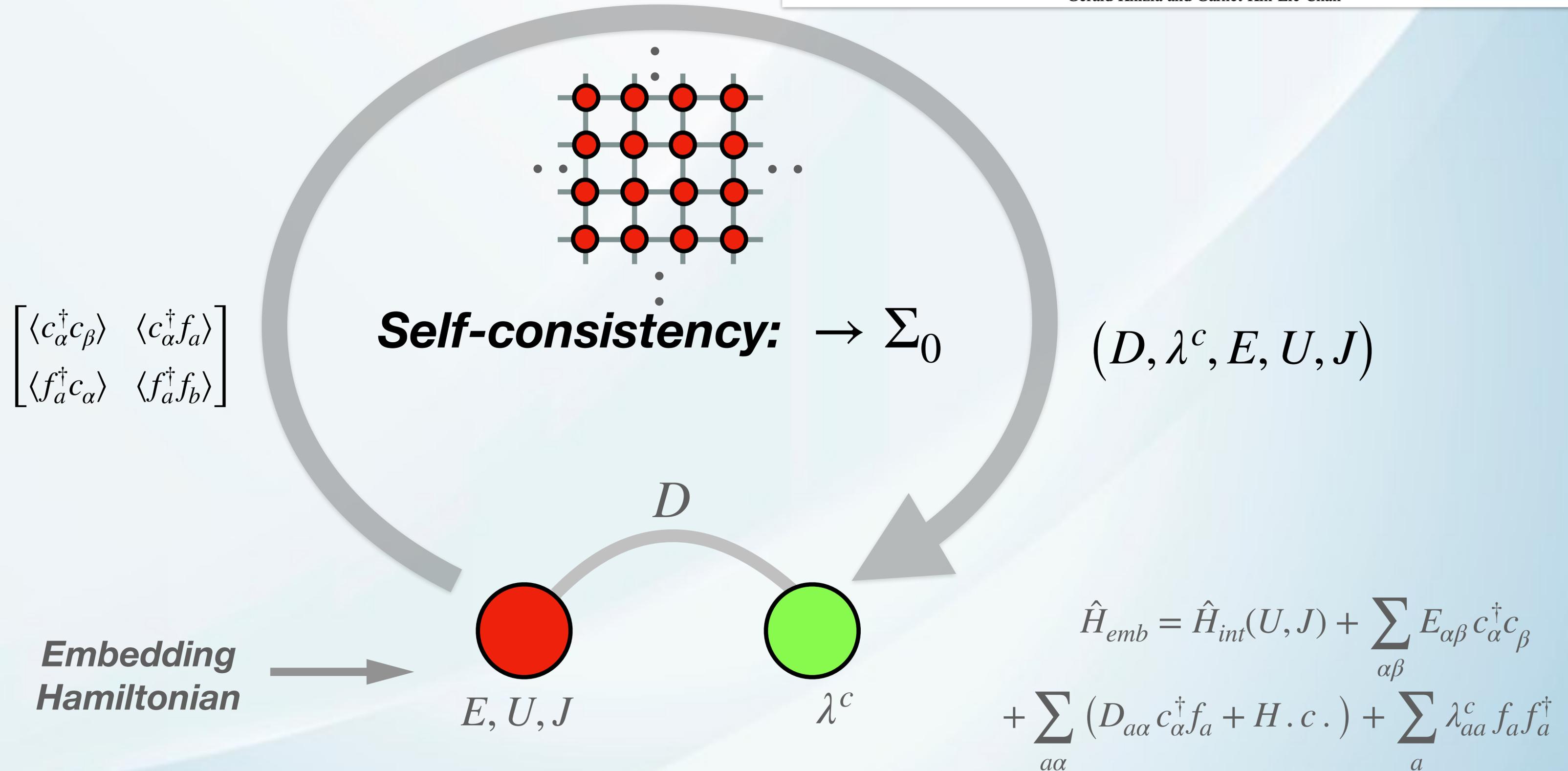
$\lambda^c$

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

# Example: DMET

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

Gerald Knizia and Garnet Kin-Lic Chan



# GA/RISB (connection with DMET)

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

## Phase Diagram and Electronic Structure of Praseodymium and Plutonium

Nicola Lanatà,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Cai-Zhuang Wang,<sup>2</sup> Kai-Ming Ho,<sup>2</sup> and Gabriel Kotliar<sup>1</sup>

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<sub>2</sub>

Nicola Lanatà,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Xiaoyu Deng,<sup>3</sup> Vladimir Dobrosavljević,<sup>1</sup> and Gabriel Kotliar<sup>3,4</sup>

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

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

Thomas Ayrál,<sup>1</sup> Tsung-Han Lee,<sup>1</sup> and Gabriel Kotliar<sup>1,2</sup>

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

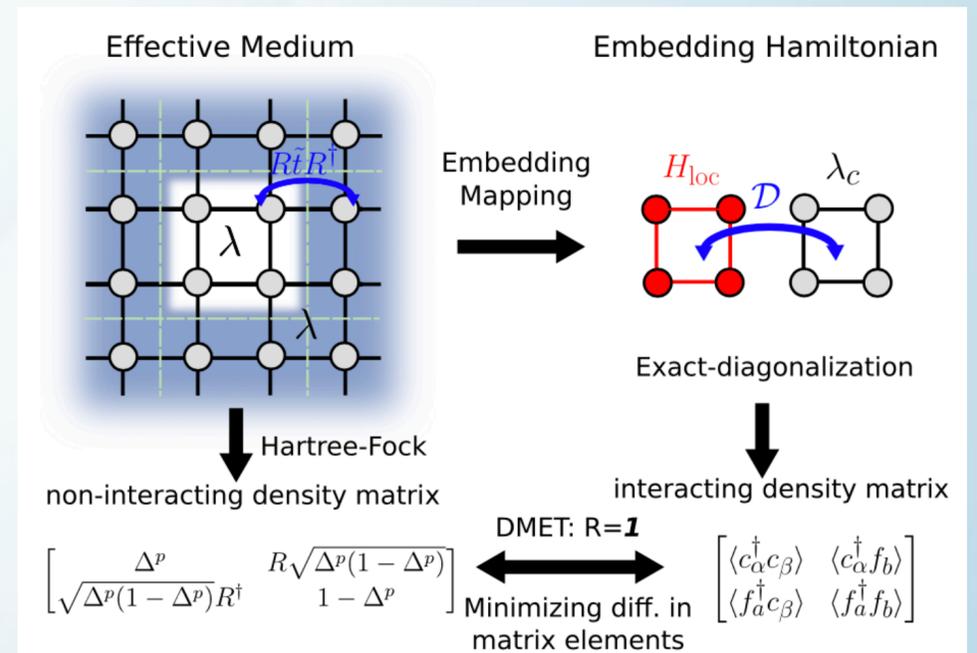
## Rotationally invariant slave-boson and density matrix embedding theory: Unified framework and comparative study on the one-dimensional and two-dimensional Hubbard model

Tsung-Han Lee,<sup>1,\*</sup> Thomas Ayrál,<sup>1,2</sup> Yong-Xin Yao,<sup>3</sup> Nicola Lanata,<sup>4</sup> and Gabriel Kotliar<sup>1,5</sup>

## Formulation of GA/RISB as QE theory



## Comparison between GA/RISB & DMET QE equations & performance



# 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.

# The Hamiltonian:

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

$\mathbf{k}$ : 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)

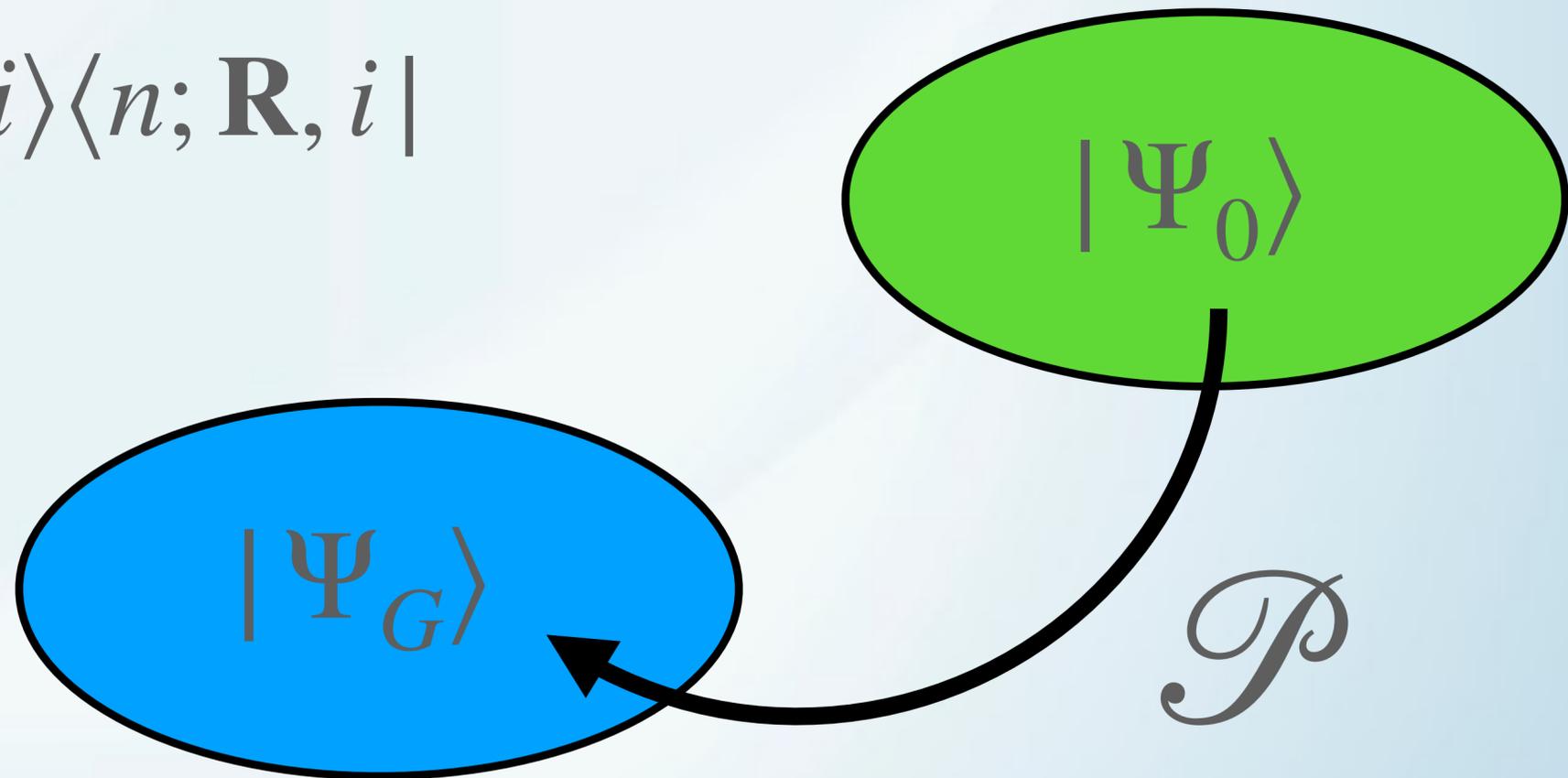
$i = 2$ : Second subset of correlated modes (e.g.  $f$  orbitals of atom 1 in unit cell)

...

# The GA variational wave function:

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

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



# The GA variational wave function:

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

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

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

$$|n; \mathbf{R}, i\rangle = [f_{\mathbf{R}i1}^\dagger]^{q_1(n)} \cdots [f_{\mathbf{R}i\nu_i}^\dagger]^{q_{\nu_i}(n)} |0\rangle$$

**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,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Cai-Zhuang Wang,<sup>2</sup> Kai-Ming Ho,<sup>2</sup> and Gabriel Kotliar<sup>1</sup>

PRL **118**, 126401 (2017)

PHYSICAL REVIEW LETTERS

week ending  
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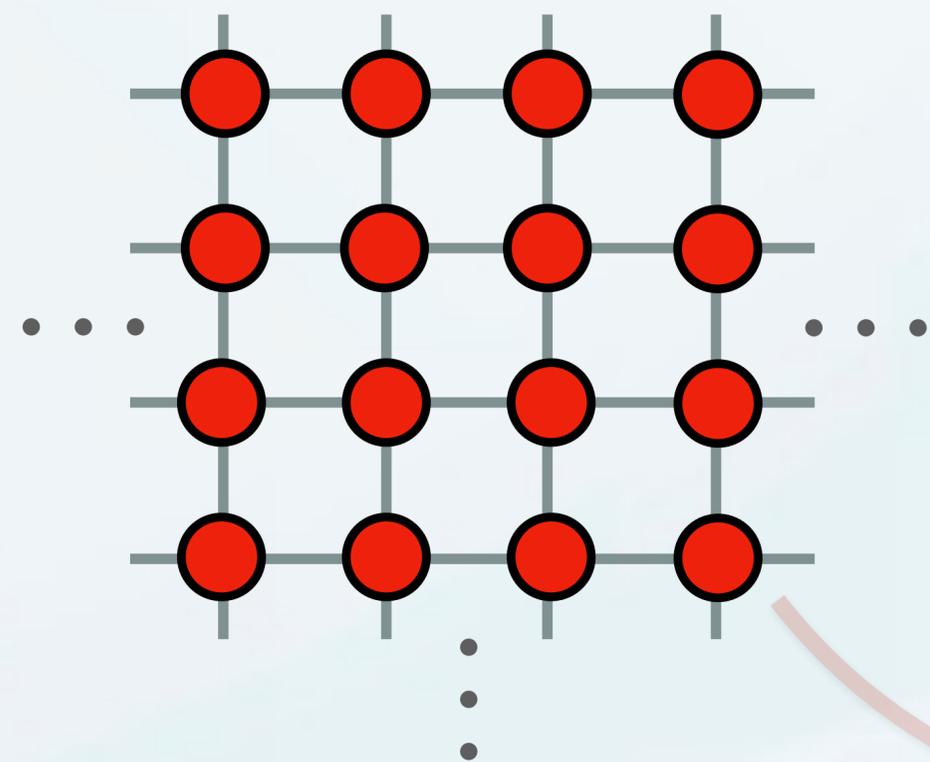
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Our goal is to minimize  $\langle \Psi_G | \hat{H} | \Psi_G \rangle$   
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$2^{\nu_i} \times 2^{\nu_i}$

*Quantum-embedding  
formulation*

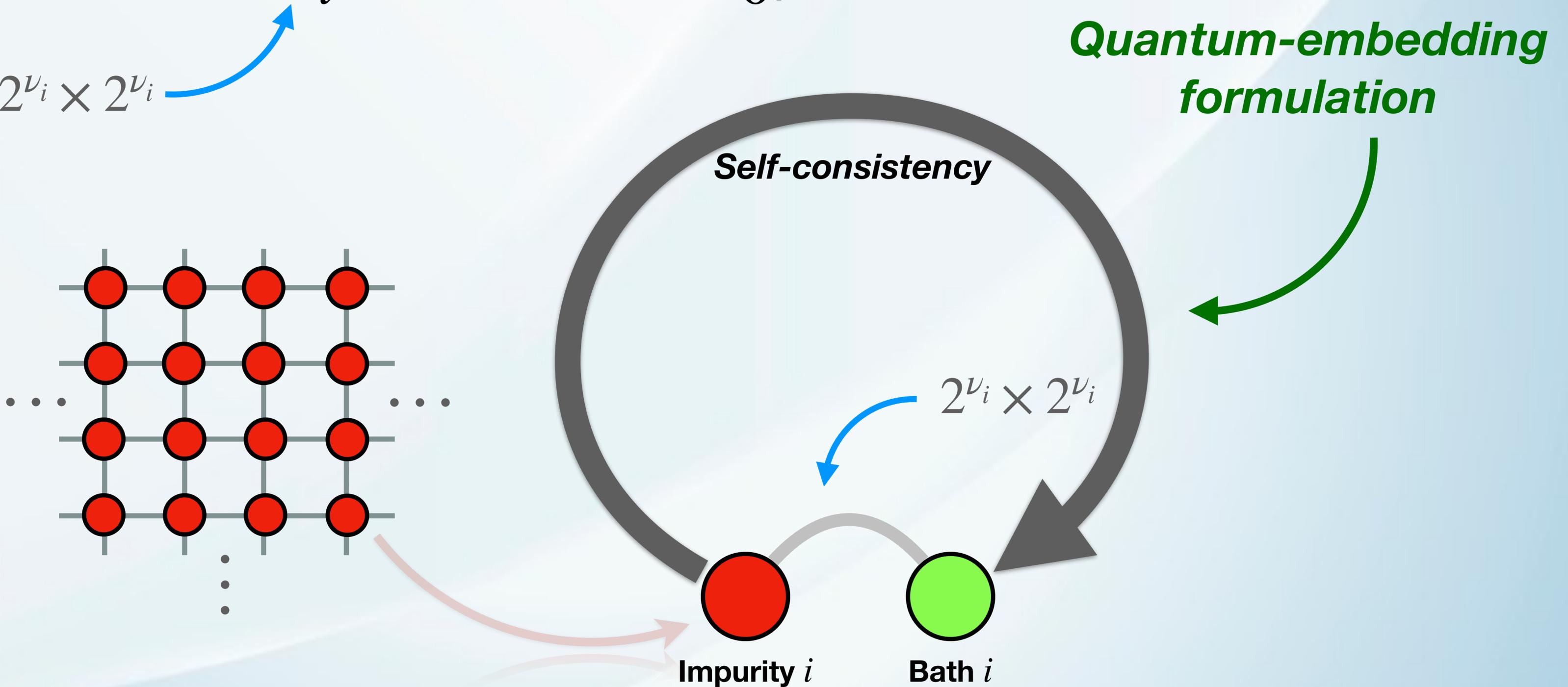


*Self-consistency*

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

Impurity  $i$

Bath  $i$



# 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.

# Gutzwiller approximation:

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

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

## Gutzwiller constraints:

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

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

# Gutzwiller approximation:

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

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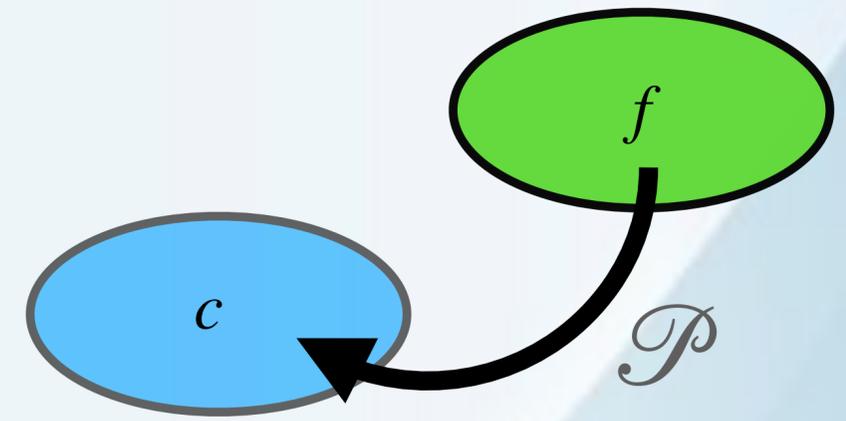
$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle \quad \forall a, b \in \{1, \dots, \nu_i\}$$

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

# Gutzwiller constraints:

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

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



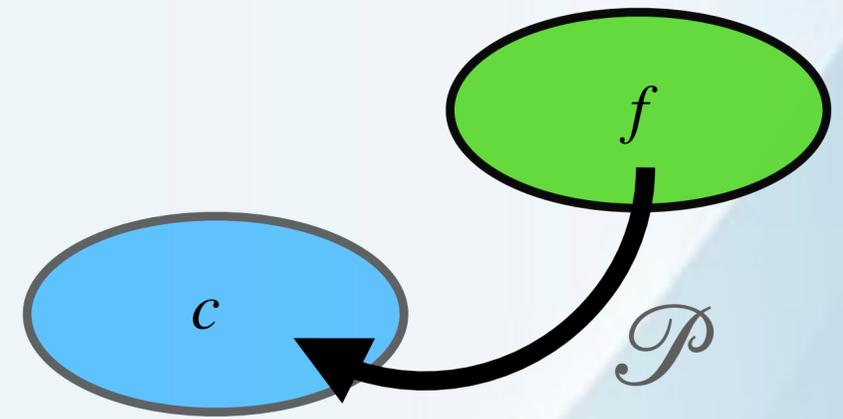
## Key consequence:

$$\begin{aligned} \langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle &= \langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle \langle \Psi_0 | f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle \\ &\quad + \langle \Psi_0 | [\mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i}] f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle_{2\text{-legs}} \end{aligned}$$

# Gutzwiller constraints:

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

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



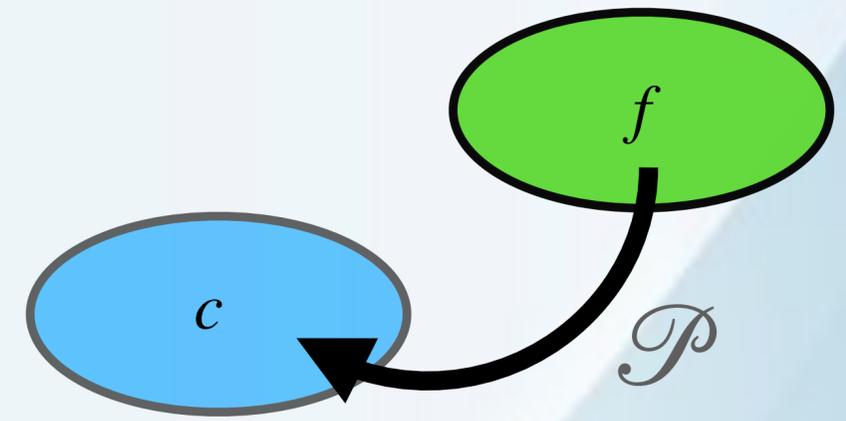
## Key consequence:

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle \langle \Psi_0 | f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle + \langle \Psi_0 | [\mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i}] f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle_{2\text{-legs}}$$

# Gutzwiller constraints:

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

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



## Key consequence:

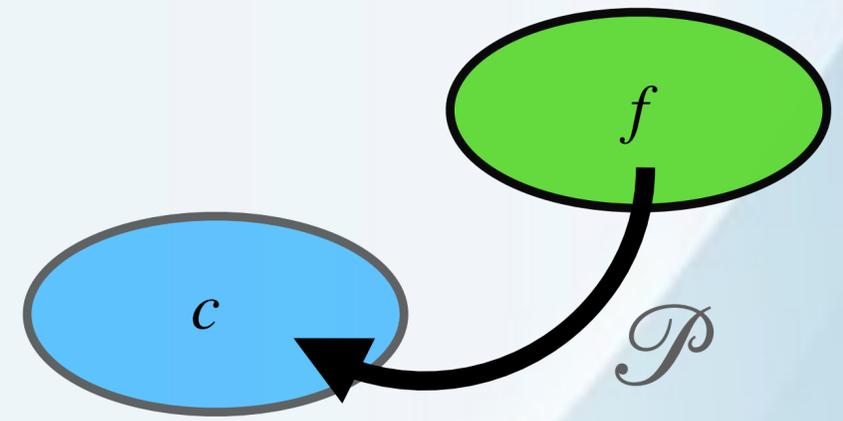
~~$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle$$

$$+ \langle \Psi_0 | [\mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i}] f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle_{2\text{-legs}}$$~~

# Gutzwiller constraints:

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

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



*Key consequence:*

$$\langle \Psi_0 | [\mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i}] f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle_{2-legs} = 0 \quad \forall a, b$$

# Gutzwiller constraints:

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

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

*Key consequence:*

$$\langle \Psi_0 | [\mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i}] f_{\mathbf{R}'ja}^\dagger f_{\mathbf{R}'jb} | \Psi_0 \rangle_{2\text{-legs}} = 0 \quad \forall a, b$$

# 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:

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

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

$\mathbf{k}$ : 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:

$$\begin{aligned} \langle \Psi_G | \hat{\mathcal{O}} [c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] | \Psi_G \rangle &= \langle \Psi_0 | \mathcal{P}^\dagger \hat{\mathcal{O}} [c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] \mathcal{P} | \Psi_0 \rangle \\ &= \langle \Psi_0 | \left[ \prod_{(\mathbf{R}', i') \neq (\mathbf{R}, i)} \mathcal{P}_{\mathbf{R}'i'}^\dagger \mathcal{P}_{\mathbf{R}'i'} \right] \mathcal{P}_{\mathbf{R}i}^\dagger \hat{\mathcal{O}} [c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle \end{aligned}$$

# Local operators: (disconnected terms)

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

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

# Local operators: (disconnected terms)

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

*(GA and G. constraints)*

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

# Local operators: (disconnected terms)

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

$$= \langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \hat{\mathcal{O}} [c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle$$

# Local operators: (connected terms)

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

The diagram illustrates the structure of the operator expression. It features a large square bracket containing a product of operators. Above the product, there are two vertical ellipses (⋮) indicating continuation. Two curved arcs connect the top of the product to the top of the operator  $\hat{\mathcal{O}}$ , suggesting a connection between the product and the operator. Another two curved arcs connect the top of the operator  $\hat{\mathcal{O}}$  to the top of the final operator  $\mathcal{P}_{\mathbf{R} i}$ , suggesting a connection between the operator and the final operator. The entire expression is enclosed in a large square bracket, with the bra  $\langle \Psi_0 |$  on the left and the ket  $| \Psi_0 \rangle$  on the right.

# Local operators: (connected terms)

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

*(GA and G. constraints)*

# Local operators:

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

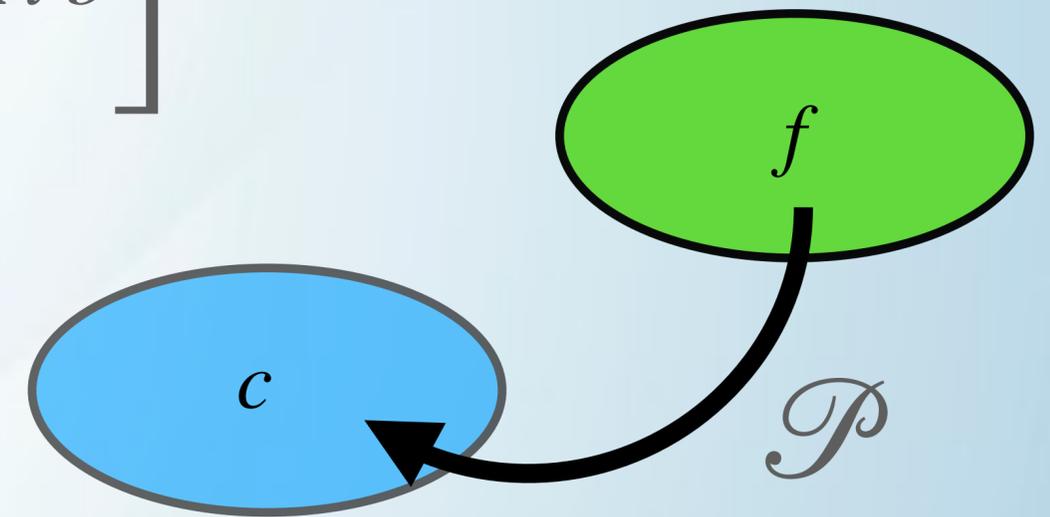
# Non-local 1-body operators, i.e., $(\mathbf{R}, i) \neq (\mathbf{R}', i')$ :

$$\langle \Psi_G | c_{\mathbf{R}i\alpha}^\dagger c_{\mathbf{R}'i'\beta} | \Psi_G \rangle = \langle \Psi_0 | [\mathcal{P}_{\mathbf{R}i}^\dagger c_{\mathbf{R}i\alpha}^\dagger \mathcal{P}_{\mathbf{R}i}] [\mathcal{P}_{\mathbf{R}'i'}^\dagger c_{\mathbf{R}'i'\beta} \mathcal{P}_{\mathbf{R}'i'}] | \Psi_0 \rangle$$

# Non-local quadratic operators:

$$\begin{aligned}
 \langle \Psi_G | c_{\mathbf{R}i\alpha}^\dagger c_{\mathbf{R}'i'\beta} | \Psi_G \rangle &= \langle \Psi_0 | \left[ \mathcal{P}_{\mathbf{R}i}^\dagger c_{\mathbf{R}i\alpha}^\dagger \mathcal{P}_{\mathbf{R}i} \right] \left[ \mathcal{P}_{\mathbf{R}'i'}^\dagger c_{\mathbf{R}'i'\beta} \mathcal{P}_{\mathbf{R}'i'} \right] | \Psi_0 \rangle \\
 &= \langle \Psi_0 | \left[ \sum_a [\mathcal{R}_i]_{a\alpha} f_{\mathbf{R}i a}^\dagger \right] \left[ \sum_b [\mathcal{R}_i]_{\beta b}^\dagger f_{\mathbf{R}'i' b} \right] | \Psi_0 \rangle
 \end{aligned}$$

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



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

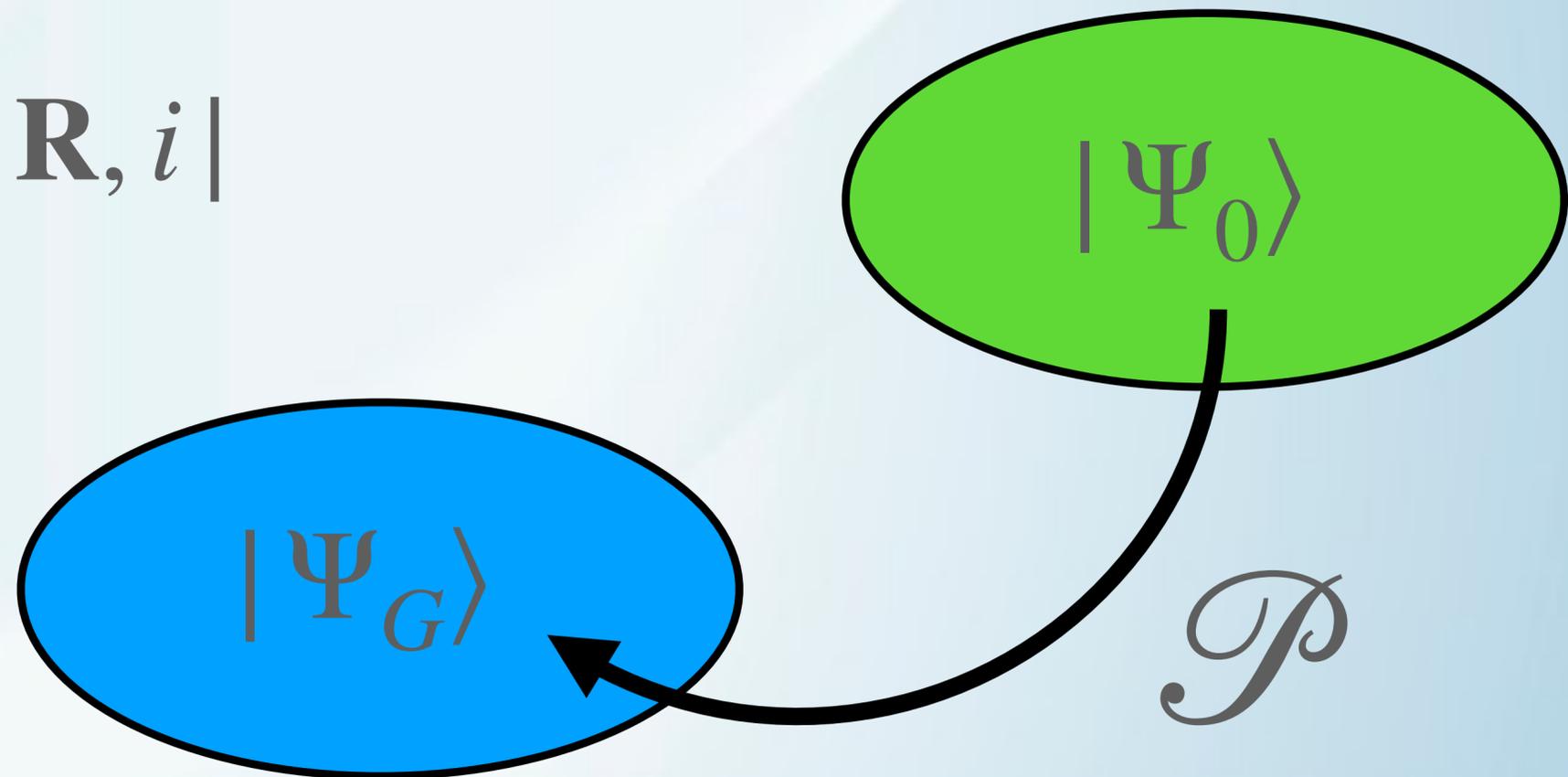
# Non-local quadratic operators:

$$\mathcal{P}_{\mathbf{R}i}^\dagger c_{\mathbf{R}i\alpha}^\dagger \mathcal{P}_{\mathbf{R}i} \rightarrow \sum_a [\mathcal{R}_i]_{a\alpha} f_{\mathbf{R}i\alpha}^\dagger$$

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

$$|\Gamma; \mathbf{R}, i\rangle = [c_{\mathbf{R}i1}^\dagger]^{q_1(\Gamma)} \cdots [c_{\mathbf{R}iv_i}^\dagger]^{q_{v_i}(\Gamma)} |0\rangle$$

$$|n; \mathbf{R}, i\rangle = [f_{\mathbf{R}i1}^\dagger]^{q_1(n)} \cdots [f_{\mathbf{R}iv_i}^\dagger]^{q_{v_i}(n)} |0\rangle$$



# Variational energy:

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

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

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

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

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle \quad \forall a, b \in \{1, \dots, \nu_i\}$$

# 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:

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

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

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

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle \quad \forall a, b \in \{1, \dots, \nu_i\}$$

# Variational energy:

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

Where:

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

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

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle \quad \forall a, b \in \{1, \dots, \nu_i\}$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger \Lambda_i] = 1$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger \Lambda_i F_{i\alpha}^\dagger F_{i\beta}] = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle =: [\Delta_i]_{\alpha\beta}$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \hat{\mathcal{O}} [c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger \hat{\mathcal{O}} [F_{i\alpha}^\dagger, F_{i\alpha}] \Lambda_i]$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger c_{\mathbf{R}i\alpha}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger F_{i\alpha}^\dagger \Lambda_i F_{i\alpha}]$$

Where:

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

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

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

$$| \Gamma; \mathbf{R}, i \rangle = [c_{\mathbf{R}i1}^\dagger]^{q_1(\Gamma)} \cdots [c_{\mathbf{R}iv_i}^\dagger]^{q_{v_i}(\Gamma)} | 0 \rangle$$

$$| n; \mathbf{R}, i \rangle = [f_{\mathbf{R}i1}^\dagger]^{q_1(n)} \cdots [f_{\mathbf{R}iv_i}^\dagger]^{q_{v_i}(n)} | 0 \rangle$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger \Lambda_i] = 1$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger \Lambda_i F_{ia}^\dagger F_{ib}] = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle =: [\Delta_i]_{ab}$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \hat{\mathcal{O}} [c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger \hat{\mathcal{O}} [F_{i\alpha}^\dagger, F_{i\alpha}] \Lambda_i]$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger c_{\mathbf{R}i\alpha}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_0 \rangle = \text{Tr} [P_i^0 \Lambda_i^\dagger F_{i\alpha}^\dagger \Lambda_i F_{ia}]$$

*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:

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

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle = \text{Tr}[\phi_i^\dagger \phi_i] = 1$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \text{Tr}[\phi_i^\dagger \phi_i F_{i\alpha}^\dagger F_{ib}] = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle =: [\Delta_i]_{ab}$$

$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \hat{\mathcal{O}}[c_{\mathbf{R}i\alpha}^\dagger, c_{\mathbf{R}i\alpha}] \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle = \text{Tr}[\phi_i \phi_i^\dagger \hat{\mathcal{O}}[F_{i\alpha}^\dagger, F_{i\alpha}]]$$

$$\text{Tr}[\phi_i^\dagger F_{i\alpha}^\dagger \phi_i F_{i\alpha}] = \sum_c [\mathcal{R}_i]_{c\alpha} [\Delta_i(1 - \Delta_i)]_{ca}^{\frac{1}{2}}$$

**Matrix of SB amplitudes:**

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

# Variational energy:

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

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

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

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

$$Tr \left[ \phi_i^\dagger \phi_i F_{i\alpha}^\dagger F_{i\beta} \right] = \langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle =: [\Delta_i]_{\alpha\beta} \quad \forall a, b \in \{1, \dots, \nu_i\}$$

# 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.

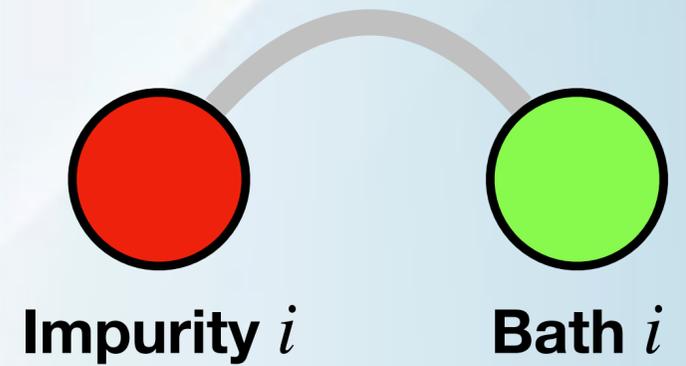
# Quantum-embedding formulation

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

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

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

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



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

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

# Quantum-embedding formulation

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

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

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

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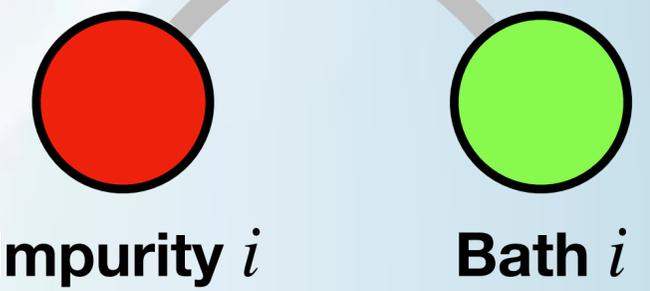
# Quantum-embedding formulation

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

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

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



$$[\mathcal{P}_{\mathbf{R}i}, \hat{N}_{\mathbf{R},i}] = 0 \iff \left[ \sum_{\alpha=1}^{\nu_i} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\alpha} + \sum_{a=1}^{\nu_i} \hat{f}_{a}^{\dagger} \hat{f}_{a} \right] |\Phi_i\rangle = \nu_i |\Phi_i\rangle$$

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

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

# Quantum-embedding formulation

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

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

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

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

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

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

# Variational energy:

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

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

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

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

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

# 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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# Variational energy:

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

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

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

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

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

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

# Variational energy:

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

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

$\langle \Psi_0 | \Psi_0 \rangle = 1$   $\xleftarrow{E}$   $E$   $\xleftarrow{[\mathcal{D}_i]_{a\alpha}}$   $[\mathcal{D}_i]_{a\alpha}$

$\langle \Phi_i | \Phi_i \rangle = 1$   $\xleftarrow{E_i^c}$   $E_i^c$

$\langle \Psi_0 | f_{\mathbf{R}i\alpha}^\dagger f_{\mathbf{R}i\beta} | \Psi_0 \rangle =: [\Delta_i]_{ab}$   $\xleftarrow{[\lambda_i]_{ab}}$   $[\lambda_i]_{ab}$

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

# Lagrange function:

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

Where:

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

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

# Lagrange equations:

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

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

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

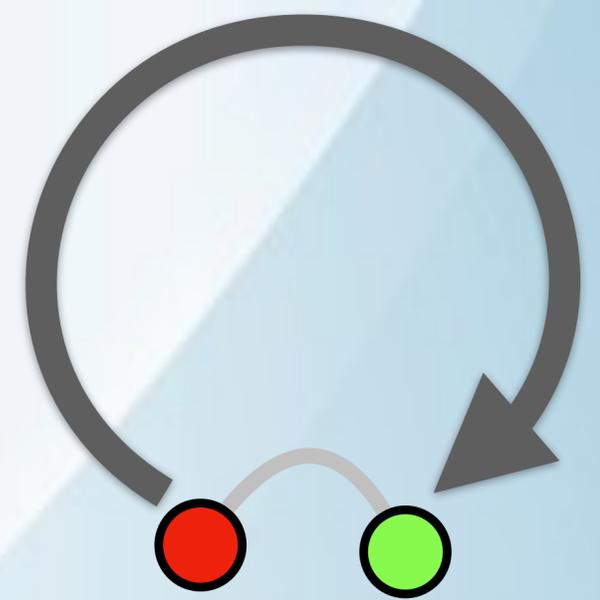
$$\hat{H}_i^{\text{emb}} |\Phi_i\rangle = E_i^c |\Phi_i\rangle \longrightarrow |\Phi_i\rangle$$

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

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

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

# Lagrange equations:



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

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

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

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

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

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

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

# Necessary steps:

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# 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,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Cai-Zhuang Wang,<sup>2</sup> Kai-Ming Ho,<sup>2</sup> and Gabriel Kotliar<sup>1</sup>

# Kohn-Sham scheme:

$$\left\{ \begin{array}{l} \mathcal{E}[\rho] = T_{KS}[\rho] + E_{HXC}[\rho] + \int \mathbf{d}\mathbf{r} V(\mathbf{r}) \rho(\mathbf{r}) \\ T_{KS}[\rho] = \min_{\Psi_0 \rightarrow \rho} \langle \Psi_0 | \hat{T} | \Psi_0 \rangle \end{array} \right.$$

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

# Kohn-Sham scheme:

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

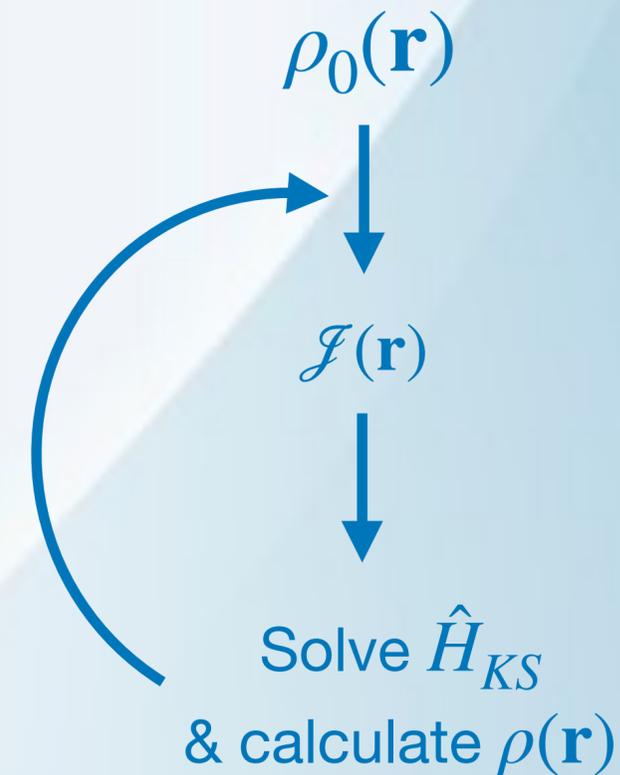
$$\mathcal{S}[\Psi_0, \rho(\mathbf{r}), \mathcal{J}(\mathbf{r})] = \langle \Psi_0 | \hat{T} + \int \mathbf{d}\mathbf{r} V(\mathbf{r}) \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle + E_{HXC}[\rho]$$

$$+ \int \mathbf{d}\mathbf{r} \mathcal{J}(\mathbf{r}) (\langle \Psi_0 | \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle - \rho(\mathbf{r}))$$

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

# Kohn-Sham scheme:

$$\left\{ \begin{array}{l} \mathcal{E}[\rho] = T_{KS}[\rho] + E_{HXC}[\rho] + \int \mathbf{dr} V(\mathbf{r}) \rho(\mathbf{r}) \\ T_{KS}[\rho] = \min_{\Psi_0 \rightarrow \rho} \langle \Psi_0 | \hat{T} | \Psi_0 \rangle \end{array} \right.$$



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

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

$\hat{H}_{KS}$

# Kohn-Sham-Hubbard scheme:

$$\left\{ \begin{array}{l}
 \mathcal{E}[\rho] = T_{KSH}[\rho] + E_{HXC}[\rho] + \int \mathbf{dr} V(\mathbf{r}) \rho(\mathbf{r}) \\
 T_{KSH}[\rho] = \min_{\Psi_G \rightarrow \rho} \langle \Psi_G | \hat{T} | \Psi_G \rangle + \sum_{i \geq 1} \hat{H}_i^{U_i, J_i}
 \end{array} \right. + \sum_{i \geq 1} E_{dc}^{U_i, J_i} (\langle \Psi_G | \hat{N}_i | \Psi_G \rangle)$$

Projectors over "correlated" degrees of freedom

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

# Kohn-Sham-Hubbard scheme:

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

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

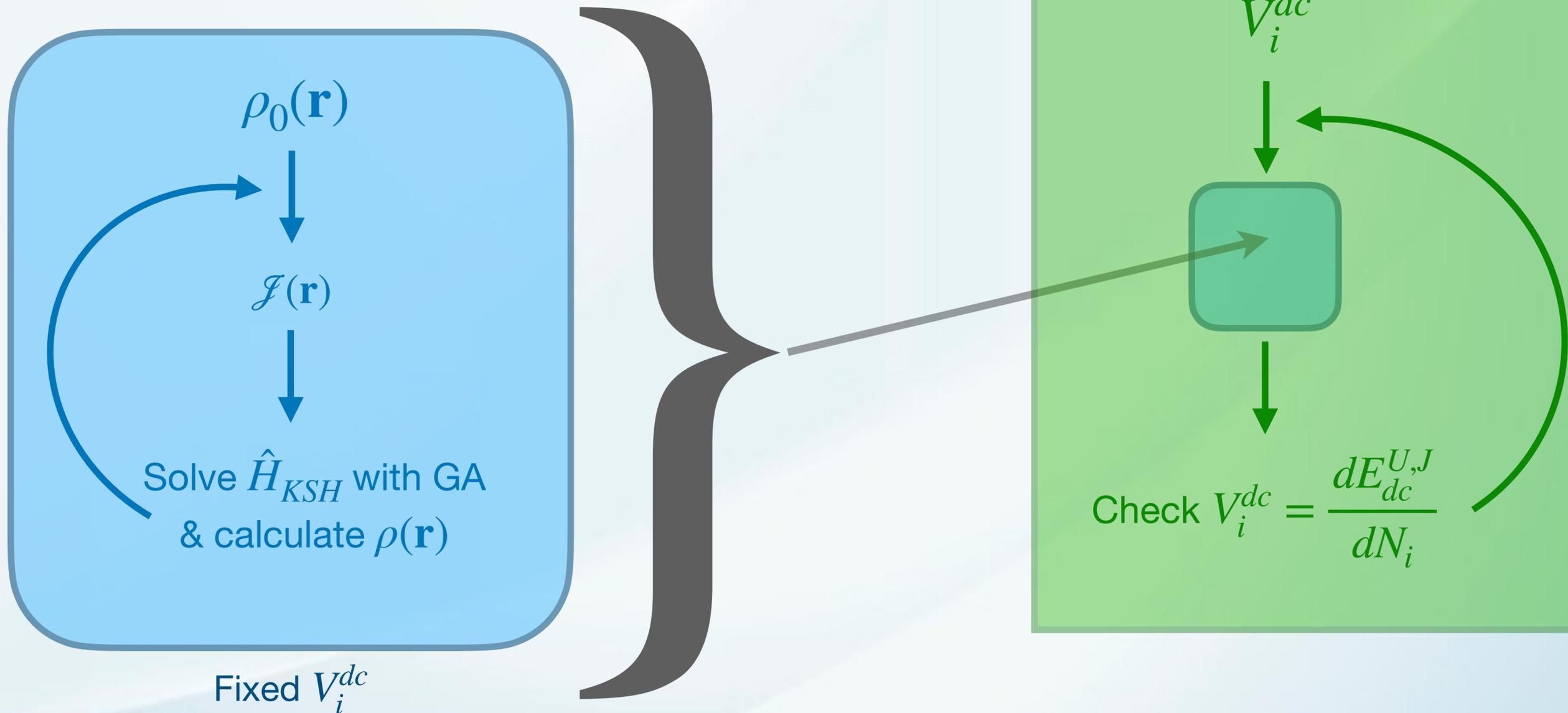
**Enforcing  
definition of  $\rho(\mathbf{r})$**

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

**Enforcing  
definition of  $N_i$**

# Algorithmic structure:

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



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# Spectral properties

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

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

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

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## Landau-Gutzwiller quasiparticles

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# Spectral properties

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

Excited states:  $|\Psi_G^{kn}\rangle = \mathcal{P} \xi_{kn}^\dagger |\Psi_0\rangle$

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

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

# Spectral properties

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

*Excited states:*  $|\Psi_G^{kn}\rangle = \mathcal{P} \xi_{kn}^\dagger |\Psi_0\rangle$

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

$$\Sigma(\omega) = \begin{pmatrix} [\mathbf{0}]_{\nu_0 \times \nu_0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \Sigma_1(\omega) & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \dots & \dots & \Sigma_M(\omega) \end{pmatrix} \quad \Sigma_i(\omega) = t_{loc} - \omega \frac{\mathbf{1} - \mathcal{R}_i^\dagger \mathcal{R}_i}{\mathcal{R}_i^\dagger \mathcal{R}_i} + [\mathcal{R}_i]^{-1} \lambda_i [\mathcal{R}_i^\dagger]^{-1}$$

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# Example: Structure, Density, Gap Theory vs Experiments

ARTICLE OPEN

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

Nicola Lanatà<sup>1</sup>, Tsung-Han Lee<sup>2,3</sup>, Yong-Xin Yao<sup>4</sup>, Vladan Stevanović<sup>5</sup> and Vladimir Dobrosavljević<sup>2</sup>

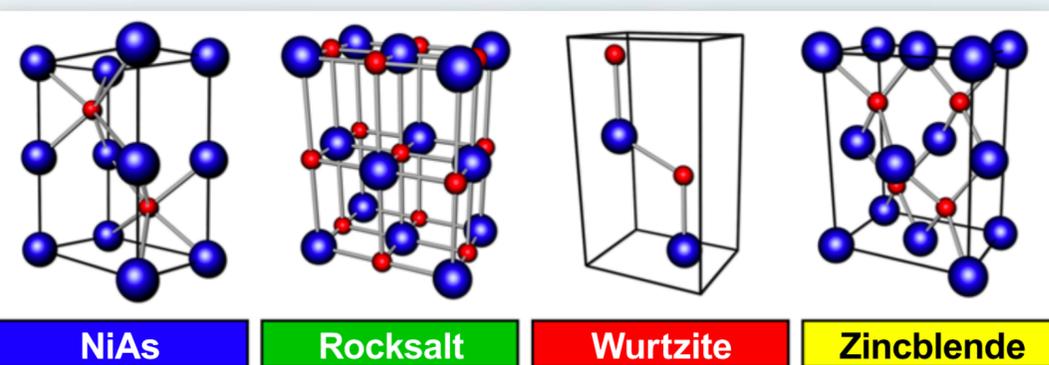
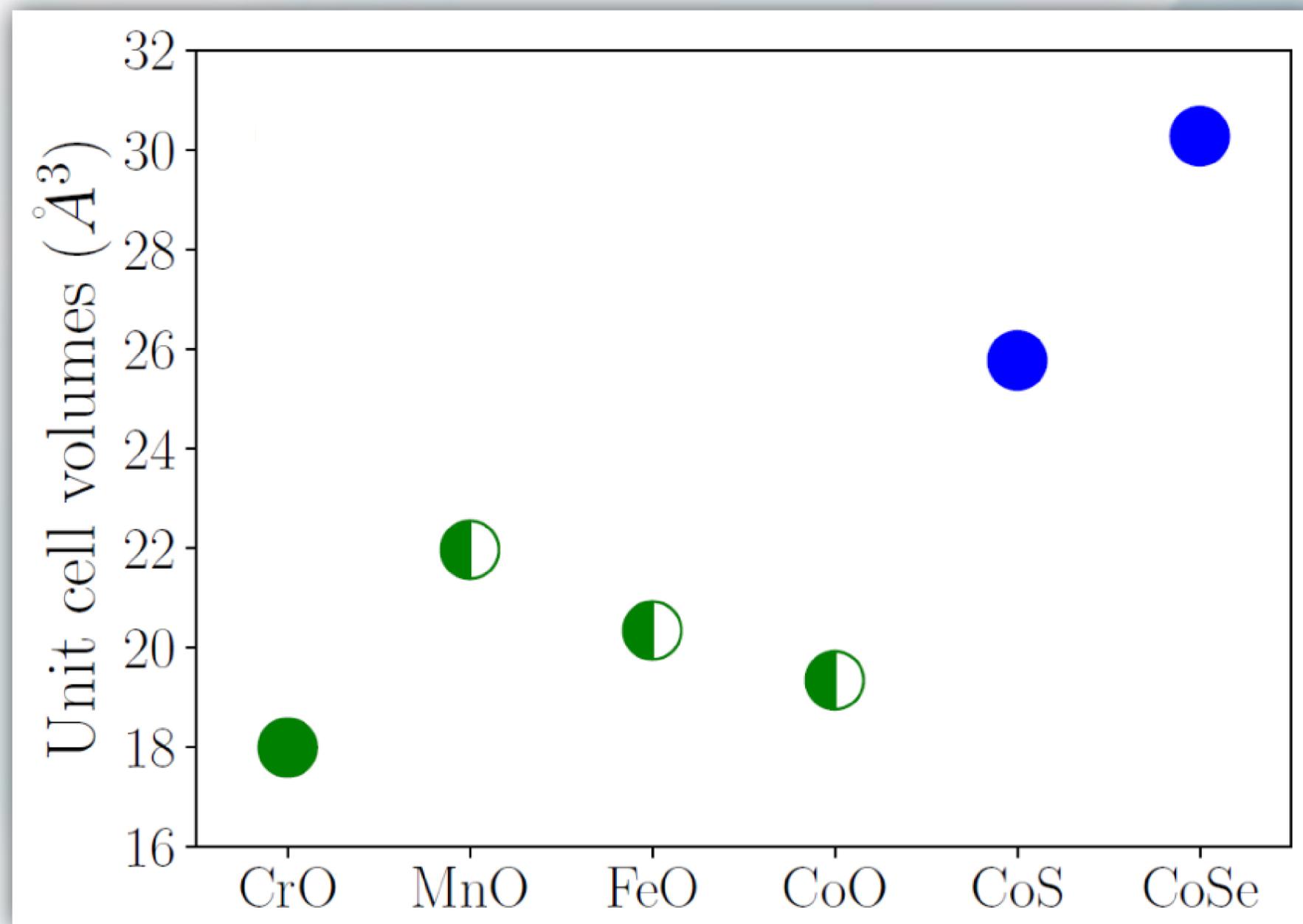
-  NiAs-type
-  Rocksalt
-  Wurtzite
-  Zinoblende

-  Experiment
-  Theory

-  Metal
-  Insulator



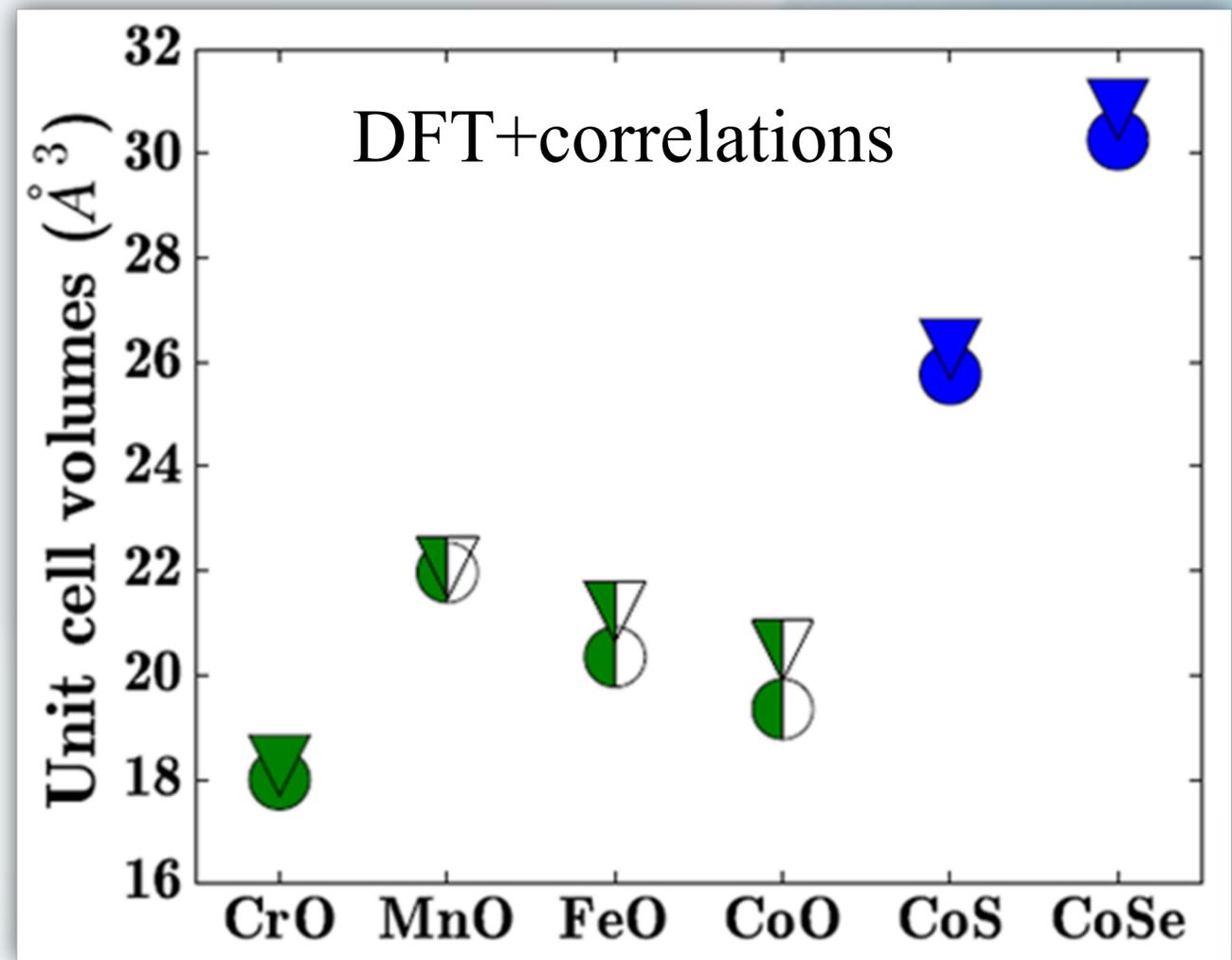
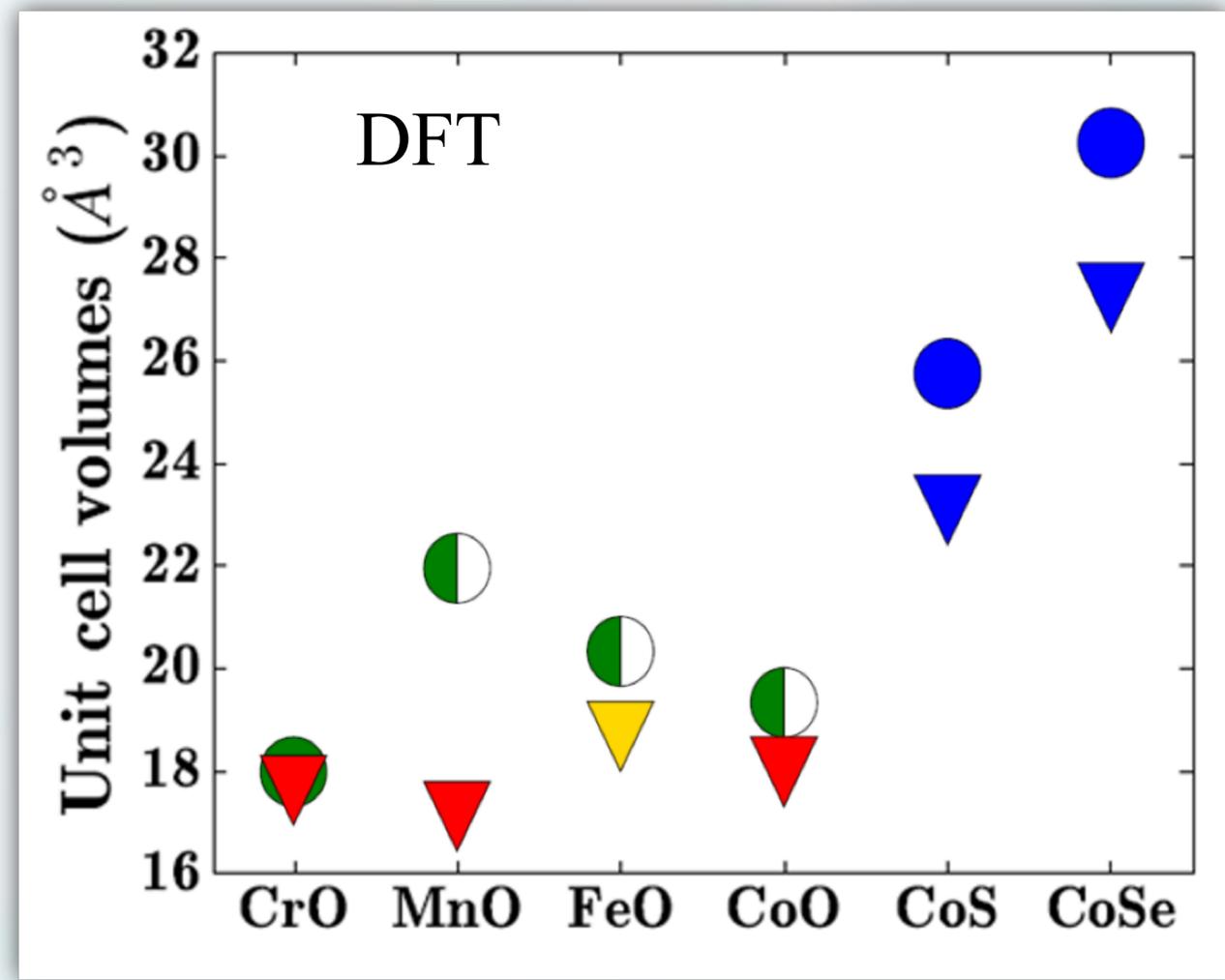
# Example: Structure, Density, Gap Theory vs Experiments

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Nicola Lanata<sup>1</sup>, Tsung-Han Lee<sup>2,3</sup>, Yong-Xin Yao<sup>4</sup>, Vladan Stevanović<sup>5</sup> and Vladimir Dobrosavljević<sup>2</sup>

- NiAs-type
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# 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.

# A more accurate extension: the g-GA method

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

## Emergent Bloch excitations in Mott matter

Nicola Lanatà,<sup>1</sup> Tsung-Han Lee,<sup>1</sup> Yong-Xin Yao,<sup>2</sup> and Vladimir Dobrosavljević<sup>1</sup>

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

Letter

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

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

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

## Operatorial formulation of the ghost rotationally invariant slave-boson theory

Nicola Lanatà<sup>\*</sup>

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

## Exciton Mott transition revisited

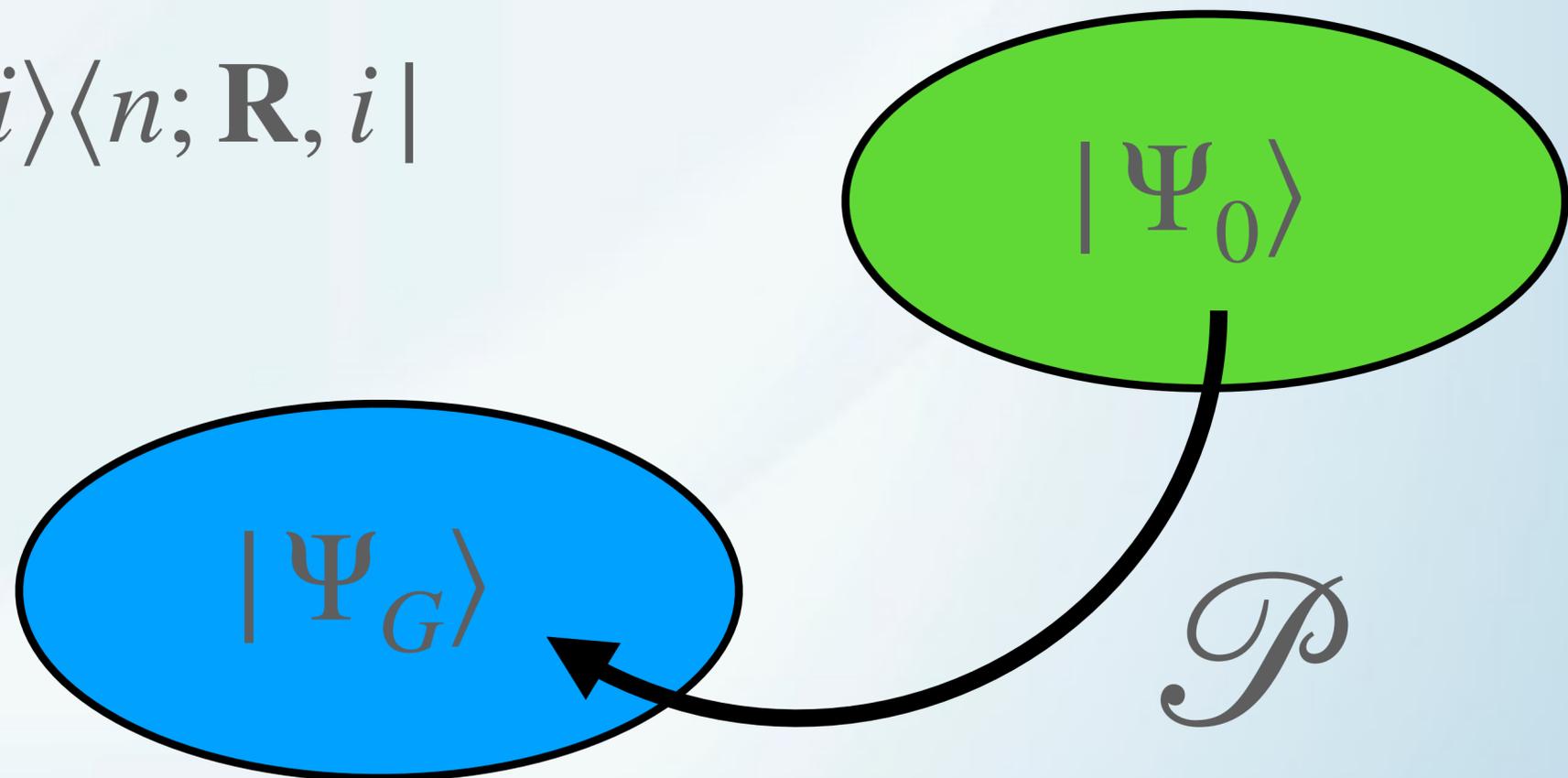
Daniele Guerci, Massimo Capone, and Michele Fabrizio

# The GA variational wave function:

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

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

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

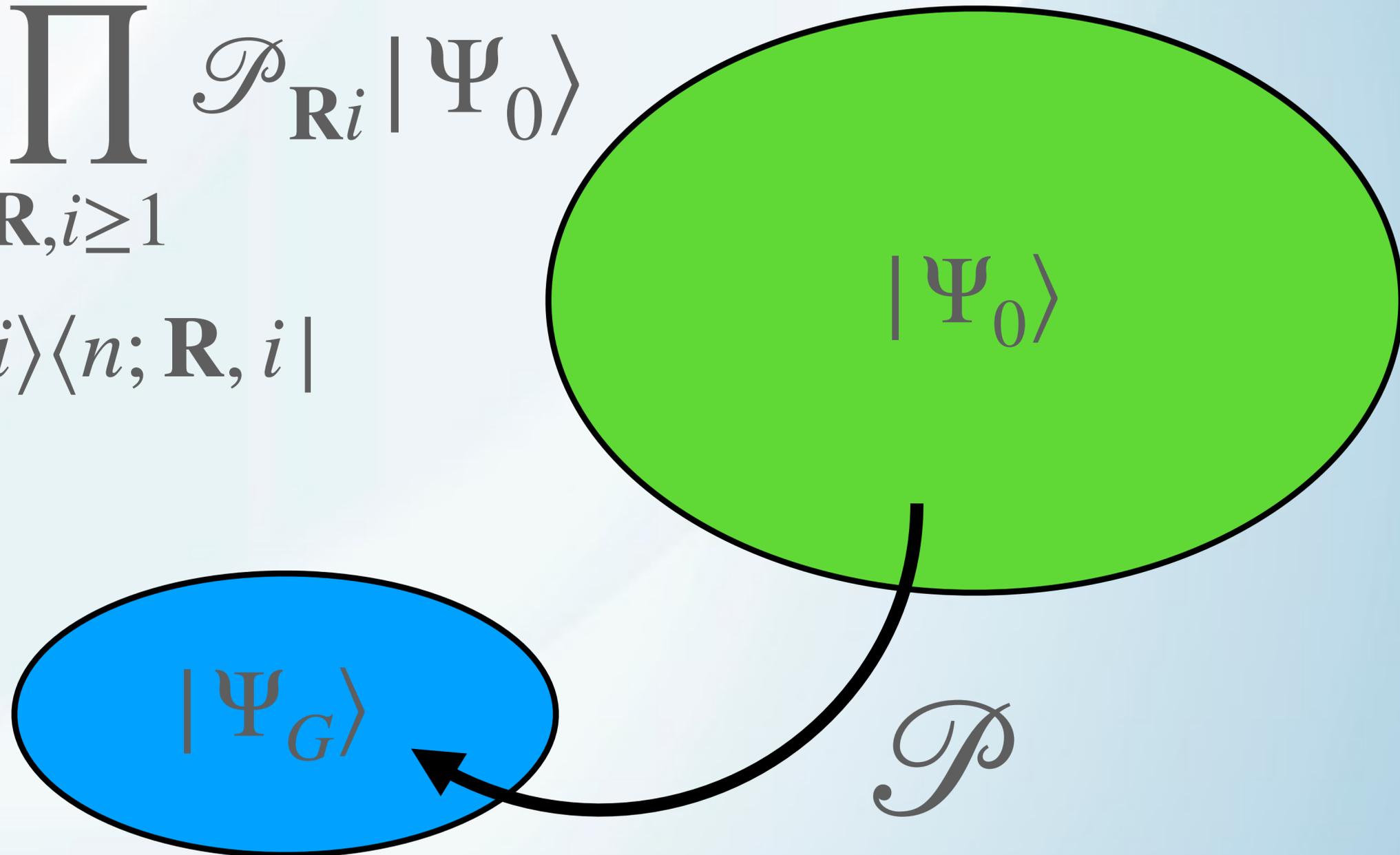


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Rectangular matrix:  $2^{\nu_i} \times 2^{\tilde{\nu}_i}$

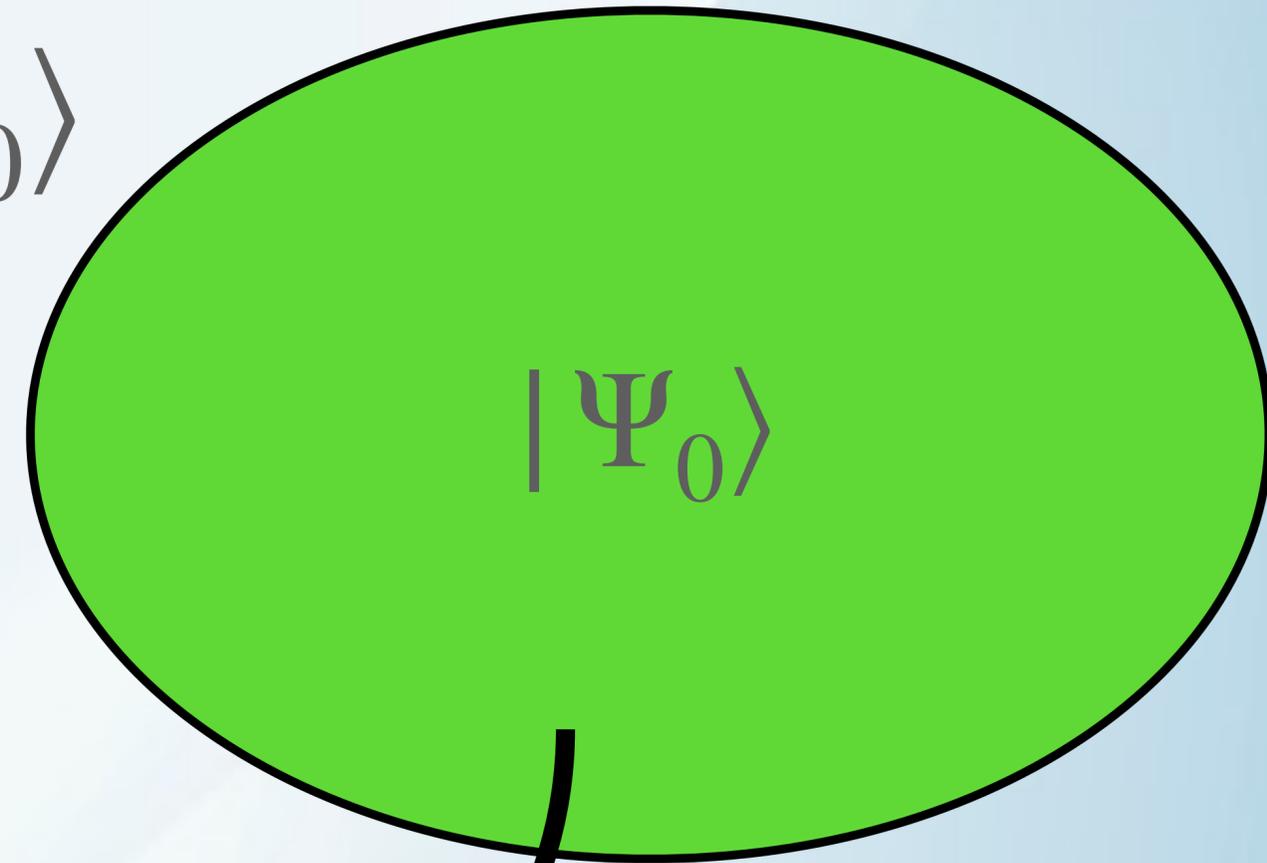
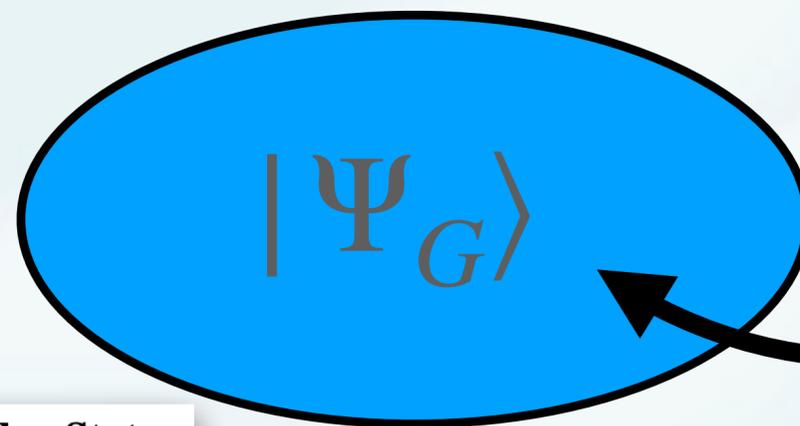


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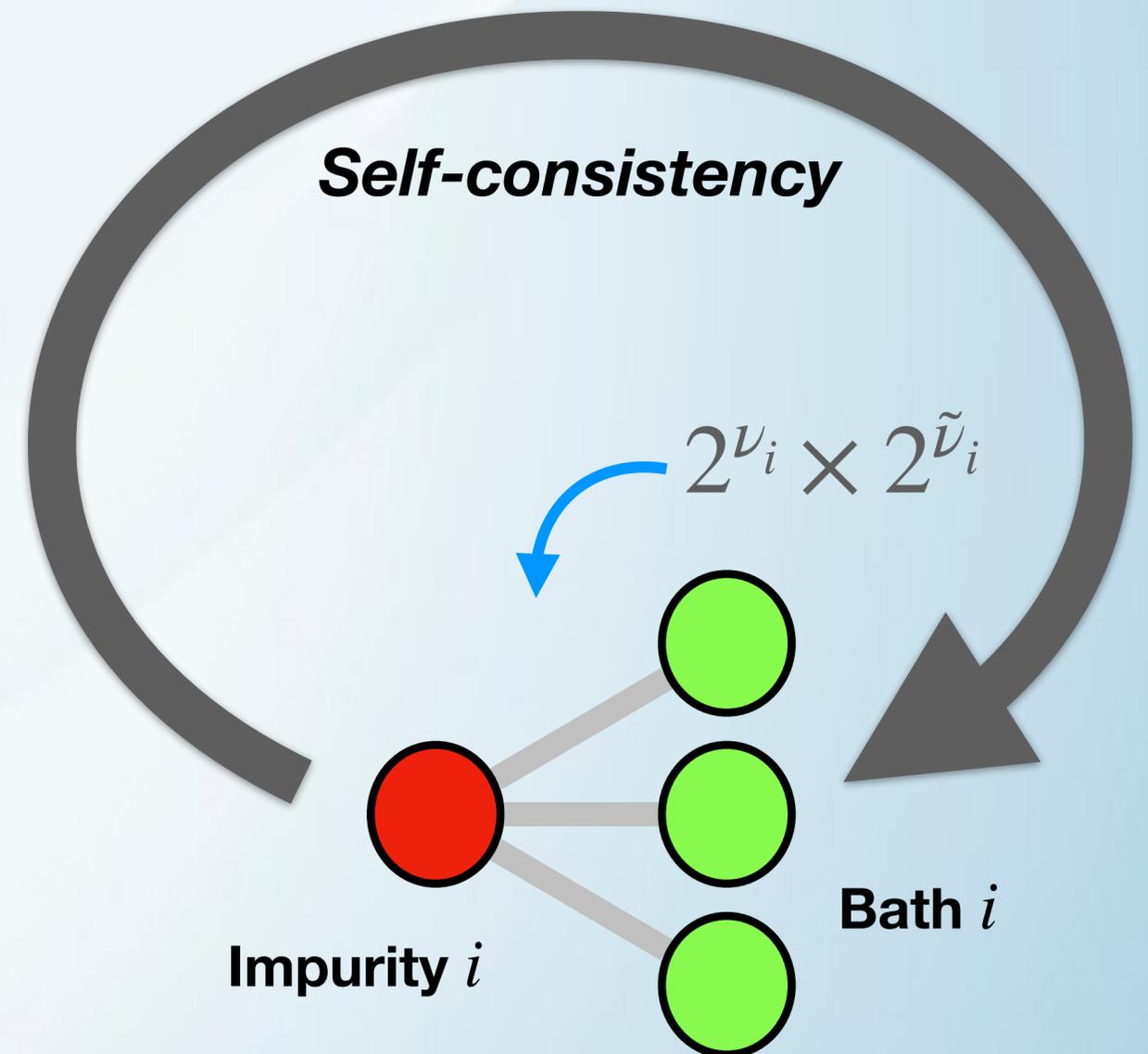
$\mathcal{P}$

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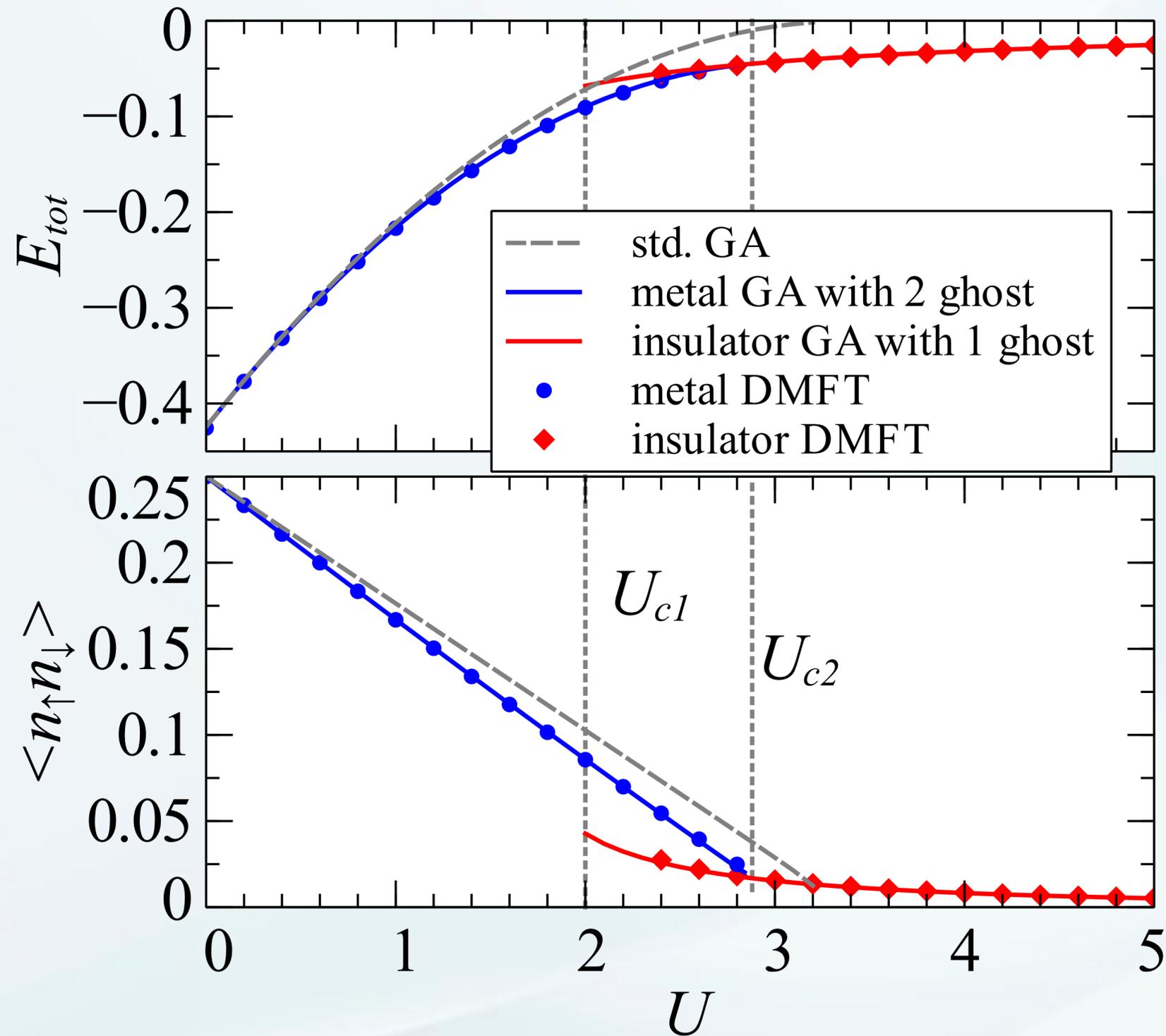
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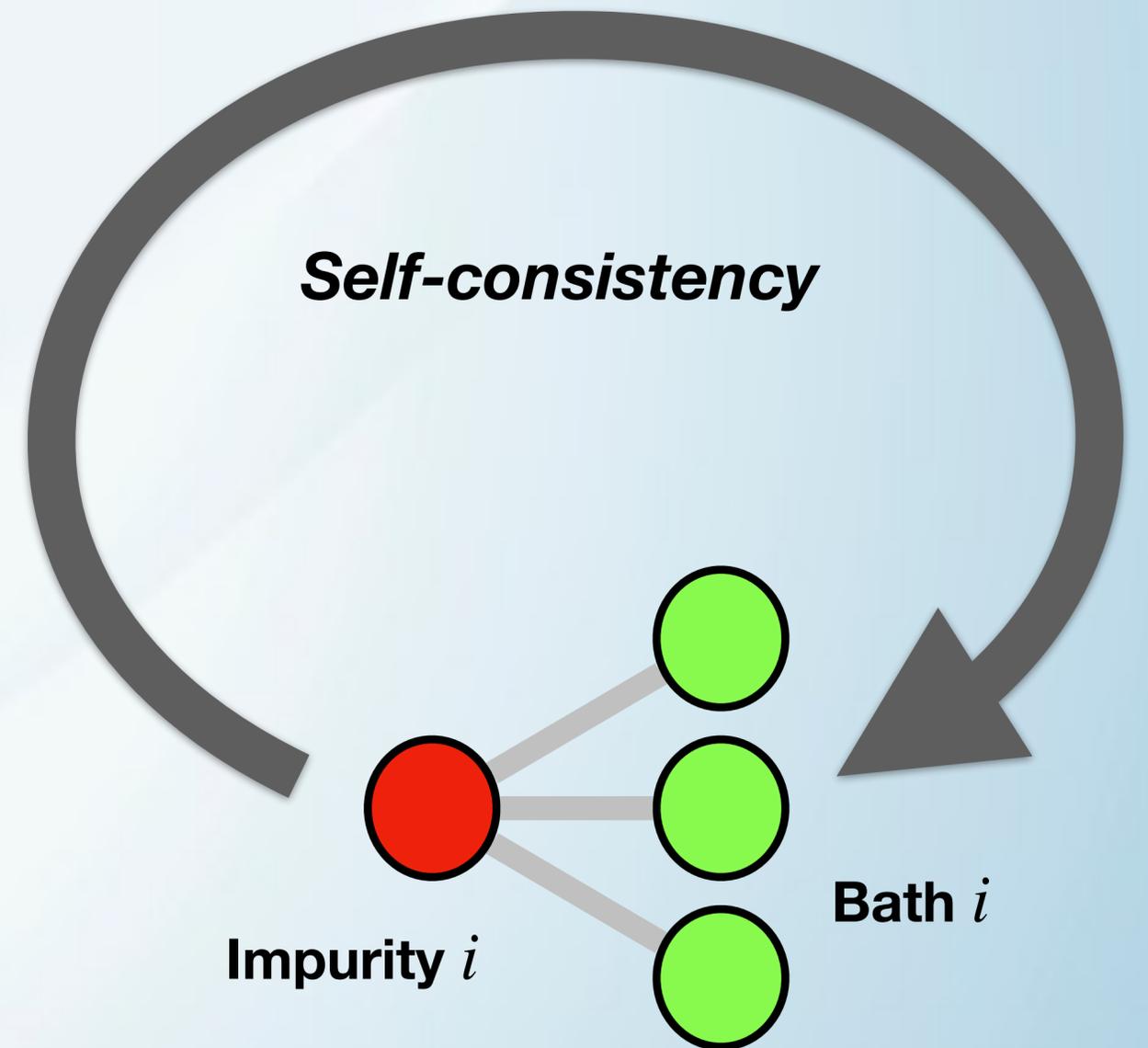
Rectangular matrix:  $2^{\nu_i} \times 2^{\tilde{\nu}_i}$



# Benchmark calculations Hubbard model:

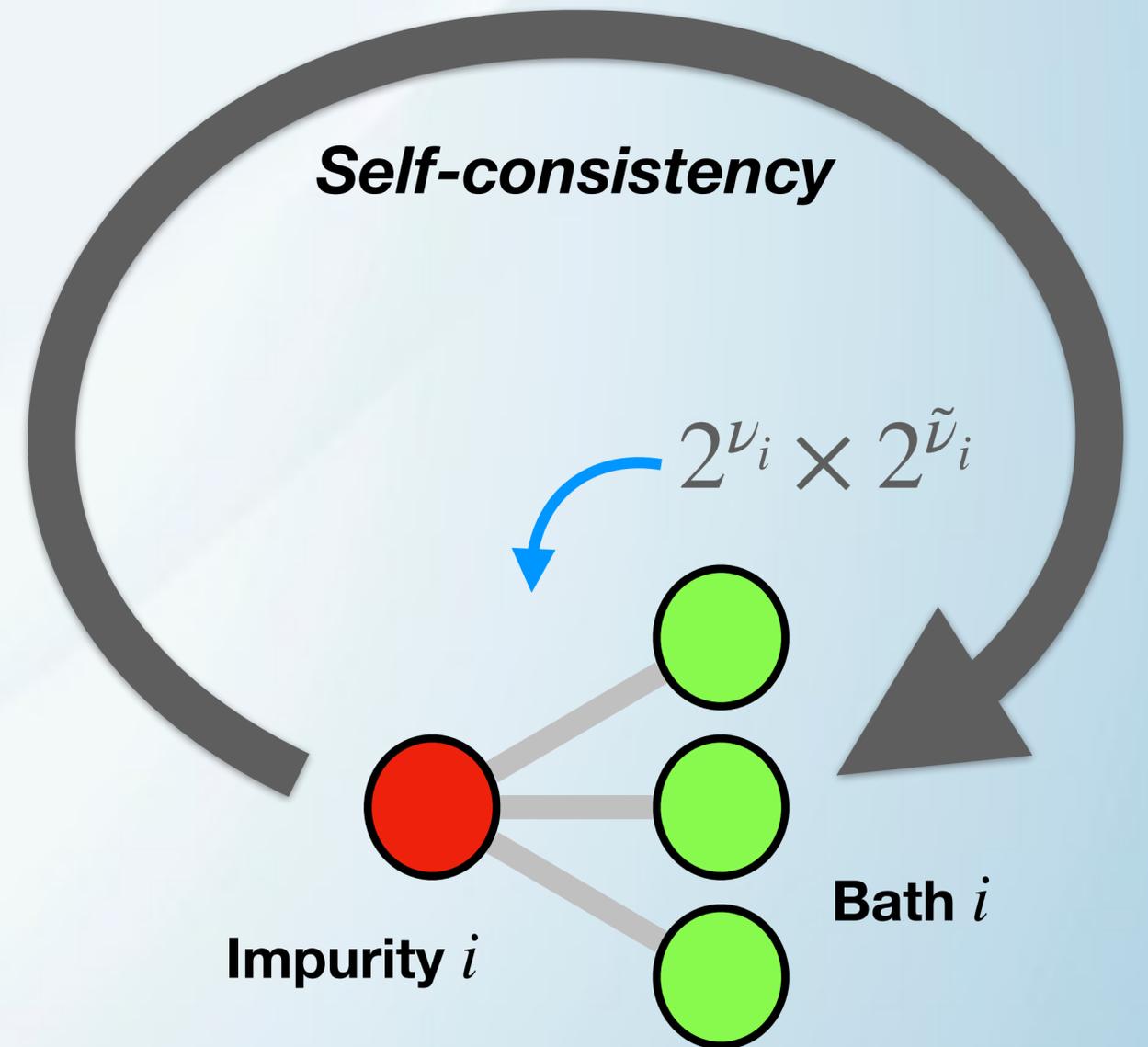
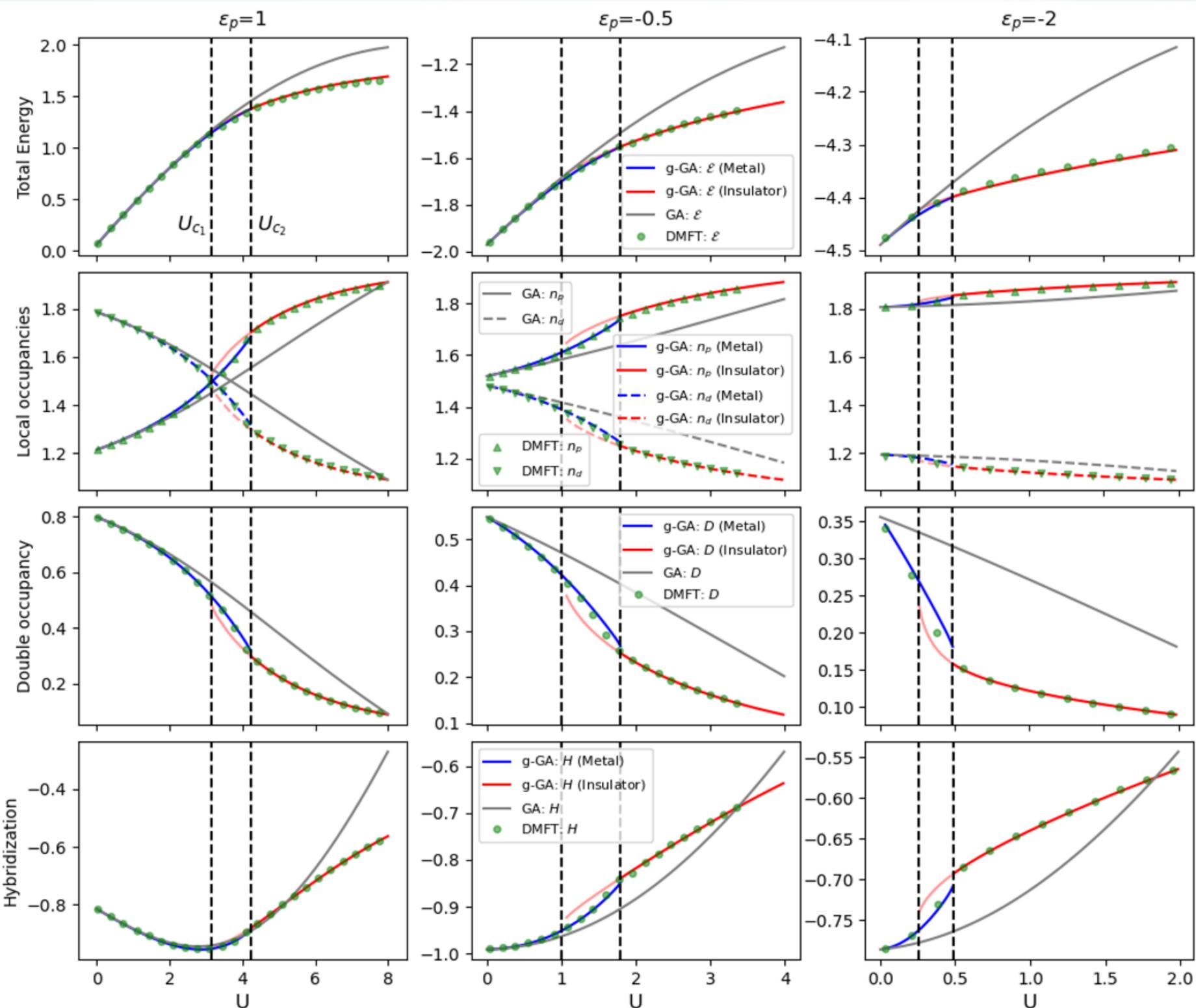


$$\hat{H} = \sum_{RR'} \sum_{\sigma} t_{RR'} c_{R\sigma}^{\dagger} c_{R'\sigma} + \sum_{R\sigma} U \hat{n}_{R\uparrow} \hat{n}_{R\downarrow}$$



# Benchmark calculations ALM:

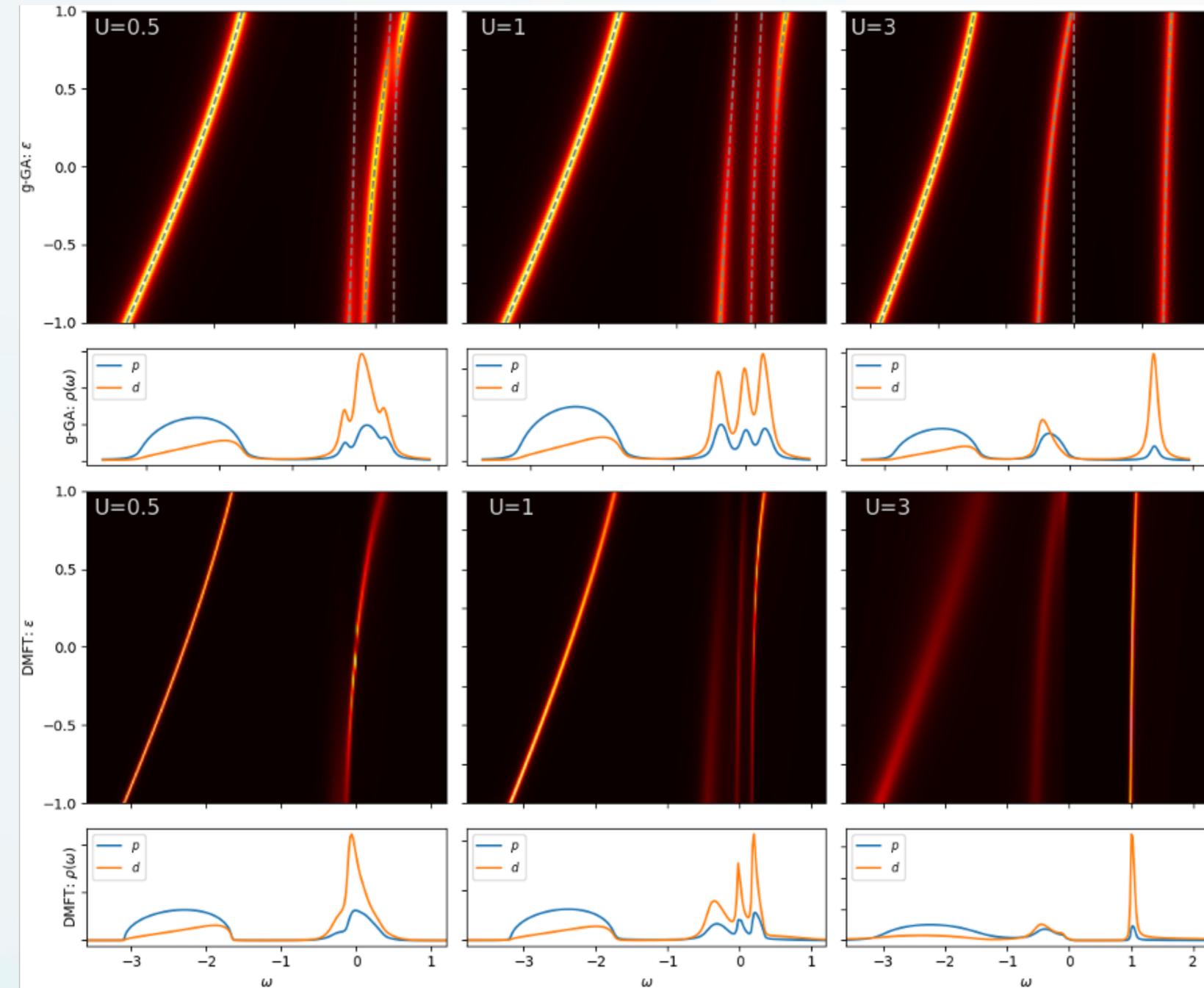
$$\hat{H} = \sum_{ij} \sum_{\sigma} (t_{ij} + \delta_{ij} \epsilon_p) p_{i\sigma}^{\dagger} p_{j\sigma} + \sum_i \frac{U}{2} (\hat{n}_{di} - 1)^2 + V \sum_{i\sigma} (p_{i\sigma}^{\dagger} d_{i\sigma} + \text{H.c.}) - \mu \sum_i \hat{N}_i$$



# Benchmark calculations ALM:

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

*Analytical (approximate) expression for self-energy*



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

# 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<sup>†</sup>, F Gebhard<sup>‡</sup> and W Weber<sup>‡</sup>

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,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Cai-Zhuang Wang,<sup>2</sup> Kai-Ming Ho,<sup>2</sup> and Gabriel Kotliar<sup>1</sup>

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<sup>(1)</sup> and Andrei E. Ruckenstein<sup>(2)</sup>

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

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

Frank Lechermann,<sup>1,2,\*</sup> Antoine Georges,<sup>2</sup> Gabriel Kotliar,<sup>2,3</sup> and Olivier Parcollet<sup>4</sup>

PRL **118**, 126401 (2017)

PHYSICAL REVIEW LETTERS

week ending  
24 MARCH 2017

## Slave Boson Theory of Orbital Differentiation with Crystal Field Effects: Application to $\text{UO}_2$

Nicola Lanatà,<sup>1,\*</sup> Yongxin Yao,<sup>2,†</sup> Xiaoyu Deng,<sup>3</sup> Vladimir Dobrosavljević,<sup>1</sup> and Gabriel Kotliar<sup>3,4</sup>

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,<sup>1</sup> Paolo Barone,<sup>1</sup> and Michele Fabrizio<sup>1,2</sup>

# Some useful references:

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

## Emergent Bloch excitations in Mott matter

Nicola Lanatà,<sup>1</sup> Tsung-Han Lee,<sup>1</sup> Yong-Xin Yao,<sup>2</sup> and Vladimir Dobrosavljević<sup>1</sup>

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

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

Letter

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

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

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

John Rogers<sup>1,2</sup>, Tsung-Han Lee<sup>3</sup>, Sahar Pakdel<sup>4</sup>, Wenhui Xu<sup>5</sup>, Vladimir Dobrosavljević<sup>2</sup>, Yong-Xin Yao<sup>6</sup>, Ove Christiansen<sup>7,\*</sup>, and Nicola Lanatà<sup>4,8,†</sup>

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<sup>1</sup> and Michele Fabrizio<sup>1,2</sup>

PHYSICAL REVIEW B **86**, 115310 (2012)

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

Nicola Lanatà<sup>1</sup> and Hugo U. R. Strand<sup>2</sup>

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

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

Nicola Lanatà,<sup>\*</sup> Xiaoyu Deng, and Gabriel Kotliar

RAPID COMMUNICATIONS

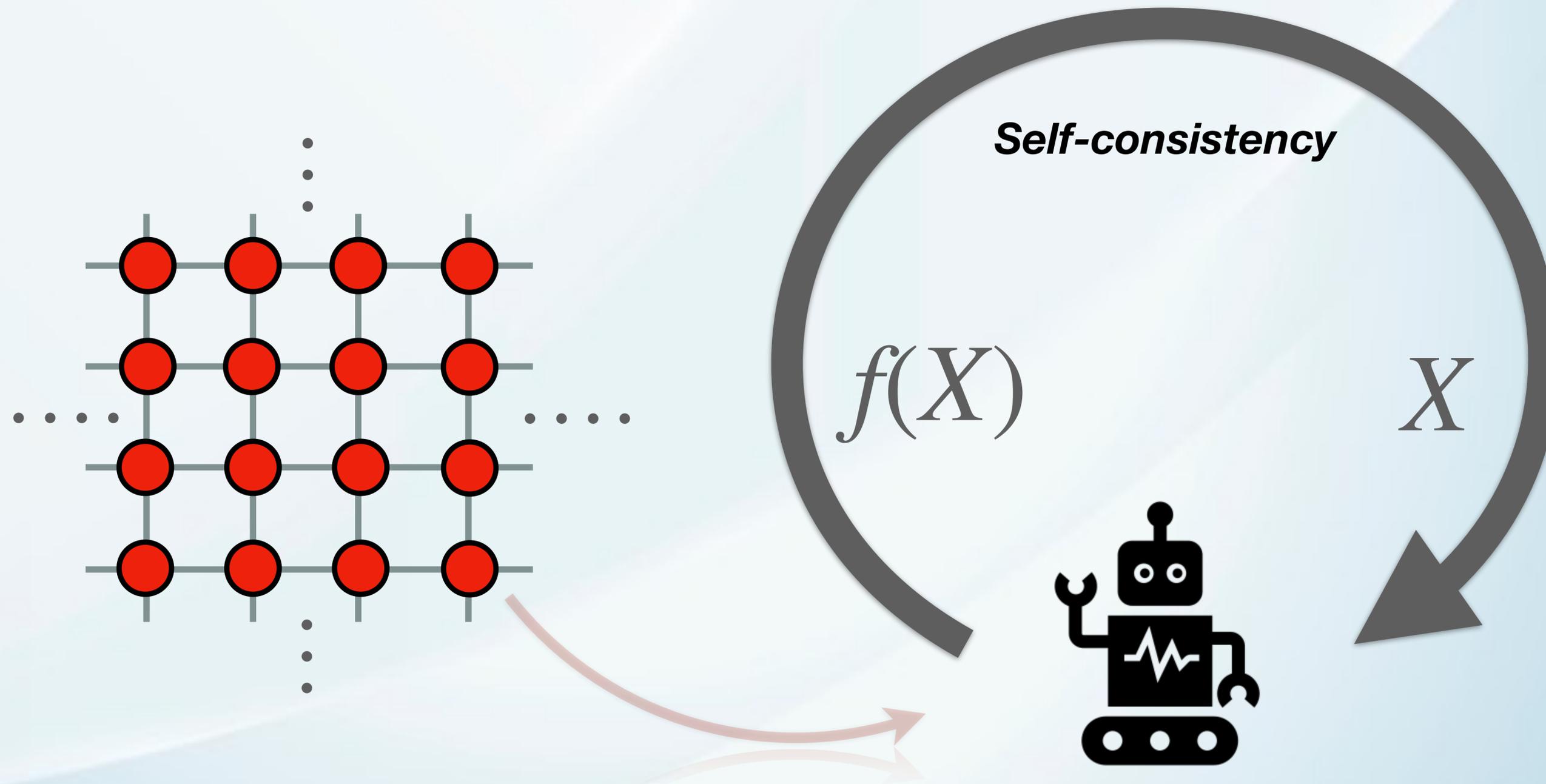
***THANK YOU FOR YOUR  
ATTENTION !!!***

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

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

Louis-François Arsenault,<sup>1,\*</sup> Alejandro Lopez-Bezanilla,<sup>2</sup> O. Anatole von Lilienfeld,<sup>3,4</sup> and Andrew J. Millis<sup>1</sup>

John Rogers<sup>1,2</sup>,,<sup>1,2</sup> Tsung-Han Lee<sup>3</sup>,,<sup>3</sup> Sahar Pakdel<sup>4</sup>,,<sup>4</sup> Wenhui Xu<sup>5</sup>,,<sup>5</sup> Vladimir Dobrosavljević<sup>2</sup>,,<sup>2</sup> Yong-Xin Yao<sup>6</sup>,,<sup>6</sup> Ove Christiansen<sup>7,\*</sup>,,<sup>7,\*</sup> and Nicola Lanà<sup>4,8,†</sup>,



# First exploratory benchmark: DFT+GA

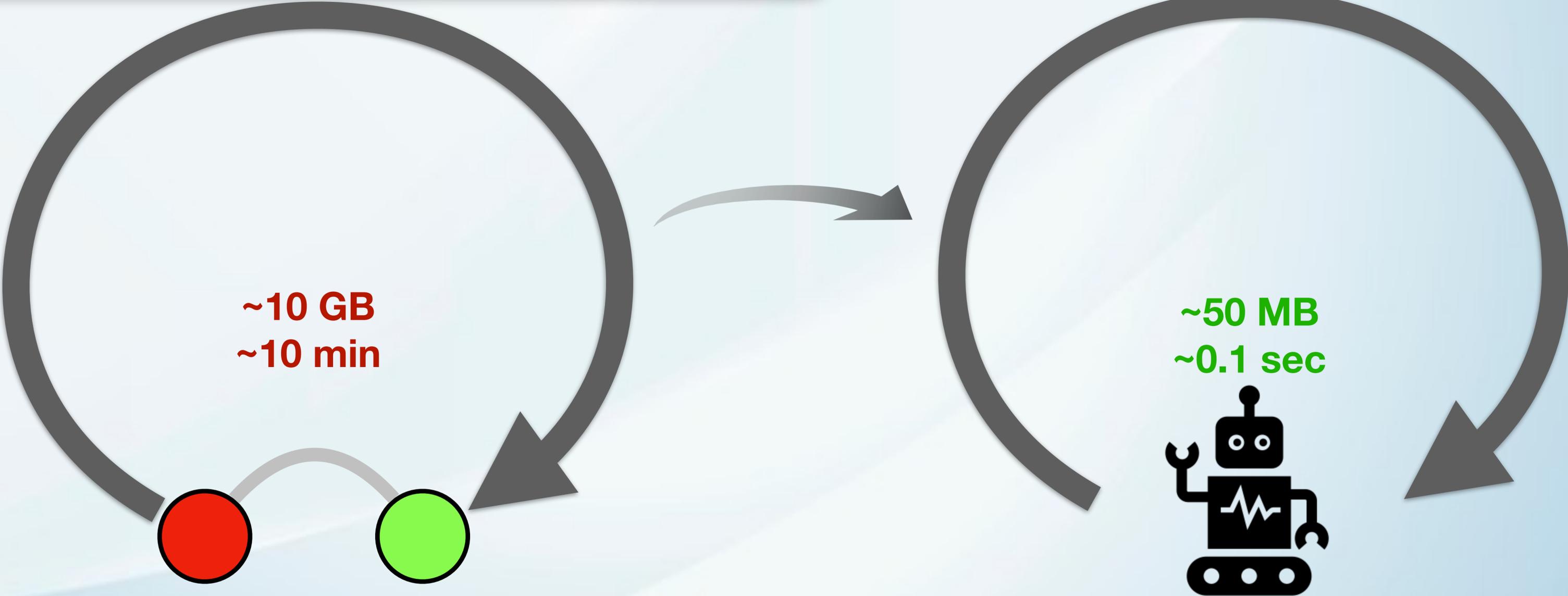
PHYSICAL REVIEW RESEARCH 3, 013101 (2021)

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

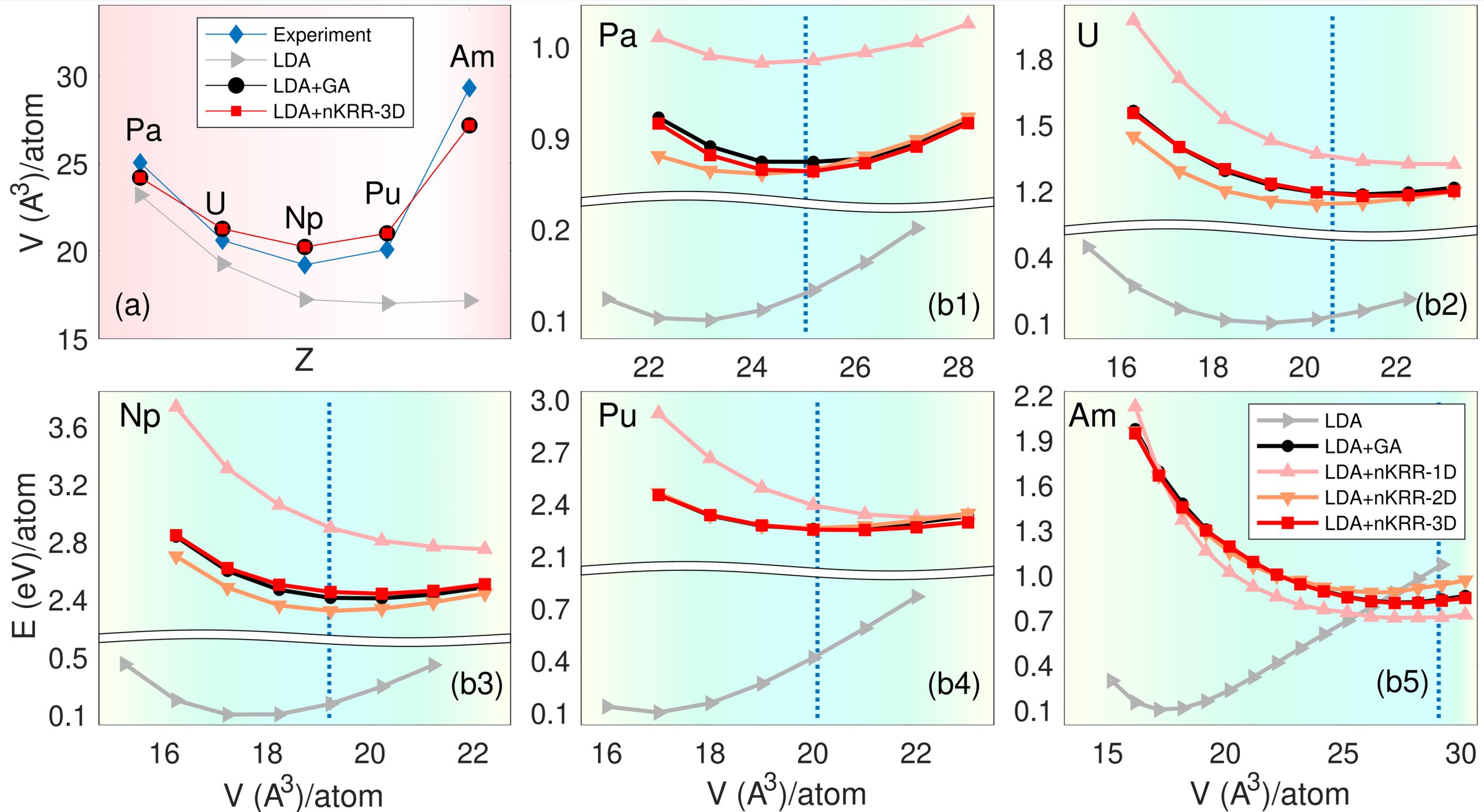
John Rogers<sup>1,2</sup>, Tsung-Han Lee<sup>3</sup>, Sahar Pakdel<sup>4</sup>, Wenhui Xu<sup>5</sup>, Vladimir Dobrosavljević<sup>2</sup>, Yong-Xin Yao<sup>6</sup>, Ove Christiansen<sup>7,\*</sup> and Nicola Lanatà<sup>4,8,†</sup>

**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:

$$\hat{H} = \sum_{ij} \sum_{\sigma} (t_{ij} + \delta_{ij} \epsilon_p) p_{i\sigma}^{\dagger} p_{j\sigma} + \sum_i \frac{U}{2} (\hat{n}_{di} - 1)^2$$

$$+ V \sum_{i\sigma} (p_{i\sigma}^{\dagger} d_{i\sigma} + \text{H.c.}) - \mu \sum_i \hat{N}_i$$

