

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.

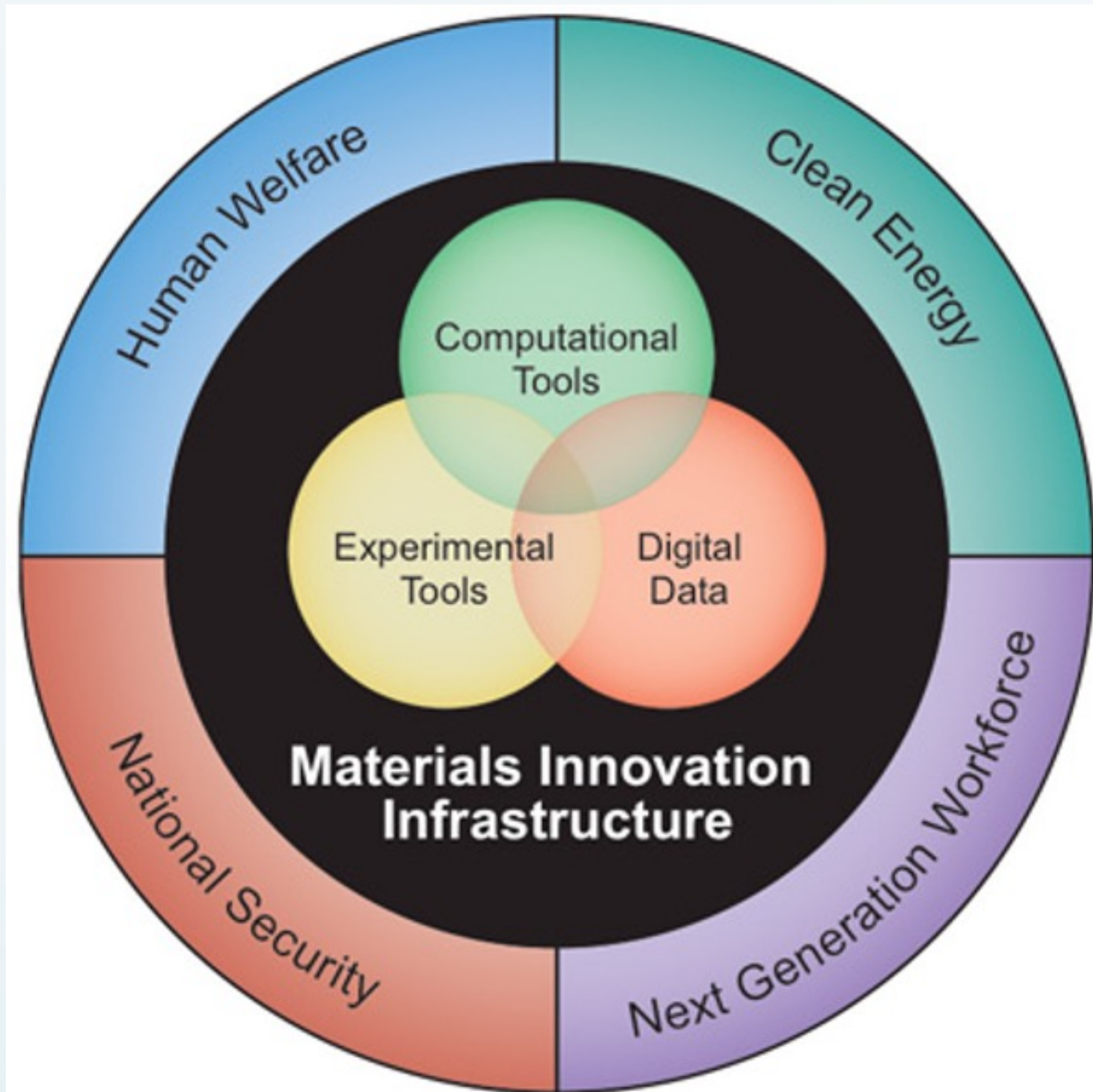
Limitations

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

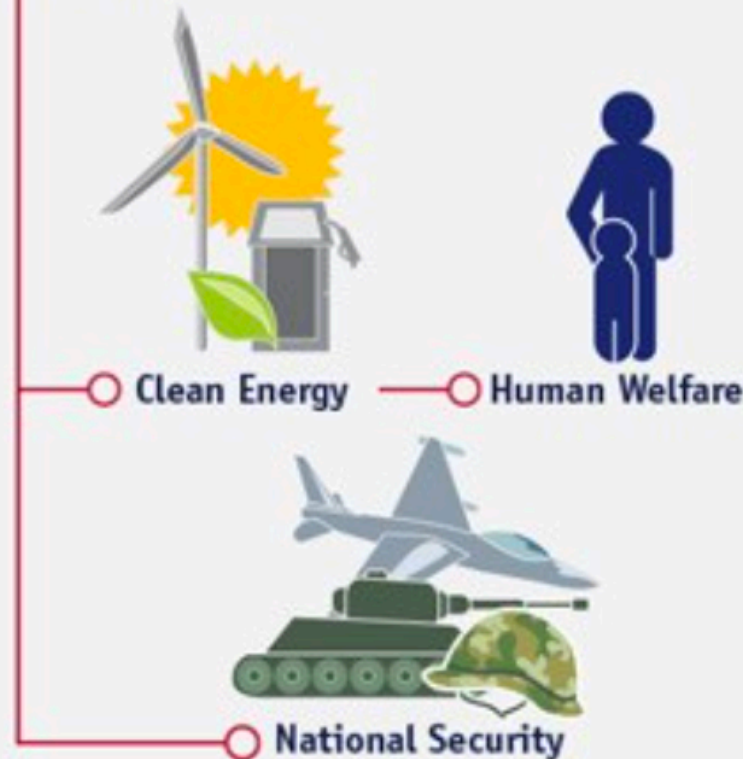


THE U.S. MATERIALS GENOME INITIATIVE

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

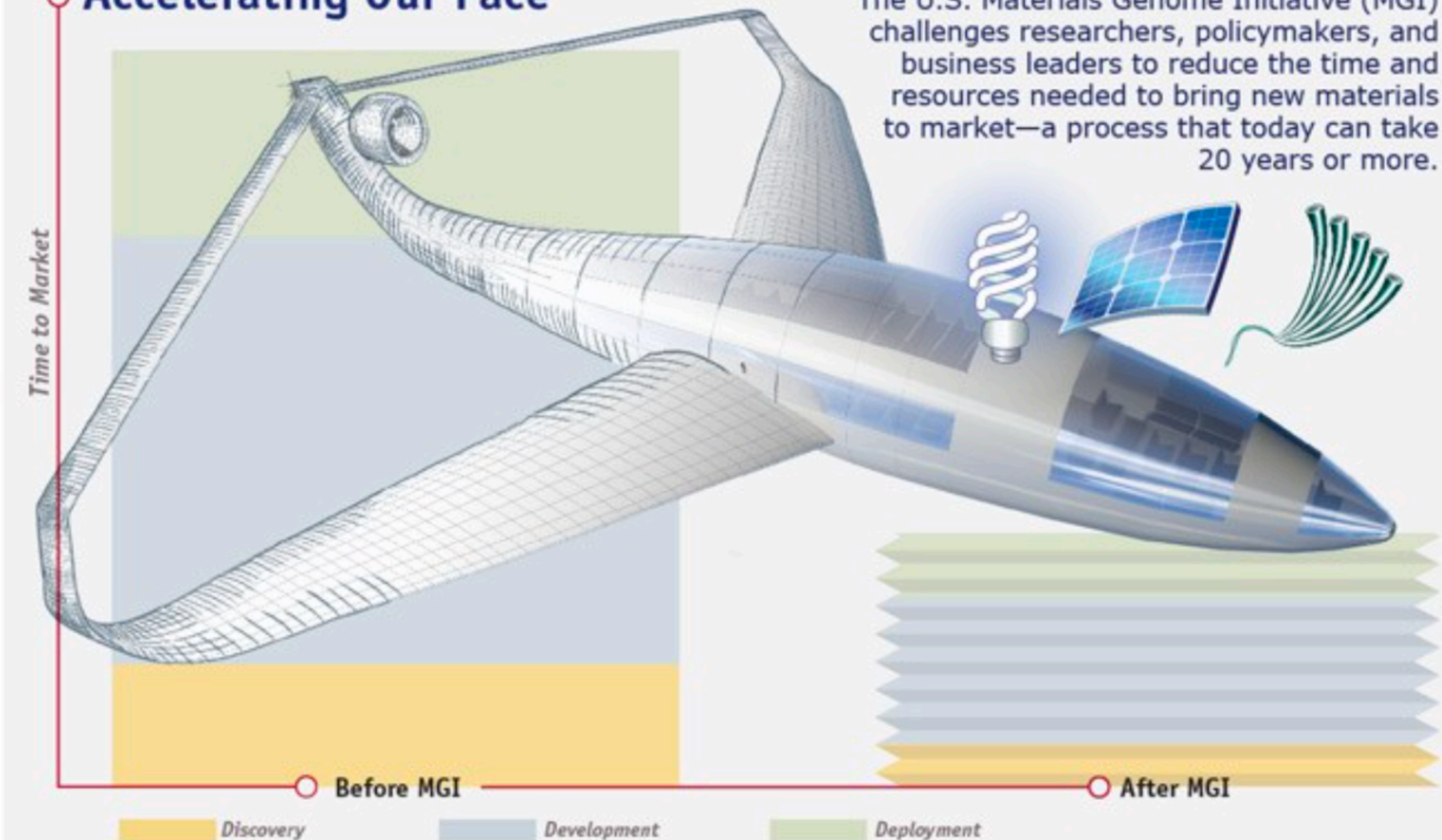
Meeting Societal Needs

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.



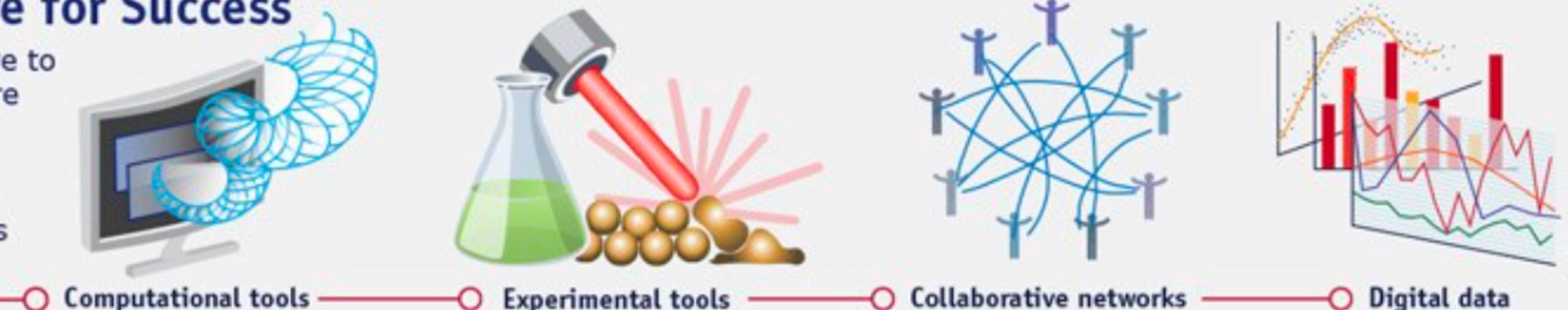
Accelerating Our Pace

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.

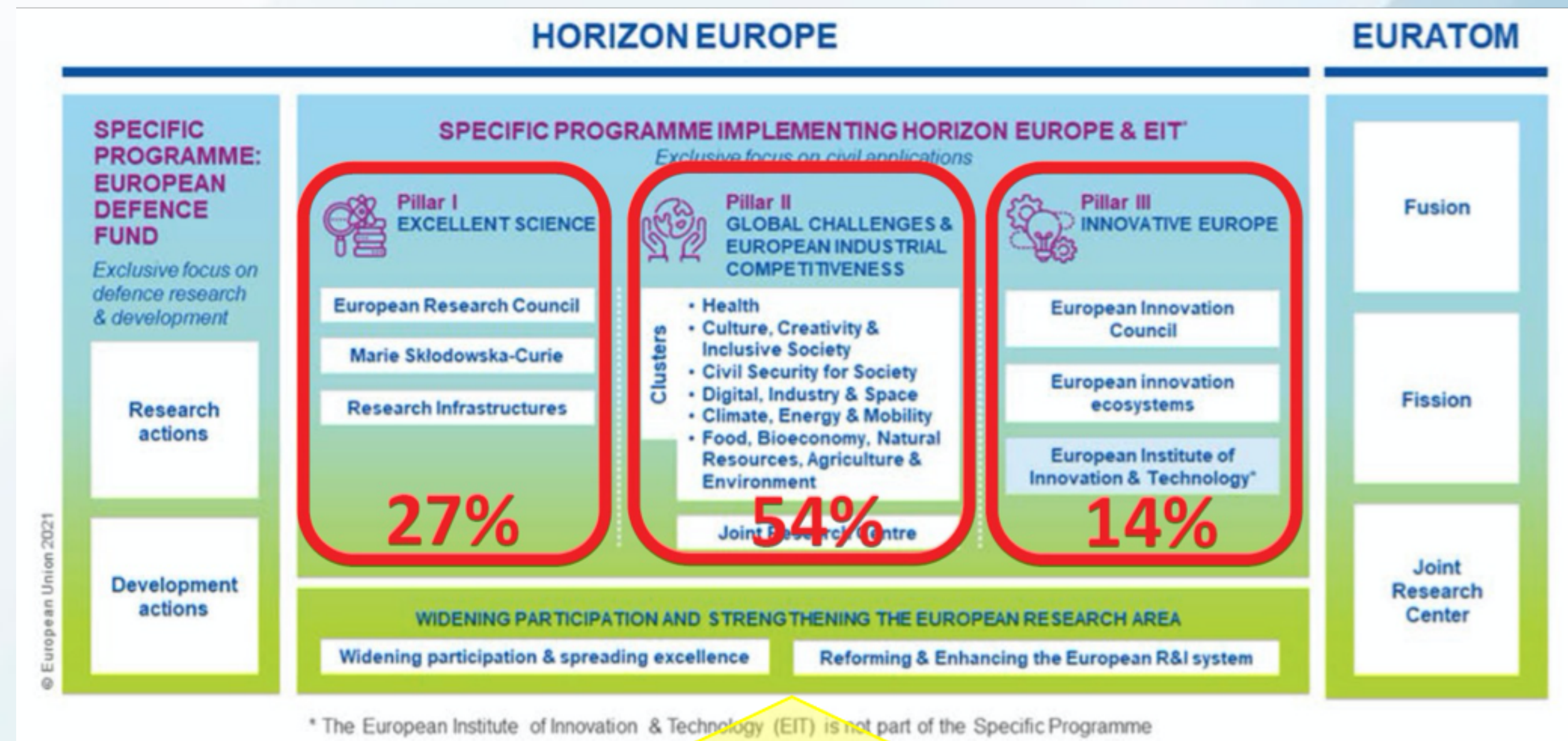


Building Infrastructure for Success

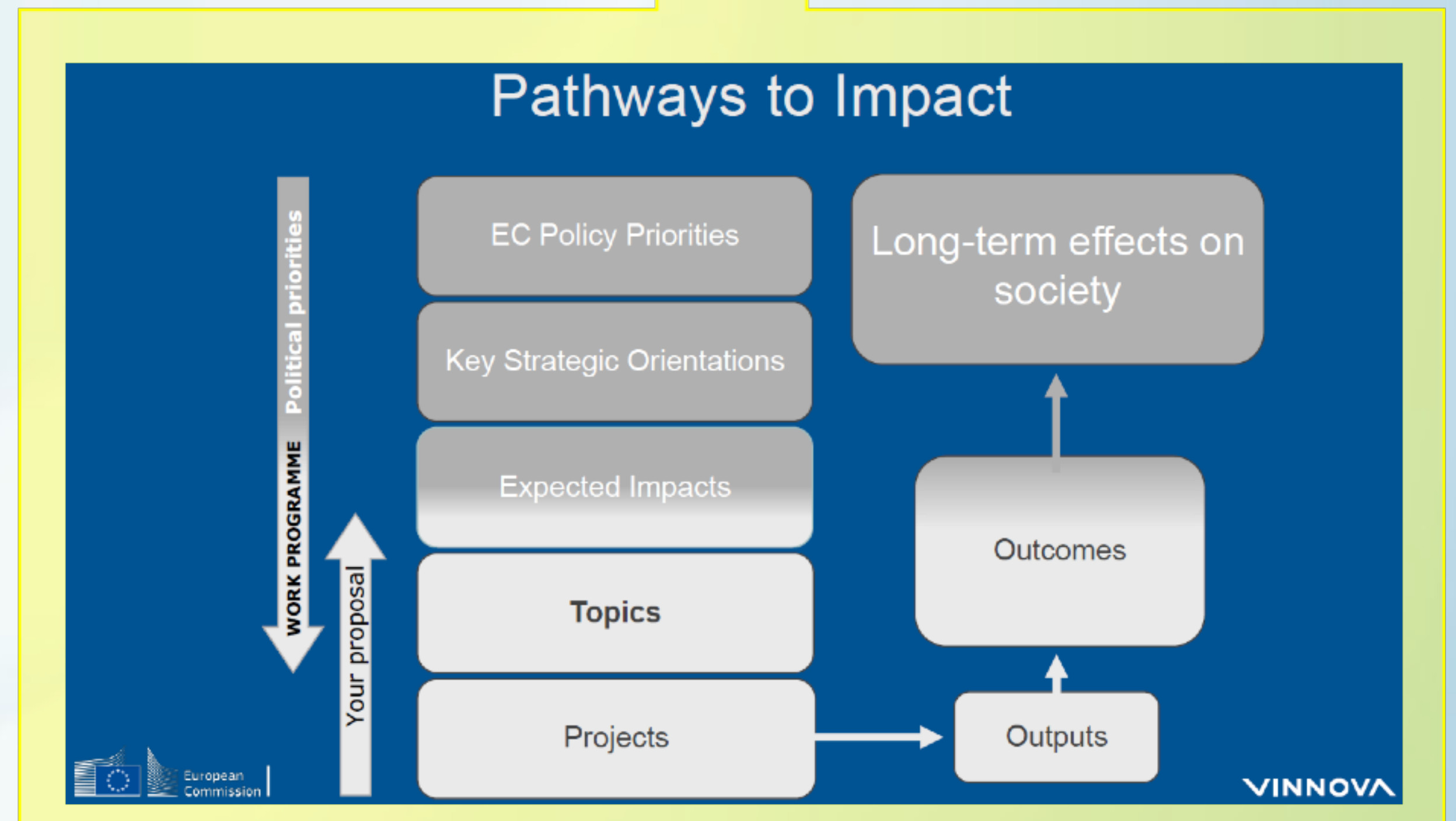
The MGI is a multi-agency initiative to renew investments in infrastructure designed for performance, and to foster a more open, collaborative approach to developing advanced materials, helping U.S. Institutions accelerate their time-to-market.



Why is computational speed important?



Increase of scientific programs prioritising research that can benefit society



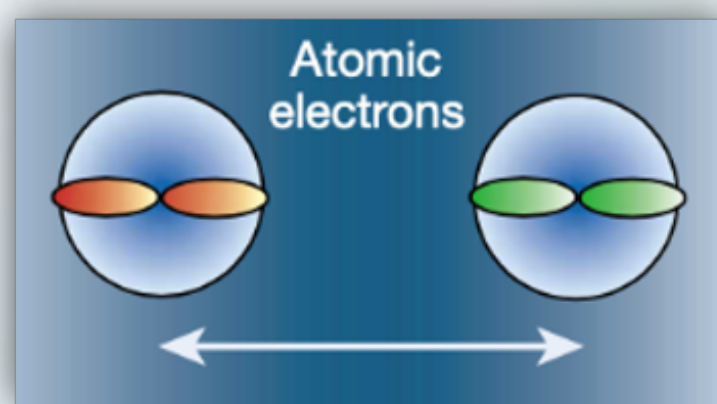
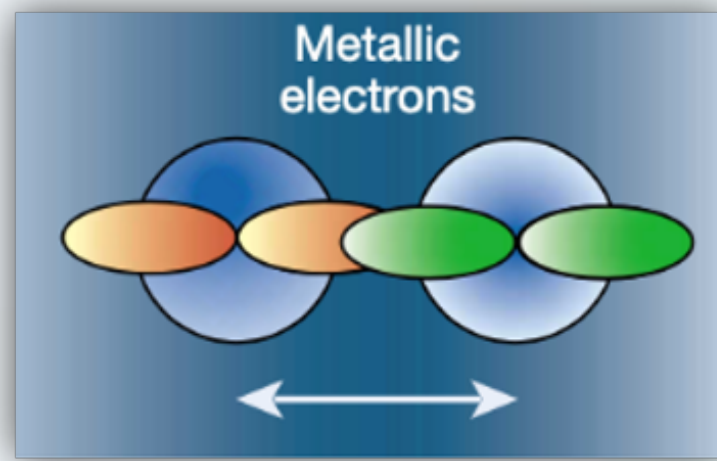
Outline

- 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).

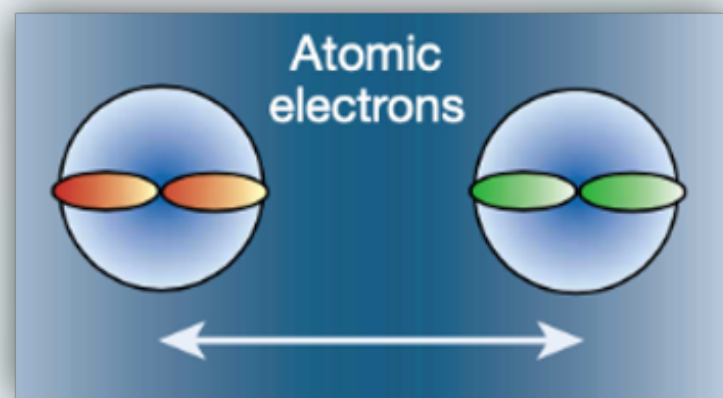
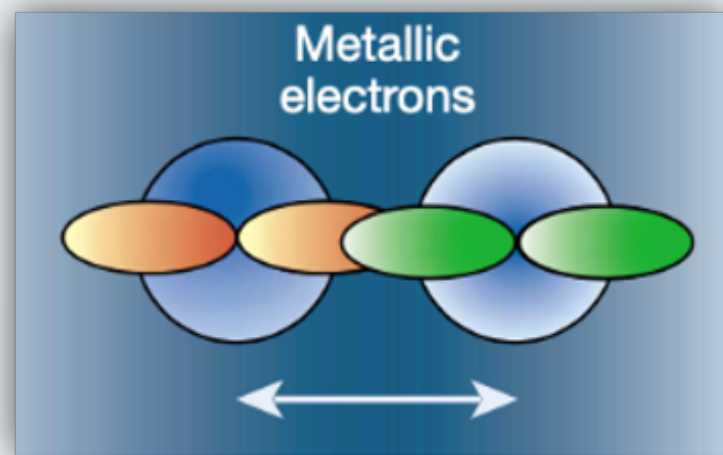
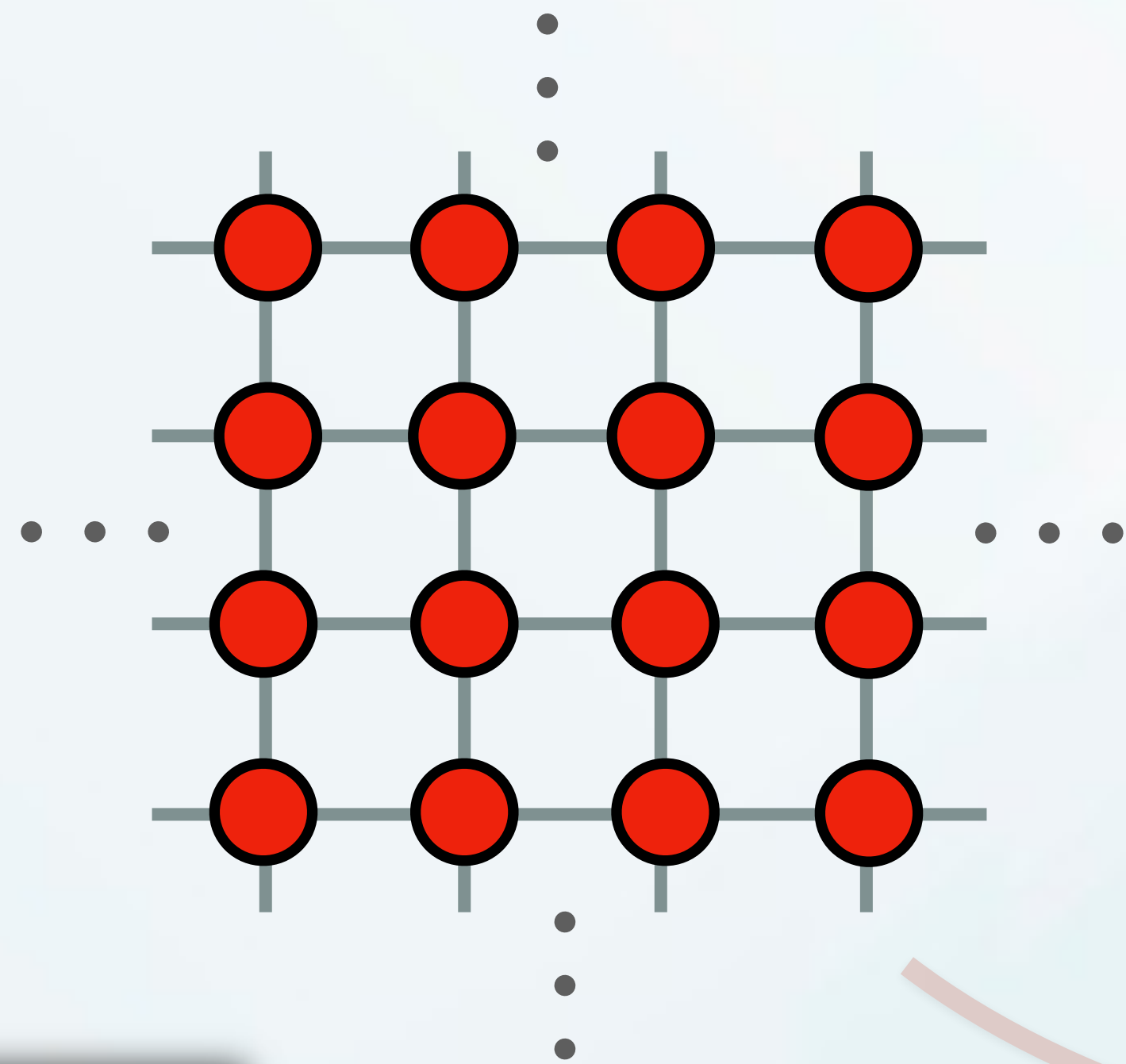
Strongly Correlated Materials

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

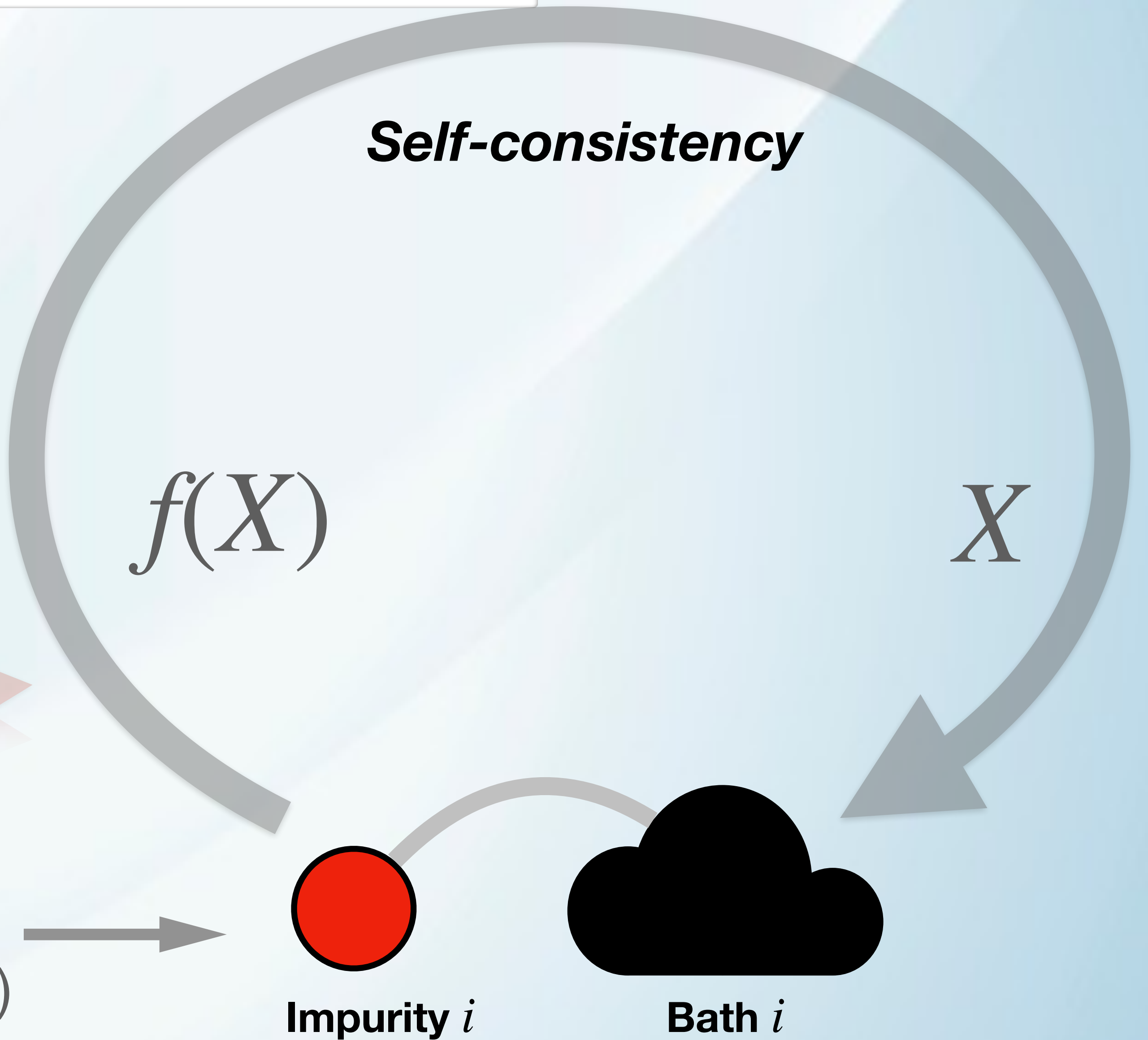
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																														
1 H Hydrogen 1.008	2 He Helium 4.002602																																														
3 Li Lithium 6.94	4 Be Beryllium 9.012182																																														
11 Na Sodium 22.989769	12 Mg Magnesium 24.305																																														
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938044	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.63	33 As Arsenic 74.9216	34 Se Selenium 78.9718	35 Br Bromine 79.904	36 Kr Krypton 83.798																														
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90637	42 Mo Molybdenum 95.95	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90545	54 Xe Xenon 131.293																														
55 Cs Caesium 132.90545	56 Ba Barium 137.327	57-71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.9804	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)																														
87 Fr Francium (223)	88 Ra Radium (226)	89-103 Actinoids	104 Rf Rutherfordium (261)	105 Db Dubnium (268)	106 Sg Seaborgium (271)	107 Bh Bohrium (272)	108 Hs Hassium (270)	109 Mt Meitnerium (276)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (280)	112 Cn Copernicium (285)	113 Nh Nihonium (284)	114 Fl Flerovium (289)	115 Mc Moscovium (288)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)																														
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																																															
<table border="1"> <tbody> <tr> <td>57 La Lanthanum 138.90547</td> <td>58 Ce Cerium 140.116</td> <td>59 Pr Praseodymium 140.90766</td> <td>60 Nd Neodymium 144.242</td> <td>61 Pm Promethium (145)</td> <td>62 Sm Samarium 150.36</td> <td>63 Eu Europium 151.964</td> <td>64 Gd Gadolinium 157.25</td> <td>65 Tb Terbium 158.92535</td> <td>66 Dy Dysprosium 162.500</td> <td>67 Ho Holmium 164.93033</td> <td>68 Er Erbium 167.259</td> <td>69 Tm Thulium 168.93403</td> <td>70 Yb Ytterbium 173.054</td> <td>71 Lu Lutetium 174.9668</td> </tr> <tr> <td>89 Ac Actinium (227)</td> <td>90 Th Thorium 232.0377</td> <td>91 Pa Protactinium 231.03688</td> <td>92 U Uranium 238.02891</td> <td>93 Np Neptunium (237)</td> <td>94 Pu Plutonium (244)</td> <td>95 Am Americium (243)</td> <td>96 Cm Curium (247)</td> <td>97 Bk Berkelium (247)</td> <td>98 Cf Californium (251)</td> <td>99 Es Einsteinium (252)</td> <td>100 Fm Fermium (257)</td> <td>101 Md Mendelevium (258)</td> <td>102 No Nobelium (259)</td> <td>103 Lr Lawrencium (262)</td> </tr> </tbody> </table>																		57 La Lanthanum 138.90547	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93403	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.9668	89 Ac Actinium (227)	90 Th Thorium 232.0377	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)
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Algorithmic structure of QE methods (DMFT, DMET, GA, g-GA,...)



*Embedding Hamiltonian
or impurity model*
(computational bottleneck)



Impurity i

Bath i

Example: DMFT

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

Antoine Georges

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Gabriel Kotliar

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

Werner Krauth and Marcelo J. Rozenberg

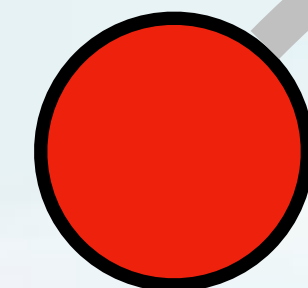
Laboratoire de Physique Statistique de l'Ecole Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France

$\Sigma(\omega)$

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

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

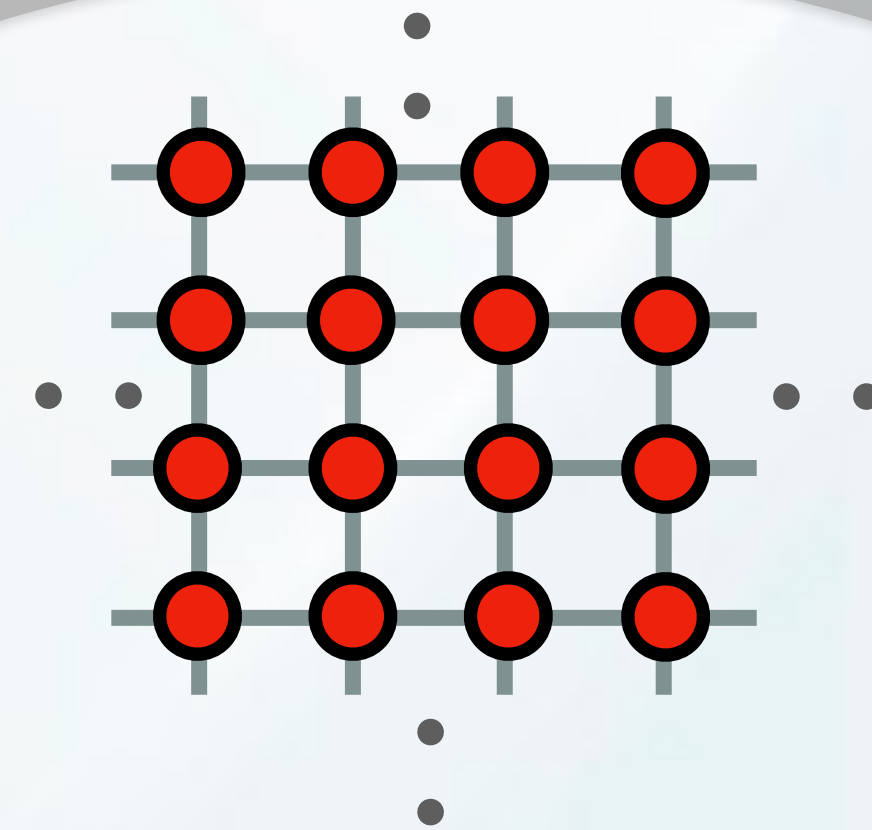
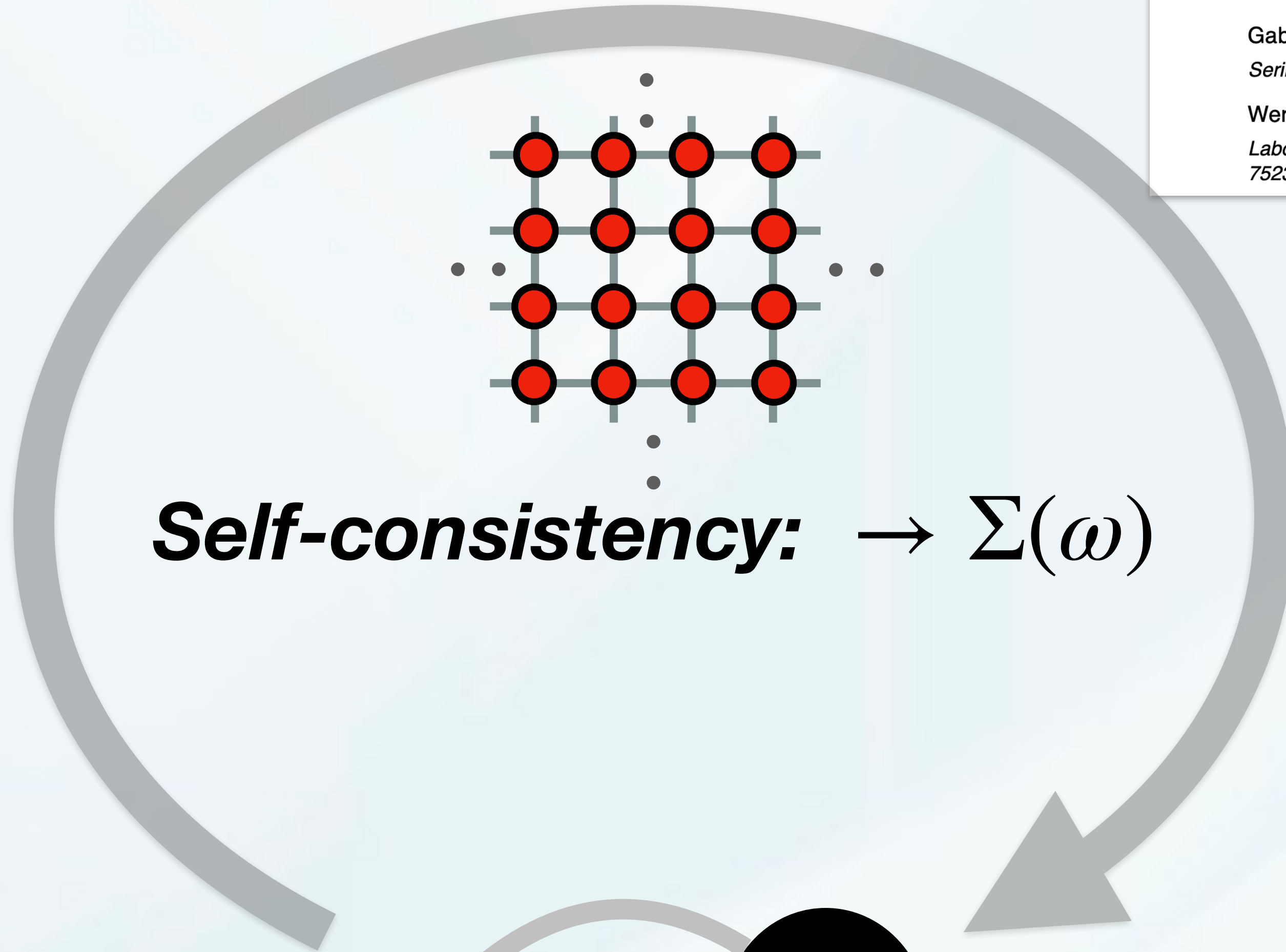
Impurity model



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,^{1,*} Yongxin Yao,^{2,†} Cai-Zhuang Wang,² Kai-Ming Ho,² and Gabriel Kotliar¹

PRL 118, 126401 (2017)

PHYSICAL REVIEW LETTERS

week ending
24 MARCH 2017

Slave Boson Theory of Orbital Differentiation with Crystal Field Effects:
Application to UO₂

Nicola Lanatà,^{1,*} Yongxin Yao,^{2,†} Xiaoyu Deng,³ Vladimir Dobrosavljević,¹ and Gabriel Kotliar^{3,4}

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

Self-consistency: $\rightarrow \Sigma_0, Z$ (D, λ^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

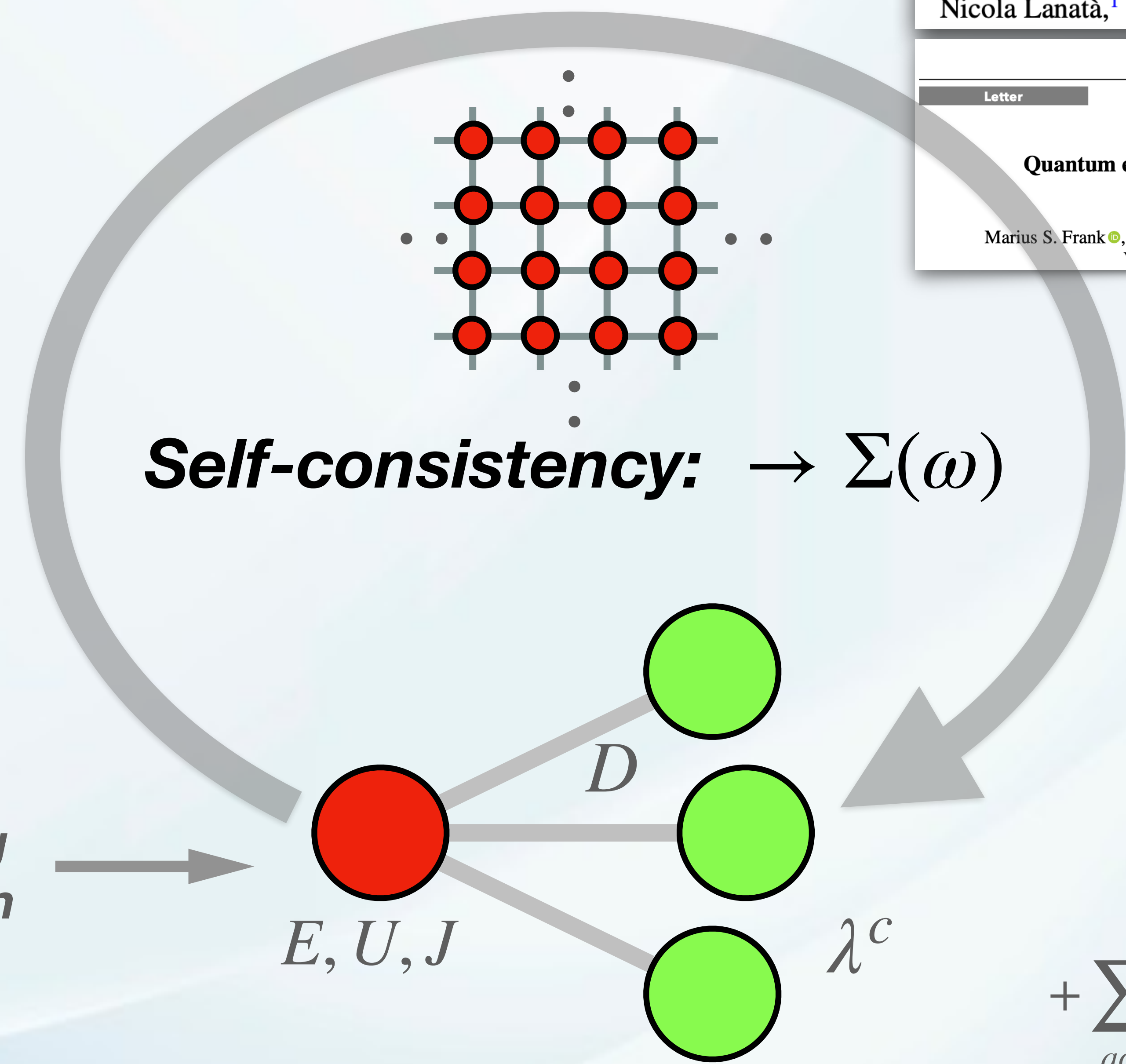
Nicola Lanatà,¹ Tsung-Han Lee,¹ Yong-Xin Yao,² and Vladimir Dobrosavljević¹

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

Letter

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

Marius S. Frank¹, Tsung-Han Lee², Gargee Bhattacharyya¹, Pak Ki Henry Tsang,³ Victor L. Quito,^{4,3} Vladimir Dobrosavljević,³ Ove Christiansen⁵ and Nicola Lanatà^{1,6,*}



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

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

Embedding Hamiltonian

E, U, J

D

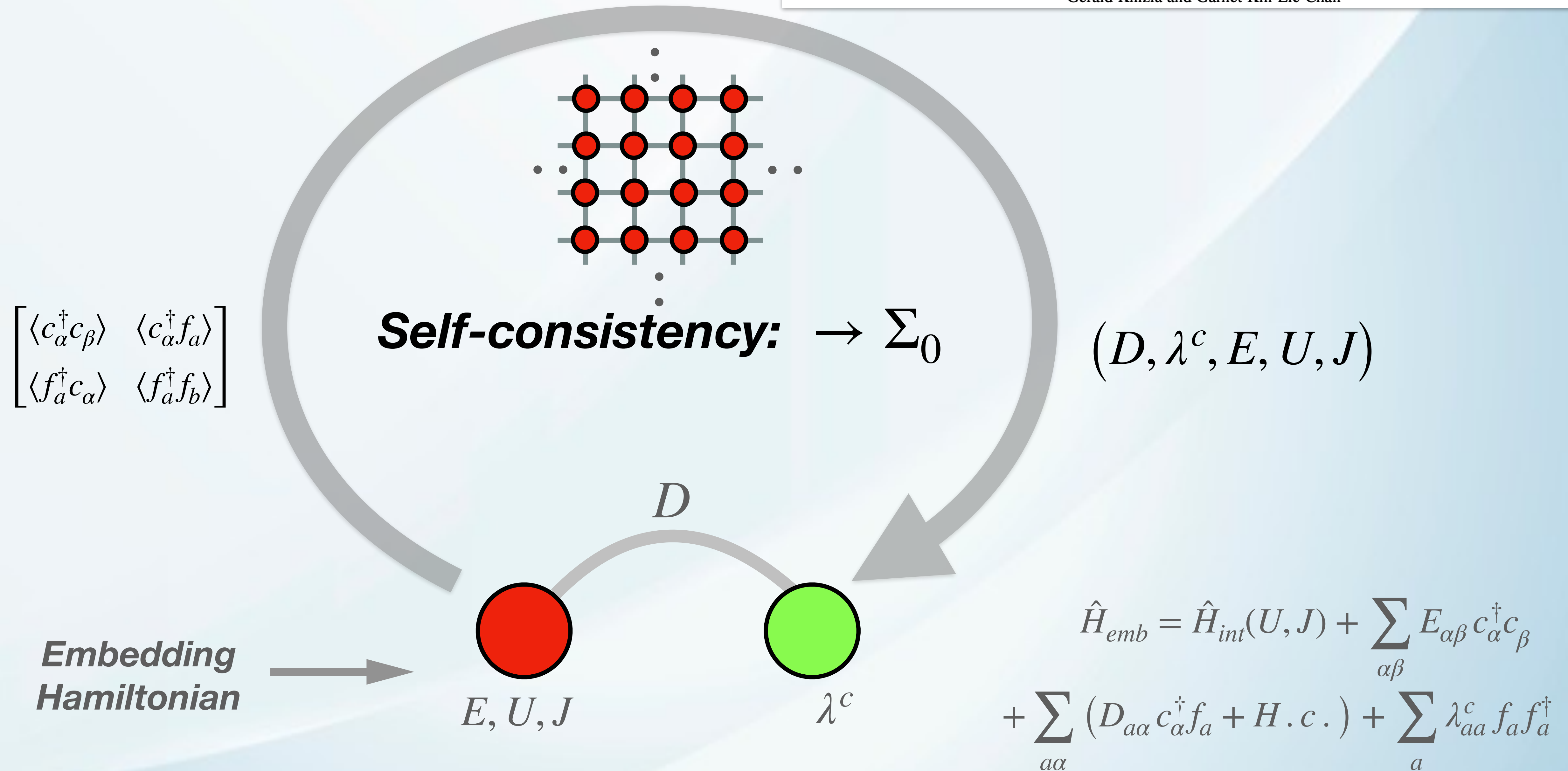
λ^c

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

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,^{1,*} Yongxin Yao,^{2,†} Cai-Zhuang Wang,² Kai-Ming Ho,² and Gabriel Kotliar¹

PRL **118**, 126401 (2017)

PHYSICAL REVIEW LETTERS

week ending
24 MARCH 2017

Slave Boson Theory of Orbital Differentiation with Crystal Field Effects: Application to UO₂

Nicola Lanatà,^{1,*} Yongxin Yao,^{2,†} Xiaoyu Deng,³ Vladimir Dobrosavljević,¹ and Gabriel Kotliar^{3,4}

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

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

Thomas Ayrál,¹ Tsung-Han Lee,¹ and Gabriel Kotliar^{1,2}

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

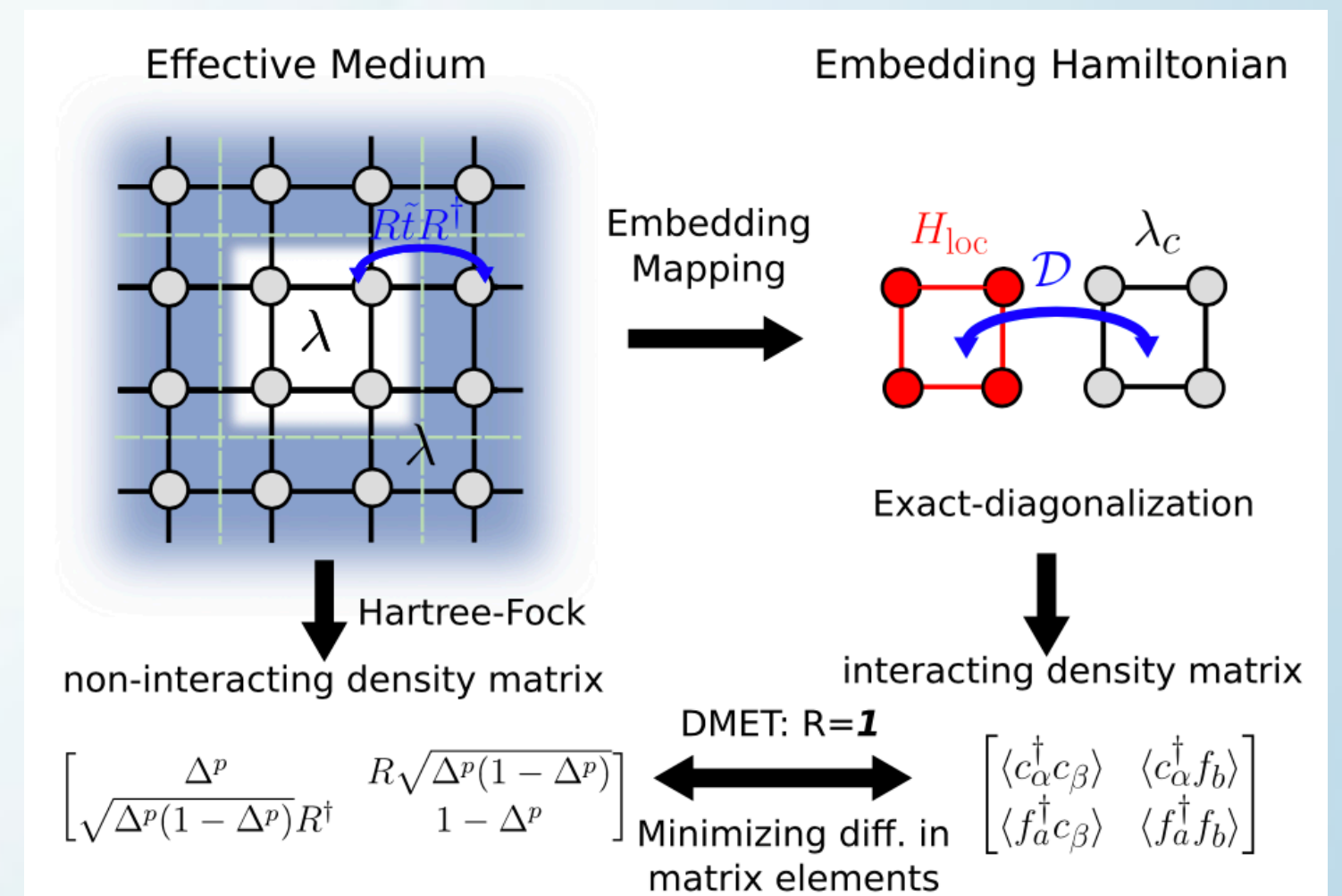
Rotationally invariant slave-boson and density matrix embedding theory: Unified framework and comparative study on the one-dimensional and two-dimensional Hubbard model

Tsung-Han Lee,^{1,*} Thomas Ayrál,^{1,2} Yong-Xin Yao,³ Nicola Lanata,⁴ and Gabriel Kotliar^{1,5}

Formulation of GA/RISB as QE theory



Comparison between GA/RISB & DMET QE equations & performance



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- A. Quantum Embedding (QE) methods.
- B. GA method (multi-orbital models): *QE formulation*.
- C. DFT+GA algorithmic structure.
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- 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)

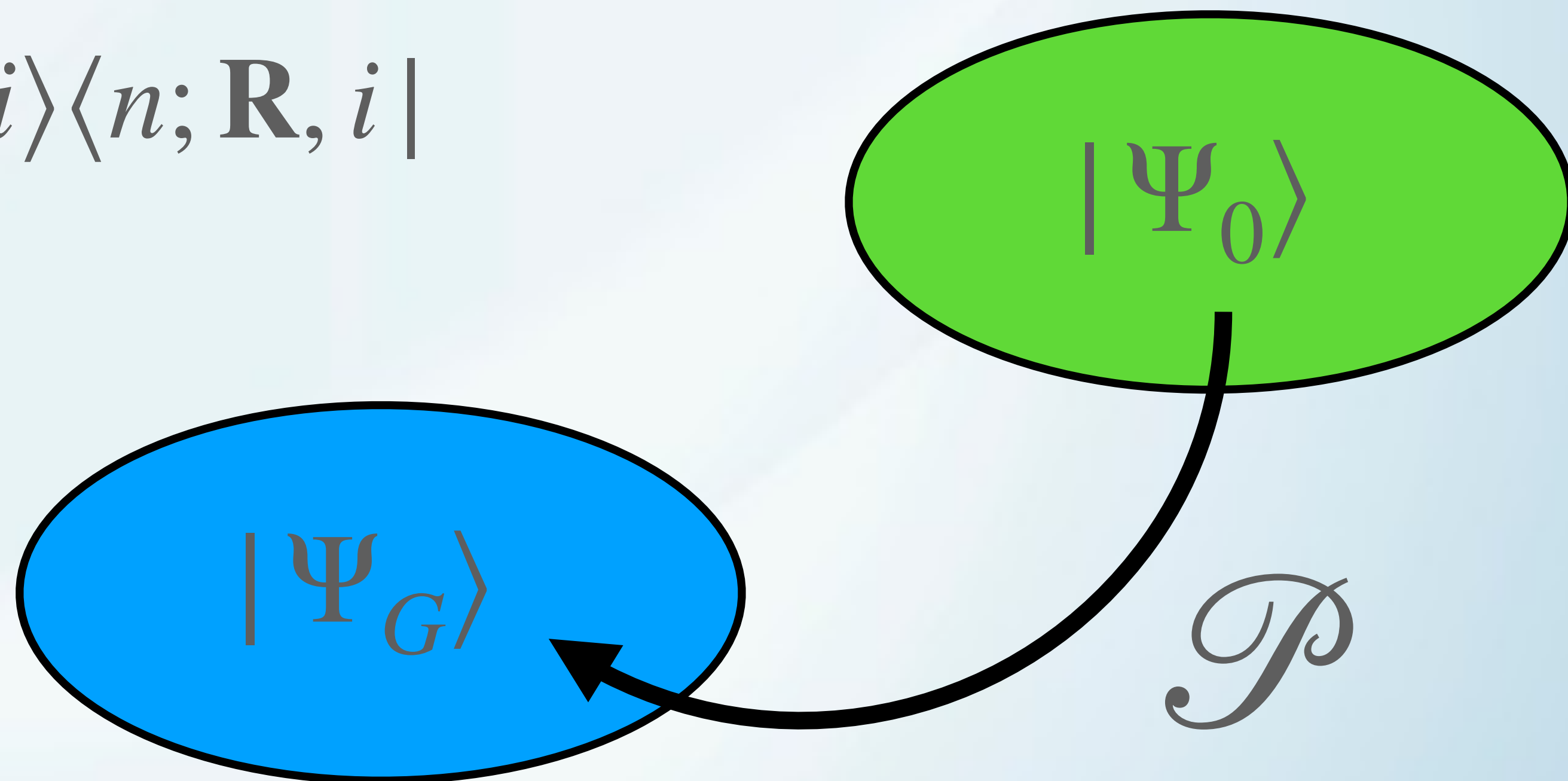
$i = 2$: Second subset of correlated modes (e.g. f orbitals of atom 1 in unit cell)

...

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:

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

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

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

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

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



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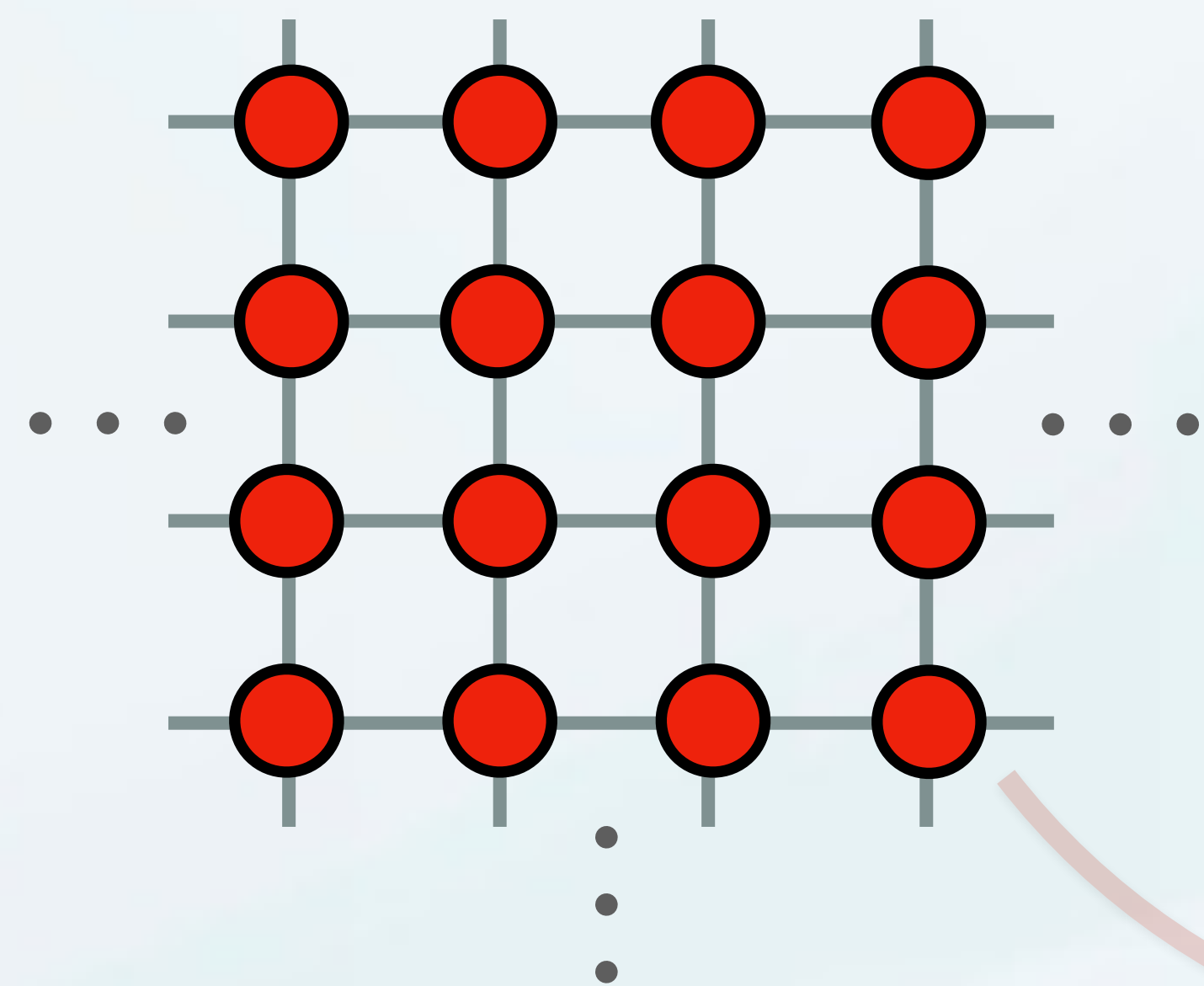
**Slave Boson Theory of Orbital Differentiation with Crystal Field Effects:
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w.r.t. $\{ \Lambda_i | i \geq 1 \}, | \Psi_0 \rangle$.

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

*Quantum-embedding
formulation*

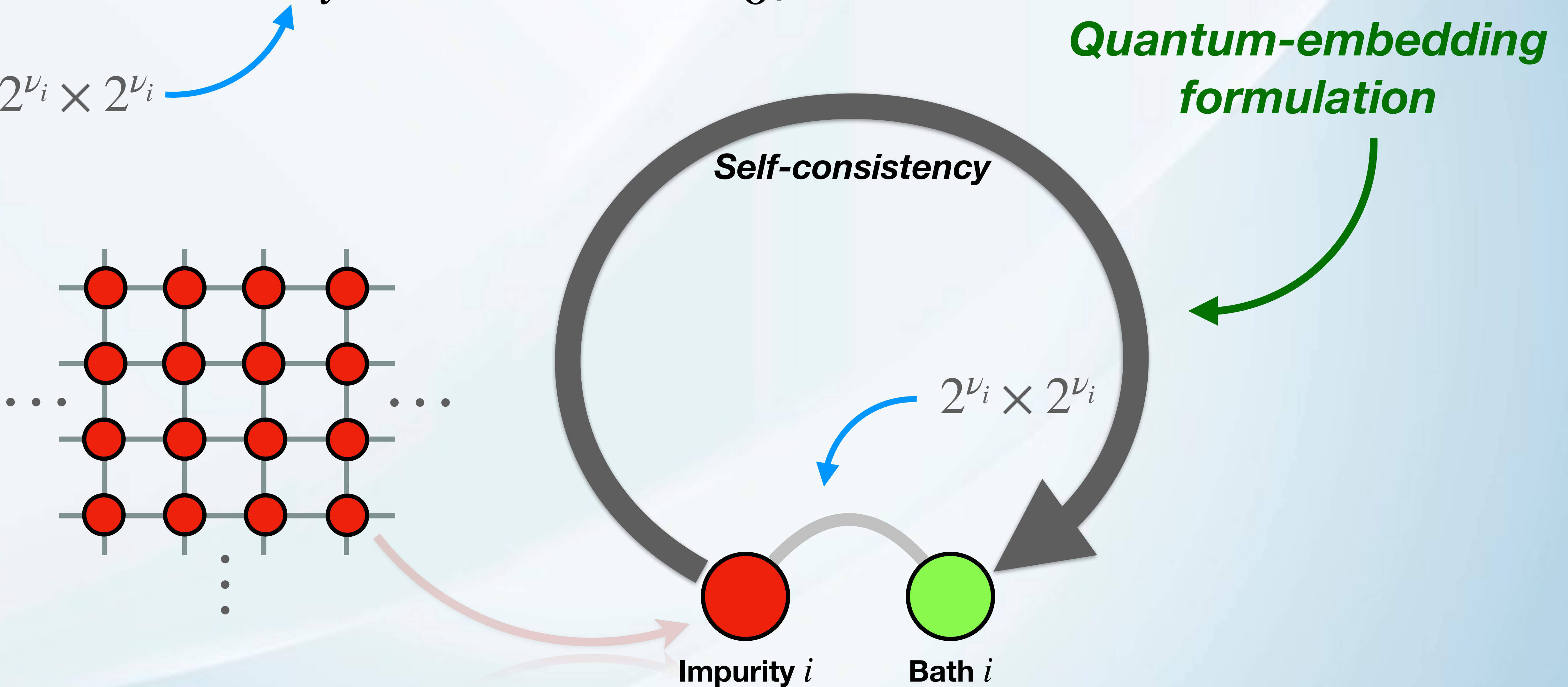


Self-consistency

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

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 ∞ -coordination lattices. In this sense, the GA is a variational approximation to DMFT.

Gutzwiller constraints:

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

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

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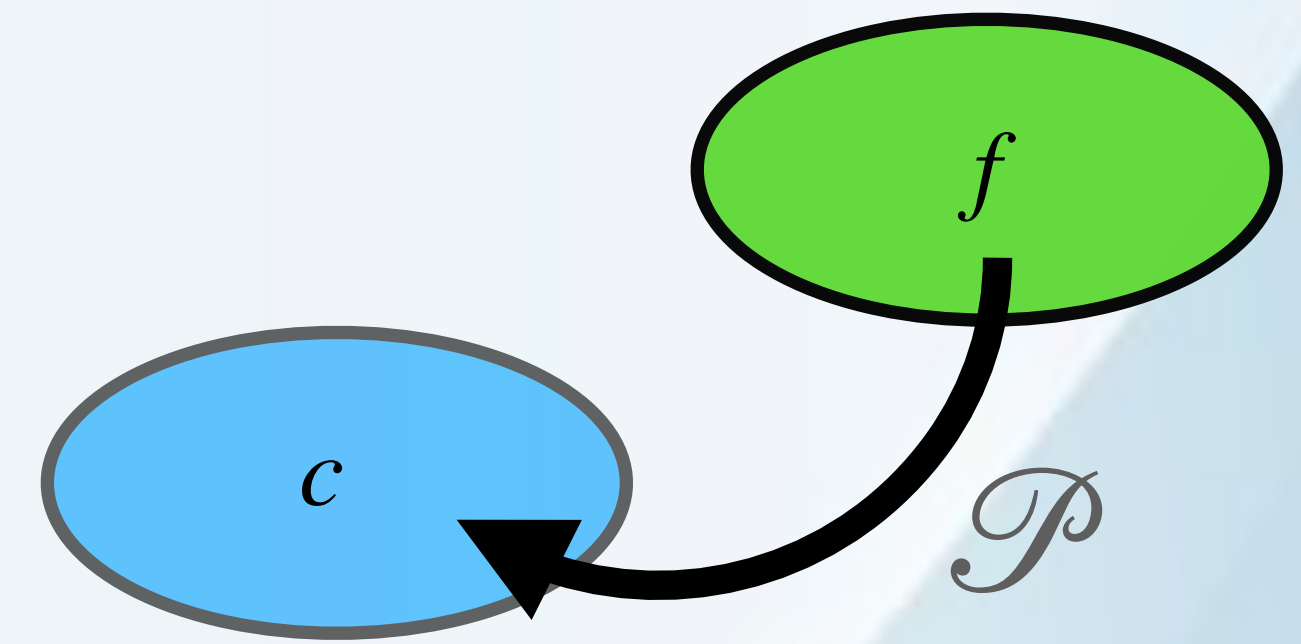
$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle \quad \forall a, b \in \{1, \dots, \nu_i\}$$

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:

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

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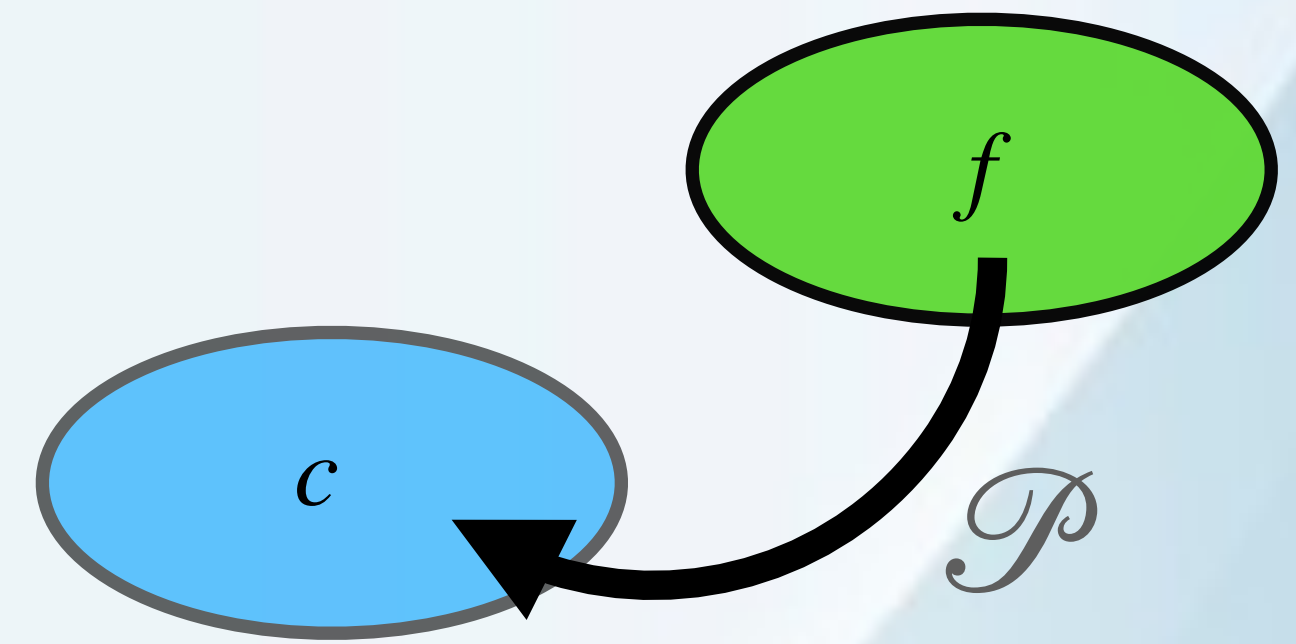
Key consequence:

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

Gutzwiller constraints:

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

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



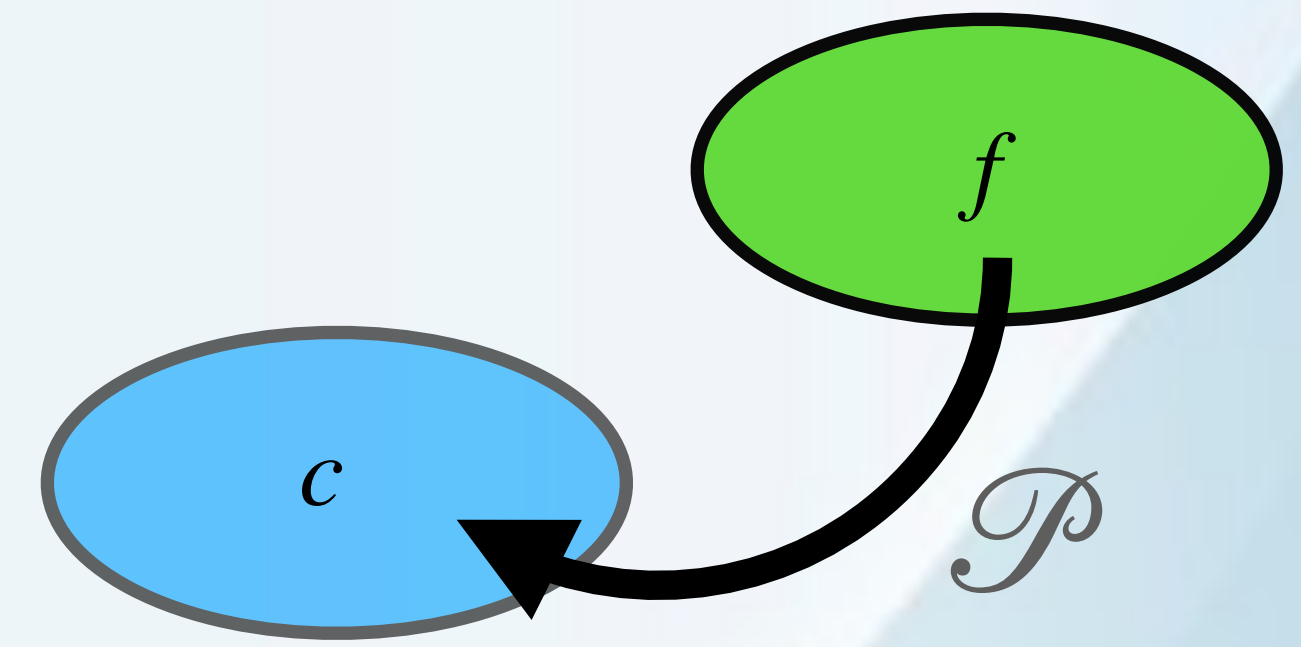
Key consequence:

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

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:

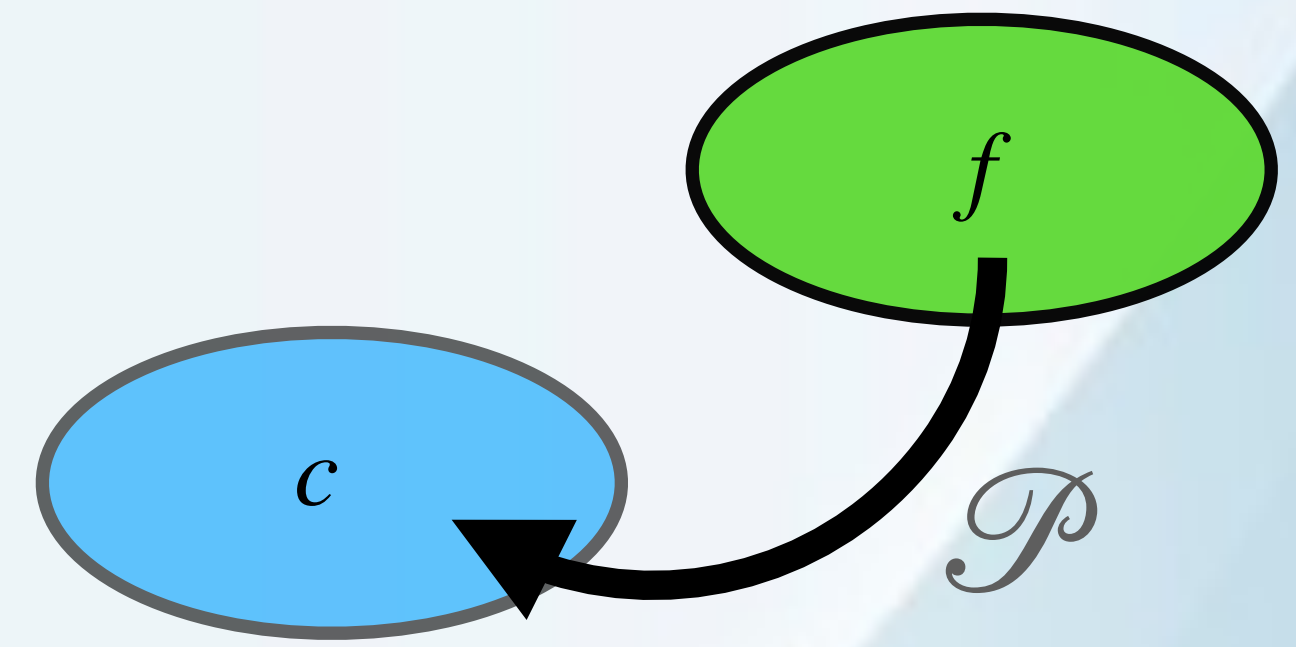
~~$$\langle \Psi_0 | \mathcal{P}_{\mathbf{R}i}^\dagger \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{\mathbf{R}ia}^\dagger f_{\mathbf{R}ib} | \Psi_0 \rangle$$

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

Gutzwiller constraints:

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

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



Key consequence:

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

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.

Local operators: (connected terms)

The diagram shows a mathematical expression for local operators, with green lines indicating connections between terms. The expression is:

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

Green lines connect the operators $\mathcal{P}_{\mathbf{R}' i'}^\dagger$ and $\mathcal{P}_{\mathbf{R}' i'}$ to the operators $\mathcal{P}_{\mathbf{R} i}^\dagger$ and $\mathcal{P}_{\mathbf{R} i}$ respectively, indicating that the operators are connected terms. The expression is enclosed in large square brackets. Above the expression, there are several curved lines and vertical ellipses, suggesting a continuation of the product or a specific configuration of operators.

(GA and G. constraints)

Local operators:

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

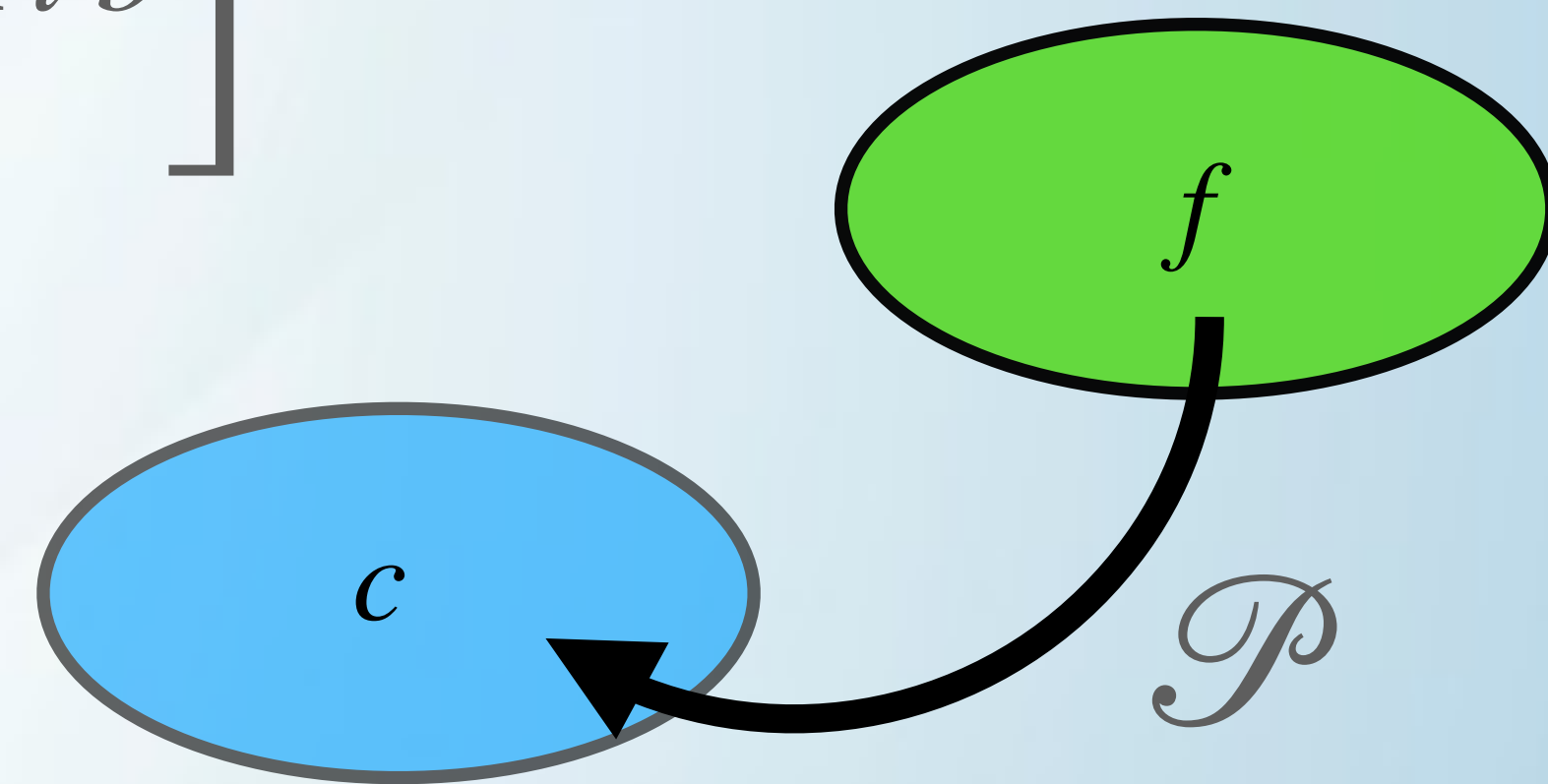
Non-local 1-body operators, i.e., $(\mathbf{R}, i) \neq (\mathbf{R}', i')$:

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

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:



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

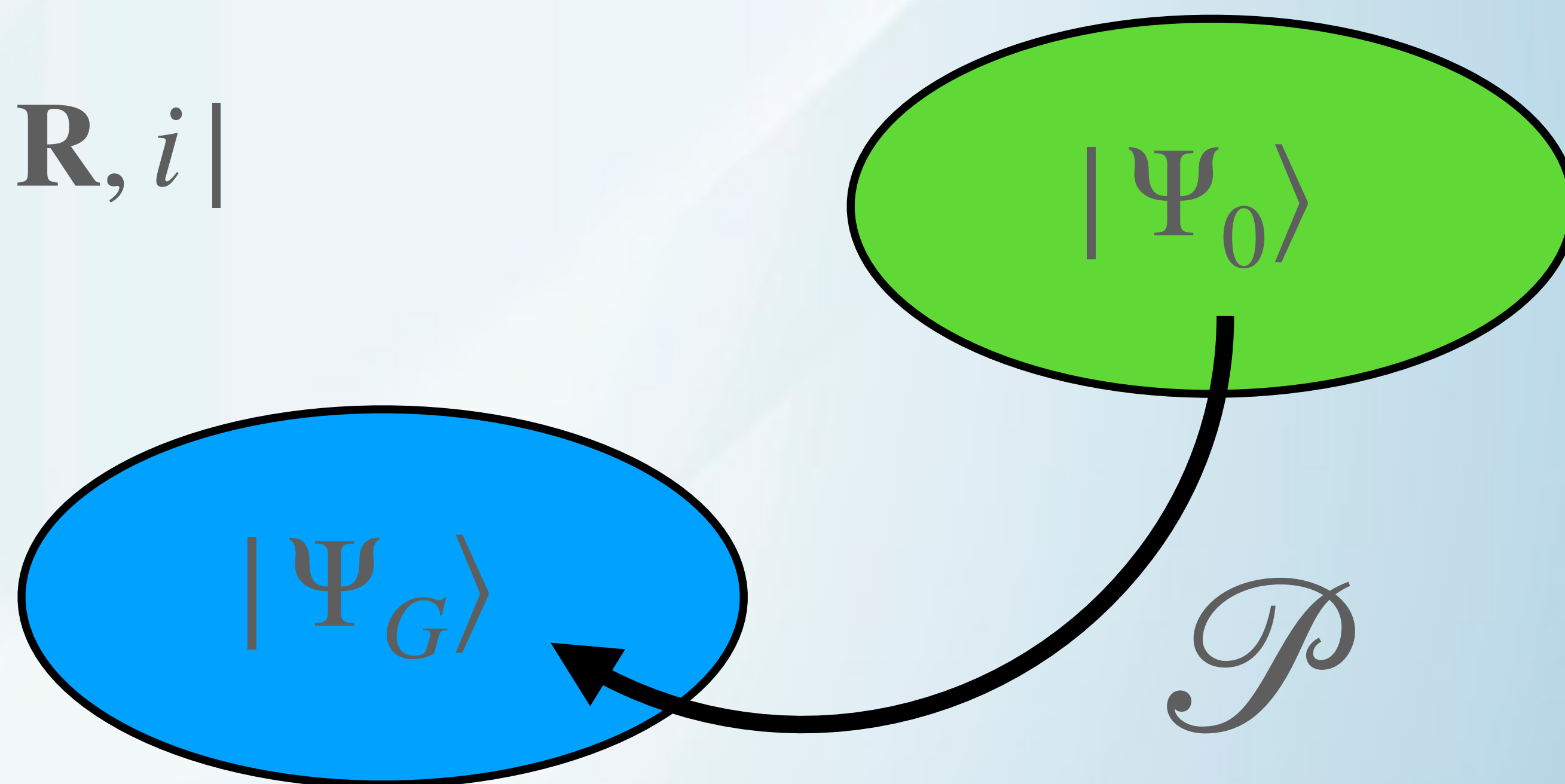
Non-local quadratic operators:

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

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

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

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



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:

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

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

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

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

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

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

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

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

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

Where:

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

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

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:

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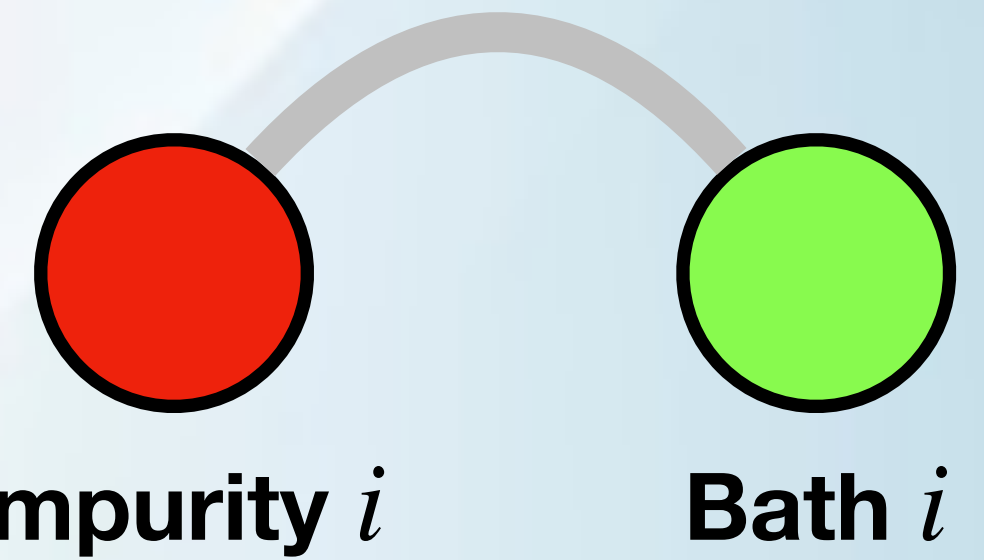
Quantum-embedding formulation

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

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

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

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



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

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

Quantum-embedding formulation

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

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

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

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

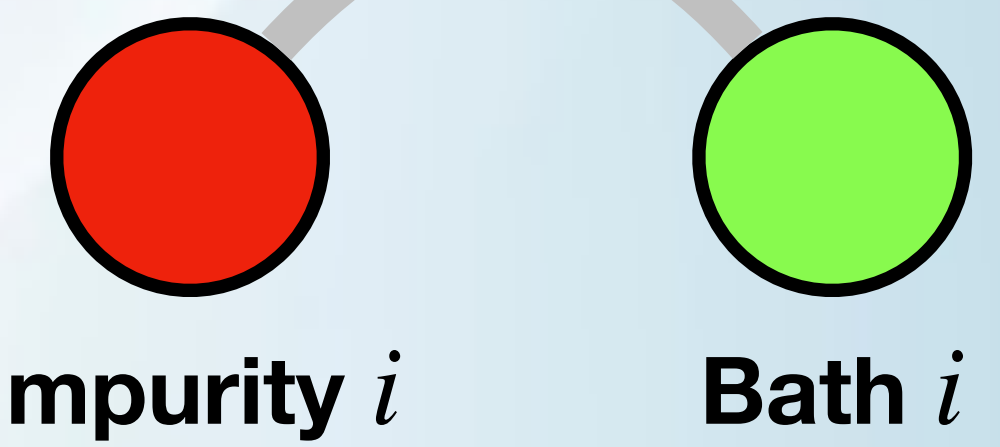
Quantum-embedding formulation

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

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

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

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



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

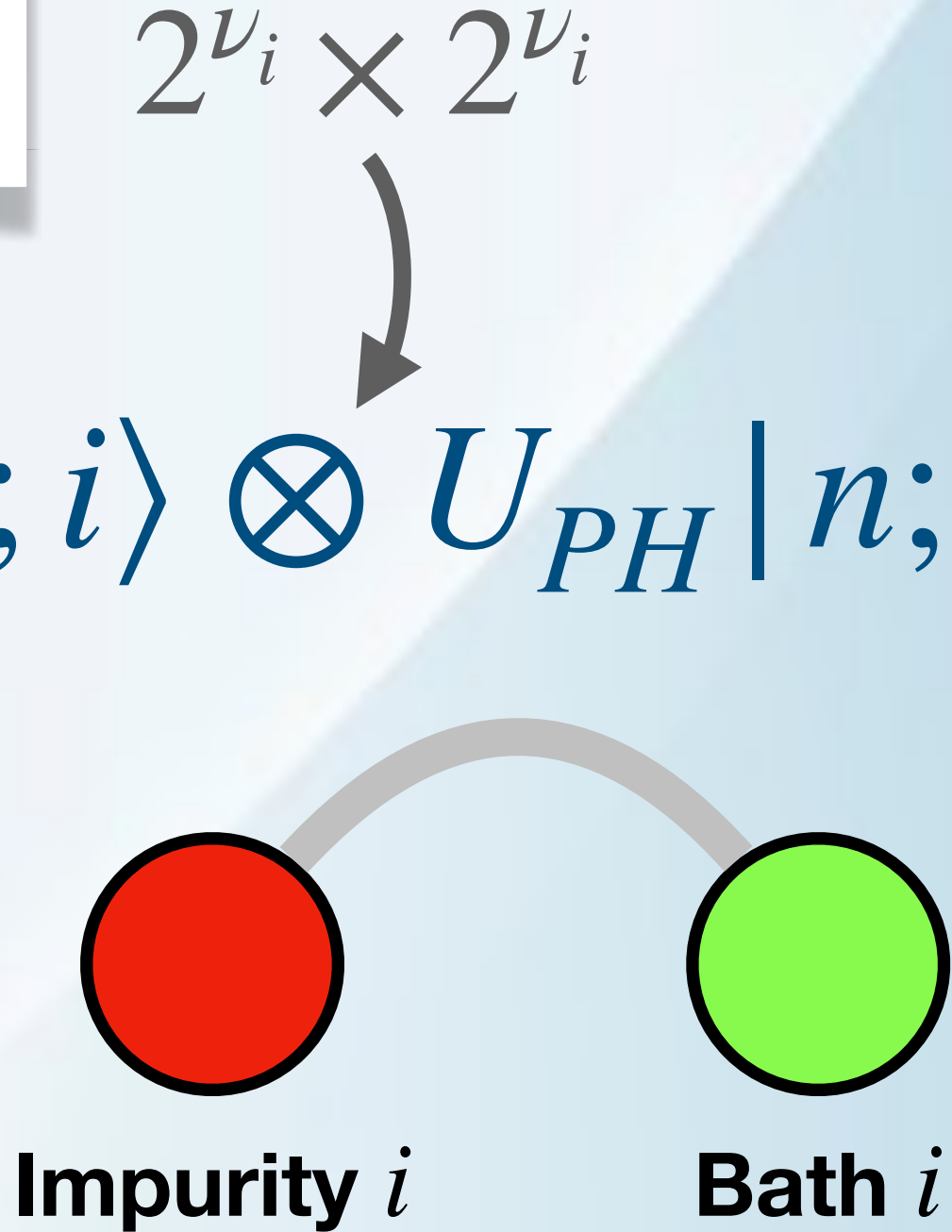
$$|\Gamma; i\rangle = [\hat{c}_{i1}^{\dagger}]^{q_1(\Gamma)} \dots [\hat{c}_{i\nu_i}^{\dagger}]^{q_{\nu_i}(\Gamma)} |0\rangle$$

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

Quantum-embedding formulation

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

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



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

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

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

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 $\{\Lambda_{i \geq 1}\}, |\Psi_0\rangle$.
3. Definition of slave-boson (SB) amplitudes.
4. Mapping from SB amplitudes to embedding states.
5. Lagrange formulation of the optimization problem.

Variational energy:

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

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:

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

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

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

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

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

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:

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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4. Mapping from SB amplitudes to embedding states.
5. Lagrange formulation of the optimization problem.

Outline

- A. Quantum Embedding (QE) methods.
- B. GA method (multi-orbital models): *QE formulation*.
- C. **DFT+GA algorithmic structure.**
- D. Spectral properties.
- E. Examples of applications.
- F. Recent formalism extensions (g-GA).

DFT+GA: algorithmic structure

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

Phase Diagram and Electronic Structure of Praseodymium and Plutonium

Nicola Lanatà,^{1,*} Yongxin Yao,^{2,†} Cai-Zhuang Wang,² Kai-Ming Ho,² and Gabriel Kotliar¹

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:

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

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

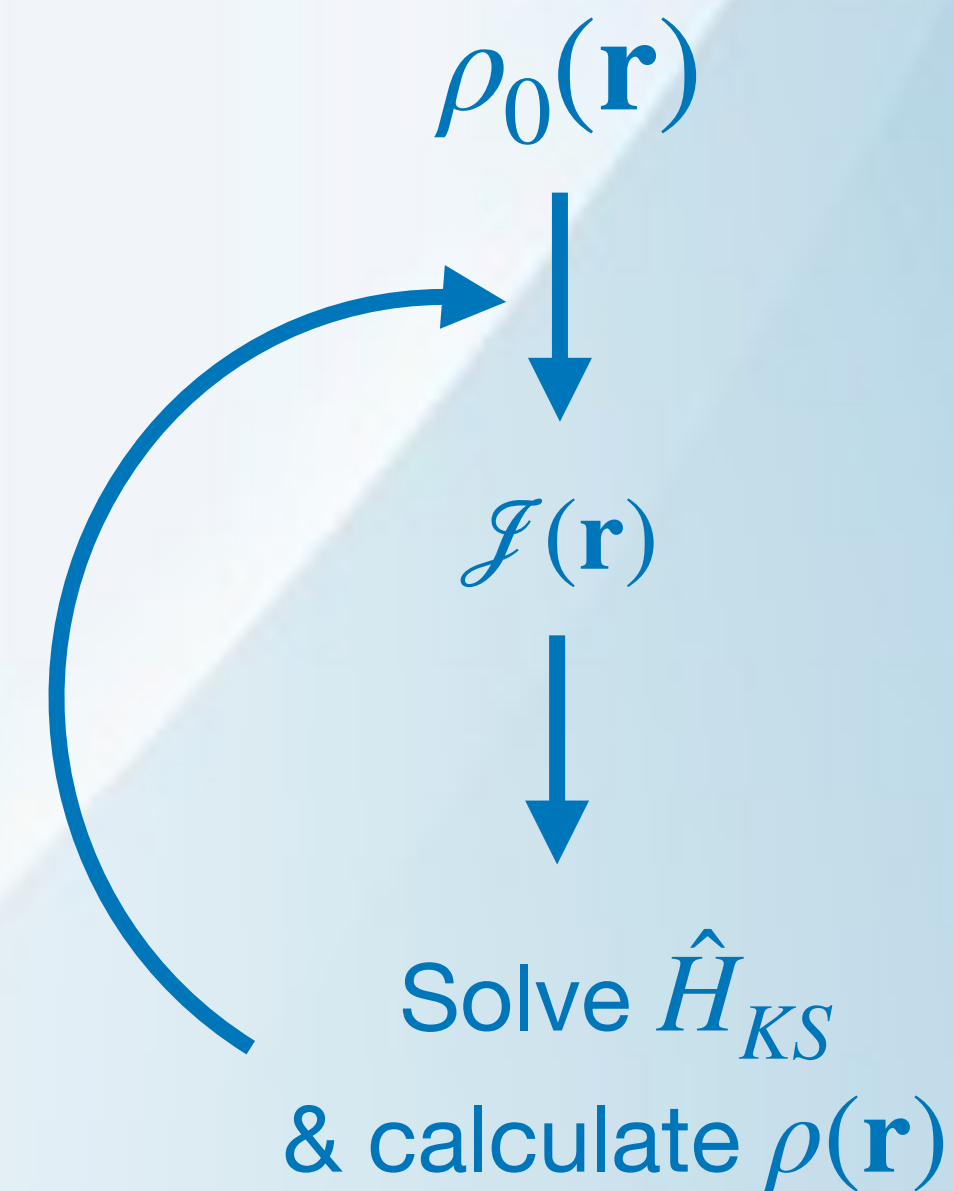
$$\mathcal{S}[\Psi_0, \rho(\mathbf{r}), \mathcal{J}(\mathbf{r})] = \langle \Psi_0 | \hat{T} + \int \mathbf{d}\mathbf{r} V(\mathbf{r}) \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle + E_{HXC}[\rho]$$

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

**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:

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

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

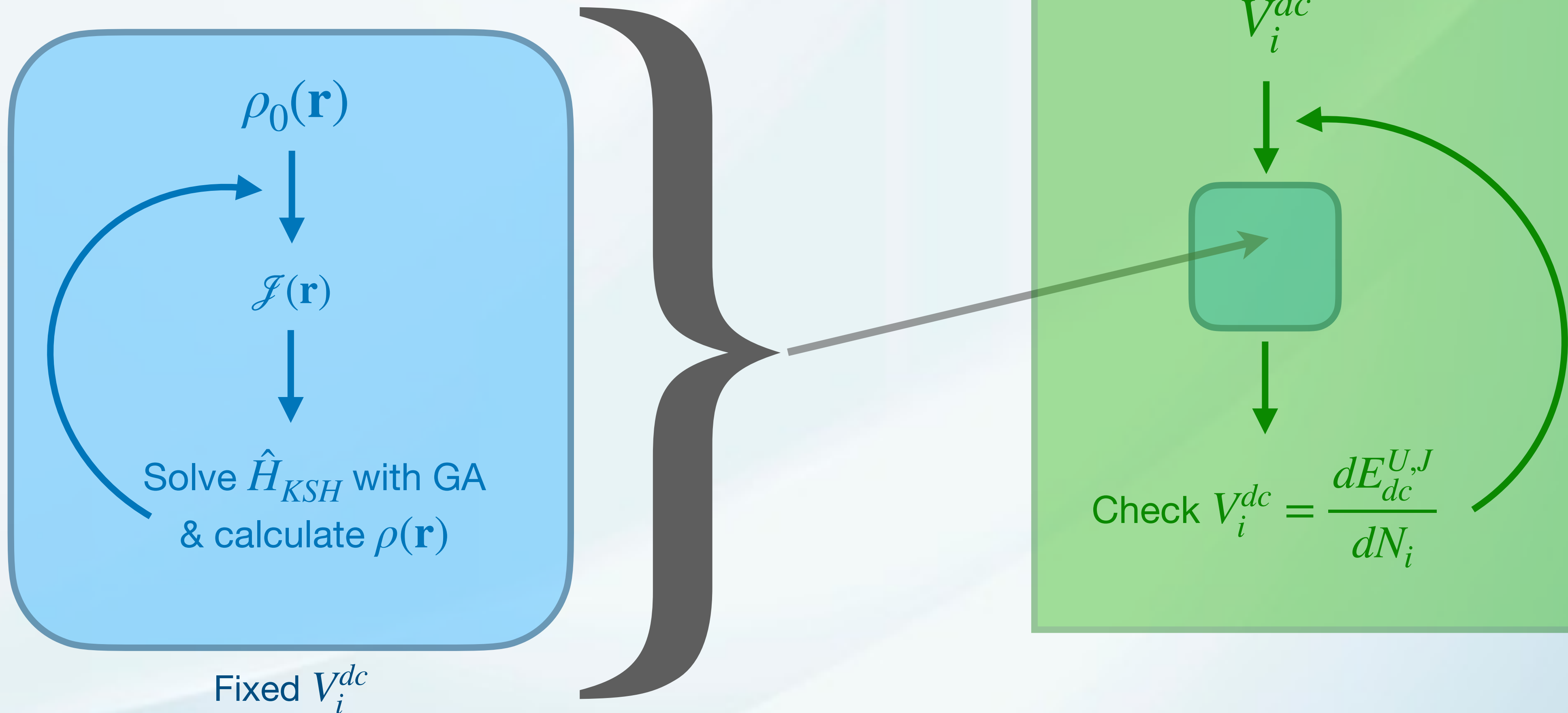
Enforcing definition of $\rho(\mathbf{r})$

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

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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- F. Recent formalism extensions.

Spectral properties

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

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

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

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

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

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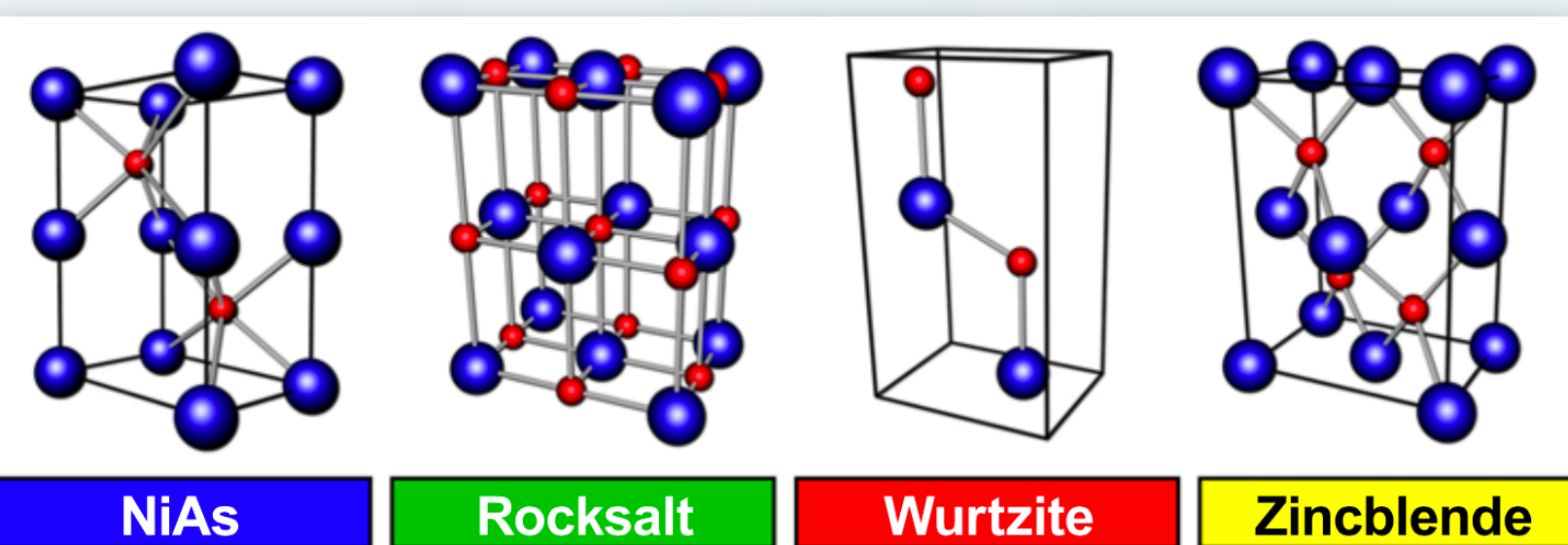
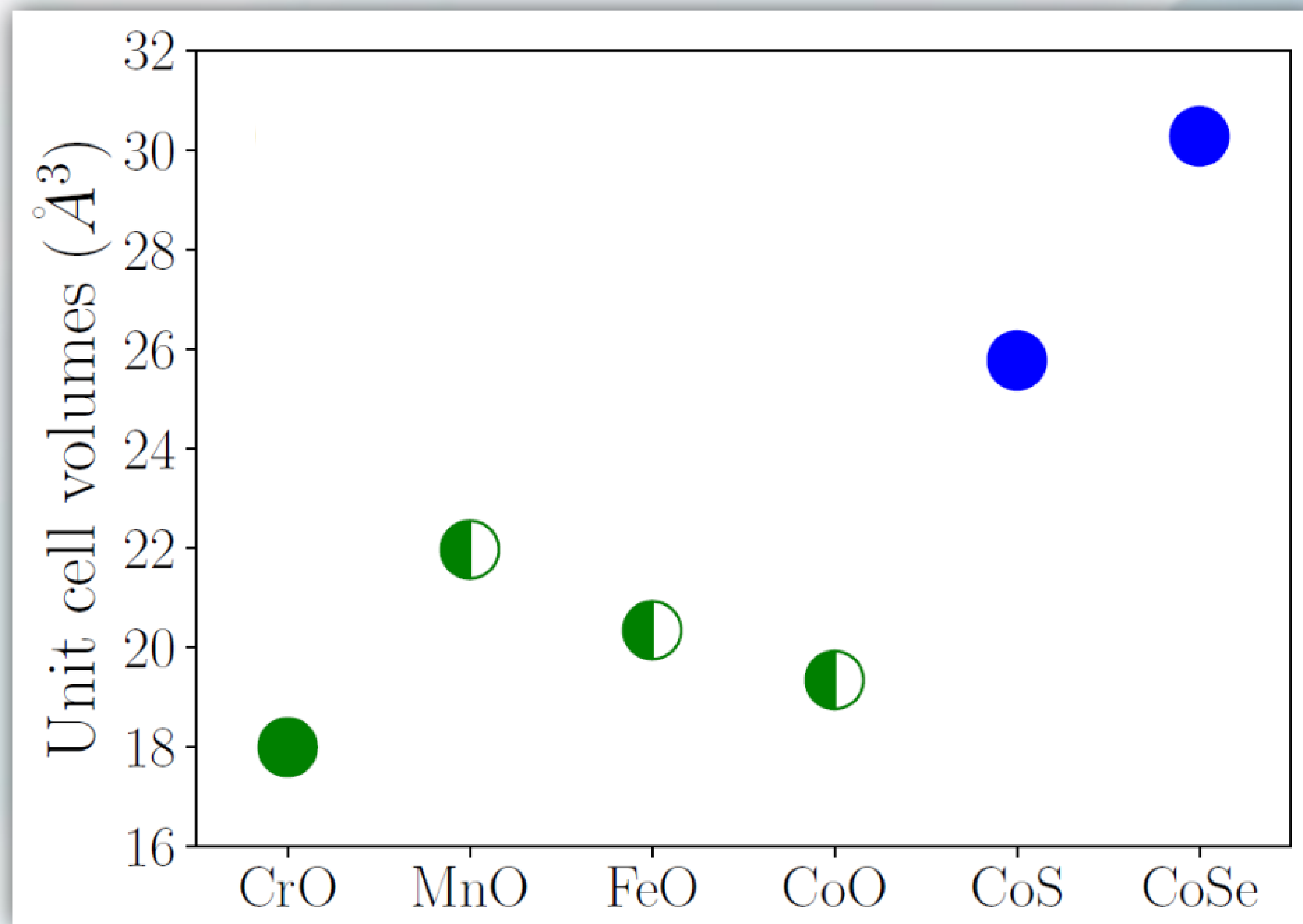
Connection between Mott physics and crystal structure in a series of transition metal binary compounds

Nicola Lanatà¹, Tsung-Han Lee^{2,3}, Yong-Xin Yao⁴, Vladan Stevanović⁵ and Vladimir Dobrosavljević²

- NiAs-type
- Rocksalt
- Wurtzite
- Zincblende

- Experiment
- Theory

- Metal
- Insulator



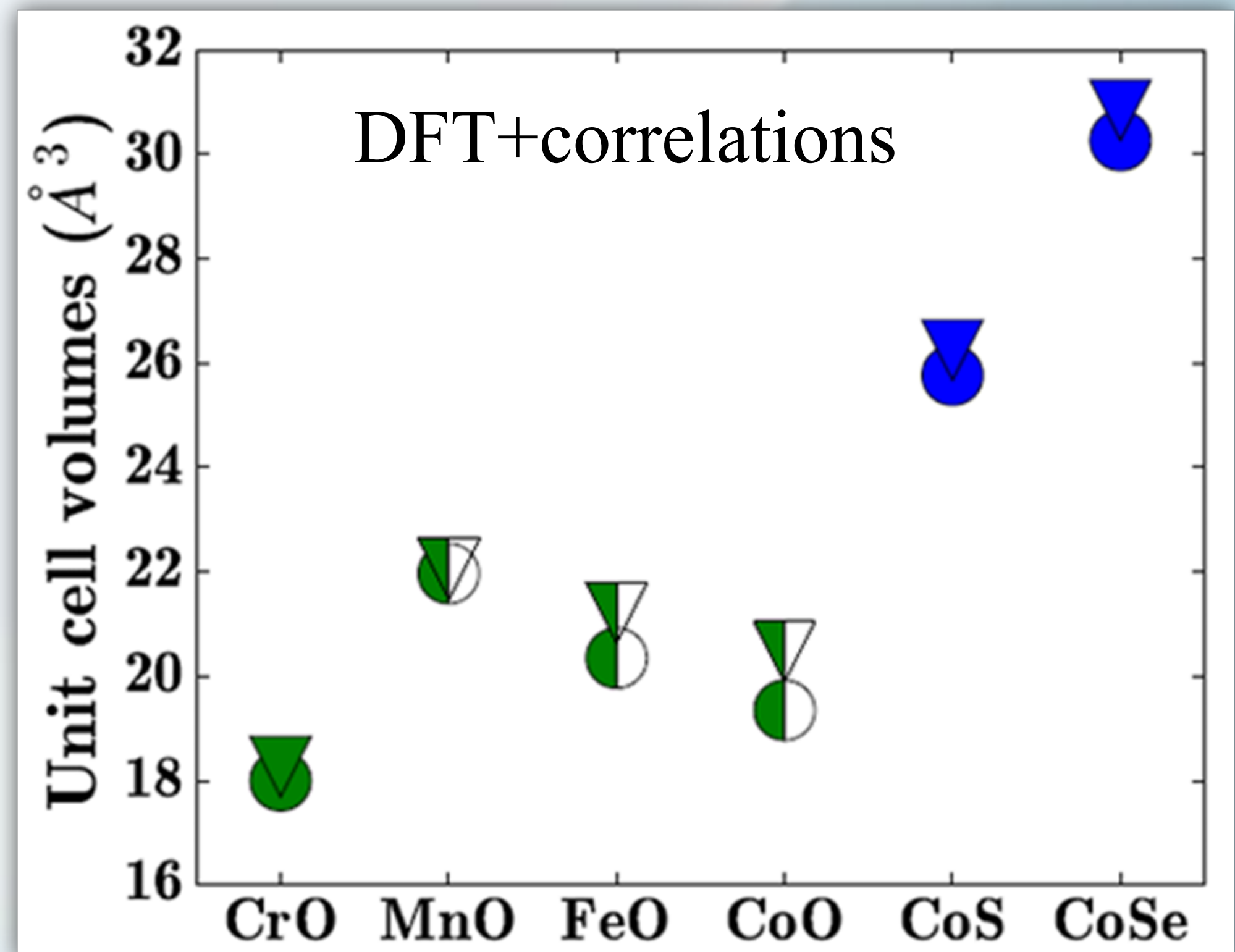
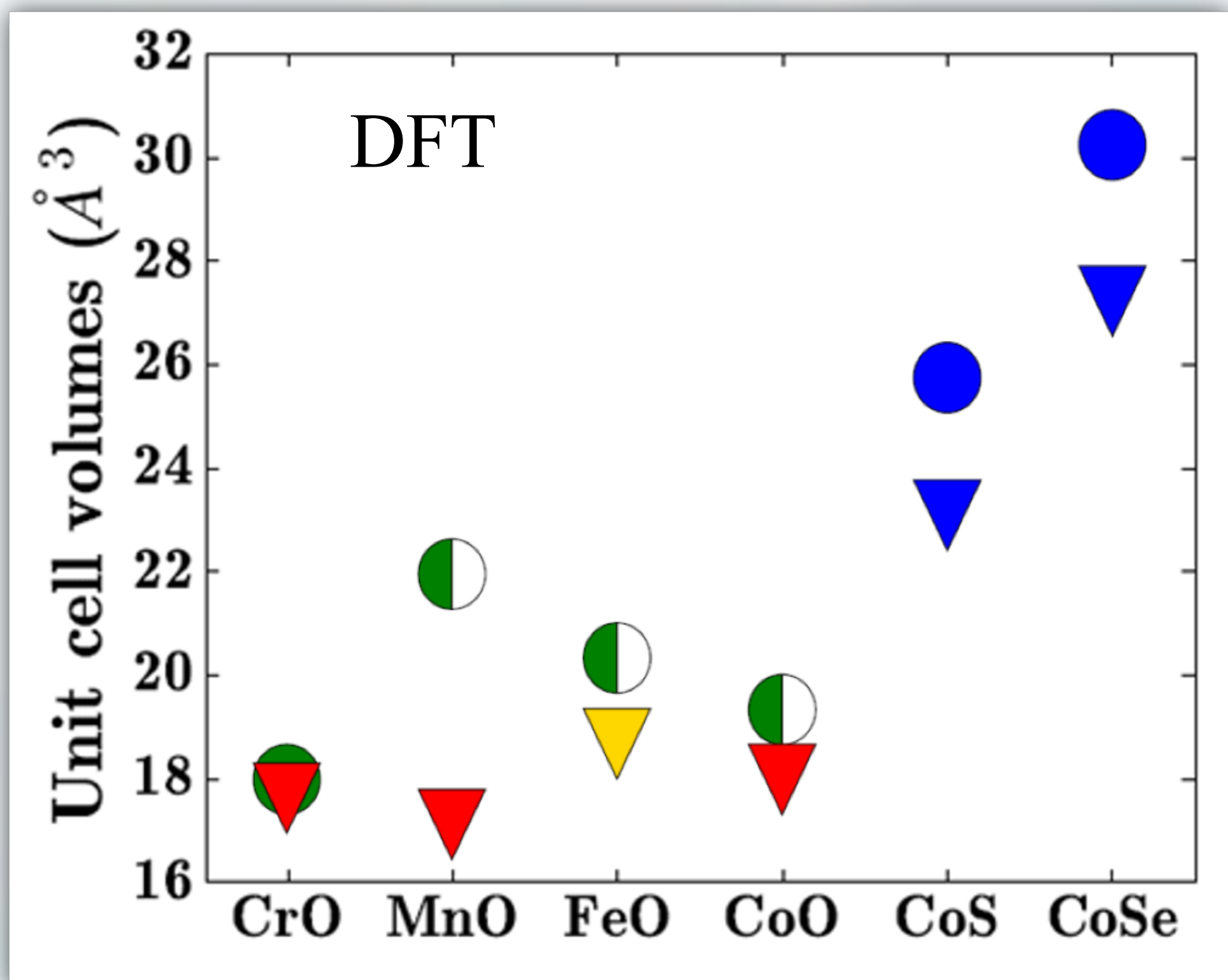
Example: Structure, Density, Gap Theory vs Experiments

ARTICLE OPEN

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

Nicola Lanatà¹, Tsung-Han Lee^{2,3}, Yong-Xin Yao⁴, Vladan Stevanović⁵ and Vladimir Dobrosavljević²

- NiAs-type
- Rocksalt
- Wurtzite
- Zincblende
- Experiment
- Theory
- Metal
- Insulator

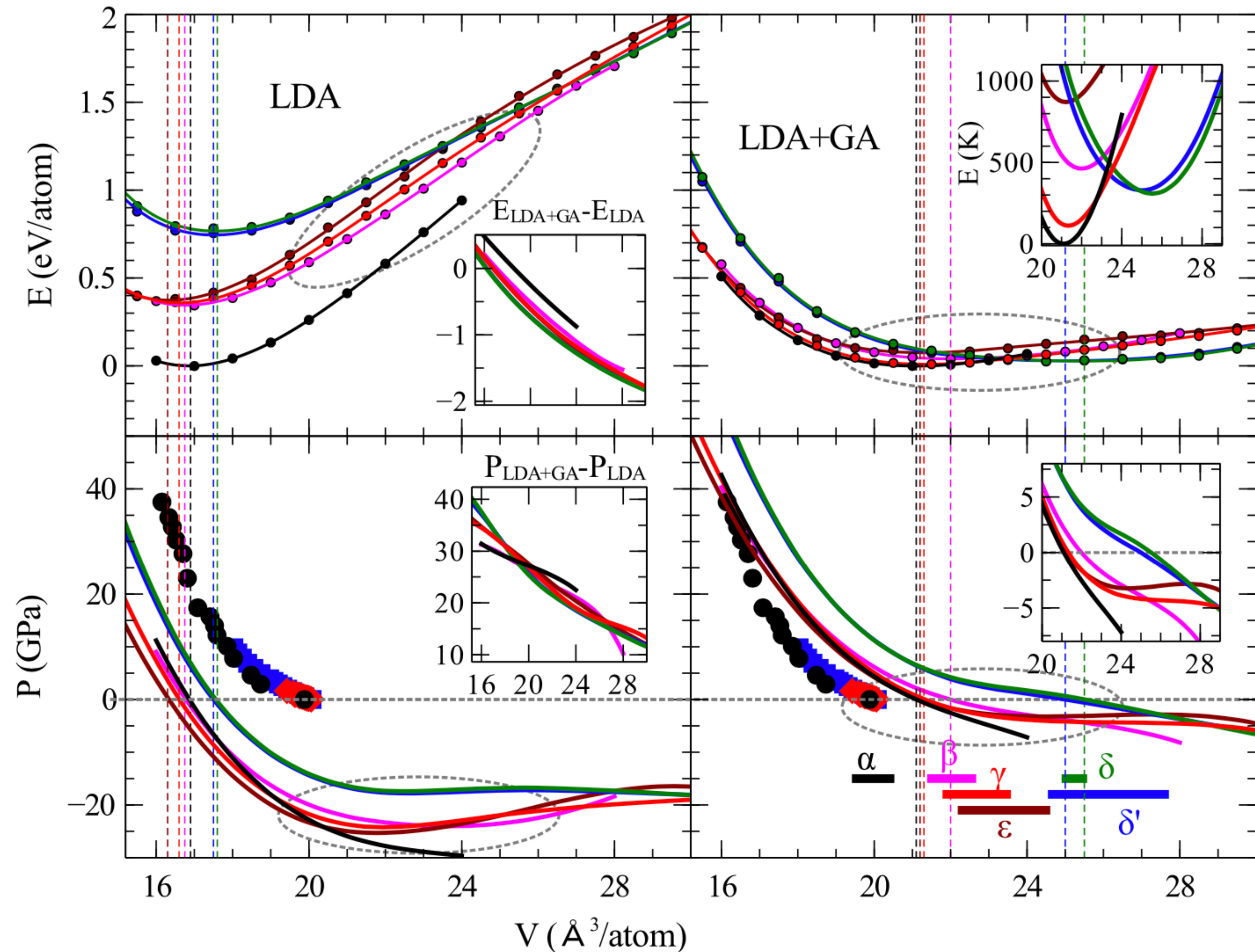
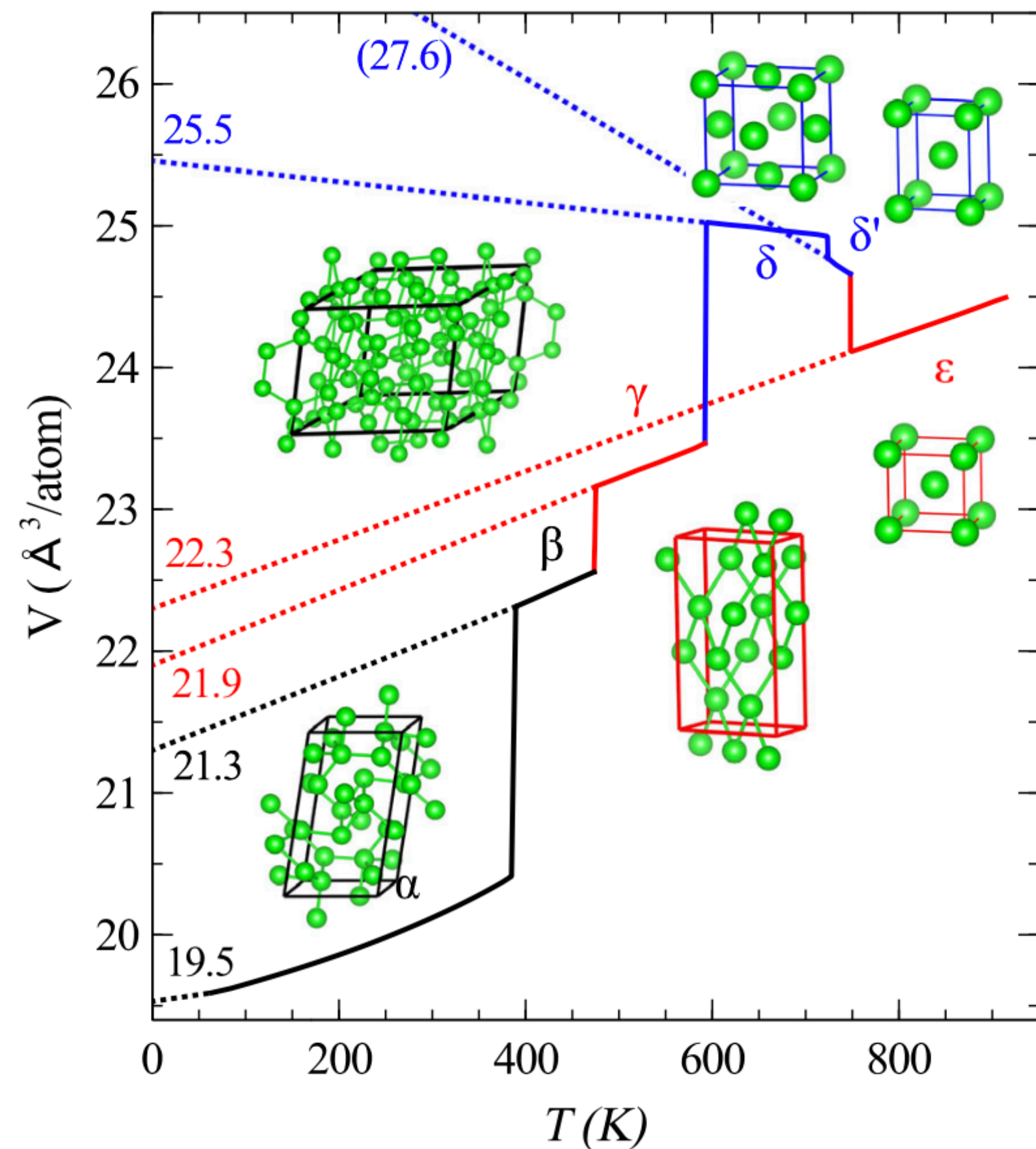


Example: phase diagram of Pu

PHYSICAL REVIEW X 5, 011008 (2015)

Phase Diagram and Electronic Structure of Praseodymium and Plutonium

Nicola Lanatà,^{1,*} Yongxin Yao,^{2,†} Cai-Zhuang Wang,² Kai-Ming Ho,² and Gabriel Kotliar¹



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,¹ Tsung-Han Lee,¹ Yong-Xin Yao,² and Vladimir Dobrosavljević¹

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

Letter

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

Marius S. Frank¹, Tsung-Han Lee², Gargee Bhattacharyya¹, Pak Ki Henry Tsang,³ Victor L. Quito^{4,3},
Vladimir Dobrosavljević,³ Ove Christiansen⁵ and Nicola Lanatà^{1,6,*}

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

Operatorial formulation of the ghost rotationally invariant slave-boson theory

Nicola Lanatà^{*}

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

Exciton Mott transition revisited

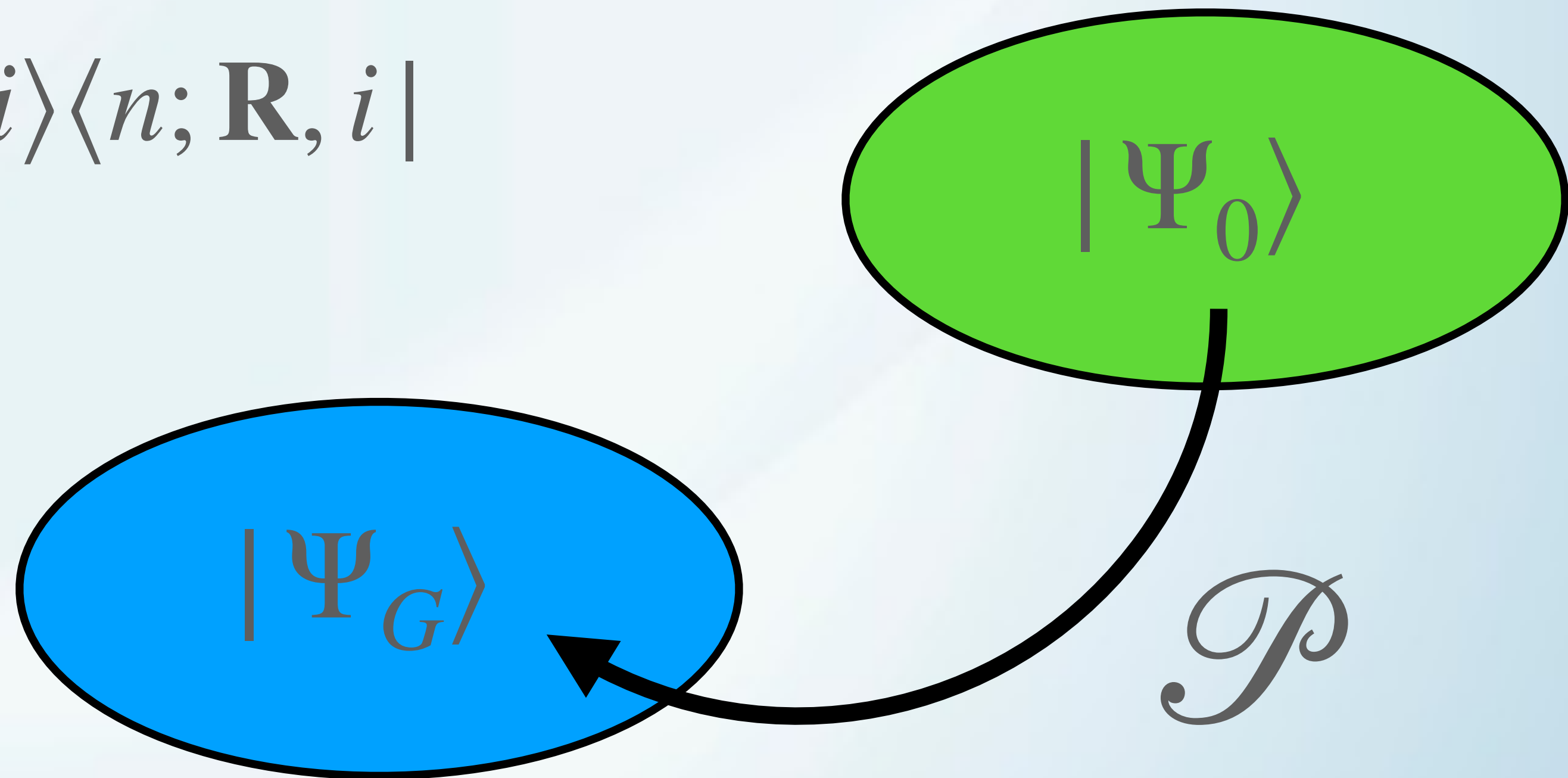
Daniele Guerci, Massimo Capone, and Michele Fabrizio

The GA variational wave function:

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

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

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

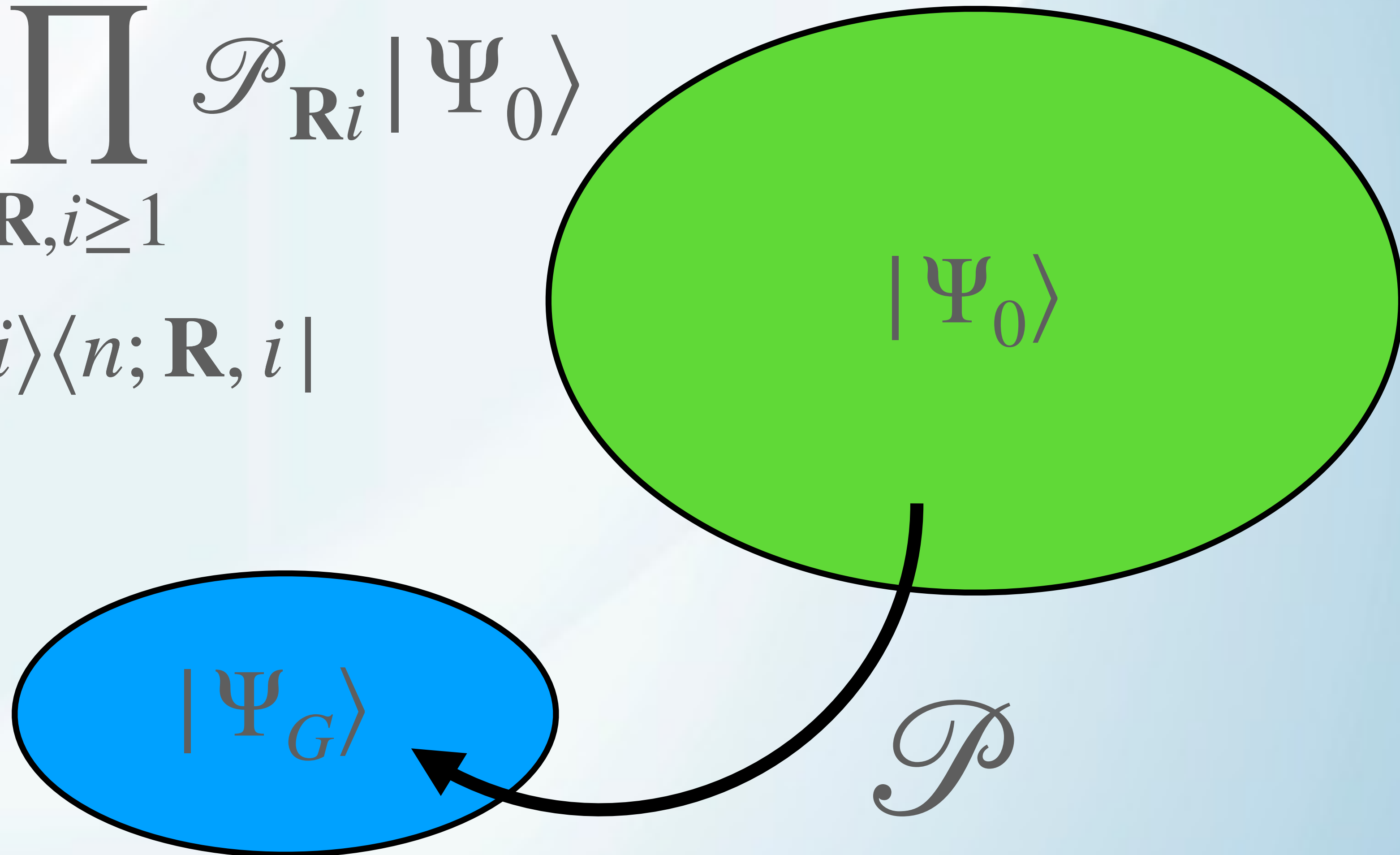


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Rectangular matrix: $2^{\nu_i} \times 2^{\tilde{\nu}_i}$

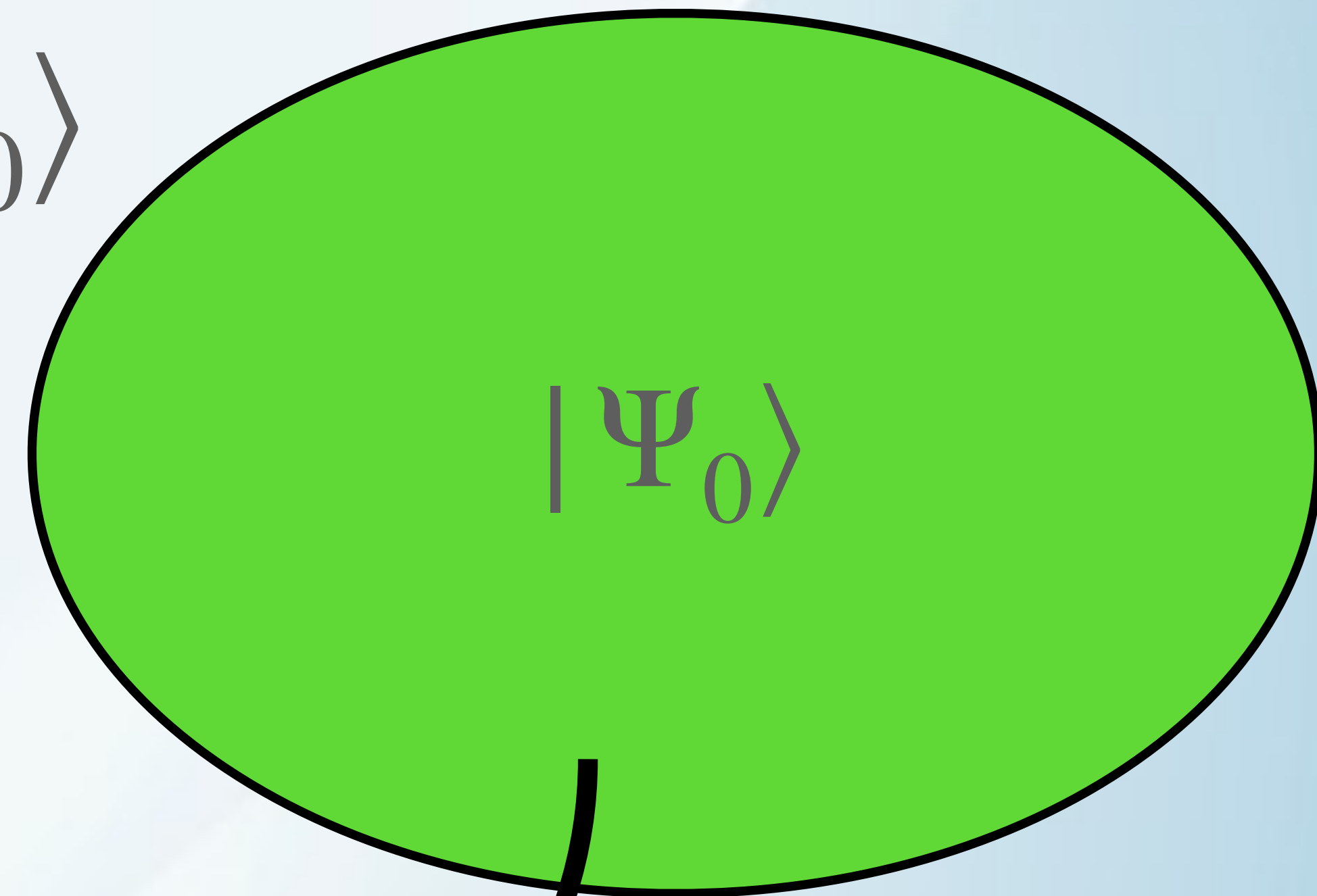
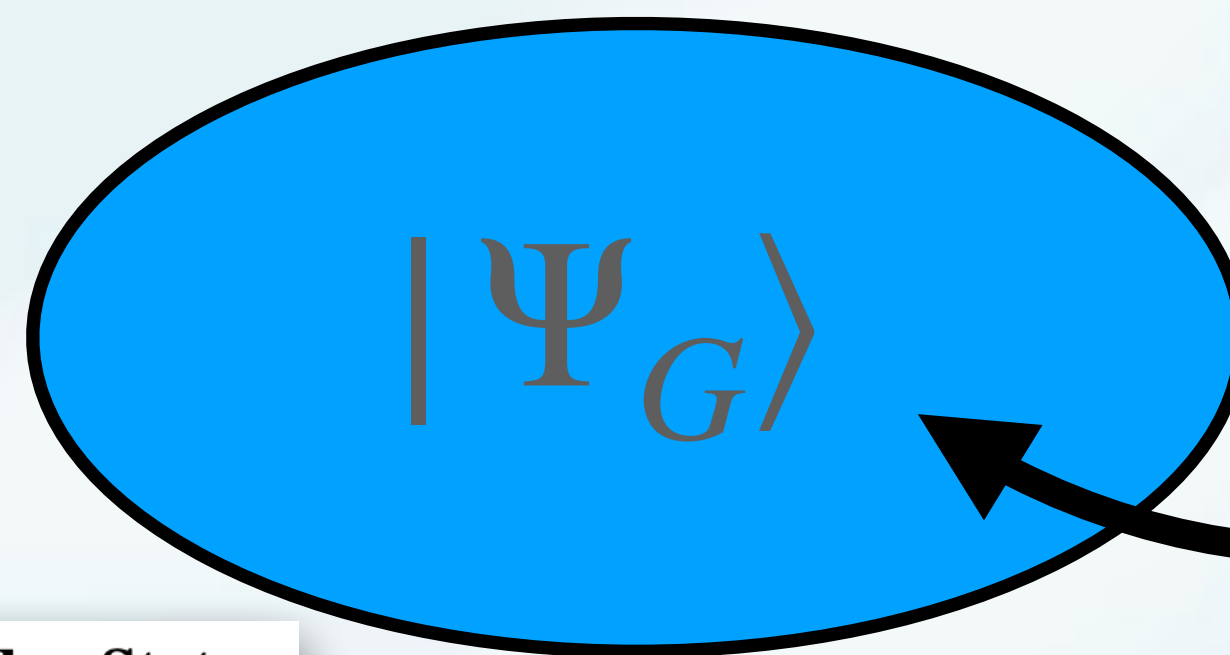


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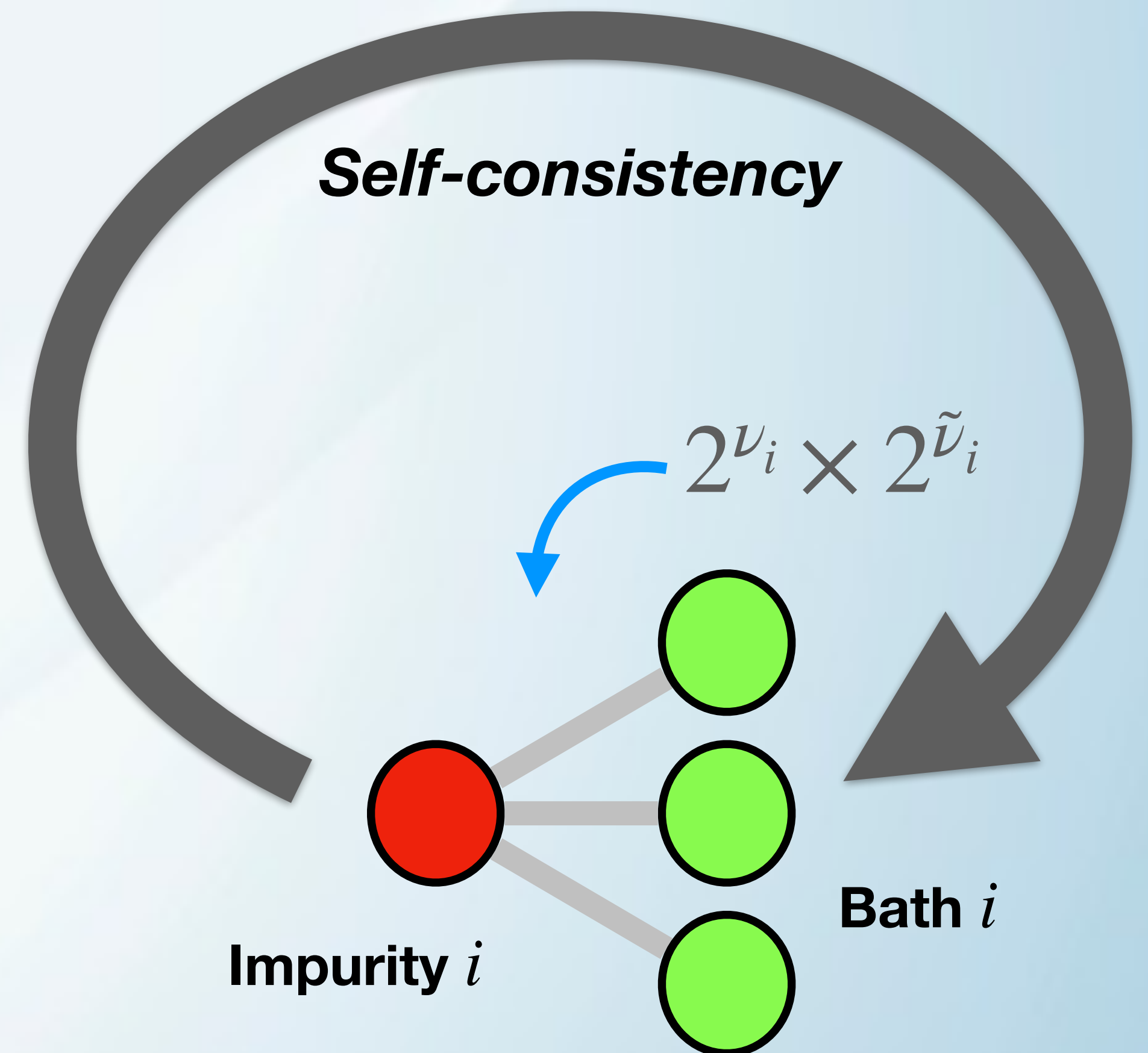
\mathcal{P}

The GA variational wave function:

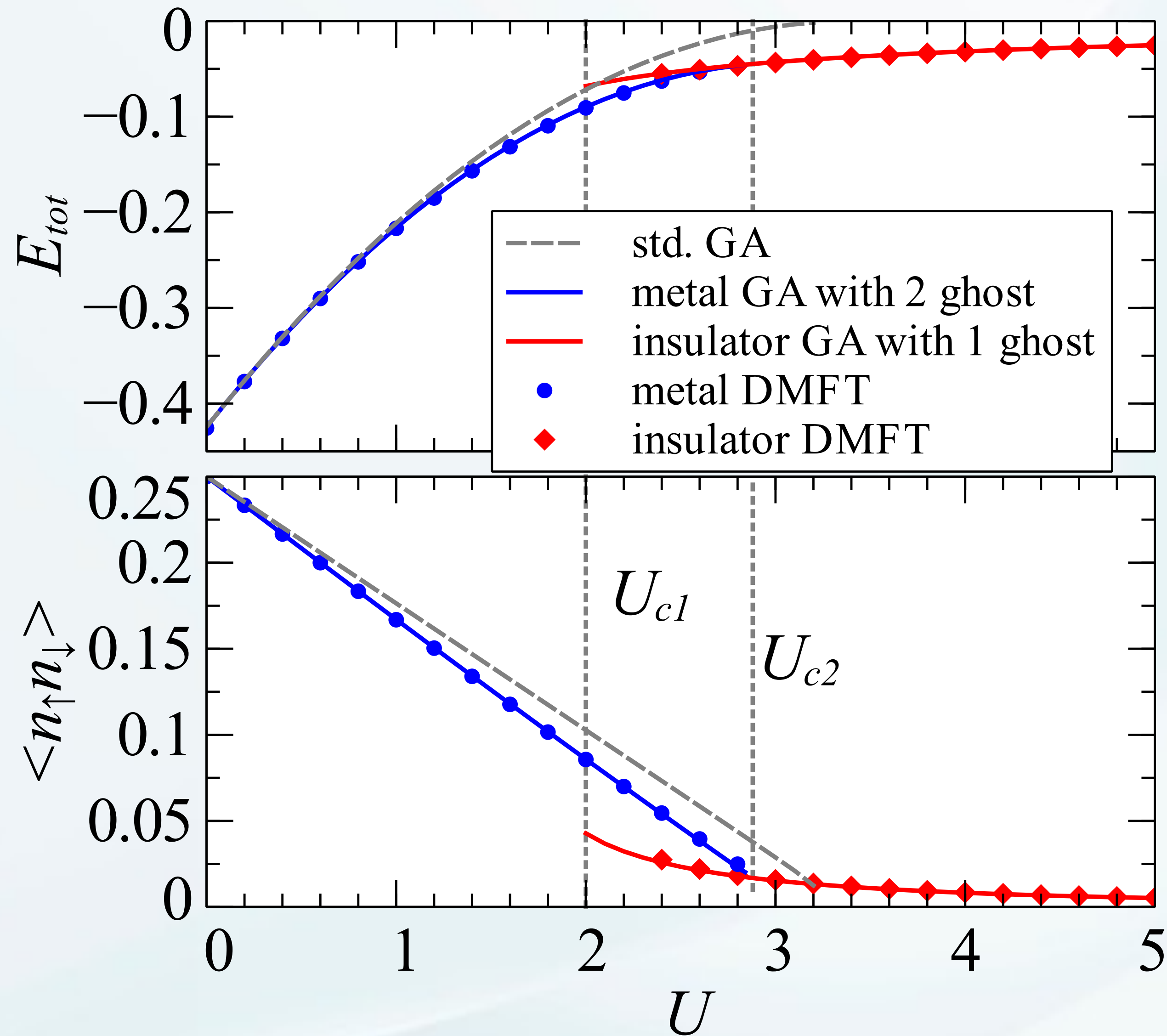
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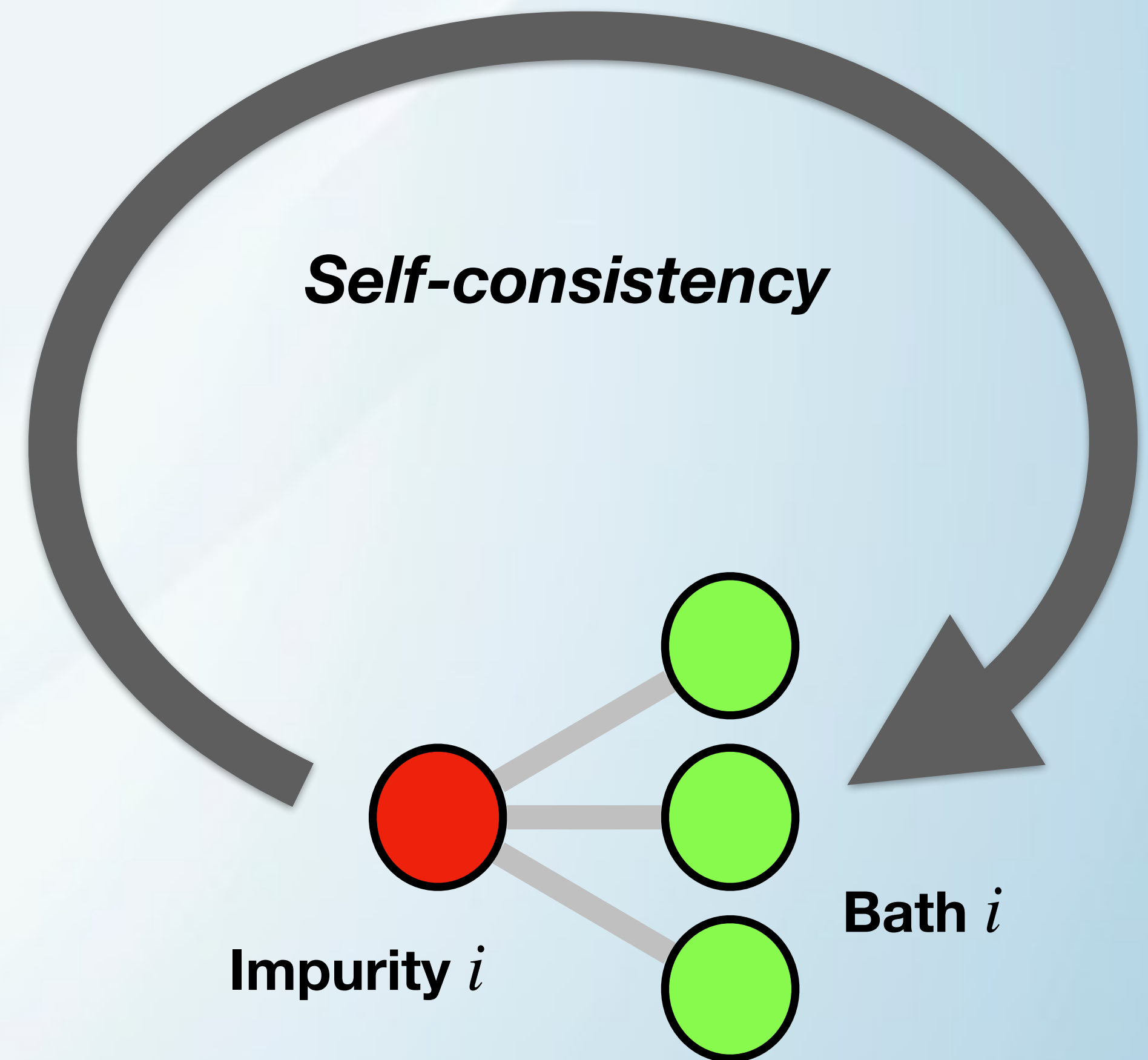
Rectangular matrix: $2^{\nu_i} \times 2^{\tilde{\nu}_i}$



Benchmark calculations Hubbard model:

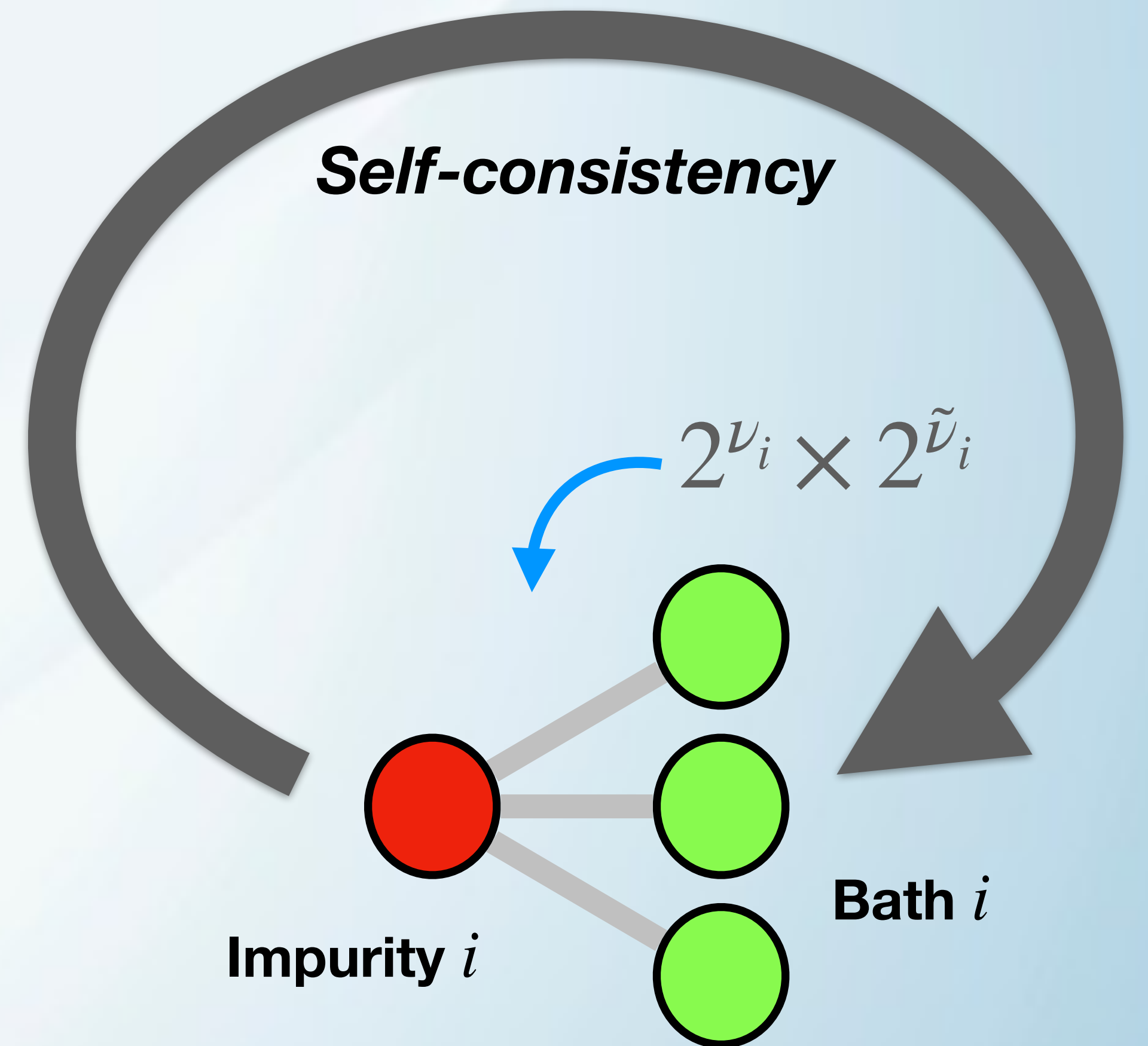
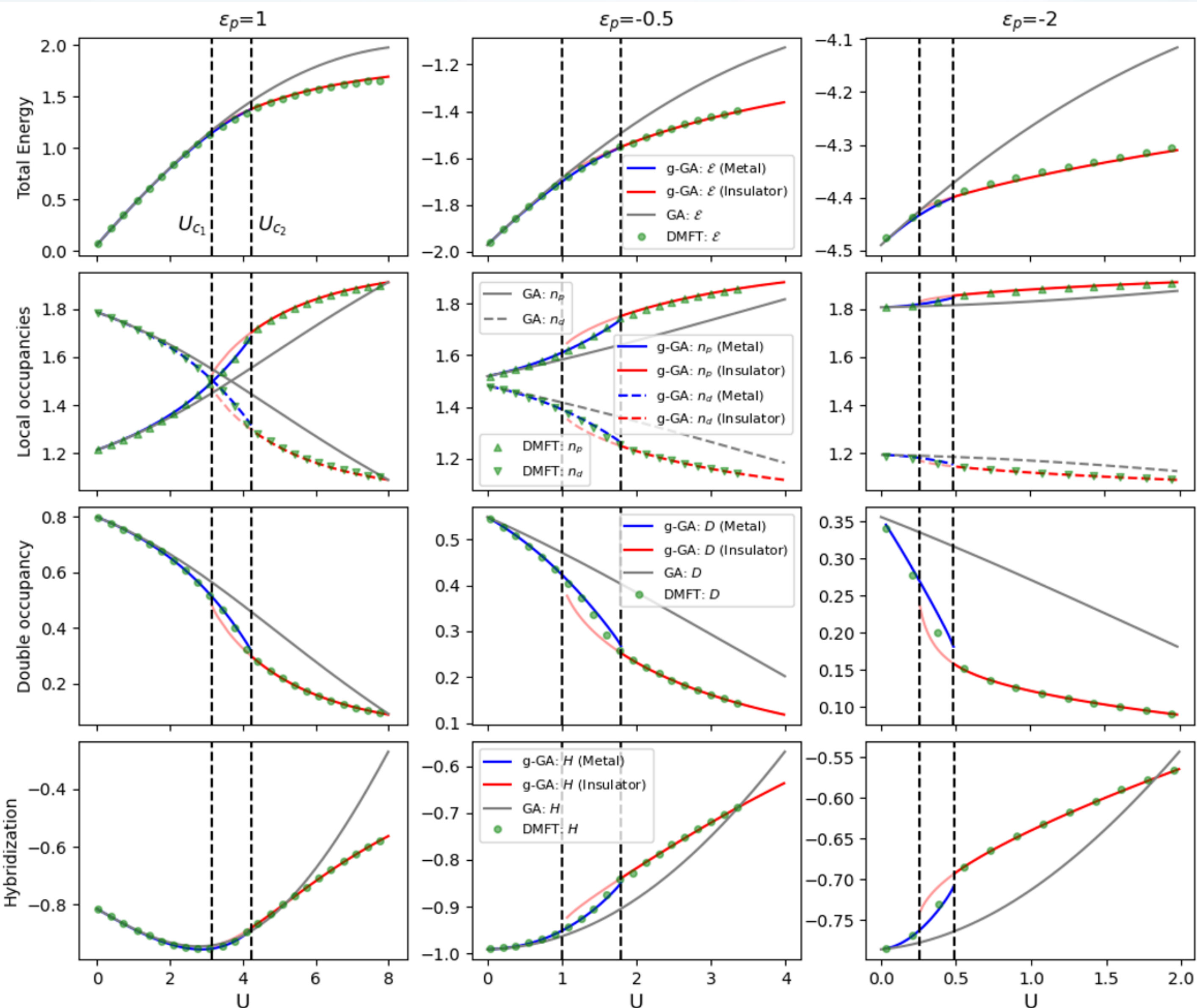


$$\hat{H} = \sum_{RR'} \sum_{\sigma} t_{RR'} c_{R\sigma}^{\dagger} c_{R'\sigma} + \sum_{R\sigma} U \hat{n}_{R\uparrow} \hat{n}_{R\downarrow}$$



Benchmark calculations ALM:

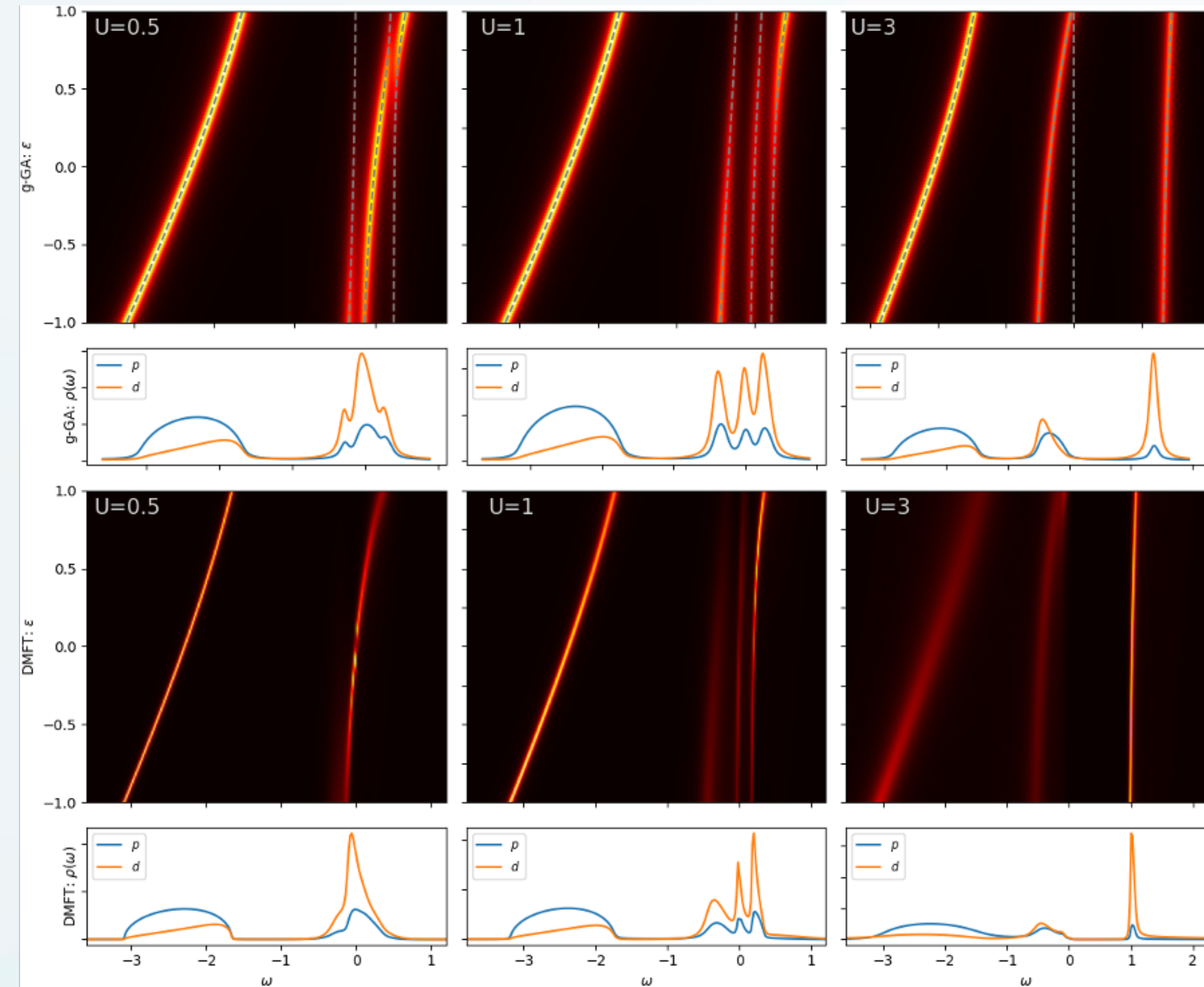
$$\hat{H} = \sum_{ij} \sum_{\sigma} (t_{ij} + \delta_{ij} \epsilon_p) p_{i\sigma}^{\dagger} p_{j\sigma} + \sum_i \frac{U}{2} (\hat{n}_{di} - 1)^2 + V \sum_{i\sigma} (p_{i\sigma}^{\dagger} d_{i\sigma} + \text{H.c.}) - \mu \sum_i \hat{N}_i$$



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



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

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[†], F Gebhard[‡] and W Weber[‡]

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

Landau-Gutzwiller quasiparticles

Jörg Bünemann

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

Florian Gebhard

Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany

Rüdiger Thul

Abteilung Theorie, Hahn-Meitner-Institut Berlin, D-14109 Berlin, Germany

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

Phase Diagram and Electronic Structure of Praseodymium and Plutonium

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VOLUME 57, NUMBER 11

PHYSICAL REVIEW LETTERS

15 SEPTEMBER 1986

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

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

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

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

Frank Lechermann,^{1,2,*} Antoine Georges,² Gabriel Kotliar,^{2,3} and Olivier Parcollet⁴

PRL **118**, 126401 (2017)

PHYSICAL REVIEW LETTERS

week ending
24 MARCH 2017

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

Nicola Lanatà,^{1,*} Yongxin Yao,^{2,†} Xiaoyu Deng,³ Vladimir Dobrosavljević,¹ and Gabriel Kotliar^{3,4}

PHYSICAL REVIEW B **76**, 193104 (2007)

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

J. Bünemann and F. Gebhard

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

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

Nicola Lanatà,¹ Paolo Barone,¹ and Michele Fabrizio^{1,2}

Some useful references:

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

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

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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^{1,2}, Tsung-Han Lee³, Sahar Pakdel⁴, Wenhui Xu⁵, Vladimir Dobrosavljević², Yong-Xin Yao⁶, Ove Christiansen^{7,*}, and Nicola Lanatà^{4,8,†}

PRL **105**, 076401 (2010)

PHYSICAL REVIEW LETTERS

week ending
13 AUGUST 2010

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

Marco Schiró¹ and Michele Fabrizio^{1,2}

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

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

Nicola Lanatà¹ and Hugo U. R. Strand²

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

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

Nicola Lanatà,^{*} Xiaoyu Deng, and Gabriel Kotliar

RAPID COMMUNICATIONS

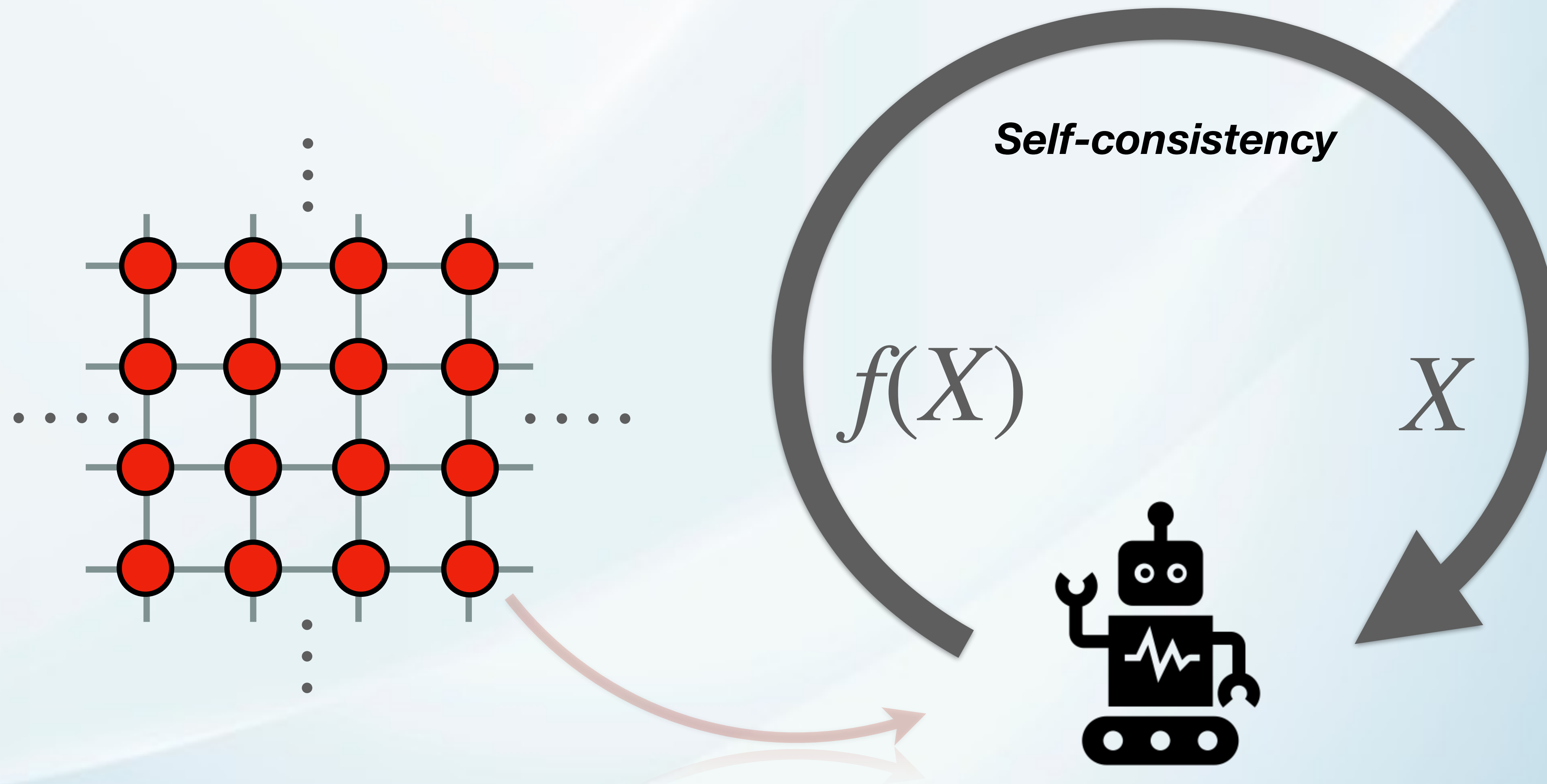
***THANK YOU FOR YOUR
ATTENTION !!!***

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,^{1,*} Alejandro Lopez-Bezanilla,² O. Anatole von Lilienfeld,^{3,4} and Andrew J. Millis¹

John Rogers^{1,2}, Tsung-Han Lee³, Sahar Pakdel⁴, Wenhui Xu⁵, Vladimir Dobrosavljević², Yong-Xin Yao⁶, Ove Christiansen^{7,*} and Nicola Lanà^{4,8,†}



First exploratory benchmark: DFT+GA

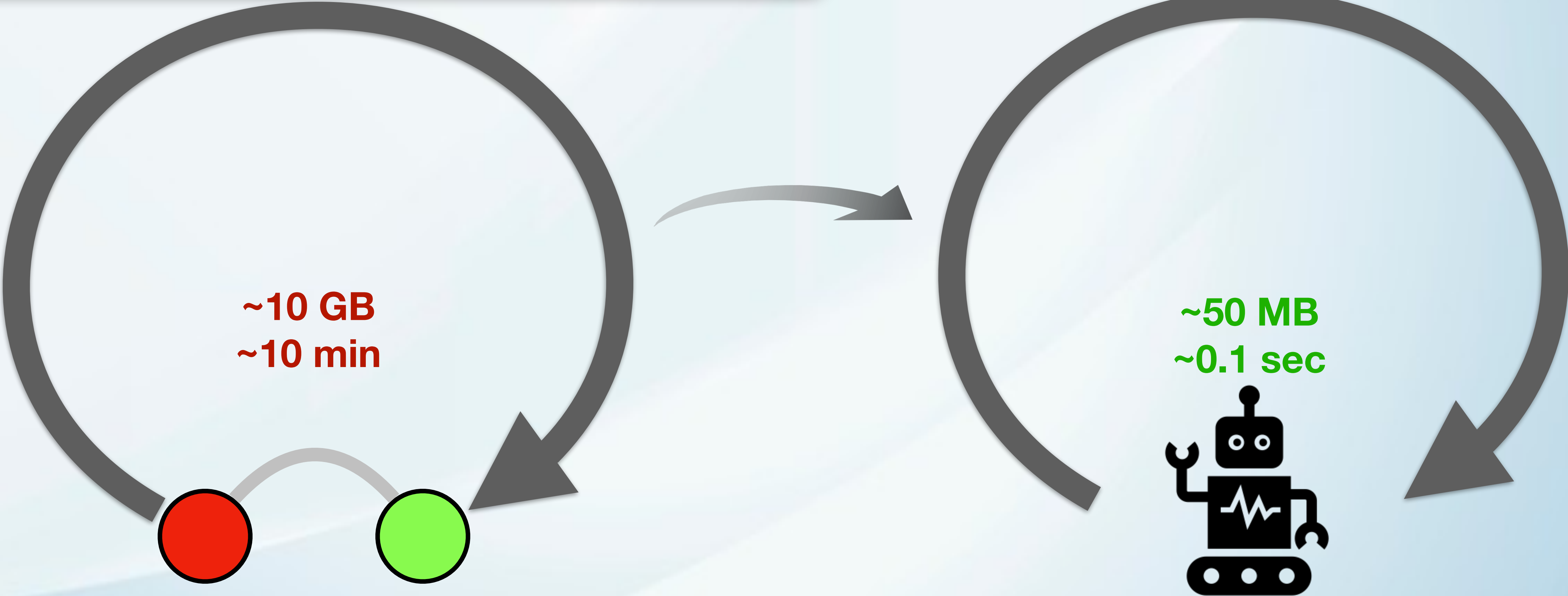
PHYSICAL REVIEW RESEARCH 3, 013101 (2021)

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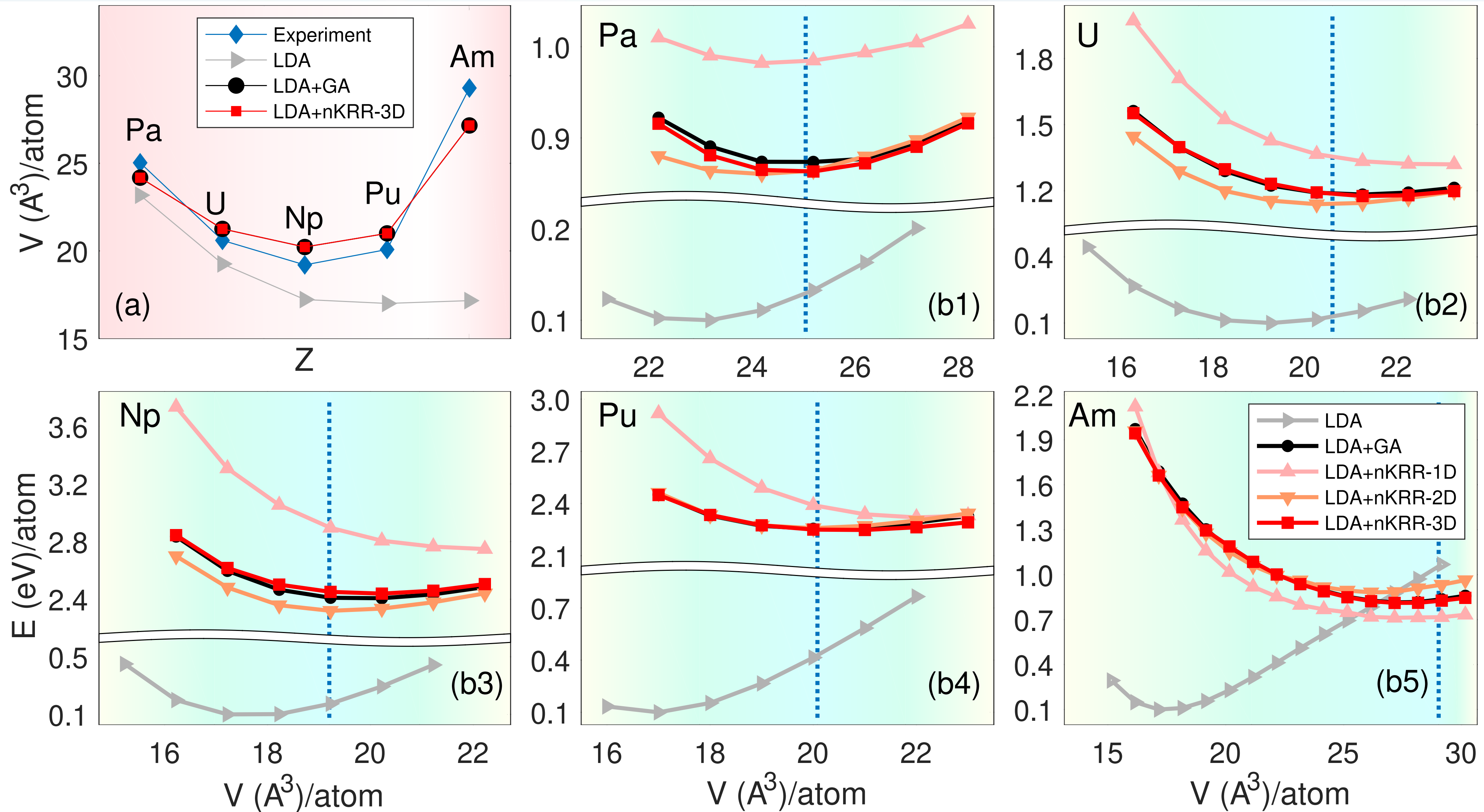
John Rogers^{1,2}, Tsung-Han Lee³, Sahar Pakdel⁴, Wenhui Xu⁵, Vladimir Dobrosavljević², Yong-Xin Yao⁶, Ove Christiansen^{7,*} and Nicola Lanatà^{4,8,†}

Study of series of actinide systems.

Simplifications from prior knowledge imbued within the regression problem



First exploratory benchmark: DFT+GA actinide systems



$n = 1$: 65

$n = 2$: 1626

$n = 3$: 19346

$n = 5$: 1410031

Benchmark calculations ALM:

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

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

