Rotationally Invariant Slave-Boson and application in combination with Density Functional Theory

Nicola Lanatà (MagLab)

Assistant for Hands-on Session: Tsung-Han Lee

E-mail: lanata@magnet.fsu.edu

NATIONAL HIGH MAGNETIC FIELD LABORATORY

ICAM-I2CAM Institute for Complex Adaptive Matter

Institute for Complex Adaptive Matter

Visit Tallahassee
A Division of Leon County

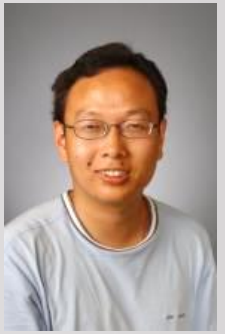
LECTURE

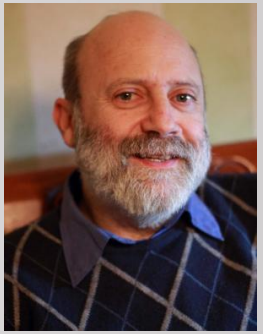
RISB formalism, numerical implementation and application in combination with DFT

N. Lanatà, Y. Yao, X. Deng, V. Dobrosavljevic and G. Kotliar, arXiv:1606.09614 (2016)
N. Lanatà, Y. Yao, C.-Z. Wang, K.-M. Ho, and G. Kotliar, PRX **5**, 011008 (2015)
N. Lanatà, H. U. R. Strand, X. Dai and B. Hellsing, Phys. Rev. B, **85**, 035133 (2012)
N. Lanatà, P. Barone and M. Fabrizio, Phys. Rev. B **78**, 155127 (2008)
F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, PRB **76**, 155102 (2007)

HANDS-ON SESSION
(assistant: Tsung-Han Lee)

Using RISB Code Developed with
Yongxin Yao (Iowa) and Gabriel Kotliar (Rutgers)





Implementation of LAPW interface with the DFT WIEN2K code adapted from DFT+DMFT code of: K. Haule et al., see Phys. Rev. B 81, 195107 (2010).

LECTURE OUTLINE:

Introduction (what is DFT+RISB useful for?)

Operatorial Formulation Rotationally Invariant Slave Boson (RISB)

- The Single-Band Hubbard Model
- Slave Boson representations Hubbard Hamiltonian
- Slave Boson Mean Field Approximation

Algorithms and Implementation RISB mean field theory

- Functional Formulation
- Stationarity Equations and Numerical Implementation

DFT + Slave Boson Approximation (DFT+RISB)

- The correlated orbitals
- DFT+RISB: Solving iteratively Kohn-Sham-Hubbard model
- Examples: low-symmetry systems (UO_2), polymorphism

Reference system to describe strongly-correlated materials (determined from K.S.)

Generic multi-band Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \sum_{ij} \sum_{\alpha\beta} \epsilon^{\alpha\beta}_{\mathbf{k},ij} \, c^{\dagger}_{\mathbf{k}i\alpha} c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}i \in \mathrm{corr}} \hat{H}^{\mathrm{loc}}_{i} [\{c^{\dagger}_{\mathbf{R}i\alpha}\}, \{c_{\mathbf{R}i\alpha}\}]$$

$$\epsilon_{\mathbf{k}} = \left[\begin{array}{c|c|c} i=0 & * & * \\ \hline * & i=1 & * \\ \hline * & * & i=2 \end{array}\right]$$

R = label unit cell
k = Fourier-conjugate of R
α, β = orbitals in R, *i*

(Example: *i* = 0: uncorrelated orbitals; *i* = 1: d orbitals atom 1
***i* = 2: *f* orbitals atom 2 …)**

What is RISB/GA good for?

RISB (mean field) Theory / GA

- Non-perturbative many-body technique which can be viewed as a ("good") approximation to DMFT.
- Largely complementary to DMFT because it is much less computationally demanding.

(The general RISB theory (before mean-field approximation) is an exact reformulation of the many-body problem.)

What is RISB/GA good for?

RISB (mean field) Theory / GA

Materials Genome Initiative

www.whitehouse.gov/mgi

About | Goals | Examples | News & Announcements | Federal Programs | External Stakeholder Activities | Contact Us

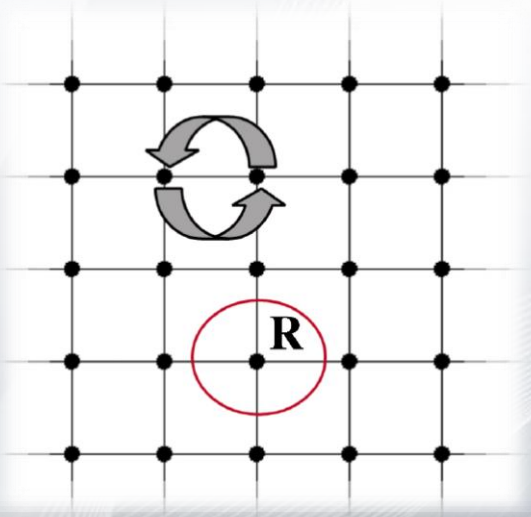
To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative. The invention of silicon circuits and lithium-ion batteries made computers and iPods and iPads possible -- but it took years to get those technologies from the drawing board to the marketplace. We can do it faster.

– President Obama, June 2011 at Carnegie Mellon University

Quadratic part correlated local orbitals included in $\mathcal{H}^{loc}$

The Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{RR}'}\sum_{\sigma} \epsilon_{\mathbf{RR}'}\, c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} U\, c^{\dagger}_{\mathbf{R}\uparrow} c_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow}$$



R = label site
σ = spin = ↑;↓
U = Hubbard strength
$\epsilon_{\mathbf{RR}'}$ = hopping coefficients

$$\mathcal{H}_F = \otimes_{\mathbf{R}} \mathcal{H}_F^{\mathbf{R}}\,; \quad \mathcal{H}_F^{\mathbf{R}} = \langle \{ |0,\mathbf{R}\rangle, |\uparrow,\mathbf{R}\rangle, |\downarrow,\mathbf{R}\rangle, |\uparrow\downarrow,\mathbf{R}\rangle, \} \rangle$$
$$= \langle \{ |0\rangle, c^{\dagger}_{\mathbf{R}\uparrow}|0\rangle, c^{\dagger}_{\mathbf{R}\downarrow}|0\rangle, c^{\dagger}_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow}|0\rangle \} \rangle$$

Focus on the local space at given R

Local Hilbert Space

$$\begin{aligned}\mathcal{H}_F^{\mathbf{R}} &= \langle\{|0,\mathbf{R}\rangle, |\uparrow,\mathbf{R}\rangle, |\downarrow,\mathbf{R}\rangle, |\uparrow\downarrow,\mathbf{R}\rangle,\}\rangle \\ &= \langle\{|0\rangle, c^\dagger_{\mathbf{R}\uparrow}|0\rangle, c^\dagger_{\mathbf{R}\downarrow}|0\rangle, c^\dagger_{\mathbf{R}\uparrow}c^\dagger_{\mathbf{R}\downarrow}|0\rangle\}\rangle\end{aligned}$$

Define unitary map from Fermionic many-body local Fock space $\mathcal{H}_F^{\mathbf{R}}$ into bigger Hilbert space $\mathcal{H}_{SB}^{\mathbf{R}}$ (generated by "artificial" Bosonic and Fermionic degrees of freedom)

(Scope: derive equivalent reformulation of the Hubbard model more suitable to define a mean-field approximation)

Defining mapping onto subspace of infinite-dimensional Hilbert space

Slave-Boson Local Hilbert Space

$\mathcal{H}^{\mathbf{R}}_{SB}$ **generated by "artificial" Bosonic and Fermionic degrees of freedom**
(dimension $\mathcal{H}^{\mathbf{R}}_{SB} = \infty$**)**

$$\mathcal{H}^{\mathbf{R}}_{F}$$

$$\langle\{|0\rangle, c^{\dagger}_{\mathbf{R}\uparrow}|0\rangle, c^{\dagger}_{\mathbf{R}\downarrow}|0\rangle, c^{\dagger}_{\mathbf{R}\uparrow}c^{\dagger}_{\mathbf{R}\downarrow}|0\rangle\}\rangle \equiv \{|A,\mathbf{R}\rangle\}$$

$$\{c^{\dagger}_{\mathbf{R}\sigma}, c_{\mathbf{R}\sigma}\}$$

$$\mathcal{H}^{\mathbf{R}}_{SB}$$

$$\langle\{|0\rangle, f^{\dagger}_{\mathbf{R}\uparrow}|0\rangle, f^{\dagger}_{\mathbf{R}\downarrow}|0\rangle, f^{\dagger}_{\mathbf{R}\uparrow}f^{\dagger}_{\mathbf{R}\downarrow}|0\rangle\}\rangle \equiv \{|n,\mathbf{R}\rangle\}$$

$$\{f^{\dagger}_{\mathbf{R}\sigma}, f_{\mathbf{R}\sigma};\ \Phi^{\dagger}_{\mathbf{R}An}, \Phi_{\mathbf{R}An}\}$$

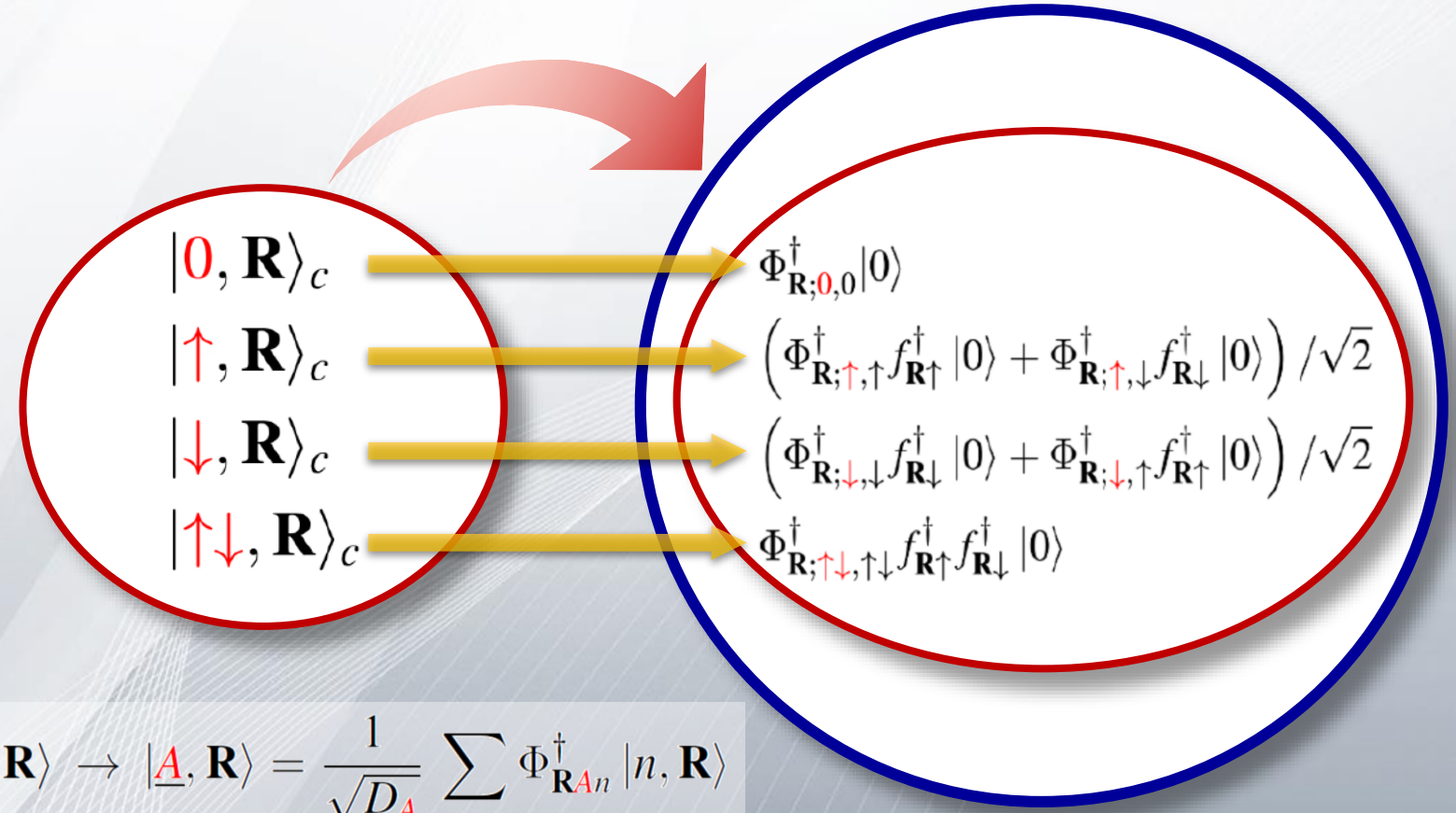
$$\left(\text{e.g.,}\quad \Phi^{\dagger}_{..}\ldots\Phi^{\dagger}_{..}f^{\dagger}_{..}\ldots f^{\dagger}_{..}|0\rangle\right)$$

$$(\ \Phi_{\mathbf{R}An} \text{ only for } N_A = N_n)$$

Quadratic part correlated local orbitals included in $\mathcal{H}^{loc}$

Slave-Boson Local Hilbert Space

$\mathcal{H}^{\mathbf{R}}_{SB}$ **generated by "artificial" Bosonic and Fermionic degrees of freedom (dimension** $\mathcal{H}^{\mathbf{R}}_{SB} = \infty$**)**

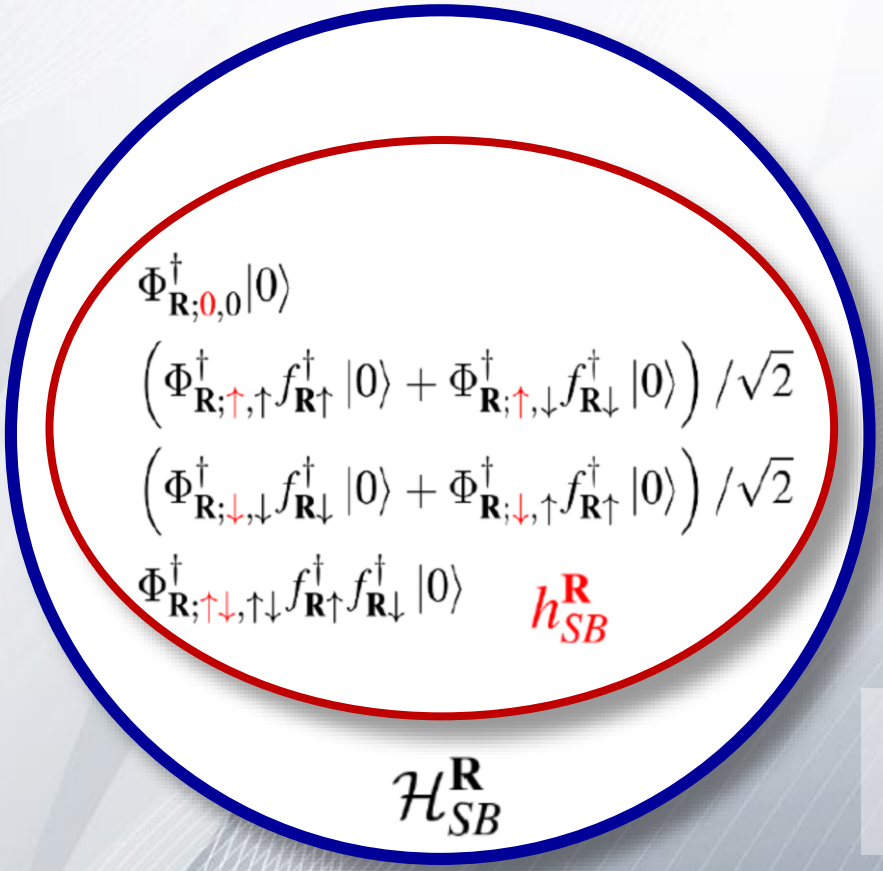


$$|A,\mathbf{R}\rangle \rightarrow |\underline{A},\mathbf{R}\rangle = \frac{1}{\sqrt{D_A}} \sum_n \Phi^{\dagger}_{\mathbf{R}An} |n,\mathbf{R}\rangle$$

Gutzwiller constraints (introducing definition F_a matrices)

Operatorial Gutzwiller Constraints

Physical subspace $h^{\mathbf{R}}_{SB}$ of $\mathcal{H}^{\mathbf{R}}_{SB}$ identified by operatorial identities



$$\sum_{An} \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}An} = 1$$

$$\sum_{Anm} [F^{\dagger}_a F_b]_{mn} \, \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Am} = f^{\dagger}_{\mathbf{R}a} f_{\mathbf{R}b}$$

$$\left([F_a]_{nm} \equiv \langle n, \mathbf{R}| f_{\mathbf{R}a} |m, \mathbf{R}\rangle \right)$$

$$|A, \mathbf{R}\rangle \rightarrow |\underline{A}, \mathbf{R}\rangle = \frac{1}{\sqrt{D_A}} \sum_n \Phi^{\dagger}_{\mathbf{R}An} |n, \mathbf{R}\rangle$$

Slave Bosons = "Local Modes" (interaction becomes *quadratic*)

The Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'} c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} U\, c^{\dagger}_{\mathbf{R}\uparrow} c_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow}$$

SB representation local interaction

$$\hat{H}^{\mathrm{loc}} \equiv \sum_{\mathbf{R}} U\, c^{\dagger}_{\mathbf{R}\uparrow} c_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow} = \sum_{\mathbf{R}} \sum_{AB} [H^{\mathrm{loc}}]_{AB} |A, \mathbf{R}\rangle \langle B, \mathbf{R}|$$

$$\underline{\hat{H}}^{\mathrm{loc}} \equiv \sum_{\mathbf{R}} \sum_{n} U\, \Phi^{\dagger}_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} = \sum_{\mathbf{R}} \sum_{AB} [H^{\mathrm{loc}}]_{AB} \sum_{n} \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Bn}$$

$\underline{\hat{H}}^{\mathrm{loc}}$ is a *faithful representation* of $\hat{H}^{\mathrm{loc}}$, i.e.:

$$\langle \underline{A}, \mathbf{R}| \underline{\hat{H}}^{\mathrm{loc}} |\underline{B}, \mathbf{R}\rangle = \langle A, \mathbf{R}| \hat{H}^{\mathrm{loc}} |B, \mathbf{R}\rangle = [H^{\mathrm{loc}}]_{AB} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{bmatrix}_{AB}$$

The Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'} \, c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} U \, c^{\dagger}_{\mathbf{R}\uparrow} c_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow}$$

SB representation hopping (non-local) term

We look for SB representation Ladder operators

We will construct Bosonic $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$ such that:

$$\underline{c}^{\dagger}_{\mathbf{R}\alpha} \equiv \sum_{a} \hat{\mathcal{R}}_{\mathbf{R}a\alpha} [\Phi_{\mathbf{R}An}, \Phi^{\dagger}_{\mathbf{R}An}] f^{\dagger}_{\mathbf{R}a} \, .$$

$$\langle \underline{A}, \mathbf{R} | \, \underline{c}^{\dagger}_{\mathbf{R}\alpha} \, | \underline{B}, \mathbf{R} \rangle = \langle A, \mathbf{R} | \, c^{\dagger}_{R\alpha} \, | B, \mathbf{R} \rangle \quad \forall A, B$$

Choice of $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$ affects mean-field approximation

Construction of $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$ such that

$$\langle \underline{A}, \mathbf{R}| \underline{c}^{\dagger}_{\mathbf{R}\alpha} |\underline{B}, \mathbf{R}\rangle = \langle A, \mathbf{R}| c^{\dagger}_{R\alpha} |B, \mathbf{R}\rangle \quad \forall A, B$$

With no loss of generality,
we can search for solution represented as:

$$\hat{\mathcal{R}}_{\mathbf{R}a\alpha} = : \left[r^{(0)}_{\mathbf{R}a\alpha} + [r^{(2)}_{\mathbf{R}a\alpha}]_{An,Bm}\, \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Bm} + \right.$$
$$\left. + \; [r^{(4)}_{\mathbf{R}a\alpha}]_{An,Bm,Cl,Dr}\, \Phi^{\dagger}_{\mathbf{R}An} \Phi^{\dagger}_{\mathbf{R}Bm} \Phi_{\mathbf{R}Cl} \Phi_{\mathbf{R}Dr} + \cdots \right] :$$

***One of the possible solutions is* (PRB 76, 155102 (2007)) :**

$$\hat{\mathcal{R}}_{\mathbf{R}a\alpha} = \sum_{AB} \sum_{nm} \frac{1}{N_A} \sqrt{\frac{D_B}{D_A}} [F^{\dagger}_{\alpha}]_{AB} [F^{\dagger}_{a}]_{nm} \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Bm}$$

Alternative $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$ suitable for MF approximation

arXiv:1606.09614 (2016)

$$\hat{\mathcal{R}}_{\mathbf{R}a\alpha} \equiv \sum_{ABnmb} \frac{1}{N_A}\sqrt{\frac{D_B}{D_A}}\,[F^{\dagger}_{\alpha}]_{AB}[F^{\dagger}_{b}]_{nm} : \Phi^{\dagger}_{\mathbf{R}An}\left[\hat{1}+\left(N_A\sqrt{\frac{D_A}{D_B}}-1\right)\sum_{Cl}\Phi^{\dagger}_{\mathbf{R}Cl}\Phi_{\mathbf{R}Cl}\right]\left[\left[\hat{1}-\hat{\Delta}_{\mathrm{p}}\right]^{[-\frac{1}{2}]}\bullet\left[\hat{1}-\hat{\Delta}_{\mathrm{h}}\right]^{[-\frac{1}{2}]}\right]_{\mathbf{R}ba}\Phi_{\mathbf{R}Bm} :$$

where:

$$[\hat{\Delta}_{\mathrm{p}}]_{\mathbf{R}ab} \equiv \sum_{Anm}[F^{\dagger}_{a}F_{b}]_{mn}\,\Phi^{\dagger}_{\mathbf{R}An}\Phi_{\mathbf{R}Am}$$

$$[\hat{\Delta}_{\mathrm{h}}]_{\mathbf{R}ab} \equiv \sum_{Anm}[F_{b}F^{\dagger}_{a}]_{mn}\,\Phi^{\dagger}_{\mathbf{R}An}\Phi_{\mathbf{R}Am}$$

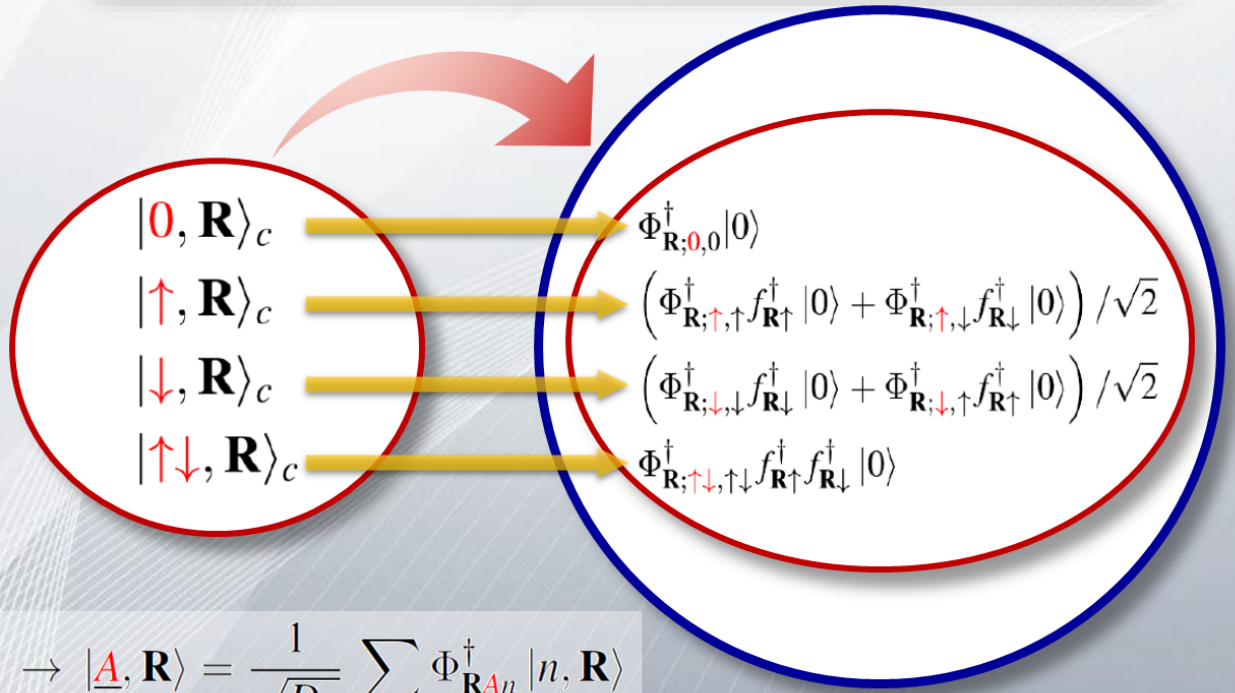
$$\left[\hat{1}-\hat{\Delta}\right]^{[-\frac{1}{2}]} \equiv \sum_{r=0}^{\infty}(-1)^r\binom{\frac{1}{2}}{r}[\hat{\Delta}]^{[r]}$$

Summary SB reformulation: quadratic interaction, "renormalized" hopping

The Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{R}\mathbf{R}'}\sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'}\, c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} U\, c^{\dagger}_{\mathbf{R}\uparrow} c_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} c_{\mathbf{R}\downarrow}$$

$$\underline{\hat{H}} = \sum_{\mathbf{R}\mathbf{R}'}\sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'}\, \underline{c}^{\dagger}_{\mathbf{R}\sigma} \underline{c}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}}\sum_{n} U\, \Phi^{\dagger}_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n}$$

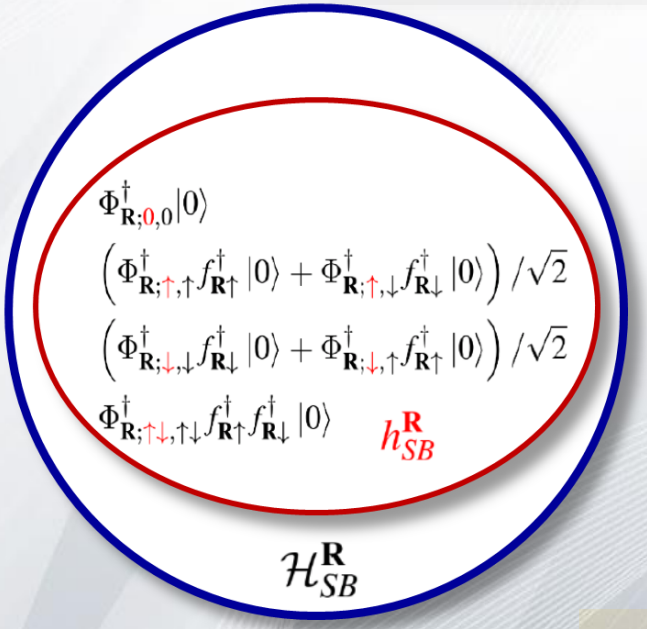


$$|A,\mathbf{R}\rangle \rightarrow |\underline{A},\mathbf{R}\rangle = \frac{1}{\sqrt{D_A}} \sum_{n} \Phi^{\dagger}_{\mathbf{R}An}\, |n,\mathbf{R}\rangle$$

Mean Field theory as a variational approximation

The Slave Boson Hubbard Hamiltonian

$$\hat{\underline{H}} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'}\, \underline{c}^{\dagger}_{\mathbf{R}\sigma} \underline{c}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} \sum_{n} U\, \Phi^{\dagger}_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n}$$



$$\sum_{An} \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}An} = 1$$

$$\sum_{Anm} [F^{\dagger}_{a} F_{b}]_{mn}\, \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Am} = f^{\dagger}_{\mathbf{R}a} f_{\mathbf{R}b}$$

$$\underline{c}^{\dagger}_{\mathbf{R}\alpha} \equiv \sum_{a} \hat{\mathcal{R}}_{\mathbf{R}a\alpha} [\Phi_{\mathbf{R}An}, \Phi^{\dagger}_{\mathbf{R}An}] f^{\dagger}_{\mathbf{R}a}$$

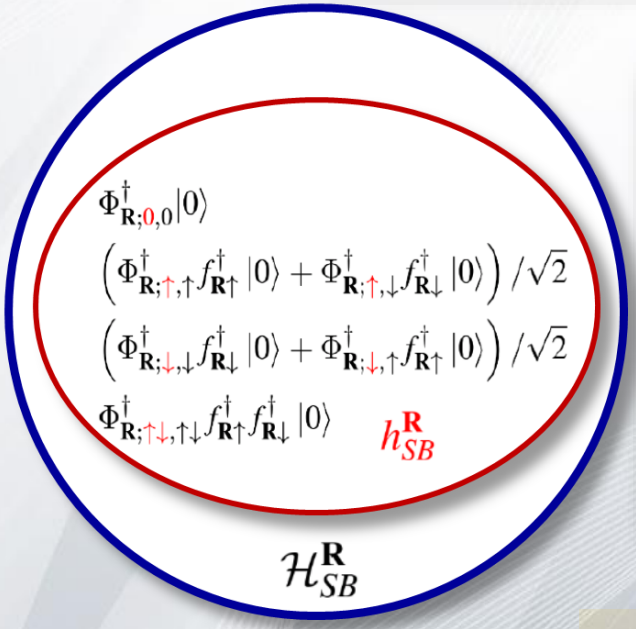
Assuming following variational ansatz:

$$|\Psi_{\mathrm{SB}}\rangle = |\Psi_0\rangle \otimes |\phi\rangle\,, \quad (\,\Phi_{\mathbf{R}An}|\phi\rangle = \phi_{An}|\phi\rangle\,)$$

We need to calculate average: 1) interaction, 2) constraints, 3) hopping

The Slave Boson Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'}\, \underline{c}^{\dagger}_{\mathbf{R}\sigma} \underline{c}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} \sum_{n} U\, \Phi^{\dagger}_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n}$$



$$\langle \Psi_{\mathrm{SB}} | \sum_{An} \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}An} - \hat{1} \, | \Psi_{\mathrm{SB}} \rangle = 0$$

$$\langle \Psi_{\mathrm{SB}} | \sum_{Anm} [F^{\dagger}_{a} F_{b}]_{mn} \, \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Am} - f^{\dagger}_{\mathbf{R}a} f_{\mathbf{R}b} \, | \Psi_{\mathrm{SB}} \rangle = 0$$

$$\underline{c}^{\dagger}_{\mathbf{R}\alpha} \equiv \sum_{a} \hat{\mathcal{R}}_{\mathbf{R}a\alpha} [\Phi_{\mathbf{R}An}, \Phi^{\dagger}_{\mathbf{R}An}] f^{\dagger}_{\mathbf{R}a}$$

Assuming following variational ansatz:

$$|\Psi_{\mathrm{SB}}\rangle = |\Psi_0\rangle \otimes |\phi\rangle \,, \quad \text{Constrained Minimization}$$

Expectation value Local Interaction ($\phi\phi^\dagger$ local reduced density matrix)

The Slave Boson Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'} \underline{c}^\dagger_{\mathbf{R}\sigma} \underline{c}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} \sum_{n} U \, \Phi^\dagger_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n}$$

Assuming following variational ansatz:

$$|\Psi_{\mathrm{SB}}\rangle = |\Psi_0\rangle \otimes |\phi\rangle$$

Local interaction:

$$\langle\phi| \sum_{\mathbf{R}} \sum_{n} U \, \Phi^\dagger_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} |\phi\rangle = \mathrm{Tr}[\phi\phi^\dagger H^{\mathrm{loc}}]$$

$$\left(H^{\mathrm{loc}}_{AB} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{bmatrix}_{AB} \right)$$

Expectation value Gutzwiller Constraints

The Slave Boson Hubbard Hamiltonian

$$\hat{\underline{H}} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'}\, \underline{c}^{\dagger}_{\mathbf{R}\sigma} \underline{c}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} \sum_{n} U\, \Phi^{\dagger}_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n}$$

Assuming following variational ansatz:

$$|\Psi_{\mathrm{SB}}\rangle = |\Psi_0\rangle \otimes |\phi\rangle$$

Gutzwiller constraints:

$$\langle \Psi_{\mathrm{SB}} | \sum_{An} \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}An} - \hat{1} \, | \Psi_{\mathrm{SB}} \rangle = \mathrm{Tr}[\phi^{\dagger}\phi] - 1 = 0$$

$$\langle \Psi_{\mathrm{SB}} | \sum_{Anm} [F^{\dagger}_a F_b]_{mn} \, \Phi^{\dagger}_{\mathbf{R}An} \Phi_{\mathbf{R}Am} - f^{\dagger}_{\mathbf{R}a} f_{\mathbf{R}b} \, | \Psi_{\mathrm{SB}} \rangle = \mathrm{Tr}[\phi^{\dagger}\phi \, F^{\dagger}_a F_b] - \langle \Psi_0 | f^{\dagger}_{\mathbf{R}a} f_{\mathbf{R}b} \, | \Psi_0 \rangle = 0$$

Expectation value Renormalization Operators

The Slave Boson Hubbard Hamiltonian

$$\hat{\underline{H}} = \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'}\, \underline{c}^{\dagger}_{\mathbf{R}\sigma} \underline{c}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} \sum_{n} U\, \Phi^{\dagger}_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n}$$

Assuming following variational ansatz:

$$|\Psi_{\mathrm{SB}}\rangle = |\Psi_0\rangle \otimes |\phi\rangle$$

Renormalization factors:

$$\langle\phi|\, \underline{c}^{\dagger}_{\mathbf{R}\alpha}\, |\phi\rangle = \sum_{a} \langle\phi|\, \hat{\mathcal{R}}_{\mathbf{R}a\alpha}[\Phi_{\mathbf{R}An}, \Phi^{\dagger}_{\mathbf{R}An}]\, |\phi\rangle\, f^{\dagger}_{\mathbf{R}a} \equiv \sum_{a} \mathcal{R}_{a\alpha}[\phi_{An}, \phi^{\dagger}_{An}]\, f^{\dagger}_{\mathbf{R}a}$$

Alternative $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$ suitable for MF approximation

$$\hat{\mathcal{R}}_{\mathbf{R}a\alpha} \equiv \sum_{ABnmb} \frac{1}{N_A}\sqrt{\frac{D_B}{D_A}}\,[F^\dagger_\alpha]_{AB}[F^\dagger_b]_{nm} : \Phi^\dagger_{\mathbf{R}An}\left[\hat{1}+\left(N_A\sqrt{\frac{D_A}{D_B}}-1\right)\sum_{Cl}\Phi^\dagger_{\mathbf{R}Cl}\Phi_{\mathbf{R}Cl}\right]\left[\left[\hat{1}-\hat{\Delta}_{\mathrm{p}}\right]^{[-\frac{1}{2}]}\bullet\left[\hat{1}-\hat{\Delta}_{\mathrm{h}}\right]^{[-\frac{1}{2}]}\right]_{\mathbf{R}ba}\Phi_{\mathbf{R}Bm} :$$

where:

$$[\hat{\Delta}_{\mathrm{p}}]_{\mathbf{R}ab} \equiv \sum_{Anm}[F^\dagger_a F_b]_{mn}\,\Phi^\dagger_{\mathbf{R}An}\Phi_{\mathbf{R}Am}$$

$$[\hat{\Delta}_{\mathrm{h}}]_{\mathbf{R}ab} \equiv \sum_{Anm}[F_b F^\dagger_a]_{mn}\,\Phi^\dagger_{\mathbf{R}An}\Phi_{\mathbf{R}Am}$$

$$\left[\hat{1}-\hat{\Delta}\right]^{[-\frac{1}{2}]} \equiv \sum_{r=0}^{\infty}(-1)^r\binom{\frac{1}{2}}{r}[\hat{\Delta}]^{[r]}$$

Mean Field renormalization factors

$$\mathcal{R}_{a\alpha} \equiv \langle\phi|\,\hat{\mathcal{R}}_{\mathbf{R}a\alpha}\,|\phi\rangle = \sum_b \mathrm{Tr}[\phi^\dagger F_\alpha^\dagger \phi F_b]\,[(1-\Delta_p)\Delta_p]^{-\frac{1}{2}}_{ba}$$

where: $\quad [\Delta_p]_{ab} = \mathrm{Tr}[\phi^\dagger\phi\, F_a^\dagger F_b]$

Consequently, in summary:

$$\langle\Psi_{SB}|\sum_{\mathbf{R}\mathbf{R}'}\sum_\sigma \epsilon_{\mathbf{R}\mathbf{R}'}\,\underline{c}^\dagger_{\mathbf{R}\sigma}\underline{c}_{\mathbf{R}'\sigma}\,|\Psi_{SB}\rangle = |\mathcal{R}(\phi)|^2\,\langle\Psi_0|\sum_{\mathbf{R}\mathbf{R}'}\sum_\sigma \epsilon_{\mathbf{R}\mathbf{R}'}\,f^\dagger_{\mathbf{R}\sigma}f_{\mathbf{R}'\sigma}\,|\Psi_0\rangle$$

$$\langle\Psi_{SB}|\sum_{\mathbf{R}n} U\,\Phi^\dagger_{\mathbf{R};\uparrow\downarrow,n}\Phi_{\mathbf{R};\uparrow\downarrow,n}\,|\Psi_{SB}\rangle = \mathrm{Tr}[\phi\phi^\dagger\,H^{\mathrm{loc}}]$$

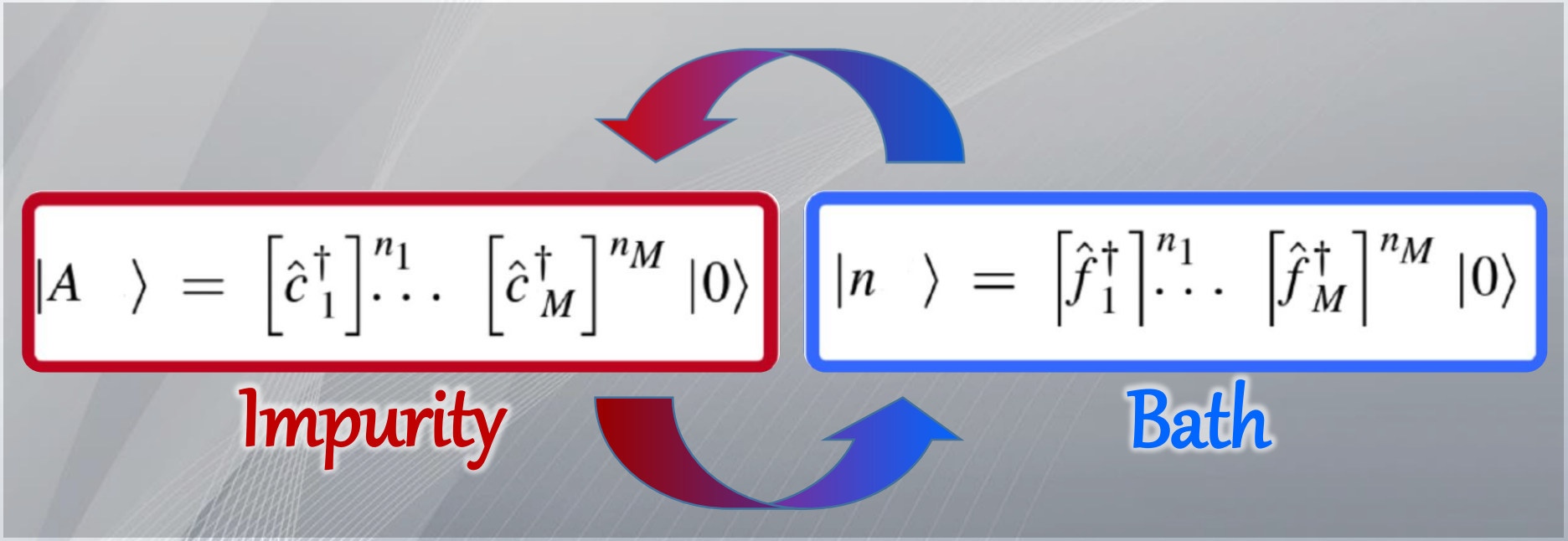
$$\langle\Psi_{\mathrm{SB}}|\sum_{An}\Phi^\dagger_{\mathbf{R}An}\Phi_{\mathbf{R}An} - \hat{1}\,|\Psi_{\mathrm{SB}}\rangle = \mathrm{Tr}[\phi^\dagger\phi] - 1 = 0$$

$$\langle\Psi_{\mathrm{SB}}|\sum_{Anm}[F_a^\dagger F_b]_{mn}\,\Phi^\dagger_{\mathbf{R}An}\Phi_{\mathbf{R}Am} - f^\dagger_{\mathbf{R}a}f_{\mathbf{R}b}\,|\Psi_{\mathrm{SB}}\rangle = \mathrm{Tr}[\phi^\dagger\phi\,F_a^\dagger F_b] - \langle\Psi_0|f^\dagger_{\mathbf{R}a}f_{\mathbf{R}b}\,|\Psi_0\rangle = 0$$

Observation: number of independent SB amplitudes (ignoring symmetry)

Number of independent complex parameters ϕ is $2^2 \times 2^2$

(as dimension "impurity model" whose bath has same dimension of the "impurity" $\mathcal{H}_F^{\mathbf{R}}$)



Quadratic part correlated local orbitals included in $\mathcal{H}^{\mathrm{loc}}$

Generic Hubbard Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \sum_{ij} \sum_{\alpha\beta} \epsilon^{\alpha\beta}_{\mathbf{k},ij} \, c^{\dagger}_{\mathbf{k}i\alpha} c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}i \in \mathrm{corr}} \hat{H}^{\mathrm{loc}}_{i} [\{c^{\dagger}_{\mathbf{R}i\alpha}\}, \{c_{\mathbf{R}i\alpha}\}]$$

$$\epsilon_{\mathbf{k}} = \left[\begin{array}{c|c|c} \mathrm{i{=}0} & * & * \\ \hline * & \mathrm{i{=}1} & * \\ \hline * & * & \mathrm{i{=}2} \end{array}\right]$$

$\mathbf{R}$ = label unit cell

$\mathbf{k}$ = Fourier-conjugate of $\mathbf{R}$

$\sum_{\mathbf{k}} \epsilon_{\mathbf{k},ii} = 0 \quad \forall\, i$ correlated

α, β = orbitals in $\mathbf{R}, i$

(Example: $i = 0$: uncorrelated orbitals; $i = 1$: d orbitals atom 1
$i = 2$: f orbitals atom 2 ...)

Constrained minimization problem, $2^{M_i} \times 2^{M_i}$ independent SB amplitudes

The variational energy

$$\hat{H} = \sum_{\mathbf{k}} \sum_{\alpha\beta} \boxed{\epsilon^{\alpha\beta}_{\mathbf{k},ij}} c^{\dagger}_{\mathbf{k}i\alpha} c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}i} \boxed{\hat{H}^{\mathrm{loc}}_{\mathbf{R}i}[\{\hat{c}^{\dagger}_{\mathbf{R}i\alpha}\}, \{\hat{c}_{\mathbf{R}i\alpha}\}]}$$

$$\mathcal{E}[\Psi_0, \{\phi_i\}] = \frac{1}{\mathcal{N}} \sum_{\mathbf{k},ij} \sum_{ab} \left[\mathcal{R}_i \, \epsilon_{\mathbf{k},ij} \mathcal{R}^{\dagger}_j\right]_{ab} \langle \Psi_0 | f^{\dagger}_{\mathbf{k}ia} f_{\mathbf{k}jb} | \Psi_0 \rangle + \sum_{i \in \mathrm{corr}} \mathrm{Tr}\left[\phi_i \, \phi^{\dagger}_i \, H^{\mathrm{loc}}_i\right]$$

where

$$[\mathcal{R}_i]_{a\alpha} = \sum_b \mathrm{Tr}\left[\phi^{\dagger}_i \, F^{\dagger}_{i\alpha} \, \phi_i \, F_{ib}\right] [\Delta_{pi}(1 - \Delta_{pi})]^{-\frac{1}{2}}_{ba}$$

to be minimized satisfying the Gutzwiller contraints:

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

$$\mathrm{Tr}\left[\phi^{\dagger}_i \phi_i \, F^{\dagger}_{ia} F_{ib}\right] = \langle \Psi_0 | f^{\dagger}_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle \equiv \Delta_{pi}$$

Step 1: promoting Δ_p, $\mathcal{R}$ to independent variables using Lagrange multipliers

Functional formulation SB

$$\mathcal{L}[\Psi_0, E; \phi, E^c; \mathcal{R}, \mathcal{R}^\dagger, \lambda; \mathcal{D}, \mathcal{D}^\dagger, \lambda^c; \Delta_p] =$$

$$\frac{1}{\mathcal{N}} \langle \Psi_0 | \hat{H}^{\rm qp}_G[\mathcal{R}, \mathcal{R}^\dagger; \lambda] | \Psi_0 \rangle + E(1 - \langle \Psi_0 | \Psi_0 \rangle) +$$

$$\sum_i \mathrm{Tr}\left[\phi_i \, \phi_i^\dagger \, H_i^{\rm loc} + \sum_{a\alpha} \left([\mathcal{D}_i]_{a\alpha} \, \phi_i^\dagger \, F_{i\alpha}^\dagger \, \phi_i \, F_{ia} + \mathrm{H.c.} \right) + \sum_{ab} [\lambda_i^c]_{ab} \, \phi_i^\dagger \phi_i \, F_{ia}^\dagger F_{ib} \right] +$$

$$\sum_i E_i^c \left(1 - \mathrm{Tr}\left[\phi_i^\dagger \phi_i \right] \right)$$

$$- \sum_i \left[\sum_{ab} \left([\lambda_i]_{ab} + [\lambda_i^c]_{ab} \right) [\Delta_{pi}]_{ab} + \sum_{ca\alpha} \left([\mathcal{D}_i]_{a\alpha} \, [\mathcal{R}_i]_{c\alpha} \, [\Delta_{pi}(1 - \Delta_{pi})]^{\frac{1}{2}}_{c\alpha} + \mathrm{c.c.} \right) \right]$$

where

$$\hat{H}^{\rm qp}_G[\mathcal{R}, \mathcal{R}^\dagger; \lambda] \equiv \sum_{k,ij} \sum_{ab} \left[\mathcal{R}_i \, \epsilon_{k,ij} \mathcal{R}_j^\dagger \right]_{ab} f^\dagger_{kia} f_{kjb} + \sum_{Ri,ab} [\lambda_i]_{ab} \, f^\dagger_{Ria} f_{Rib}$$

Now *quadratic* functional of ϕ (linear in ϕ and $\phi^\dagger$)!
($\frac{\delta \mathcal{L}}{\delta \phi} = 0$ same complexity of ground-state eigenvalue problem ...)

Step 2: Eliminating (formally) $|\Psi_0\rangle$ and E

Functional formulation SB

$$\mathcal{L}[\,\Psi_0, E\,;\phi, E^c;\ \mathcal{R}, \mathcal{R}^\dagger, \lambda;\ \mathcal{D}, \mathcal{D}^\dagger, \lambda^c;\ \Delta_p] =$$

$$\frac{1}{\mathcal{N}}\langle\Psi_0|\,\hat{H}^{\rm qp}_G[\mathcal{R}, \mathcal{R}^\dagger;\lambda]\,|\Psi_0\rangle + E(1-\langle\Psi_0|\Psi_0\rangle) +$$

$$\sum_i \mathrm{Tr}\left[\phi_i\,\phi_i^\dagger\,H_i^{\rm loc} + \sum_{a\alpha}\left([\mathcal{D}_i]_{a\alpha}\ \phi_i^\dagger\,F_{i\alpha}^\dagger\,\phi_i\ F_{ia} + \text{H.c.}\right) + \sum_{ab}[\lambda_i^c]_{ab}\ \phi_i^\dagger\phi_i\ F_{ia}^\dagger F_{ib}\right] +$$

$$\sum_i E_i^c\left(1-\mathrm{Tr}\left[\phi_i^\dagger\phi_i\right]\right)$$

$$-\sum_i\left[\sum_{ab}\left([\lambda_i]_{ab}+[\lambda_i^c]_{ab}\right)[\Delta_{pi}]_{ab} + \sum_{ca\alpha}\left([\mathcal{D}_i]_{a\alpha}\,[\mathcal{R}_i]_{c\alpha}\,[\Delta_{pi}(1-\Delta_{pi})]^{\frac{1}{2}}_{c\alpha} + \text{c.c.}\right)\right]$$

where

$$\hat{H}^{\rm qp}_G[\mathcal{R}, \mathcal{R}^\dagger;\lambda] \equiv \sum_{k,ij}\sum_{ab}\left[\mathcal{R}_i\,\epsilon_{k,ij}\mathcal{R}_j^\dagger\right]_{ab} f_{kia}^\dagger f_{kjb} + \sum_{Ri,ab}[\lambda_i]_{ab}\,f_{Ria}^\dagger f_{Rib}$$

Step 2: Eliminating (formally) $|\Psi_0\rangle$ and E

Functional formulation SB

$$\mathcal{L}[\phi, E^c;\ \mathcal{R}, \mathcal{R}^\dagger, \lambda;\ \mathcal{D}, \mathcal{D}^\dagger, \lambda^c;\ \Delta_p] =$$

$$\frac{\mathcal{T}}{\mathcal{N}} \sum_{k,\omega} \mathrm{Tr}\log\left(\frac{1}{i\omega - \mathcal{R}\epsilon_k\mathcal{R}^\dagger - \lambda}\right) e^{i\omega 0^+} +$$

$$\sum_i \mathrm{Tr}\left[\phi_i\ \phi_i^\dagger\ H_i^{\mathrm{loc}} + \sum_{a\alpha}\left([\mathcal{D}_i]_{a\alpha}\ \phi_i^\dagger\ F_{i\alpha}^\dagger\ \phi_i\ F_{ia} + \mathrm{H.c.}\right) + \sum_{ab}[\lambda_i^c]_{ab}\ \phi_i^\dagger\phi_i\ F_{ia}^\dagger F_{ib}\right] +$$

$$\sum_i E_i^c\left(1 - \mathrm{Tr}\left[\phi_i^\dagger\phi_i\right]\right)$$

$$-\sum_i\left[\sum_{ab}\left([\lambda_i]_{ab} + [\lambda_i^c]_{ab}\right)[\Delta_{pi}]_{ab} + \sum_{ca\alpha}\left([\mathcal{D}_i]_{a\alpha}\,[\mathcal{R}_i]_{c\alpha}\,[\Delta_{pi}(1-\Delta_{pi})]^{\frac{1}{2}}_{c\alpha} + \mathrm{c.c.}\right)\right]$$

where

$$\epsilon_{\mathbf{k}} = \left[\begin{array}{c|c|c} i=0 & * & * \\ \hline * & i=1 & * \\ \hline * & * & i=2 \end{array}\right] ;\quad \mathcal{R} = \left[\begin{array}{c|c|c} \mathbb{1} & 0 & 0 \\ \hline 0 & \mathcal{R}_{i=1} & 0 \\ \hline 0 & 0 & \mathcal{R}_{i=2} \end{array}\right] ;\quad \lambda = \left[\begin{array}{c|c|c} 0 & 0 & 0 \\ \hline 0 & \lambda_{i=1} & 0 \\ \hline 0 & 0 & \lambda_{i=2} \end{array}\right]$$

Step 3: Re-interpretation ϕ_i using Schmidt decomposition

Functional formulation SB

$$\mathcal{L}[\phi, E^c; \mathcal{R}, \mathcal{R}^\dagger, \lambda; \mathcal{D}, \mathcal{D}^\dagger, \lambda^c; \Delta_p] = \frac{\mathcal{T}}{\mathcal{N}} \sum_{k,\omega} \mathrm{Tr}\log\left(\frac{1}{i\omega - \mathcal{R}\epsilon_k\mathcal{R}^\dagger - \lambda}\right) e^{i\omega 0^+} +$$

$$\sum_i \mathrm{Tr}\left[\phi_i\, \phi_i^\dagger\, H_i^{\mathrm{loc}} + \sum_{a\alpha}\left([\mathcal{D}_i]_{a\alpha}\, \phi_i^\dagger\, F_{i\alpha}^\dagger\, \phi_i\, F_{ia} + \mathrm{H.c.}\right) + \sum_{ab}[\lambda_i^c]_{ab}\, \phi_i^\dagger \phi_i\, F_{ia}^\dagger F_{ib}\right] +$$

$$\sum_i E_i^c\left(1 - \mathrm{Tr}\left[\phi_i^\dagger \phi_i\right]\right)$$

$$-\sum_i\left[\sum_{ab}\left([\lambda_i]_{ab} + [\lambda_i^c]_{ab}\right)[\Delta_{pi}]_{ab} + \sum_{ca\alpha}\left([\mathcal{D}_i]_{a\alpha}\,[\mathcal{R}_i]_{c\alpha}\,[\Delta_{pi}(1-\Delta_{pi})]^{\frac{1}{2}}_{c\alpha} + \mathrm{c.c.}\right)\right]$$

Elements ϕ_i can be viewed as coefficients Schmidt decomposition:

$$|\Phi_i\rangle \equiv \sum_{An} e^{i\frac{\pi}{2}N_n(N_n-1)}\,[\phi_i]_{An}\;|A,i\rangle\, U_{\mathrm{PH}}|n,i\rangle$$

$$|A\rangle = \left[\hat{c}_1^\dagger\right]^{n_1}\cdots\left[\hat{c}_M^\dagger\right]^{n_M}|0\rangle \qquad |n\rangle = \left[\hat{f}_1^\dagger\right]^{n_1}\cdots\left[\hat{f}_M^\dagger\right]^{n_M}|0\rangle$$

Impurity Bath

Step 3: Re-interpretation ϕ_i using Schmidt decomposition

Functional formulation SB

$$\mathcal{L}[\Phi, E^c;\ \mathcal{R}, \mathcal{R}^\dagger, \lambda;\ \mathcal{D}, \mathcal{D}^\dagger, \lambda^c;\ \Delta_p] = \frac{\mathcal{T}}{\mathcal{N}} \sum_{k,\omega} \mathrm{Tr}\log\left(\frac{1}{i\omega - \mathcal{R}\epsilon_k\mathcal{R}^\dagger - \lambda}\right) e^{i\omega 0^+} +$$

$$\sum_i \left[\langle\Phi_i|\,\mathcal{H}_i^{\mathrm{emb}}[\mathcal{D}_i, \mathcal{D}_i^\dagger; \lambda_i^c]\,|\Phi_i\rangle + E_i^c(1 - \langle\Phi_i|\Phi_i\rangle)\right]$$

$$-\sum_i \left[\sum_{ab}\left([\lambda_i]_{ab} + [\lambda_i^c]_{ab}\right)[\Delta_{pi}]_{ab} + \sum_{ca\alpha}\left([\mathcal{D}_i]_{a\alpha}\,[\mathcal{R}_i]_{c\alpha}\,[\Delta_{pi}(1-\Delta_{pi})]^{\frac{1}{2}}_{c\alpha} + \mathrm{c.c.}\right)\right]$$

where

$$\begin{aligned}\mathcal{H}_i^{\mathrm{emb}}[\mathcal{D}_i, \mathcal{D}_i^\dagger; \lambda_i^c] \;&\equiv\; \hat{H}_i^{\mathrm{loc}}[\{\hat{c}_{i\alpha}^\dagger\}, \{\hat{c}_{i\alpha}\}] \\ &+\; \sum_{a\alpha}\left([\mathcal{D}_i]_{a\alpha}\,\hat{c}_{i\alpha}^\dagger\hat{f}_{ia} + \mathrm{H.c.}\right) + \sum_{ab}[\lambda_i^c]_{ab}\hat{f}_{ib}\hat{f}_{ia}^\dagger\end{aligned}$$

Stationarity equations: λ, R, Δ_p; $\langle\Phi|\&E^c$; D, λ^c

SB stationarity equations

$$(\mathcal{R},\lambda) \longrightarrow \frac{1}{\mathcal{N}}\left[\sum_k \Pi_i f\left(\mathcal{R}\epsilon_k\mathcal{R}^\dagger+\lambda\right)\Pi_i\right]_{ba} = [\Delta_{pi}]_{ab} \tag{1}$$

$$\frac{1}{\mathcal{N}}\left[\frac{1}{\mathcal{R}_i}\sum_k \Pi_i\,\mathcal{R}\epsilon_k\mathcal{R}^\dagger f\left(\mathcal{R}\epsilon_k\mathcal{R}^\dagger+\lambda\right)\Pi_i\right]_{\alpha a} = \sum_c [\mathcal{D}_i]_{c\alpha}\,[\Delta_{ip}\,(1-\Delta_{ip})]^{\frac{1}{2}}_{ac} \tag{2}$$

$$\left[\sum_{cb\alpha}\frac{\partial}{\partial d^p_{is}}\,[\Delta_{pi}\,(1-\Delta_{pi})]^{\frac{1}{2}}_{cb}\,[\mathcal{D}_i]_{b\alpha}[\mathcal{R}_i]_{c\alpha}+\text{c.c.}\right]+\left[l+l^c\right]_{is}=0 \tag{3}$$

$$\mathcal{H}^{\text{emb}}_i[\mathcal{D}_i,\mathcal{D}_i^\dagger;\lambda^c_i]\,|\Phi_i\rangle = E^c_i\,|\Phi_i\rangle \tag{4}$$

$$\left[\mathcal{F}^{(1)}_i\right]_{\alpha a} \equiv \langle\Phi_i|\,\hat{c}^\dagger_{i\alpha}\hat{f}_{ia}\,|\Phi_i\rangle - \sum_c [\Delta_{ip}\,(1-\Delta_{ip})]^{\frac{1}{2}}_{ca}\,[\mathcal{R}_i]_{c\alpha}=0 \tag{5}$$

$$\left[\mathcal{F}^{(2)}_i\right]_{ab} \equiv \langle\Phi_i|\,\hat{f}_{ib}\hat{f}^\dagger_{ia}\,|\Phi_i\rangle - [\Delta_{pi}]_{ab}=0 \tag{6}$$

where

$$\Delta_{pi}=\sum_s d^p_{is}\,{}^t h_{is}\,;\quad \lambda^c_i=\sum_s l^c_{is}\,h_{is}\,;\quad \lambda_i=\sum_s l_{is}\,h_{is}\,;\quad \mathcal{R}_i=\sum_s r_{is}\,h_{is}$$

"Adding interaction" to KS (only for selected correlated orbitals)

The Projector: Definition of the Correlated Orbitals

$$\hat{\Xi}(\mathbf{r},\sigma) = \sum_{\sigma'} \sum_{ki,\pi\in P} \xi_{ki,\pi}(\mathbf{r})\chi_{\sigma'}(\sigma)\, c_{ki\pi\sigma} + \hat{\Xi}_Q(\mathbf{r},\sigma) \equiv \sum_i \hat{\Xi}_{Pi}(\mathbf{r},\sigma) + \hat{\Xi}_Q(\mathbf{r},\sigma)$$

$$\hat{A} = \sum_\sigma \int d\mathbf{r}\, \hat{\Xi}^\dagger(\mathbf{r},\sigma)\, A\, \hat{\Xi}(\mathbf{r},\sigma) \equiv \sum_i \hat{A}_i^{\mathrm{loc}} + \hat{A}^{\mathrm{hop}}$$

where

$$\hat{A}_i^{\mathrm{loc}} \equiv \sum_\sigma \int d\mathbf{r}\, \hat{\Xi}_{Pi}^\dagger(\mathbf{r},\sigma)\, A\, \hat{\Xi}_{Pi}(\mathbf{r},\sigma)\,; \quad \hat{A}^{\mathrm{hop}} \equiv \hat{A} - \sum_i \hat{A}_i^{\mathrm{loc}}\,.$$

$$A = \left[\begin{array}{c|c|c} A^{\mathrm{hop}} & A^{\mathrm{hop}} & A^{\mathrm{hop}} \\ \hline A^{\mathrm{hop}} & A_{i=1}^{\mathrm{loc}} & A^{\mathrm{hop}} \\ \hline A^{\mathrm{hop}} & A^{\mathrm{hop}} & A_{i=2}^{\mathrm{loc}} \end{array}\right]$$

K. Haule et al., Phys. Rev. B **81**, 195107 (2010)

LDA+SB as solving iteratively Kohn-Sham-Hubbard Hamiltonian

Functional formulation LDA+SB for non-linear double-counting

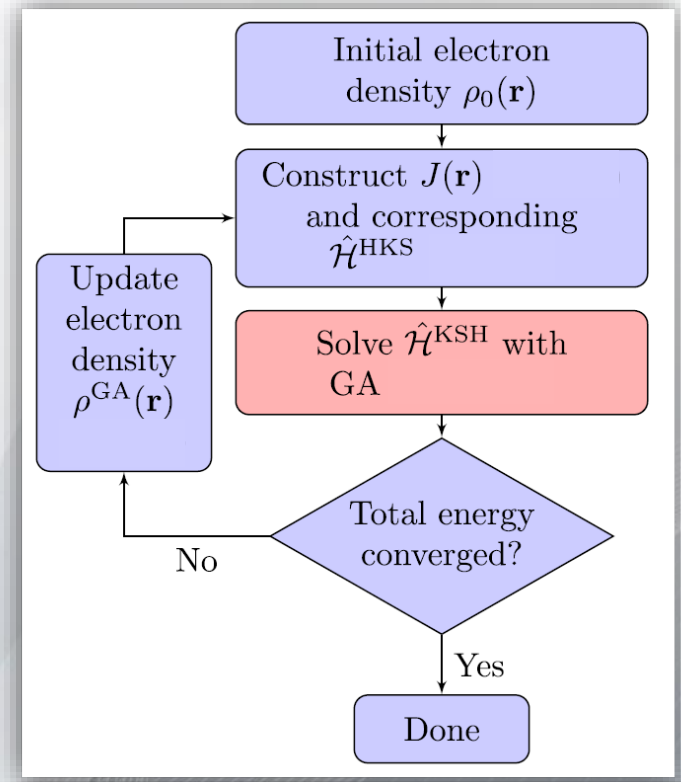
$$\Omega_{E^{\rm dc},N}[N^{\rm loc}, V^{\rm dc};\ \rho(\mathbf{r}), J(\mathbf{r});\ \Phi, E^c, \mathcal{R}, \mathcal{R}^\dagger, \lambda, \mu, \mathcal{D}, \mathcal{D}^\dagger, \lambda^c, \Delta_p] =$$
$$\mathcal{L}_{\rm KSH}[J(\mathbf{r});\ \phi, E^c;\ \mathcal{R}, \mathcal{R}^\dagger, \lambda;\ \mathcal{D}, \mathcal{D}^\dagger, \lambda^c;\ \Delta_p\ , \mu] +$$
$$\int d\mathbf{r} J(\mathbf{r})\rho(\mathbf{r}) + E^{\rm LDA}_{\rm Hxc}[\rho(\mathbf{r})] + E_{\rm ion}[\rho(\mathbf{r})] + E_{\text{ion-ion}}$$
$$+\sum_i \left[E_i^{\rm dc}[N_i^{\rm loc}] - V_i^{\rm dc} N_i^{\rm loc}\right]$$

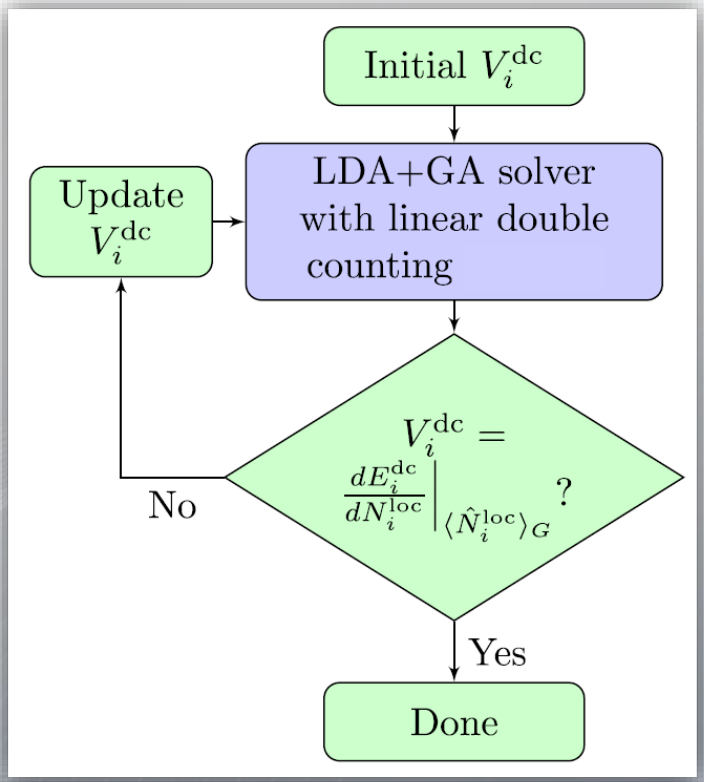
where $\mathcal{L}_{\rm KSH}$ is the SB functional of:

$$\hat{H}^{\rm KSH}_{V^{\rm dc}}[J(\mathbf{r})] \equiv -\hat{\Delta} + \frac{\delta E^{\rm LDA}_{\rm Hxc}}{\delta\rho(\mathbf{r})} + \frac{\delta E_{\rm ion}}{\delta\rho(\mathbf{r})} + \sum_i \hat{H}_i^{\rm int} - \sum_i V_i^{\rm dc}\hat{N}_i^{\rm loc}$$

LDA+SB as solving iteratively Kohn-Sham-Hubbard Hamiltonian

Functional formulation LDA+SB for non-linear double-counting





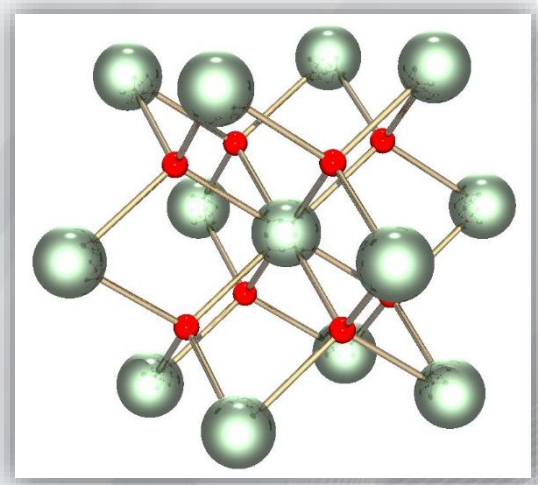
$$\hat{H}^{\mathrm{KSH}}_{V^{\mathrm{dc}}}[J(\mathbf{r})] \equiv -\hat{\Delta} + \frac{\delta E^{\mathrm{LDA}}_{\mathrm{Hxc}}}{\delta \rho(\mathbf{r})} + \frac{\delta E_{\mathrm{ion}}}{\delta \rho(\mathbf{r})} + \sum_i \hat{H}_i^{\mathrm{int}} - \sum_i V_i^{\mathrm{dc}} \hat{N}_i^{\mathrm{loc}}$$

An example: Orbital Differentiation with Crystal Field Effects in UO_2

UO_2 (arXiv:1606.09614 (2016))

Cubic fluorite structure

Point symmetry U atoms "double O point group" (low symmetry)



$$
\begin{aligned}
|\Gamma_6, 7/2, \pm\rangle &= \sqrt{5/12}\,|7/2, \pm 7/2\rangle + \sqrt{7/12}\,|7/2, \mp 1/2\rangle \\
|\Gamma_7, 7/2, \pm\rangle &= \mp\sqrt{3/4}\,|7/2, \pm 5/2\rangle \pm \sqrt{1/4}\,|7/2, \mp 3/2\rangle \\
|\Gamma_8^{(1)}, 7/2, \pm\rangle &= \pm\sqrt{7/12}\,|7/2, \pm 7/2\rangle \mp \sqrt{5/12}\,|7/2, \mp 1/2\rangle \\
|\Gamma_8^{(2)}, 7/2, \pm\rangle &= \mp\sqrt{1/4}\,|7/2, \pm 5/2\rangle \mp \sqrt{3/4}\,|7/2, \mp 3/2\rangle \\
|\Gamma_7, 5/2, \pm\rangle &= \sqrt{5/6}\,|5/2, \pm 3/2\rangle - \sqrt{1/6}\,|5/2, \mp 5/2\rangle \\
|\Gamma_8^{(1)}, 5/2, \pm\rangle &= \sqrt{1/6}\,|5/2, \pm 3/2\rangle + \sqrt{5/6}\,|5/2, \mp 5/2\rangle \\
|\Gamma_8^{(2)}, 5/2, \pm\rangle &= |5/2, \pm 1/2\rangle\,,
\end{aligned}
$$

Self Energy $\Sigma(\omega)$ non diagonal (less symmetry → less selection rules)

An example: Orbital Differentiation with Crystal Field Effects in UO_2

UO_2 (arXiv:1606.09614 (2016))

Eigenvalues of the 5*f* quasi-particle matrix *Z* and corresponding orbital occupations for LDA+RISB calculations. Theoretical results obtained by taking into account the crystal field splittings and by neglecting them.

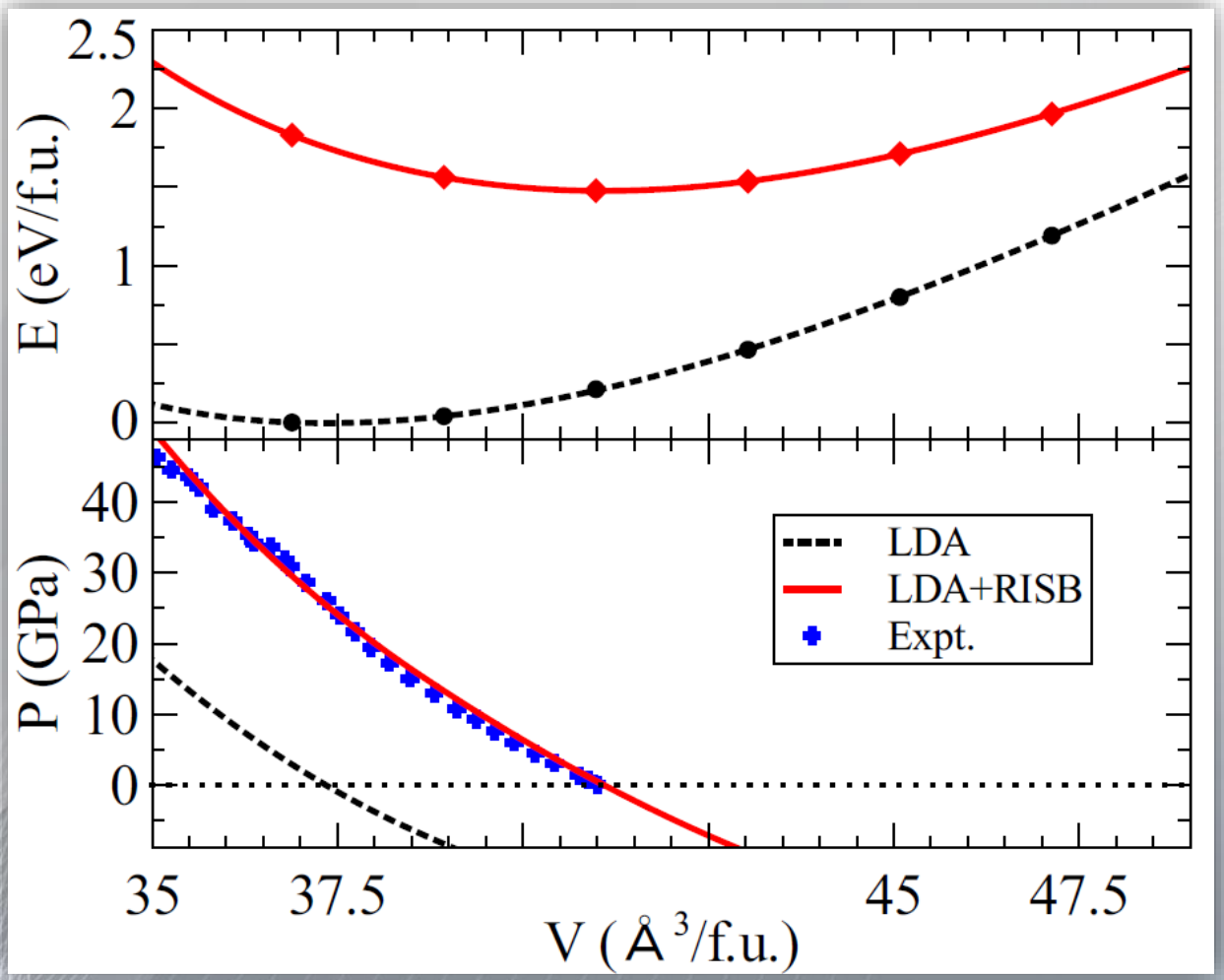
Crystal Field Splitting essential in order to capture the correct pattern of orbital differentiation in UO_2

w/ CFS	$\Gamma_8(4)$	$\Gamma_7(2)$	$\Gamma_8(4)$	$\Gamma_7(2)$	$\Gamma_6(2)$
Z	0	0.92	0.92	0.95	0.95
n	1.92	0.14	0.08	0.06	0.04

w/o CFS	5/2	7/2
Z	0	0.96
n	1.98	0.16

An example: Orbital Differentiation with Crystal Field Effects in UO_2

UO_2 (arXiv:1606.09614 (2016))



An example: Polymorphism in Strongly Correlated Materials

Polymorphism

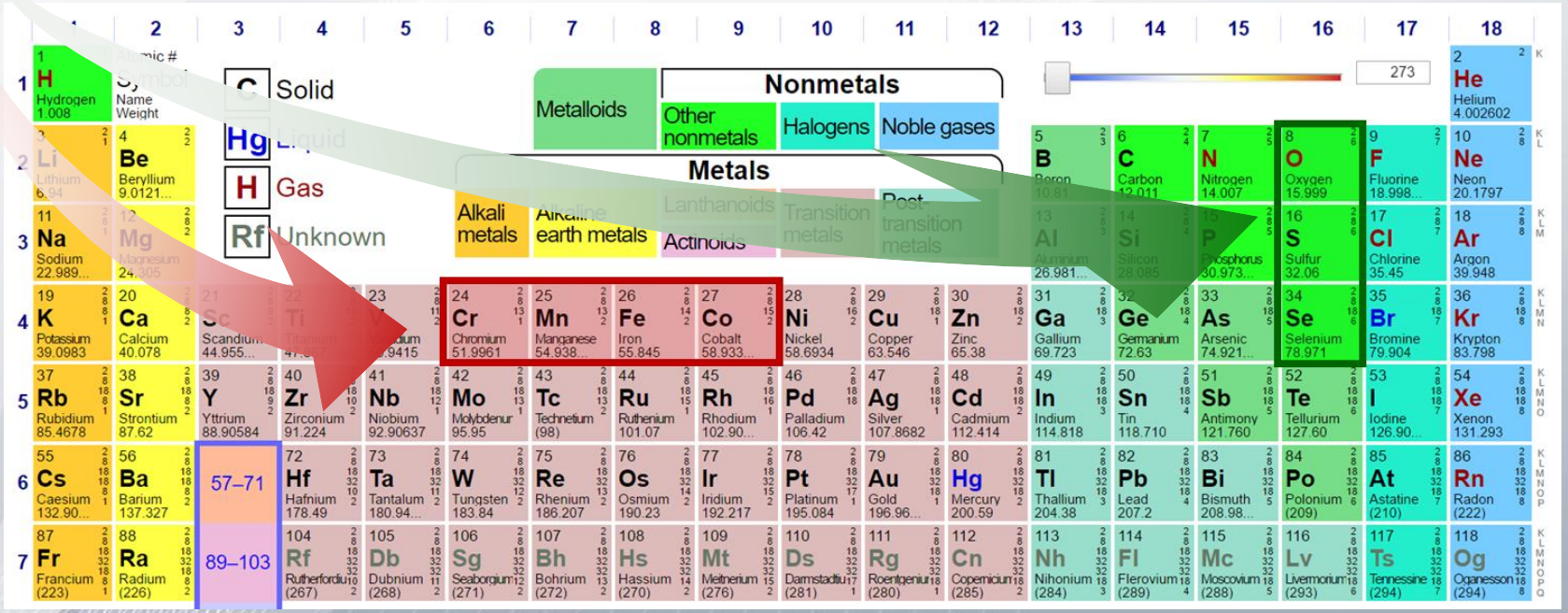
- **Carbon**: Graphite, Diamond (different mechanical, optical, electronic properties)
- **TiO_2**: Anatase, Rutile (enhance photocatalytic activity in Anatase with respect to Rutile)
- **White and Grey Tin** (different electronic and mechanical properties)

LDA-like functionals lead systematically to wrong predictions for correlated materials, e.g., involving transition-metal atoms.

An example: Polymorphism in Strongly Correlated Materials

Ground state structures and equilibrium volumes predicted by LDA and LDA+GA/RISB

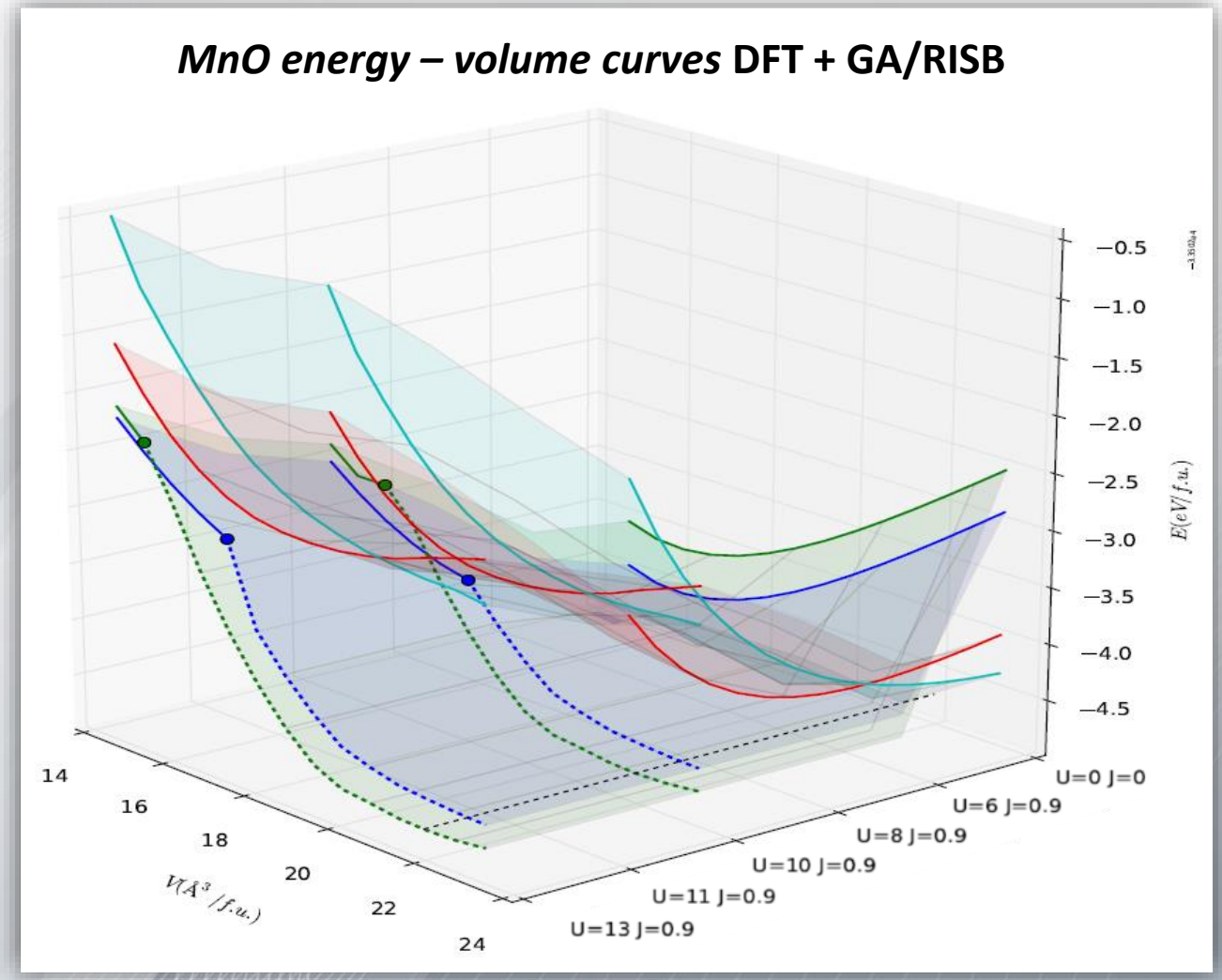
	LDA			LDA+SB $U = 13$ $J = 0.9$			experiment		
	g.s. structure	g.s. phase	V_0 ($Å^3/f.u.$)	g.s. structure	g.s. phase	V_0 ($Å^3/f.u.$)	g.s. structure	g.s. phase	V_0 ($Å^3/f.u.$)
CoO	Wurtzite	Metal	17.64	Rocksalt	Insulator	20.48	Rocksalt	Insulator	19.35
CoS	NiAs	Metal	23.11	NiAs	Metal	25.93	NiAs	Metal	25.77
CoSe	NiAs	Metal	27.25	NiAs	Metal	30.99	NiAs	Metal	30.27
CrO	Wurtzite	Metal	17.64	Rocksalt	Metal	18.27	Rocksalt		18
MnO	Wurtzite	Metal	17.13	Rocksalt	Insulator	22.06	Rocksalt	Insulator	21.97
FeO	Zincblende	Metal	18.69	Rocksalt	Insulator	21.23	Rocksalt	Insulator	20.35

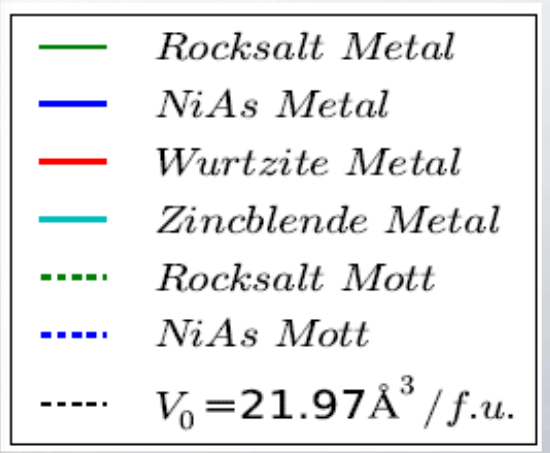


An example: Polymorphism in Strongly Correlated Materials

Energy Profile MnO

MnO energy – volume curves **DFT + GA/RISB**

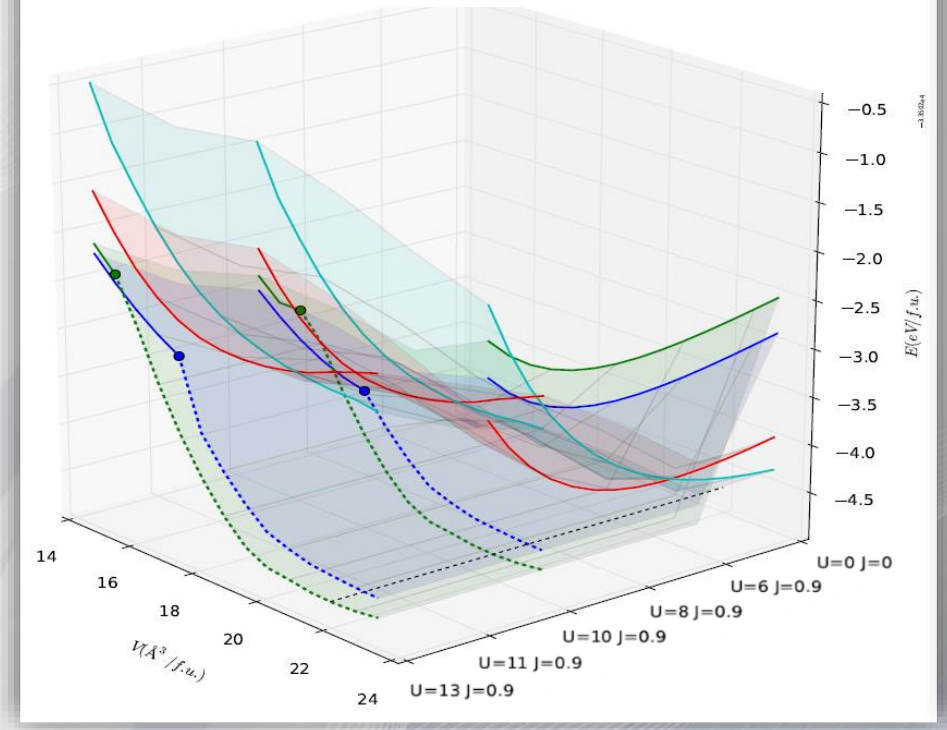




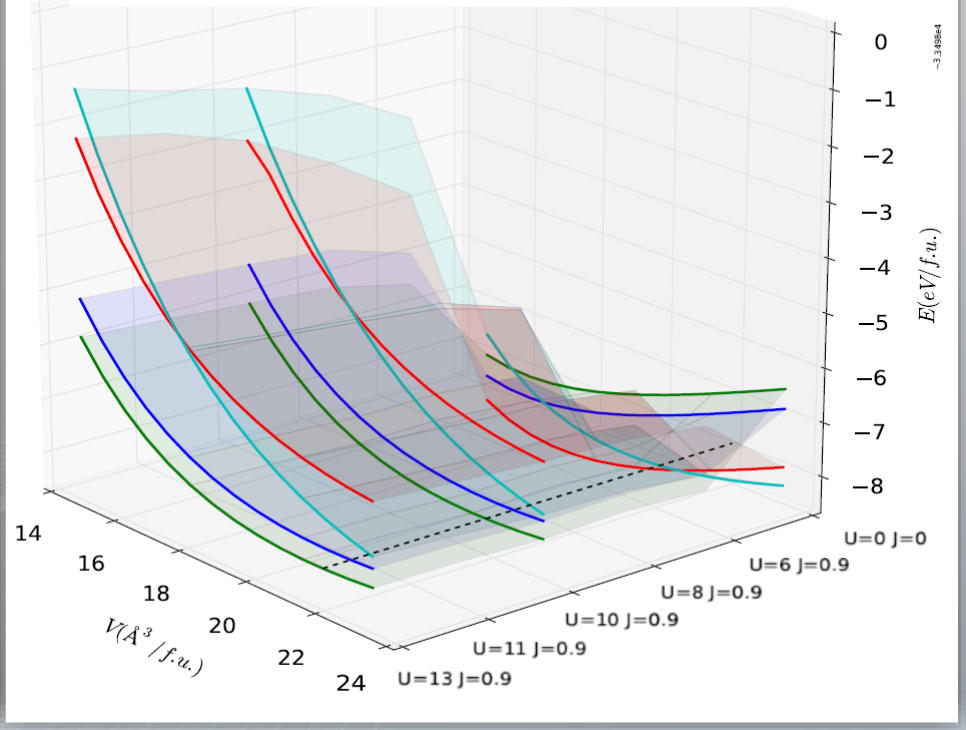
An example: Polymorphism in Strongly Correlated Materials

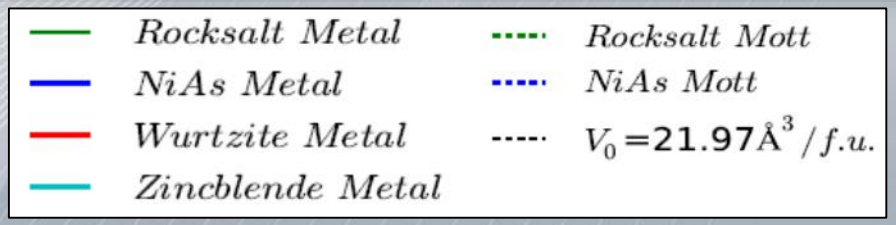
Energy Profile MnO

MnO energy – volume curves DFT + GA/RISB



MnO energy – volume curves DFT + U

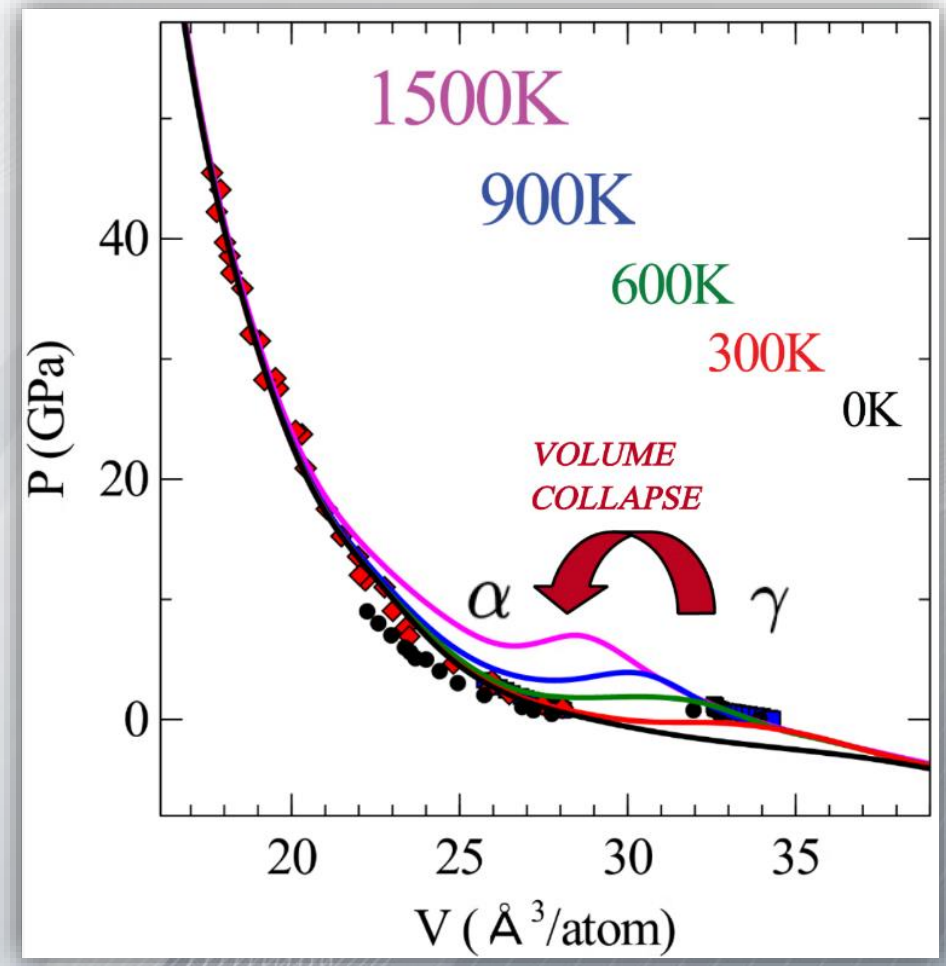


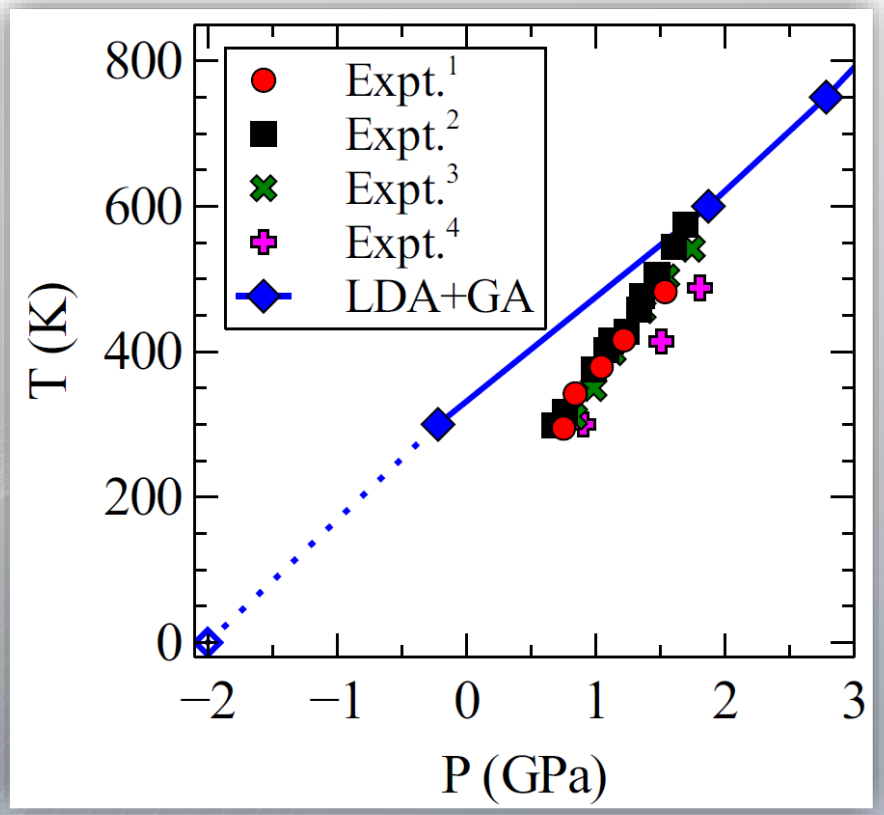


Thank you for your attention!

An example: The γ-α transition of Ce

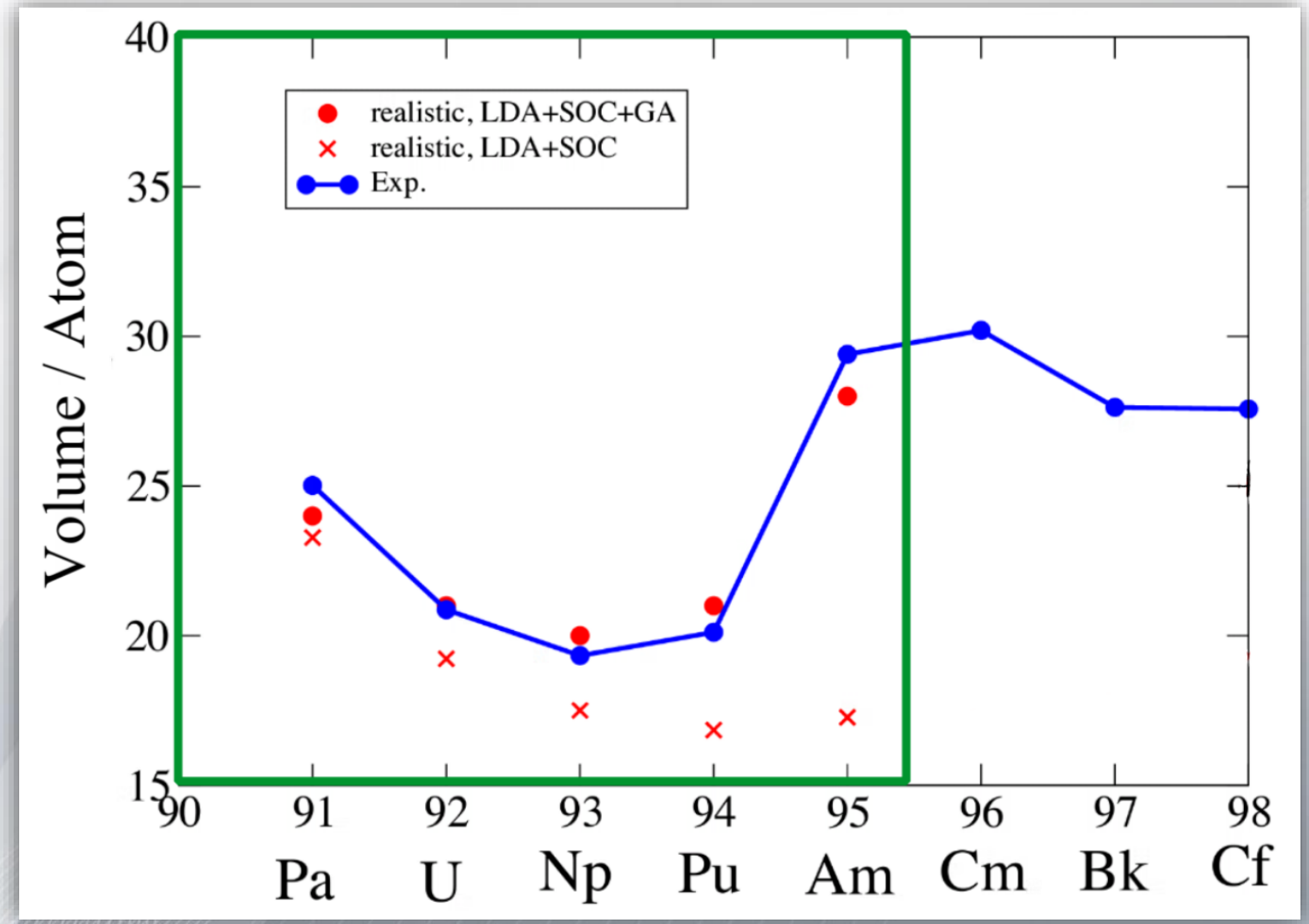
Phys. Rev. Lett. 111, 196801 (2013), Phys. Rev. B 90, 161104(R) (2014), Phys. Rev. Lett. 113, 036402 (2014)





Experimental data at room temperature

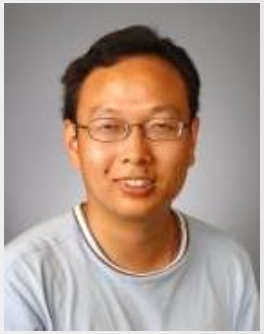
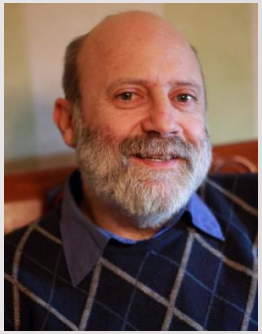
Actinides Transition



HANDS-ON SESSION
(assistant: Tsung-Han Lee)

Using RISB Code Developed with Yongxin Yao (Iowa) and Gabriel Kotliar (Rutgers):

N. Lanatà, Y. Yao, C.-Z. Wang, K.-M. Ho, and G. Kotliar, PRX **5**, 011008 (2015)
N. Lanatà, Y. Yao, X. Deng, V. Dobrosavljevic and G. Kotliar, arXiv:1606.09614 (2016).

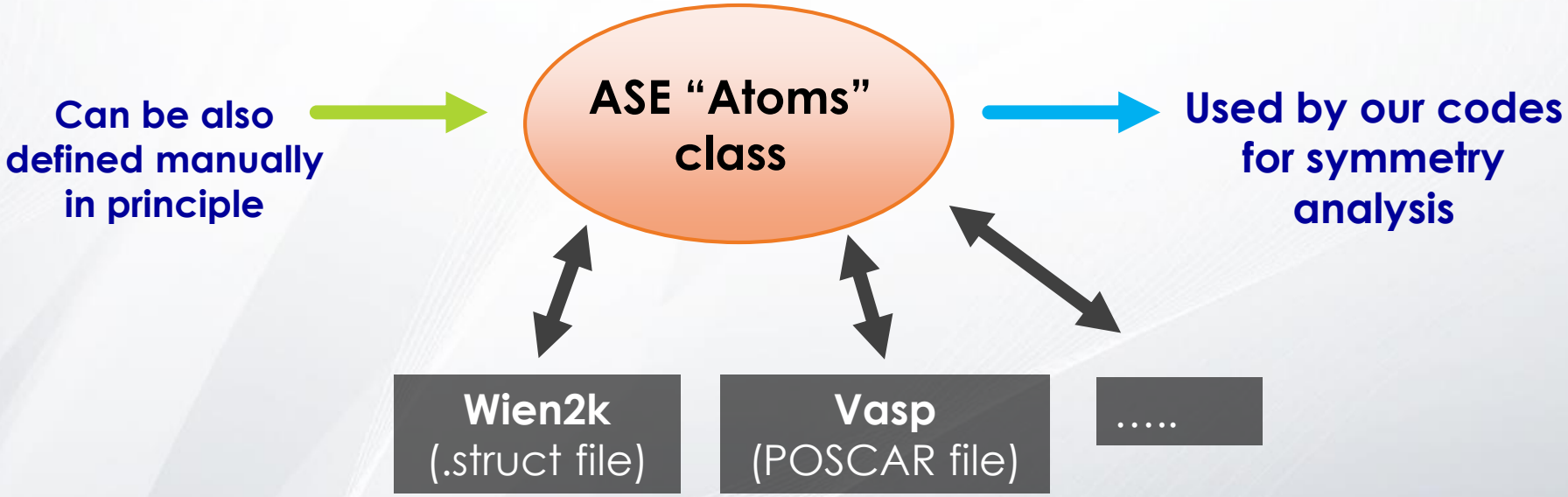
Implementation of LAPW interface with the DFT WIEN2K code adapted from DFT+DMFT code of:

K. Haule et al., see Phys. Rev. B **81**, 195107 (2010).

CyGutz User Guide

For details, please refer to CyGutz user guide:
http://ykent.public.iastate.edu/cygutz/

Fundamental object encoding material structure processed by our symmetry-analysis codes:
ASE (Atomic Simulation Environment, GNU LGPL license) class "Atoms"



In our DFT (Wien2k) + X (GA/RISB, DMFT,…) "Atoms" class automatically created from Wien2k structure file

But our symmetry codes elaborate the ASE (GNU LGPL license) "Atoms" class (which does not depend on Wien2k)

Example where “Atoms” class is created manually

lanata@Phoenix: ~/scratch/VideoConference/Preparation structure files

lanata@Phoenix: ~/scratch/VideoConference/Preparation structure files 103x33

File Edit Options Buffers Tools Python Help

```
import sys
import numpy as np
from numpy.linalg import det
```

Manual preparation “Atoms” class of MnBi

```
symbols=['Mn','Mn','Bi','Bi']
cell = [ (4.29, 0, 0), (0, 4.29, 0), (0, 0, 6.13) ]
scaled_positions=[(0,0,0), (0,0,1.0/2.0), (1.0/3.0,2.0/3.0,1.0/4.0), (2.0/3.0,1.0/3.0,3.0/4.0)]

from ase import Atoms
Material = Atoms( symbols=symbols, cell=cell, scaled_positions=scaled_positions, pbc=True )

##############################################################################

import os
from ase.io.wien2k import write_struct

path = os.getcwd()

material = 'MnBi'
name = material + '.struct'
fullname = path + '/' + material + '/' + name
print fullname

write_struct(name, atoms2=Material, rmt=None, lattice='P', zza=None)
```

Corresponding Wien2k structure file automatically written in proper format

-UU-:----F1 **auto_struct.py** All L27 (Python) ----------

Example where “Atoms” class is written/read from different structure files

lanata@Phoenix: ~/scratch/VideoConference/Preparation structure files

lanata@Phoenix: ~/scratch/VideoConference/Preparation structure files 103x33

File Edit Options Buffers Tools Python Help

```
import sys
import numpy as np
from numpy.linalg import det

from ase import Atoms

##############################################################################

import os
from ase.io.wien2k import write_struct
from ase.io import read
```

Creating “Atoms” classes from existing Vasp POSCAR files

```
MnO_RS = read('POSCAR_MnO_RS', index=None, format='vasp')
MnO_ZB = read('POSCAR_MnO_ZB', index=None, format='vasp')
write_struct('MnO_RS.struct', atoms2=MnO_RS, rmt=None, lattice='P', zza=None)
write_struct('MnO_ZB.struct', atoms2=MnO_ZB, rmt=None, lattice='P', zza=None)
```

Corresponding Wien2k structure files automatically written from “Atoms” classes

-UU-:----F1 **convert_struct.py** All L23 (Python) ----------

End of buffer

Work done by our symmetry code: Part 1

Detect: **(I) symmetry group lattice, (II) equivalent atoms in unit cell, (III) point symmetry groups of inequivalent correlated atoms (3x3 matrices representing 3-dimensional space isometries).**

"Easy": Essentially real-space geometry.
Automatically done by "pymatgen" (ASE-based open-source software)

Starting point for actual symmetry analysis (see the next slide).

Work done by our symmetry code: Part 2

Use theory of group representations to split single-particle space and many-body local space of strongly correlated electrons in irreducible representations.

More complicated: Depends on whether we treat "d" or "f" electrons, whether we neglect or not SOC/CF, single-particle space or many-body space, etc… In general. It depends on how the quantum configurations considered transform with respect to the group transformations. Additional complications of "double groups" (2π rotations not identity for half-integer J).

This enables us to obtain: (I) "symmetry basis" in which the *local self-energy* and the *many-body local density matrix* of the correlated electrons are as simple as possible (block diagonal, inequivalent representations not coupled, ecc…).

Interactive user interface

Given a folder with a completed DFT job, the python script "init_ga.py" asks questions to the user concerning the desired approximations.

(The symmetry analysis depends on whether the correlated shell is "d" or "f" and whether the SOC or the CFS are negligible)

Examples:

♦ If SOC is neglected a rotation within the single-particle (or many-body) space is represented as **exp(iLθ)**, where **L** is the orbital angular momentum. If instead both SOC and CFS are important, a rotation within the same space is represented as **exp(iJθ)**, where **J=L+S** is the total angular momentum.

♦ If J is half-integer a rotation of 2π is not the identity (but the identity multiplied by -1). This requires to duplicate the group (double groups). For instance, the Koster symbols in our paper about UO_2 [arXiv:1606.09614 (2016)] correspond to irreducible representations of a double group.

Our code can deal with all of these possibilities automatically. The user does not need to know anything about group theory, but simply describe the physical problem and the desired approximation scheme.

Initialization UO_2: LDA

Initialization UO_2 : LDA

henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... ×

```
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_k2000/UO2$ init_lapw -b -vxc 5 -ecut 8 -rkmax 9 -numk 2000
```

Initialization UO_2 : LDA

henhans@henhans-Satellite-C55-C: ~ | henhans@henhans-Satellite-C55-C: ~/cygutz/UO2/LDA/UO2 | henhans@henhans-Satellite-C55-C: ~/git/cygutz_release/t...

```
    ATOM  2  O          ATOM  1  U
 RMT(  2)=2.09000 AND RMT(  1)=2.36000
 SUMS TO 4.45000  LT.  NN-DIST= 4.47760
NN ENDS
0.0u 0.0s 0:00.00 0.0% 0+0k 0+40io 0pf+0w
>   sgroup      (12:51:05) 0.0u 0.0s 0:00.00 0.0% 0+0k 0+8io 0pf+0w
  Names of point group: m-3m   4/m -3 2/m   Oh
  Names of point group: -43m  -43m    Td
Number and name of space group: 225 (F m -3 m)
>   symmetry    (12:51:05) 0.0u 0.0s 0:00.00 0.0% 0+0k 0+72io 0pf+0w
 2 Atoms found: U O
generate atomic configuration for atom 1 : U
generate atomic configuration for atom 2 : O
  SELECT XCPOT:
  recommended: 13: PBE-GGA (Perdew-Burke-Ernzerhof 96)
                5: LSDA
               11: WC-GGA (Wu-Cohen 2006)
               19: PBEsol-GGA (Perdew etal. 2008)
  SELECT ENERGY to separate core and valence states:
  recommended: -6.0 Ry (check how much core charge leaks out of MT-sphere)
  ALTERNATIVELY: specify charge localization
  (between 0.97 and 1.0) to select core state

WARNING: R0=0.000100 for atom    1 Z= 92.00 too big. Use 0.00005

LSTART ENDS
WARNING: R0=0.000100 for atom    1 Z= 92.00 too big. Use 0.00005
>   inputfiles prepared (12:51:05)
  NUMBER OF K-POINTS IN WHOLE CELL: (0 allows to specify 3 divisions of G)
 length of reciprocal lattice vectors:   1.052   1.052   1.052  17.100  17.100  17.100
         165  k-points generated, ndiv=          17          17          17
KGEN ENDS
>   dstart      (12:51:05) DSTART ENDS
0.9u 0.0s 0:00.99 98.9% 0+0k 0+424io 0pf+0w
-----> new UO2.in0 generated
init_lapw finished ok

henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA/UO2$ initso_lapw
```

Initialization UO_2 : LDA

henhans@henhans-Satellite-C55-C: ~ × | henhans@henhans-Satellite-C55-C: ~/cygutz/UO2/LDA/UO2 × | henhans@henhans-Satellite-C55-C: ~/git/cygutz_release/t... ×

```
The file UO2.in2c has been generated automatically

---->Please select the direction of the moment ( h k l )
              (For R-lattice in R coordinates)(default 0 0 1):
```

Initialization UO_2 : LDA

henhans@henhans-Satellite-C55-C: ~ | henhans@henhans-Satellite-C55-C: ~/cygutz/UO2/LDA/UO2 | henhans@henhans-Satellite-C55-C: ~/git/cygutz_release/t...

```
The file UO2.in2c has been generated automatically

---->Please select the direction of the moment ( h k l )
              (For R-lattice in R coordinates)(default 0 0 1):
atom 1 is U
atom 2 is O

Select  atom-numbers (1,2,3) or "ranges of atoms" (1-3,9-12) (without blanks)
for which you would NOT like to add SO interaction
 (default none, just press "enter" ): 1
```

Initialization UO_2 : LDA

henhans@henhans-Satellite-C55-C: ~ | henhans@henhans-Satellite-C55-C: ~/cygutz/UO2/LDA/UO2 | henhans@henhans-Satellite-C55-C: ~/git/cygutz_release/t...

```
For large spin orbit effects it might be necessary to include many more
eigenstates from lapw1 by increasing EMAX in case.in1(c).

---->Please enter EMAX(default 5.0 Ryd):
```

Initialization UO_2 : LDA

henhans@henhans-Satellite-C55-C: ~ | henhans@henhans-Satellite-C55-C: ~/cygutz/UO2/LDA/UO2 | henhans@henhans-Satellite-C55-C: ~/git/cygutz_release/t...

```
For large spin orbit effects it might be necessary to include many more
eigenstates from lapw1 by increasing EMAX in case.in1(c).

---->Please enter EMAX(default 5.0 Ryd):

The radial basis set for heavy atoms with p-semicore states is very
limited. One can improve this by adding RLOs. Note: you MUST NOT add
RLOs for atoms like oxygen,.... therefore the default is set to NONE
---->Add RLO for NONE, ALL, CHOOSE elements? (N/a/c) :
```

Initialization UO_2 : LDA

henhans@henhans-Satellite-C55-C: ~ | henhans@henhans-Satellite-C55-C: ~/cygutz/UO2/LDA/UO2 | henhans@henhans-Satellite-C55-C: ~/git/cygutz_release/t...

```
For large spin orbit effects it might be necessary to include many more
eigenstates from lapw1 by increasing EMAX in case.in1(c).

---->Please enter EMAX(default 5.0 Ryd):

The radial basis set for heavy atoms with p-semicore states is very
limited. One can improve this by adding RLOs. Note: you MUST NOT add
RLOs for atoms like oxygen,.... therefore the default is set to NONE
---->Add RLO for NONE, ALL, CHOOSE elements? (N/a/c) :
cat: .ieds: No such file or directory
 Check the generated UO2.inso file (RLOs,...)
 Check the generated UO2.in1 file (Emax at the bottom of the file)

In spinpolarized case SO may reduce symmetry.

The program symmetso dedects the proper symmetry and creates new struct and
input files. (Note, equivalent atoms could become inequivalent in some cases).

Do you have a spinpolarized case (and want to run symmetso) ? (y/N)
```

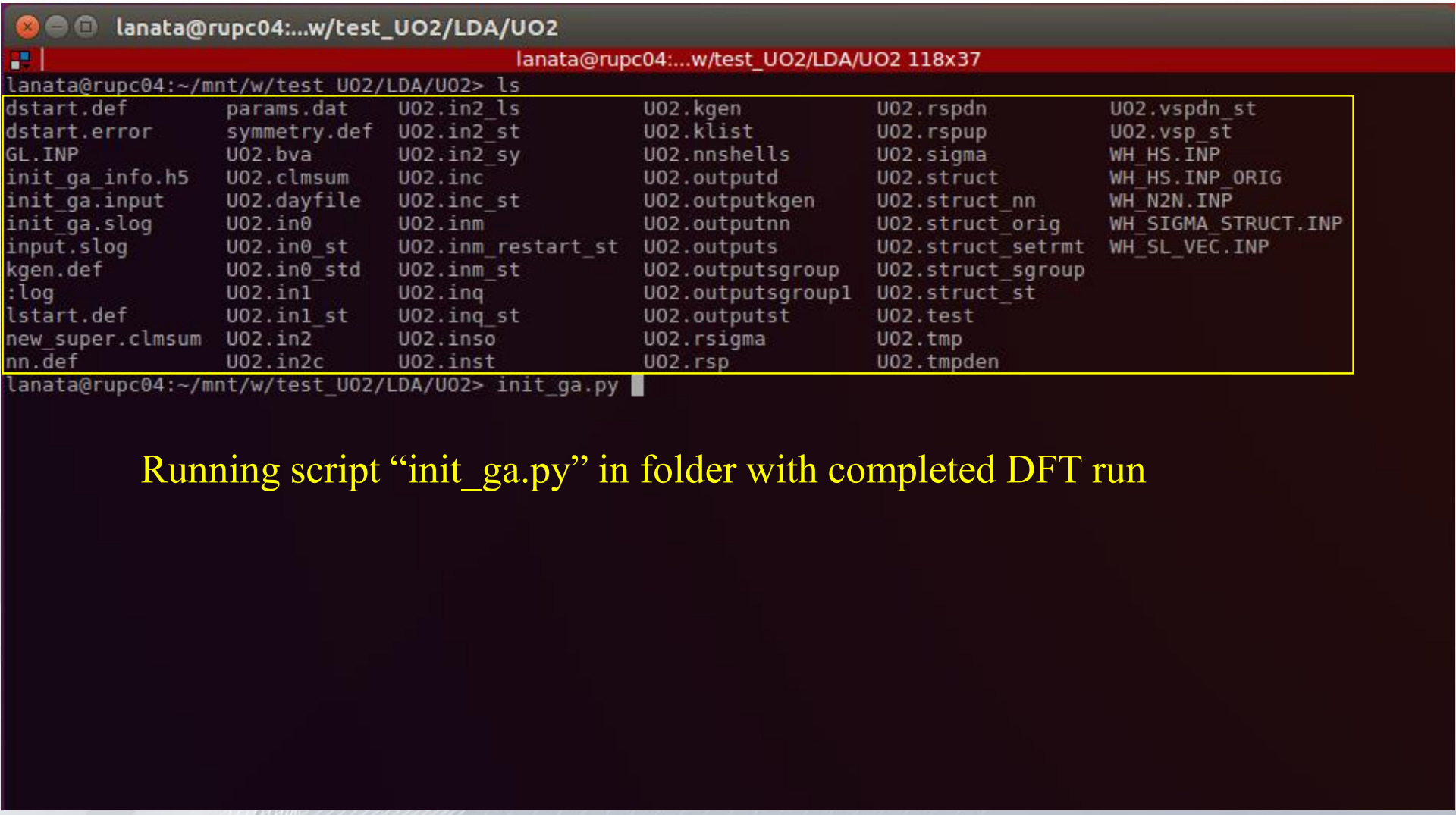
Initialization UO_2 : LDA

henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... ×

```
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_k2000/UO2$ run_lapw -so
```

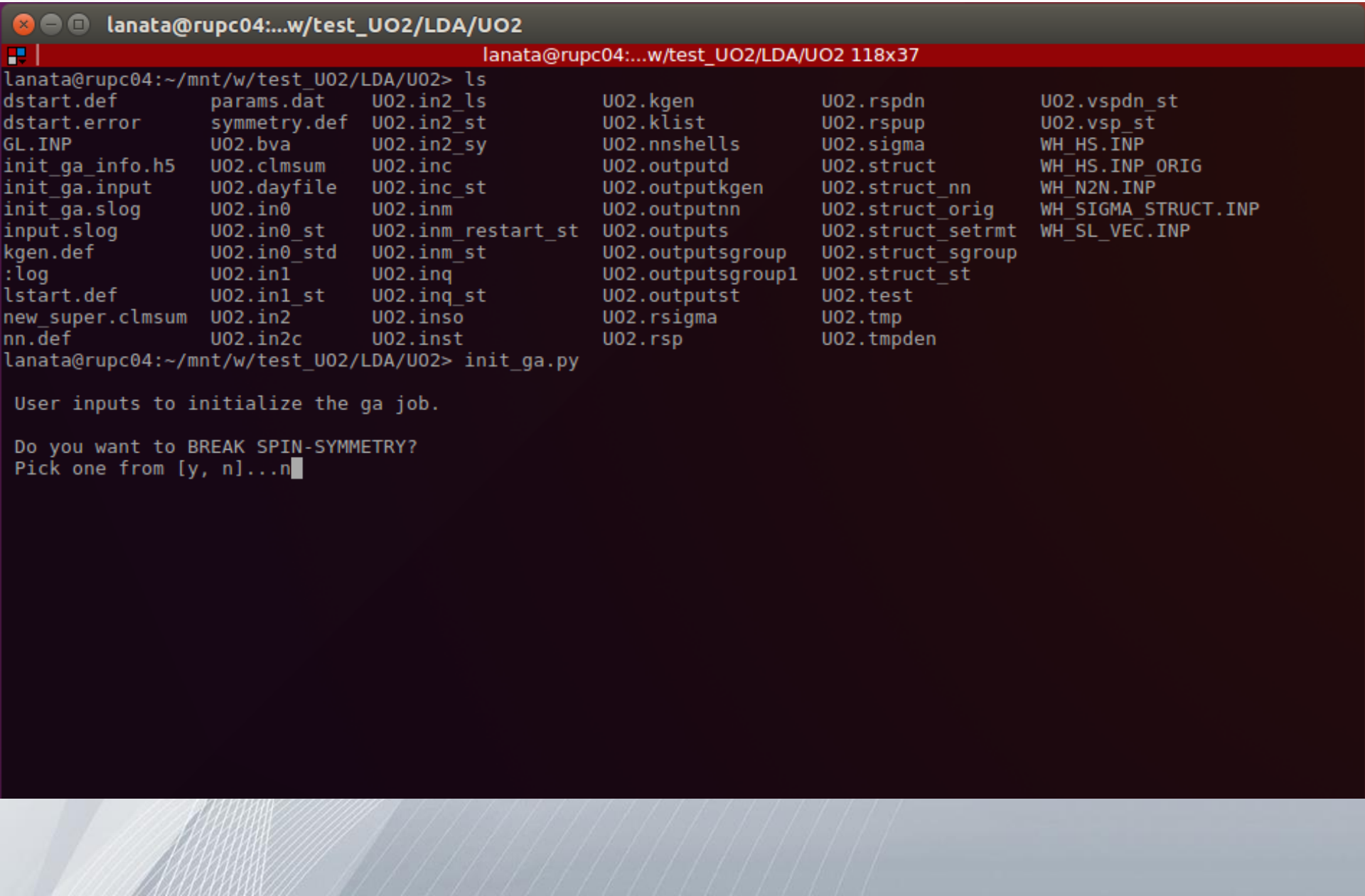
Initialization UO_2: LDA + RISB

Initialization UO_2 : LDA + RISB



Running script “init_ga.py” in folder with completed DFT run

Initialization UO_2 : LDA + RISB



Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> ls
dstart.def        params.dat    UO2.in2_ls          UO2.kgen          UO2.rspdn          UO2.vspdn_st
dstart.error      symmetry.def  UO2.in2_st          UO2.klist         UO2.rspup          UO2.vsp_st
GL.INP            UO2.bva       UO2.in2_sy          UO2.nnshells      UO2.sigma          WH_HS.INP
init_ga_info.h5   UO2.clmsum    UO2.inc             UO2.outputd       UO2.struct         WH_HS.INP_ORIG
init_ga.input     UO2.dayfile   UO2.inc_st          UO2.outputkgen    UO2.struct_nn      WH_N2N.INP
init_ga.slog      UO2.in0       UO2.inm             UO2.outputnn      UO2.struct_orig    WH_SIGMA_STRUCT.INP
input.slog        UO2.in0_st    UO2.inm_restart_st  UO2.outputs       UO2.struct_setrmt  WH_SL_VEC.INP
kgen.def          UO2.in0_std   UO2.inm_st          UO2.outputsgroup  UO2.struct_sgroup
:log              UO2.in1       UO2.inq             UO2.outputsgroup1 UO2.struct_st
lstart.def        UO2.in1_st    UO2.inq_st          UO2.outputst      UO2.test
new_super.clmsum  UO2.in2       UO2.inso            UO2.rsigma        UO2.tmp
nn.def            UO2.in2c      UO2.inst            UO2.rsp           UO2.tmpden
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> init_ga.py

 User inputs to initialize the ga job.

Do you want to BREAK SPIN-SYMMETRY?
Pick one from [y, n]...n

Do you want to COMPLETELY BREAK ORBITAL-SYMMETRY?
Pick one from [y, n]...n
```

Answer “y” only if looking for solution breaking local spin/orbital symmetry spontaneously (e.g., we may need it for URu_2Si_2)

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> ls
dstart.def        params.dat    UO2.in2_ls          UO2.kgen          UO2.rspdn          UO2.vspdn_st
dstart.error      symmetry.def  UO2.in2_st          UO2.klist         UO2.rspup          UO2.vsp_st
GL.INP            UO2.bva       UO2.in2_sy          UO2.nnshells      UO2.sigma          WH_HS.INP
init_ga_info.h5   UO2.clmsum    UO2.inc             UO2.outputd       UO2.struct         WH_HS.INP_ORIG
init_ga.input     UO2.dayfile   UO2.inc_st          UO2.outputkgen    UO2.struct_nn      WH_N2N.INP
init_ga.slog      UO2.in0       UO2.inm             UO2.outputnn      UO2.struct_orig    WH_SIGMA_STRUCT.INP
input.slog        UO2.in0_st    UO2.inm_restart_st  UO2.outputs       UO2.struct_setrmt  WH_SL_VEC.INP
kgen.def          UO2.in0_std   UO2.inm_st          UO2.outputsgroup  UO2.struct_sgroup
:log              UO2.in1       UO2.inq             UO2.outputsgroup1 UO2.struct_st
lstart.def        UO2.in1_st    UO2.inq_st          UO2.outputst      UO2.test
new_super.clmsum  UO2.in2       UO2.inso            UO2.rsigma        UO2.tmp
nn.def            UO2.in2c      UO2.inst            UO2.rsp           UO2.tmpden
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> init_ga.py

 User inputs to initialize the ga job.

 Do you want to BREAK SPIN-SYMMETRY?
 Pick one from [y, n]...n

 Do you want to COMPLETELY BREAK ORBITAL-SYMMETRY?
 Pick one from [y, n]...n

 Symmetrically-equivalent atom indices:  0  1  1
 (note: '0 0 0 1 1' means 1-3 and 4-5 are two inequivalent atoms).
 Accept?
 Pick one from [y, n]...y
```

Pymatgen detects automatically equivalent atoms (information used to avoid solving repeatedly equivalent impurity problems)

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> ls
dstart.def        params.dat    UO2.in2_ls          UO2.kgen          UO2.rspdn          UO2.vspdn_st
dstart.error      symmetry.def  UO2.in2_st          UO2.klist         UO2.rspup          UO2.vsp_st
GL.INP            UO2.bva       UO2.in2_sy          UO2.nnshells      UO2.sigma          WH_HS.INP
init_ga_info.h5   UO2.clmsum    UO2.inc             UO2.outputd       UO2.struct         WH_HS.INP_ORIG
init_ga.input     UO2.dayfile   UO2.inc_st          UO2.outputkgen    UO2.struct_nn      WH_N2N.INP
init_ga.slog      UO2.in0       UO2.inm             UO2.outputnn      UO2.struct_orig    WH_SIGMA_STRUCT.INP
input.slog        UO2.in0_st    UO2.inm_restart_st  UO2.outputs       UO2.struct_setrmt  WH_SL_VEC.INP
kgen.def          UO2.in0_std   UO2.inm_st          UO2.outputsgroup  UO2.struct_sgroup
:log              UO2.in1       UO2.inq             UO2.outputsgroup1 UO2.struct_st
lstart.def        UO2.in1_st    UO2.inq_st          UO2.outputst      UO2.test
new_super.clmsum  UO2.in2       UO2.inso            UO2.rsigma        UO2.tmp
nn.def            UO2.in2c      UO2.inst            UO2.rsp           UO2.tmpden
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> init_ga.py

 User inputs to initialize the ga job.

 Do you want to BREAK SPIN-SYMMETRY?
 Pick one from [y, n]...n

 Do you want to COMPLETELY BREAK ORBITAL-SYMMETRY?
 Pick one from [y, n]...n

 Symmetrically-equivalent atom indices:  0  1  1
 (note: '0 0 0 1 1' means 1-3 and 4-5 are two inequivalent atoms).
 Accept?
 Pick one from [y, n]...y

------------
atom  0   U

Is this atom correlated?
Pick one from [y, n]...y
```

Code asking user if atom with label “0” (which is U) is correlated or not

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> ls
dstart.def        params.dat    UO2.in2_ls          UO2.kgen          UO2.rspdn          UO2.vspdn_st
dstart.error      symmetry.def  UO2.in2_st          UO2.klist         UO2.rspup          UO2.vsp_st
GL.INP            UO2.bva       UO2.in2_sy          UO2.nnshells      UO2.sigma          WH_HS.INP
init_ga_info.h5   UO2.clmsum    UO2.inc             UO2.outputd       UO2.struct         WH_HS.INP_ORIG
init_ga.input     UO2.dayfile   UO2.inc_st          UO2.outputkgen    UO2.struct_nn      WH_N2N.INP
init_ga.slog      UO2.in0       UO2.inm             UO2.outputnn      UO2.struct_orig    WH_SIGMA_STRUCT.INP
input.slog        UO2.in0_st    UO2.inm_restart_st  UO2.outputs       UO2.struct_setrmt  WH_SL_VEC.INP
kgen.def          UO2.in0_std   UO2.inm_st          UO2.outputsgroup  UO2.struct_sgroup
:log              UO2.in1       UO2.inq             UO2.outputsgroup1 UO2.struct_st
lstart.def        UO2.in1_st    UO2.inq_st          UO2.outputst      UO2.test
new_super.clmsum  UO2.in2       UO2.inso            UO2.rsigma        UO2.tmp
nn.def            UO2.in2c      UO2.inst            UO2.rsp           UO2.tmpden
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> init_ga.py

 User inputs to initialize the ga job.

 Do you want to BREAK SPIN-SYMMETRY?
 Pick one from [y, n]...n

 Do you want to COMPLETELY BREAK ORBITAL-SYMMETRY?
 Pick one from [y, n]...n

 Symmetrically-equivalent atom indices:  0  1  1
 (note: '0 0 0 1 1' means 1-3 and 4-5 are two inequivalent atoms).
 Accept?
 Pick one from [y, n]...y

 ------------
 atom  0   U

 Is this atom correlated?
 Pick one from [y, n]...y

 Enter correlated shells?
 Pick one or combinations separated by blank space
 from [s, p, d, f]...f
```

U atom has *f* correlated electrons

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
init_ga.slog      UO2.in0       UO2.inm             UO2.outputnn       UO2.struct_orig    WH_SIGMA_STRUCT.INP
input.slog        UO2.in0_st    UO2.inm_restart_st  UO2.outputs        UO2.struct_setrmt  WH_SL_VEC.INP
kgen.def          UO2.in0_std   UO2.inm_st          UO2.outputsgroup   UO2.struct_sgroup
:log              UO2.in1       UO2.inq             UO2.outputsgroup1  UO2.struct_st
lstart.def        UO2.in1_st    UO2.inq_st          UO2.outputst       UO2.test
new_super.clmsum  UO2.in2       UO2.inso            UO2.rsigma         UO2.tmp
nn.def            UO2.in2c      UO2.inst            UO2.rsp            UO2.tmpden
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> init_ga.py

 User inputs to initialize the ga job.

 Do you want to BREAK SPIN-SYMMETRY?
 Pick one from [y, n]...n

 Do you want to COMPLETELY BREAK ORBITAL-SYMMETRY?
 Pick one from [y, n]...n

 Symmetrically-equivalent atom indices:  0  1  1
 (note: '0 0 0 1 1' means 1-3 and 4-5 are two inequivalent atoms).
 Accept?
 Pick one from [y, n]...y

 ------------
 atom  0   U

 Is this atom correlated?
 Pick one from [y, n]...y

 Enter correlated shells?
 Pick one or combinations separated by blank space
 from [s, p, d, f]...f

 Do you want to take into account the SPIN-ORBIT interaction?
 Pick one from [y, n]...y

 Do you want to take into account the CRYSTAL FIELD effect?
 Pick one from [y, n]...y
```

SOC and CFS not negligible: System not spin rotationally-invariant. Discrete group with rotations generated by J=L+S

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
nn.def            UO2.in2c      UO2.inst            UO2.rsp            UO2.tmpden
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> init_ga.py

 User inputs to initialize the ga job.

 Do you want to BREAK SPIN-SYMMETRY?
 Pick one from [y, n]...n

 Do you want to COMPLETELY BREAK ORBITAL-SYMMETRY?
 Pick one from [y, n]...n

 Symmetrically-equivalent atom indices:  0  1  1
 (note: '0 0 0 1 1' means 1-3 and 4-5 are two inequivalent atoms).
 Accept?
 Pick one from [y, n]...y

 ------------
 atom  0   U

 Is this atom correlated?
 Pick one from [y, n]...y

 Enter correlated shells?
 Pick one or combinations separated by blank space
 from [s, p, d, f]...f

 Do you want to take into account the SPIN-ORBIT interaction?
 Pick one from [y, n]...y

 Do you want to take into account the CRYSTAL FIELD effect?
 Pick one from [y, n]...y

 ------------
 atom  1   O

 Is this atom correlated?
 Pick one from [y, n]...n
```

Code asking user if atom with label “1” (which is O) is correlated or not (it’s not)

Initialization UO_2 : LDA + RISB

lanata@rupc04:...w/test_UO2/LDA/UO2

lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

```
Accept?
Pick one from [y, n]...y

------------
atom  0   U

Is this atom correlated?
Pick one from [y, n]...y

Enter correlated shells?
Pick one or combinations separated by blank space
from [s, p, d, f]...f

Do you want to take into account the SPIN-ORBIT interaction?
Pick one from [y, n]...y

Do you want to take into account the CRYSTAL FIELD effect?
Pick one from [y, n]...y

------------
atom  1   O

Is this atom correlated?
Pick one from [y, n]...n

LHUB = 1: Slater-Condo parametrization.
       2: Kanamori parametrization (useful for models).
       0: U_{i,j,k,l} (NO SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          V(|r-r'|) phi(r_k) phi(r'_l)}}
          will be provided by file V2AO.INP
      -1: U_{i,j,k,l} (INCLUDING SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          phi(r_k) phi(r'_l)}}
          will be provided by file V2H.INP
Please select LHUB:
Pick one from [1, -1, 0, 2]...1
```

Other questions not related with symmetry analysis

We choose Slater parametrization local interaction (consequently values of U,J will be asked)

Initialization UO_2 : LDA + RISB

lanata@rupc04:...w/test_UO2/LDA/UO2

lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

```
Do you want to take into account the SPIN-ORBIT interaction?
Pick one from [y, n]...y

Do you want to take into account the CRYSTAL FIELD effect?
Pick one from [y, n]...y

------------
atom  1   O

Is this atom correlated?
Pick one from [y, n]...n

LHUB = 1: Slater-Condo parametrization.
       2: Kanamori parametrization (useful for models).
       0: U_{i,j,k,l} (NO SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          V(|r-r'|) phi(r_k) phi(r'_l)}}
          will be provided by file V2AO.INP
      -1: U_{i,j,k,l} (INCLUDING SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          phi(r_k) phi(r'_l)}}
          will be provided by file V2H.INP
Please select LHUB:
Pick one from [1, -1, 0, 2]...1

LDC = 12: Recommended. Standard double counting
          (updating Vdc at each charge iteration,
          initial n0 to be provided.)
       2: Fix double counting potential
          (keep same Vdc/n0 at each charge iteration,
          n0 to be provided.)
       1: Standard double counting potential
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12
```

Other questions not related with symmetry analysis

We generally choose standard (quadratic) double counting in all of our calculations

Initialization UO_2 : LDA + RISB

lanata@rupc04:...w/test_UO2/LDA/UO2

lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

```
Do you want to take into account the CRYSTAL FIELD effect?
Pick one from [y, n]...y

------------
atom  1   O

Is this atom correlated?
Pick one from [y, n]...n

LHUB = 1: Slater-Condo parametrization.
       2: Kanamori parametrization (useful for models).
       0: U_{i,j,k,l} (NO SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          V(|r-r'|) phi(r_k) phi(r'_l)}}
          will be provided by file V2AO.INP
      -1: U_{i,j,k,l} (INCLUDING SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          phi(r_k) phi(r'_l)}}
          will be provided by file V2H.INP
Please select LHUB:
Pick one from [1, -1, 0, 2]...1

LDC = 12: Recommended. Standard double counting
          (updating Vdc at each charge iteration,
          initial n0 to be provided.)
       2: Fix double counting potential
          (keep same Vdc/n0 at each charge iteration,
          n0 to be provided.)
       1: Standard double counting potential
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12

Please enter the tolerance of solving the equations of {R, \lambda}
(recommend 1.e-5 or smaller)...5.e-6
```

Other questions not related with symmetry analysis

Question specific for GA/RISB solver (precision requested for self-energy self consistency, which is formulated as a root problem)

Initialization UO_2 : LDA + RISB

lanata@rupc04:...w/test_UO2/LDA/UO2

lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

```
Is this atom correlated?
Pick one from [y, n]...n

LHUB = 1: Slater-Condo parametrization.
       2: Kanamori parametrization (useful for models).
       0: U_{i,j,k,l} (NO SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          V(|r-r'|) phi(r_k) phi(r'_l)}}
          will be provided by file V2AO.INP
      -1: U_{i,j,k,l} (INCLUDING SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          phi(r_k) phi(r'_l)}}
          will be provided by file V2H.INP
Please select LHUB:
Pick one from [1, -1, 0, 2]...1

LDC = 12: Recommended. Standard double counting
          (updating Vdc at each charge iteration,
          initial n0 to be provided.)
       2: Fix double counting potential
          (keep same Vdc/n0 at each charge iteration,
          n0 to be provided.)
       1: Standard double counting potential
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12

Please enter the tolerance of solving the equations of {R, \lambda}
(recommend 1.e-5 or smaller)...5.e-6

LNEWTON = 0: Recommended. Modified Powell hybrid method (HYDRD1).
         -1: Broyden method. Faster for solutions with Z
             much larger than 0, e.g., magnetic calculations.
Please select LNEWTON:
Pick one from [-1, 0]...0
```

Other questions not related with symmetry analysis

Question specific for GA/RISB solver (solver used for root problem, basically better to use default option in all cases)

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
       2: Kanamori parametrization (useful for models).
       0: U_{i,j,k,l} (NO SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          V(|r-r'|) phi(r_k) phi(r'_l)}}
          will be provided by file V2AO.INP
      -1: U_{i,j,k,l} (INCLUDING SPIN INDEX) =
          int_{dr int_{dr' phi^{*}(r_i) phi^{*}(r'_j)
          phi(r_k) phi(r'_l)}}
          will be provided by file V2H.INP
Please select LHUB:
Pick one from [1, -1, 0, 2]...1

LDC = 12: Recommended. Standard double counting
          (updating Vdc at each charge iteration,
          initial n0 to be provided.)
       2: Fix double counting potential
          (keep same Vdc/n0 at each charge iteration,
          n0 to be provided.)
       1: Standard double counting potential
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12

Please enter the tolerance of solving the equations of {R, \lambda}
(recommend 1.e-5 or smaller)...5.e-6

LNEWTON = 0: Recommended. Modified Powell hybrid method (HYDRD1).
         -1: Broyden method. Faster for solutions with Z
             much larger than 0, e.g., magnetic calculations.
Please select LNEWTON:
Pick one from [-1, 0]...0

LCLUSTER = 0: Single-atom impurity.
           1: Multi-atom (cluster) impurity.
Please select LCLUSTER:
Pick one from [0, 1]...0
```

Other questions not related with symmetry analysis

The cluster impurity (option 1) is not even implemented. Answer “0” to apply standard single-site approximation scheme

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

LDC = 12: Recommended. Standard double counting
          (updating Vdc at each charge iteration,
          initial n0 to be provided.)
       2: Fix double counting potential
          (keep same Vdc/n0 at each charge iteration,
          n0 to be provided.)
       1: Standard double counting potential
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12

Please enter the tolerance of solving the equations of {R, \lambda}
(recommend 1.e-5 or smaller)...5.e-6

LNEWTON = 0: Recommended. Modified Powell hybrid method (HYDRD1).
         -1: Broyden method. Faster for solutions with Z
             much larger than 0, e.g., magnetic calculations.
Please select LNEWTON:
Pick one from [-1, 0]...0

LCLUSTER = 0: Single-atom impurity.
           1: Multi-atom (cluster) impurity.
Please select LCLUSTER:
Pick one from [0, 1]...0

Solution embedding system:
LEIGV = 0: Choose automatically solver depending
           on the size of the problem (DEFAULT)
        1: Exact diagonalization (ZHEEV) in LAPACK
        2: Lanczos (zhdrv1) in ARPACK
        3: Exact diagonalization (ZHEEVX,
           selective lowest two eigen-vectors) in LAPACK
        5: PRIMME (Recommended for large dimension.)
Please select LEIGV:
Pick one from [5, 0, 1, 2, 3]...5
```

Other questions not related with symmetry analysis

Option “5” is basically a robust implementation of Lanczos (best option for now).

Currently testing new solvers (DMRG, CISD, etc.…). Big room for improvement with respect to Lanczos.

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
       2: Fix double counting potential
          (keep same Vdc/n0 at each charge iteration,
          n0 to be provided.)
       1: Standard double counting potential
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12

Please enter the tolerance of solving the equations of {R, \lambda}
(recommend 1.e-5 or smaller)...5.e-6

LNEWTON = 0: Recommended. Modified Powell hybrid method (HYDRD1).
         -1: Broyden method. Faster for solutions with Z
             much larger than 0, e.g., magnetic calculations.
Please select LNEWTON:
Pick one from [-1, 0]...0

LCLUSTER = 0: Single-atom impurity.
           1: Multi-atom (cluster) impurity.
Please select LCLUSTER:
Pick one from [0, 1]...0

Solution embedding system:
LEIGV = 0: Choose automatically solver depending
           on the size of the problem (DEFAULT)
        1: Exact diagonalization (ZHEEV) in LAPACK
        2: Lanczos (zhdrv1) in ARPACK
        3: Exact diagonalization (ZHEEVX,
           selective lowest two eigen-vectors) in LAPACK
        5: PRIMME (Recommended for large dimension.)
Please select LEIGV:
Pick one from [5, 0, 1, 2, 3]...5

INFORMATION FOR f ELECTRONS OF U :
Please provide interaction parameters U,J
separated by a space: 9 0.6
```

Other questions not related with symmetry analysis

Provide U,J parameters for atom indicated (U in this case)

Initialization UO_2 : LDA + RISB

lanata@rupc04:...w/test_UO2/LDA/UO2

lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

```
          (n0 self-consistently determined.)
       0:  No double counting.
Please select LDC:
Pick one from [12, 0, 1, 2]...12

Please enter the tolerance of solving the equations of {R, \lambda}
(recommend 1.e-5 or smaller)...5.e-6

LNEWTON = 0: Recommended. Modified Powell hybrid method (HYDRD1).
         -1: Broyden method. Faster for solutions with Z
             much larger than 0, e.g., magnetic calculations.
Please select LNEWTON:
Pick one from [-1, 0]...0

LCLUSTER = 0: Single-atom impurity.
           1: Multi-atom (cluster) impurity.
Please select LCLUSTER:
Pick one from [0, 1]...0

Solution embedding system:
LEIGV = 0: Choose automatically solver depending
           on the size of the problem (DEFAULT)
        1: Exact diagonalization (ZHEEV) in LAPACK
        2: Lanczos (zhdrv1) in ARPACK
        3: Exact diagonalization (ZHEEVX,
           selective lowest two eigen-vectors) in LAPACK
        5: PRIMME (Recommended for large dimension.)
Please select LEIGV:
Pick one from [5, 0, 1, 2, 3]...5

INFORMATION FOR f ELECTRONS OF U :
Please provide interaction parameters U,J
separated by a space: 9 0.6
Please provide N1,N2 defining valence range [N1,N2]
separated by a space ( 0 < N1 < N2 < 14 ): 0 4
Please provide guess n0 for valence
(0 < n0 < 4 overwritten by GL_NELF1.INP): 2.1
```

Other questions not related with symmetry analysis

Relevant valence range of U atom. Embedding problem computationally challenging when CFS and SOC both non-negligible. Valence truncation necessary with Lanczos (and fortunately licit for this system).

Initialization UO_2 : LDA + RISB

lanata@rupc04:...w/test_UO2/LDA/UO2

lanata@rupc04:...w/test_UO2/LDA/UO2 118x37

```
 21 -1.00  0.00 -0.00
    -0.00 -0.00  1.00
     0.00  1.00  0.00
 22 -0.00  1.00  0.00
     1.00  0.00 -0.00
    -0.00  0.00 -1.00
 23  0.00 -1.00 -0.00
    -1.00 -0.00  0.00
    -0.00  0.00 -1.00
Error in sum_chi2 = 24.0
 Please run ga_init_dmft.py with parameters given in init_ga.slog
 The default dist_cut for extracting a centered cluster
 for symmetry evaluation =  3.9044007499
 Molecule extracted O_8 U_13 :
 atom    x       y       z     distance
   O   -1.35   -1.35   -1.35     2.3297
   O    1.35    1.35   -1.35     2.3297
   O    1.35   -1.35    1.35     2.3297
   U   -0.00   -2.69   -2.69     3.8044
   O    1.35   -1.35   -1.35     2.3297
   U    2.69    0.00   -2.69     3.8044
   U    2.69   -2.69    0.00     3.8044
   O   -1.35    1.35    1.35     2.3297
   U   -2.69   -0.00   -2.69     3.8044
   O   -1.35    1.35   -1.35     2.3297
   U    0.00    2.69   -2.69     3.8044
   U   -2.69   -2.69    0.00     3.8044
   O   -1.35   -1.35    1.35     2.3297
   U    0.00    0.00    0.00     0.0000
   O    1.35    1.35    1.35     2.3297
   U    2.69    2.69    0.00     3.8044
   U    0.00   -2.69    2.69     3.8044
   U    2.69    0.00    2.69     3.8044
   U   -2.69    2.69    0.00     3.8044
   U   -2.69    0.00    2.69     3.8044
   U    0.00    2.69    2.69     3.8044
lanata@rupc04:~/mnt/w/test_UO2/LDA/UO2> less init_ga.slog
```

Initialization completed. Corresponding information given (and part of the processed information) dumped in file “init_ga.slog”.

Initialization UO_2 : LDA + RISB

```
lanata@rupc04:...w/test_UO2/LDA/UO2
lanata@rupc04:...w/test_UO2/LDA/UO2 118x37
The executed commant line is:
/home/ykent/WIEN_GUTZ/bin/tools/Gutzwiller/init_ga.py
 Cell:
[[  3.29444387e-16   2.69011757e+00   2.69011757e+00]
 [  2.69011757e+00   1.64722193e-16   2.69011757e+00]
 [  2.69011757e+00   2.69011757e+00   0.00000000e+00]]
 Symbols:  ['U', 'O', 'O']
 Scaled_positions:
[[ 0.    0.    0.  ]
 [ 0.75  0.75  0.75]
 [ 0.25  0.25  0.25]]
 Mapping-table equivalent atoms:  [0 1 1]
 Labels correlated atoms:  [0]
 Orbital angular momentums of correlated electrons:  ['f']
 Take into accout SOC or not:  ['y']
 Take into accout crystal-fields or not:  ['y']
 Cut-off distance for symmetry analysis:  -1.0
 LGPRJ = 11:  Assuming only that  $[\phi,N] = 0$ (allowing simultaneously SOC, magnetism and crystal field)
( the value of n0 will be overwritten by GL_NELF1.INP & GL_NELF1.OUT during the calculation )
self_energy  0
[[1 2 0 0 0 0 0 0 0 0 0 0 0 0]
 [3 4 0 0 0 0 0 0 0 0 0 0 0 0]
 [0 0 1 2 0 0 0 0 0 0 0 0 0 0]
 [0 0 3 4 0 0 0 0 0 0 0 0 0 0]
 [0 0 0 0 5 6 0 0 0 0 0 0 0 0]
 [0 0 0 0 7 8 0 0 0 0 0 0 0 0]
 [0 0 0 0 0 0 5 6 0 0 0 0 0 0]
 [0 0 0 0 0 0 7 8 0 0 0 0 0 0]
 [0 0 0 0 0 0 0 0 5 6 0 0 0 0]
 [0 0 0 0 0 0 0 0 7 8 0 0 0 0]
 [0 0 0 0 0 0 0 0 0 0 5 6 0 0]
 [0 0 0 0 0 0 0 0 0 0 7 8 0 0]
 [0 0 0 0 0 0 0 0 0 0 0 0 9 0]
 [0 0 0 0 0 0 0 0 0 0 0 0 0 9]]
 Please run ga_init_dmft.py with the following parameters.
init_ga.slog lines 1-36/54 76%
```

Initialization completed. Corresponding information given (and part of the processed information) dumped in file "init_ga.slog".

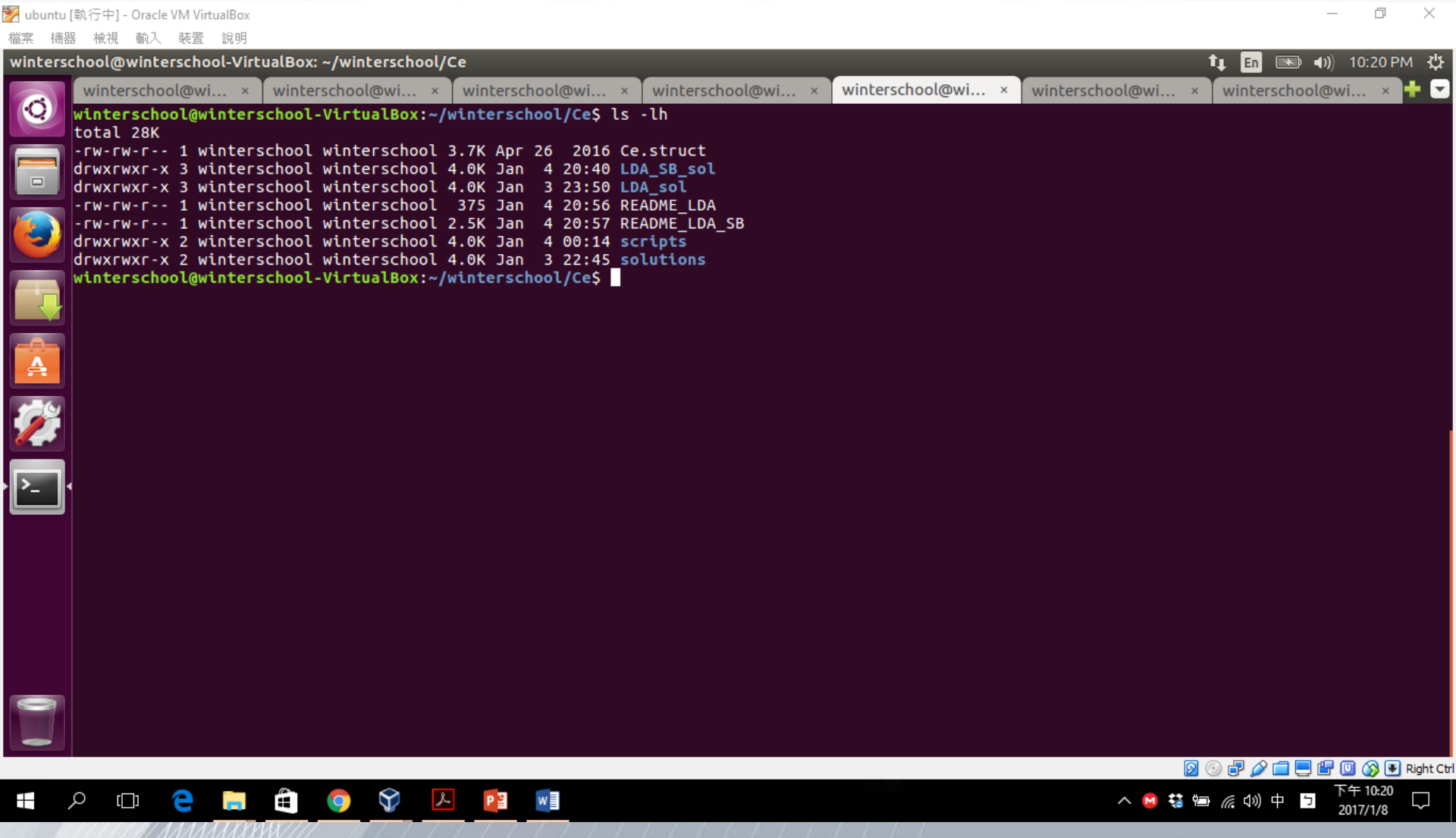
Block structure of self energy of *f* electrons of U atom in symmetry basis accordingly to Shur Lemma (calculated by our symmetry code)

Hands-on Session: Outline

- α-Ce LDA+SB calculation:
  density of state, multiplets histogram, band structure.
- α-Fe LDA+SB spin polarized calculation:
  density of state, band structure.
- (Optional) Energy-Volume scan for α-Ce.

Hands-on Session: α-Ce

Folder structure:



Hands-on Session: α-Ce

- Perform a LDA+spin orbit calculation with vxc=5(LDA), numk 5000, rkmax=9.
- Copy the converged LDA folder to LDA+SB and perform a LDA+SB calculation.
- Plot density of state(using plot_dos.py in ./scripts).
- Plot multiplet histogram(using multiplets_analysis_soc.py in ./scripts).
- Perform one shot calculation for band structure with fcc k-path.
- Plot band structure(using plot_bands.py in ./scripts).

Please refer to the README files or http://ykent.public.iastate.edu/cygutz/tutorials.html#ce-with-spin-orbit-interaction for details

Hands-on Session: α-Fe

Folder structure:

ubuntu [執行中] - Oracle VM VirtualBox

檔案 機器 檢視 輸入 裝置 說明

winterschool@winterschool-VirtualBox: ~/winterschool/Fe

8:06 PM

```
winterschool@winterschool-VirtualBox:~/winterschool/Fe$ ls -lh
total 28K
-rw-rw-r-- 1 winterschool winterschool 3.7K Apr 26  2016 Fe.struct
drwxrwxr-x 3 winterschool winterschool 4.0K Jan  3 23:03 LDA_SB_sol
drwxrwxr-x 3 winterschool winterschool 4.0K Jan  3 11:33 LDA_sol
-rw-rw-r-- 1 winterschool winterschool  265 Jan  6 22:36 README_LDA
-rw-rw-r-- 1 winterschool winterschool 2.2K Jan  4 20:57 README_LDA_SB
drwxrwxr-x 2 winterschool winterschool 4.0K Jan  7 04:55 scripts
drwxrwxr-x 2 winterschool winterschool 4.0K Jan  3 22:52 solutions
winterschool@winterschool-VirtualBox:~/winterschool/Fe$
```

Right Ctrl

下午 08:06
2017/1/8

Hands-on Session: α-Fe

- Perform a LDA calculation with vxc=5(LDA), numk 5000, rkmax=8.
- Copy the converged LDA folder to LDA+SB and perform a spin ploarized LDA+SB calculation.
- Plot density of state(using plot_dos.py in ./scripts).
- Perform one shot calculation for band structure with bcc k-path.
- Plot band structure(using plot_bands.py in ./scripts).

Please refer to the README files or http://ykent.public.iastate.edu/cygutz/tutorials.html#ferromagnetic-calculation-for-fe for details

Hands-on Session: (optional) α-Ce E-V plot

- Change the RMT in Ce.struct to 2.3.
- Create structure files for different volume using gen_struct_folders.py in ${WIEN_GUTZ_ROOT}/tools/WIEN2k/.
- Perform LDA+SB for each volume.
- Plot EV curve using analysis_total_energy.py in ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/.

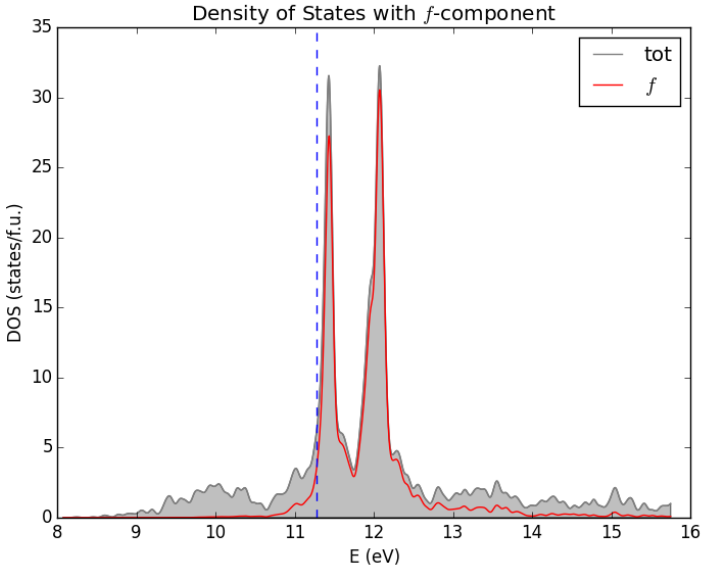
γ-α Isostructural Transition in Cerium, N. Lanata et. al
http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.111.196801

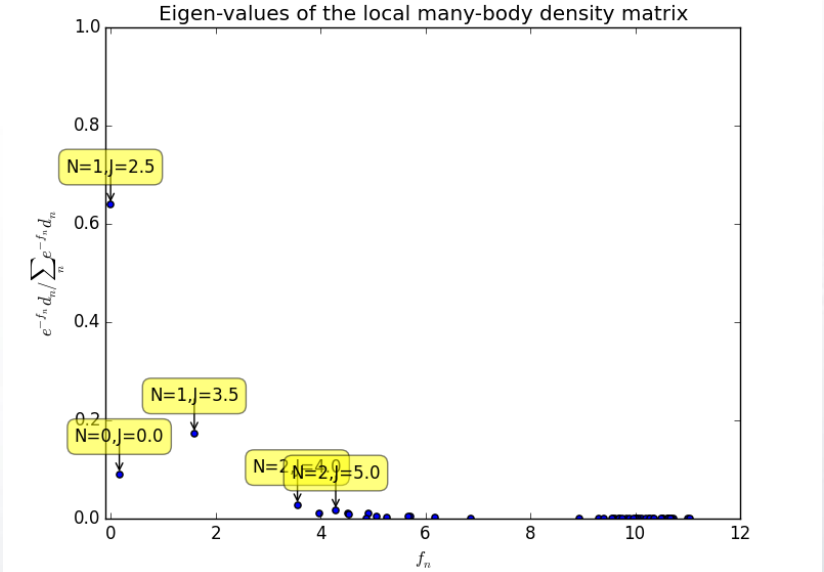
Extract important quantities

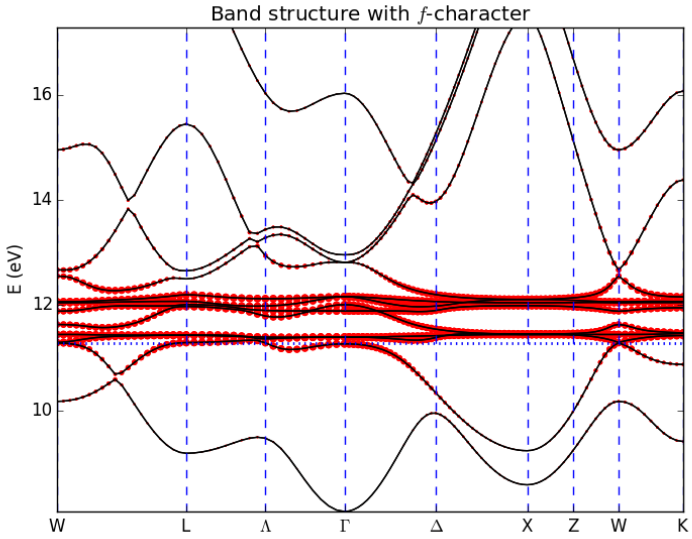
- Total energy: grep :ENE case.scf.
- Quasiaprticle weight: grep -A 26 daggerR GUTZ.LOG.
- Magnetic moment: grep MOMENT GUTZ.LOG.
- Quasiparticle occupancy: grep –A 26 NKS-UNSYM GUTZ.LOG
- Physical occupancy: grep -A 26 NCP_RENORM GUTZ.LOG.
- Check convergence: grep :ENE case.dayfile
- Check CyGutz convergence: grep MAXERR GUTZ.LOG.

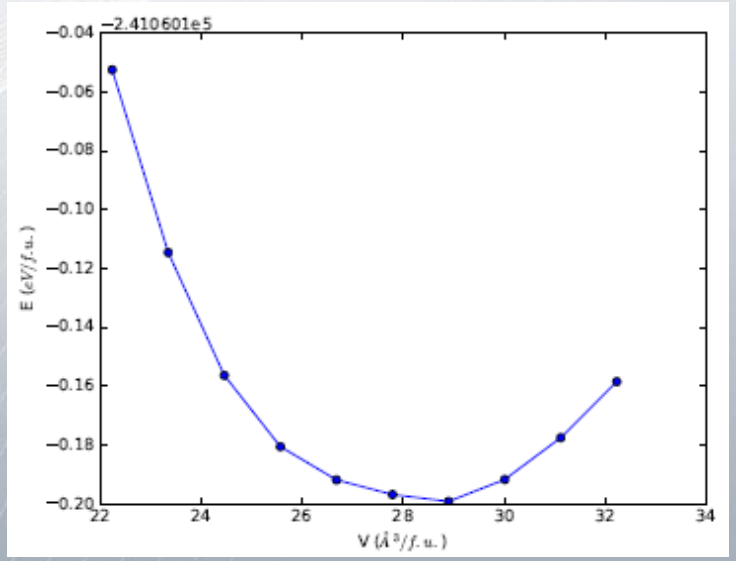
NOTE: One can grep either GL_LOG.OUT or GUTZ.LOG for CyGutz information.

Hands-on Session: α-Ce

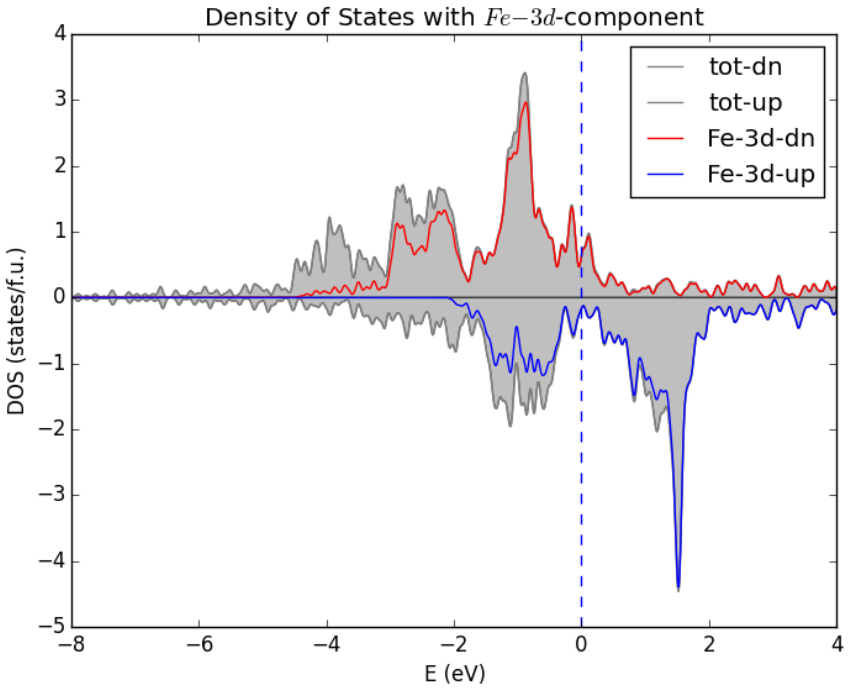


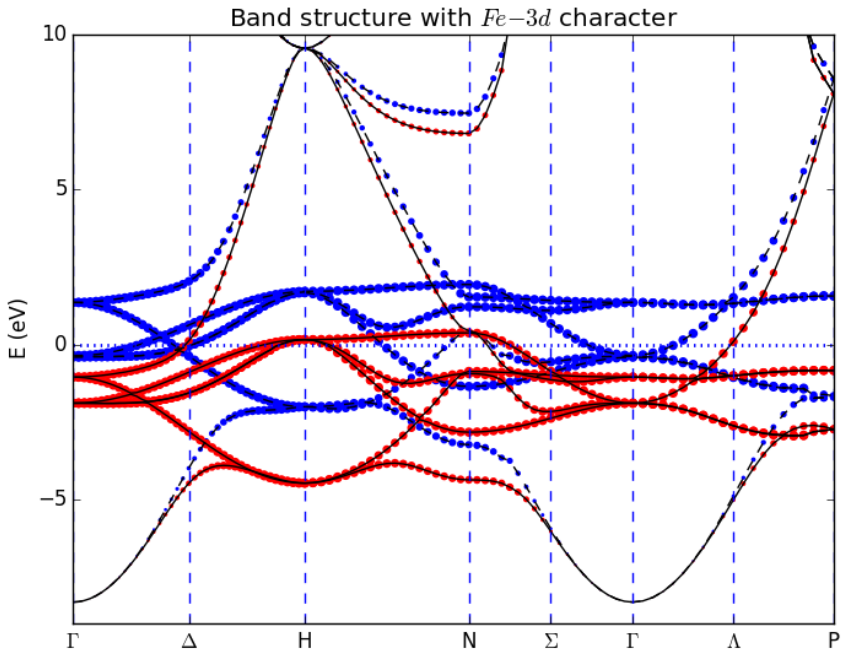






Hands-on Session: α-Fe





Gutzwiller approximation

The variational wavefunction

$$|\Psi_G\rangle = \mathcal{P}|\Psi_0\rangle = \prod_{\mathbf{R},\, i\in\text{corr}} \mathcal{P}_{\mathbf{R}i}\,|\Psi_0\rangle$$

- $|\Psi_0\rangle$: ***Slater determinant*** (hybridizing bands)
- $\mathcal{P}_{\mathbf{R}i}$: ***Local operator*** that modifies the weights of the local electronic configurations

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

Local Fock configurations:

$$|\Gamma;\mathbf{R},i\rangle = \left(c^\dagger_{\mathbf{R}i1}\right)^{n_1}\cdots\left(c^\dagger_{\mathbf{R}iM}\right)^{n_M}|0\rangle$$

$$|n;\mathbf{R},i\rangle = \left(f^\dagger_{\mathbf{R}i1}\right)^{n'_1}\cdots\left(f^\dagger_{\mathbf{R}iM}\right)^{n'_M}|0\rangle \quad \left(\langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle \equiv n^0_{iab} = \delta_{ab}\,n^0_{ibb}\right)$$

Calculations considerably simplified by the following assumptions:

Gutzwiller Approximation:

$|\Psi_G\rangle$ can be dealt only numerically unless in the limit of ∞-coordination lattices

(as in DMFT)

Gutzwiller constraints:

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

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

("slightly" reduce variational freedom)

Considerable simplification of the calculations

Gutzwiller constraints:

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

$$\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle = \langle \Psi_0 | f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ib} | \Psi_0 \rangle \quad (\forall a, b)$$

Key consequence:

$$\langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ia} | \Psi_0 \rangle = \langle \Psi_0 | \mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} | \Psi_0 \rangle \langle \Psi_0 | f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ia} | \Psi_0 \rangle + \langle \Psi_0 | \left[\mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} \right] \left(f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ia} \right) | \Psi_0 \rangle_{\text{2-legs contracted}}$$

$$\langle \Psi_0 | \left[\mathcal{P}^\dagger_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} \right] \left(c^\dagger_{\mathbf{R}'j\alpha} c_{\mathbf{R}'j\alpha} \right) | \Psi_0 \rangle_{\text{2-legs contracted}} = 0 \quad \forall \mathbf{R}, i; \mathbf{R}', j$$

Local operators:

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

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

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

$$+ \langle \Psi_0 | \left[\prod_{\mathbf{R}', i' \neq \mathbf{R}', i} \mathcal{P}^\dagger_{\mathbf{R}'i'} \mathcal{P}_{\mathbf{R}'i'} \right] \left(\mathcal{P}^\dagger_{\mathbf{R}i} \, \hat{\mathcal{O}}_{\mathbf{R}i}[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}] \, \mathcal{P}_{\mathbf{R}i} \right) \, | \Psi_0 \rangle_{\text{2-legs}}$$

$$+ \langle \Psi_0 | \left[\prod_{\mathbf{R}', i' \neq \mathbf{R}', i} \mathcal{P}^\dagger_{\mathbf{R}'i'} \mathcal{P}_{\mathbf{R}'i'} \right] \left(\mathcal{P}^\dagger_{\mathbf{R}i} \, \hat{\mathcal{O}}_{\mathbf{R}i}[c^\dagger_{\mathbf{R}i\alpha}, c_{\mathbf{R}i\alpha}] \, \mathcal{P}_{\mathbf{R}i} \right) \, | \Psi_0 \rangle_{(N \geq 4)\text{-legs}}$$

Local operators:

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

Inter-site single-particle quadratic operators:

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

where $\mathcal{P}_{\mathbf{R}i} = \sum_{\Gamma n}\,\lambda_{i,\Gamma n}\,|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i|$

Inter-site single-particle density matrix operators:

$$\begin{aligned}
\langle\Psi_0|\,\mathcal{P}^\dagger\, c^\dagger_{\mathbf{R}i\alpha} c_{\mathbf{R}'j\beta}\,\mathcal{P}\,|\Psi_0\rangle &= \langle\Psi_0|\,[\mathcal{P}^\dagger_{\mathbf{R}i}\, c^\dagger_{\mathbf{R}i\alpha}\,\mathcal{P}_{\mathbf{R}i}]\,[\mathcal{P}^\dagger_{\mathbf{R}'j}\, c_{\mathbf{R}'j\beta}\,\mathcal{P}_{\mathbf{R}'j}]\,|\Psi_0\rangle \\
&= \langle\Psi_0|\,[\mathcal{P}^\dagger_{\mathbf{R}i}\, c^\dagger_{\mathbf{R}i\alpha}\,\mathcal{P}_{\mathbf{R}i}]\,[\mathcal{P}^\dagger_{\mathbf{R}'j}\, c_{\mathbf{R}'j\beta}\,\mathcal{P}_{\mathbf{R}'j}]\,|\Psi_0\rangle_{\text{1-leg}} \\
&\equiv \sum_{ab} \langle\Psi_0|\,\left([\mathcal{R}_i]_{a\alpha}\, f^\dagger_{\mathbf{R}ia}\right)\left([\mathcal{R}_j]^*_{b\beta}\, f_{\mathbf{R}'jb}\right)\,|\Psi_0\rangle
\end{aligned}$$

Original ladder operators effectively transform as

$$c^\dagger_{\mathbf{R}i\alpha} \rightarrow \sum_a [\mathcal{R}_i]_{a\alpha}\, f^\dagger_{\mathbf{R}ia}$$

under the action of the Gutzwiller projector, where:

$$\begin{aligned}
[\mathcal{R}_i]_{a\alpha} &= \boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,[c^\dagger_{\mathbf{R}i\alpha}\,\mathcal{P}_{\mathbf{R}i}\, f_{\mathbf{R}ia}\,|\Psi_0\rangle}\,] \,/\, \langle\Psi_0|f^\dagger_{\mathbf{R}ia} f_{\mathbf{R}ia}\,|\Psi_0\rangle \\
\mathcal{P}_{\mathbf{R}i} &= \sum_{\Gamma n} \lambda_{i,\Gamma n}\,|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i|
\end{aligned}$$

Important $|\Psi_0\rangle$-averages of local operators expressed as traces: step 1

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,\mathcal{P}_{\mathbf{R}i}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[P^0_i\lambda^\dagger_i\lambda_i\Big] = 1$$

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,\mathcal{P}_{\mathbf{R}i}\,f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[P^0_i\lambda^\dagger_i\lambda_i\,F^\dagger_{ia}F_{ib}\Big] = \langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle \equiv n^0_{iab}\,\delta_{ab}$$

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,c^\dagger_{\mathbf{R}i\alpha}\,\mathcal{P}_{\mathbf{R}i}\,f_{\mathbf{R}ia}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[P^0_i\lambda^\dagger_i\,F^\dagger_{i\alpha}\,\lambda_i\;F_{ia}\Big]$$

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,\hat{\mathcal{O}}_{\mathbf{R}i}\,\mathcal{P}_{\mathbf{R}i}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[P^0_i\lambda^\dagger_i\,O\,\lambda_i\Big]$$

$$\mathcal{P}_{\mathbf{R}i} \equiv \sum_{\Gamma n}\lambda_{i,\Gamma n}\,|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i|$$

$$|\Gamma;R,i\rangle \equiv \Big[c^\dagger_{Ri1}\Big]^{n_1}\cdots\Big[c^\dagger_{RiM}\Big]^{n_M}\,|0\rangle\,;\quad |n;R,i\rangle \equiv \Big[f^\dagger_{Ri1}\Big]^{n_1}\cdots\Big[f^\dagger_{RiM}\Big]^{n_M}\,|0\rangle$$

$$\Big[P^0_i\Big]_{nn'} \equiv \langle\Psi_0|\,|n',Ri\rangle\langle n,Ri|\,|\Psi_0\rangle\,\delta_{nn'}$$

$$[F_{ib}]_{nn'} = \langle\Gamma,Ri\,|\,c_{Rib}\,|\,\Gamma',Ri\rangle = \langle n,Ri\,|f_{Rib}\,|\,n',Ri\rangle$$

$$[O]_{\Gamma\Gamma'} = \langle\Gamma,Ri\,|\,\hat{\mathcal{O}}_{\mathbf{R}i}\,|\,\Gamma',Ri\rangle$$

Important $|\Psi_0\rangle$-averages of local operators expressed as traces: step 2

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,\mathcal{P}_{\mathbf{R}i}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[\phi_i\,\phi_i^\dagger\Big] = 1$$

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,\mathcal{P}_{\mathbf{R}i}\,f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[\phi_i^\dagger\phi_i\;F^\dagger_{ia}F_{ib}\Big] = \langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ib}\,|\Psi_0\rangle \equiv n^0_{iab}\,\delta_{ab}$$

$$\boxed{[\mathcal{R}_i]_{a\alpha}} \equiv \boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,c^\dagger_{\mathbf{R}i\alpha}\,\mathcal{P}_{\mathbf{R}i}\,f_{\mathbf{R}ia}\,|\Psi_0\rangle} \Big/ \langle\Psi_0|f^\dagger_{\mathbf{R}ia}f_{\mathbf{R}ia}\,|\Psi_0\rangle$$

$$= \mathrm{Tr}\Big[\phi_i^\dagger\,F^\dagger_{i\alpha}\,\phi_i\;F_{ia}\Big] \Big/ \sqrt{n^0_{iaa}\left(1-n^0_{iaa}\right)}$$

$$\boxed{\langle\Psi_0|\,\mathcal{P}^\dagger_{\mathbf{R}i}\,\hat{\mathcal{O}}_{\mathbf{R}i}\,\mathcal{P}_{\mathbf{R}i}\,|\Psi_0\rangle} = \mathrm{Tr}\Big[\phi_i\,\phi_i^\dagger\,O\Big]$$

$$\mathcal{P}_{\mathbf{R}i} \equiv \sum_{\Gamma n}\lambda_{i,\Gamma n}\,|\Gamma;\mathbf{R},i\rangle\langle n;\mathbf{R},i|$$

$$\Big[P^0_i\Big]_{nn'} \equiv \langle\Psi_0|\,|n',Ri\rangle\langle n,Ri|\,|\Psi_0\rangle\,\delta_{nn'}$$

$$[F_{ib}]_{nn'} = \langle\Gamma,Ri\,|\,c_{Rib}\,|\,\Gamma',Ri\rangle = \langle n,Ri\,|\,f_{Rib}\,|\,n',Ri\rangle$$

$$[O]_{\Gamma\Gamma'} = \langle\Gamma,Ri\,|\,\hat{\mathcal{O}}_{\mathbf{R}i}\,|\,\Gamma',Ri\rangle$$

$$\boxed{\phi_i} = \lambda_i\sqrt{P^0_i}$$

Initialization UO_2: LDA + RISB Mott

Initialization UO_2 : LDA + RISB Mott

henhans@henhans-Satellite-C55-C: ~ × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | henhans@henhans-Satellite-C55-C: ~/cyg... ×

```
[thlee@zakynthos UO2]$ python ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/init_mott.py
```

Initialization UO_2 : LDA + RISB Mott

henhans@henhans-Satellite-C55-C: ~ × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | henhans@henhans-Satellite-C55-C: ~/cyg... ×

```
[thlee@zakynthos UO2]$ python ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/init_mott.py
**********  Impurity 0  **********
 Sigma structure:
index     0    1    2    3    4    5    6    7    8    9   10   11   12   13

   0      1    2    0    0    0    0    0    0    0    0    0    0    0    0
   1      3    4    0    0    0    0    0    0    0    0    0    0    0    0
   2      0    0    1    2    0    0    0    0    0    0    0    0    0    0
   3      0    0    3    4    0    0    0    0    0    0    0    0    0    0
   4      0    0    0    0    5    6    0    0    0    0    0    0    0    0
   5      0    0    0    0    7    8    0    0    0    0    0    0    0    0
   6      0    0    0    0    0    0    5    6    0    0    0    0    0    0
   7      0    0    0    0    0    0    7    8    0    0    0    0    0    0
   8      0    0    0    0    0    0    0    0    5    6    0    0    0    0
   9      0    0    0    0    0    0    0    0    7    8    0    0    0    0
  10      0    0    0    0    0    0    0    0    0    0    5    6    0    0
  11      0    0    0    0    0    0    0    0    0    0    7    8    0    0
  12      0    0    0    0    0    0    0    0    0    0    0    0    9    0
  13      0    0    0    0    0    0    0    0    0    0    0    0    0    9
 Please provide the indices of orbitals to be Mott localized
 (e.g., 0 2 ): 4 6 8 10
```

Initialization UO_2 : LDA + RISB Mott

henhans@henhans-Satellite-C55-C: ~ × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | henhans@henhans-Satellite-C55-C: ~/cyg... ×

```
[thlee@zakynthos UO2]$ python ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/init_mott.py
**********  Impurity 0  **********
 Sigma structure:
index     0    1    2    3    4    5    6    7    8    9   10   11   12   13

   0      1    2    0    0    0    0    0    0    0    0    0    0    0    0
   1      3    4    0    0    0    0    0    0    0    0    0    0    0    0
   2      0    0    1    2    0    0    0    0    0    0    0    0    0    0
   3      0    0    3    4    0    0    0    0    0    0    0    0    0    0
   4      0    0    0    0    5    6    0    0    0    0    0    0    0    0
   5      0    0    0    0    7    8    0    0    0    0    0    0    0    0
   6      0    0    0    0    0    0    5    6    0    0    0    0    0    0
   7      0    0    0    0    0    0    7    8    0    0    0    0    0    0
   8      0    0    0    0    0    0    0    0    5    6    0    0    0    0
   9      0    0    0    0    0    0    0    0    7    8    0    0    0    0
  10      0    0    0    0    0    0    0    0    0    0    5    6    0    0
  11      0    0    0    0    0    0    0    0    0    0    7    8    0    0
  12      0    0    0    0    0    0    0    0    0    0    0    0    9    0
  13      0    0    0    0    0    0    0    0    0    0    0    0    0    9
 Please provide the indices of orbitals to be Mott localized
 (e.g., 0 2 ): 4 6 8 10
 You selected [4 6 8 10] to be Mott localized, right? (y/n):y
```

Initialization UO_2 : LDA + RISB Mott

henhans@henhans-Satellite-C55-C: ~ × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | henhans@henhans-Satellite-C55-C: ~/cyg... ×

```
[thlee@zakynthos UO2]$ python ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/init_mott.py
**********  Impurity 0  **********
 Sigma structure:
index     0    1    2    3    4    5    6    7    8    9   10   11   12   13

   0      1    2    0    0    0    0    0    0    0    0    0    0    0    0
   1      3    4    0    0    0    0    0    0    0    0    0    0    0    0
   2      0    0    1    2    0    0    0    0    0    0    0    0    0    0
   3      0    0    3    4    0    0    0    0    0    0    0    0    0    0
   4      0    0    0    0    5    6    0    0    0    0    0    0    0    0
   5      0    0    0    0    7    8    0    0    0    0    0    0    0    0
   6      0    0    0    0    0    0    5    6    0    0    0    0    0    0
   7      0    0    0    0    0    0    7    8    0    0    0    0    0    0
   8      0    0    0    0    0    0    0    0    5    6    0    0    0    0
   9      0    0    0    0    0    0    0    0    7    8    0    0    0    0
  10      0    0    0    0    0    0    0    0    0    0    5    6    0    0
  11      0    0    0    0    0    0    0    0    0    0    7    8    0    0
  12      0    0    0    0    0    0    0    0    0    0    0    0    9    0
  13      0    0    0    0    0    0    0    0    0    0    0    0    0    9
 Please provide the indices of orbitals to be Mott localized
 (e.g., 0 2 ): 4 6 8 10
 You selected [4 6 8 10] to be Mott localized, right? (y/n):y
 Please provide the total number of Mott localized electrons (per unit cell): 2
```

Initialization UO_2 : LDA + RISB Mott

henhans@henhans-Satellite-C55-C: ~ × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | thlee@zakynthos:~/cygutz/UO2/LDA_SB... × | henhans@henhans-Satellite-C55-C: ~/cyg... ×

```
[thlee@zakynthos UO2]$ python ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/init_mott.py
**********  Impurity 0  **********
 Sigma structure:
index     0    1    2    3    4    5    6    7    8    9   10   11   12   13

   0      1    2    0    0    0    0    0    0    0    0    0    0    0    0
   1      3    4    0    0    0    0    0    0    0    0    0    0    0    0
   2      0    0    1    2    0    0    0    0    0    0    0    0    0    0
   3      0    0    3    4    0    0    0    0    0    0    0    0    0    0
   4      0    0    0    0    5    6    0    0    0    0    0    0    0    0
   5      0    0    0    0    7    8    0    0    0    0    0    0    0    0
   6      0    0    0    0    0    0    5    6    0    0    0    0    0    0
   7      0    0    0    0    0    0    7    8    0    0    0    0    0    0
   8      0    0    0    0    0    0    0    0    5    6    0    0    0    0
   9      0    0    0    0    0    0    0    0    7    8    0    0    0    0
  10      0    0    0    0    0    0    0    0    0    0    5    6    0    0
  11      0    0    0    0    0    0    0    0    0    0    7    8    0    0
  12      0    0    0    0    0    0    0    0    0    0    0    0    9    0
  13      0    0    0    0    0    0    0    0    0    0    0    0    0    9
 Please provide the indices of orbitals to be Mott localized
 (e.g., 0 2 ): 4 6 8 10
 You selected [4 6 8 10] to be Mott localized, right? (y/n):y
 Please provide the total number of Mott localized electrons (per unit cell): 2
 Total 2 electrons will be Mott localized, right? (y/n):y
```

Initialization UO_2 : LDA + RISB Mott

henhans@henhans-Satellite-C55-C: ~ | thlee@zakynthos:~/cygutz/UO2/LDA_SB... | thlee@zakynthos:~/cygutz/UO2/LDA_SB... | henhans@henhans-Satellite-C55-C: ~/cyg...

```
 (e.g., 0 2 ): 4 6 8 10
 You selected [4 6 8 10] to be Mott localized, right? (y/n):y
 Please provide the total number of Mott localized electrons (per unit cell): 2
 Total 2 electrons will be Mott localized, right? (y/n):y
 R structure:
index     0    1    2    3    4    5    6    7    8    9   10   11   12   13

   0      1    2    0    0    0    0    0    0    0    0    0    0    0    0
   1      3    4    0    0    0    0    0    0    0    0    0    0    0    0
   2      0    0    1    2    0    0    0    0    0    0    0    0    0    0
   3      0    0    3    4    0    0    0    0    0    0    0    0    0    0
   4      0    0    0    0    5    0    0    0    0    0    0    0    0    0
   5      0    0    0    0    6    7    0    0    0    0    0    0    0    0
   6      0    0    0    0    0    0    5    0    0    0    0    0    0    0
   7      0    0    0    0    0    0    6    7    0    0    0    0    0    0
   8      0    0    0    0    0    0    0    0    5    0    0    0    0    0
   9      0    0    0    0    0    0    0    0    6    7    0    0    0    0
  10      0    0    0    0    0    0    0    0    0    0    5    0    0    0
  11      0    0    0    0    0    0    0    0    0    0    6    7    0    0
  12      0    0    0    0    0    0    0    0    0    0    0    0    8    0
  13      0    0    0    0    0    0    0    0    0    0    0    0    0    8
 Lambda structure:
index     0    1    2    3    4    5    6    7    8    9   10   11   12   13

   0      1    2    0    0    0    0    0    0    0    0    0    0    0    0
   1      3    4    0    0    0    0    0    0    0    0    0    0    0    0
   2      0    0    1    2    0    0    0    0    0    0    0    0    0    0
   3      0    0    3    4    0    0    0    0    0    0    0    0    0    0
   4      0    0    0    0    5    0    0    0    0    0    0    0    0    0
   5      0    0    0    0    0    6    0    0    0    0    0    0    0    0
   6      0    0    0    0    0    0    5    0    0    0    0    0    0    0
   7      0    0    0    0    0    0    0    6    0    0    0    0    0    0
   8      0    0    0    0    0    0    0    0    5    0    0    0    0    0
   9      0    0    0    0    0    0    0    0    0    6    0    0    0    0
  10      0    0    0    0    0    0    0    0    0    0    5    0    0    0
  11      0    0    0    0    0    0    0    0    0    0    0    6    0    0
  12      0    0    0    0    0    0    0    0    0    0    0    0    7    0
  13      0    0    0    0    0    0    0    0    0    0    0    0    0    7
[thlee@zakynthos UO2]$ python ${WIEN_GUTZ_ROOT}/ga_run_dmft.py
```

Initialization UO_2: LDA + RISB Mott (DOS Band Structure)

Initialization UO_2 : LDA + RISB Mott (DOS Band Structure)

henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... × | henhans@henhans-Satel... ×

```
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ ${WIEN_GUTZ_ROOT}/tools/Gutzwiller/save_lapwg -a -d UO2_SCF
```

Initialization UO_2 : LDA + RISB Mott (DOS Band Structure)

```
henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... ×

   UO2.nmat_only -> Ce_SCF/UO2.nmat_only
   UO2.vsp -> Ce_SCF/UO2.vsp
   UO2.vspup -> Ce_SCF/UO2.vspup
   UO2.vspdn -> Ce_SCF/UO2.vspdn
   UO2.r2v -> Ce_SCF/UO2.r2v
   UO2.r2vdn -> Ce_SCF/UO2.r2vdn
   params.dat -> Ce_SCF/params.dat
   EFLDA.INP -> Ce_SCF/EFLDA.INP
   EFLDA.OUT -> Ce_SCF/EFLDA.OUT
   WH_HS.INP -> Ce_SCF/WH_HS.INP
   WH_HS_L.INP -> Ce_SCF/WH_HS_L.INP
   WH_HS_R.INP -> Ce_SCF/WH_HS_R.INP
   WH_N2N.INP -> Ce_SCF/WH_N2N.INP
   WH_RLNEF.INP -> Ce_SCF/WH_RLNEF.INP
   WH_SIGMA_STRUCT.INP -> Ce_SCF/WH_SIGMA_STRUCT.INP
   WH_SIGMA_STRUCT_L.INP -> Ce_SCF/WH_SIGMA_STRUCT_L.INP
   WH_SIGMA_STRUCT_R.INP -> Ce_SCF/WH_SIGMA_STRUCT_R.INP
   WH_SL_VEC.INP -> Ce_SCF/WH_SL_VEC.INP
   WH_EL0.OUT -> Ce_SCF/WH_EL0.OUT
   WH_RLNEF.OUT -> Ce_SCF/WH_RLNEF.OUT
   GL.INP -> Ce_SCF/GL.INP
   GL_NELF1.INP -> Ce_SCF/GL_NELF1.INP
   GMPI_0.INP -> Ce_SCF/GMPI_0.INP
   GUTZ1.INP -> Ce_SCF/GUTZ1.INP
   GUTZ2.INP -> Ce_SCF/GUTZ2.INP
   GUTZ3.INP -> Ce_SCF/GUTZ3.INP
   GUTZ4.INP -> Ce_SCF/GUTZ4.INP
   GUTZ5.INP -> Ce_SCF/GUTZ5.INP
   GL_LOG.OUT -> Ce_SCF/GL_LOG.OUT
   GL_NELF1.OUT -> Ce_SCF/GL_NELF1.OUT
   GLPJC_1.OUT -> Ce_SCF/GLPJC_1.OUT
   FROZEN.INP -> Ce_SCF/FROZEN.INP
   glog.h5 -> Ce_SCF/glog.h5
   init_ga_info.h5 -> Ce_SCF/init_ga_info.h5

broyden files deleted, clm*, dmat*, vorb*, vresp*, eece*, scf, struct and input files saved under Ce_SCF/init_ga_info

henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ sed -i 's/.*LSCF.*/LSCF = 2/' GL.INP && sed -i 's/.*LSCF.*/&\nLEL0 = 1/' GL
.INP && sed -i 's/.*LSCF.*/&\nLEFERMI = 1/' GL.INP
```

Initialization UO_2 : LDA + RISB Mott (DOS Band Structure)

henhans@henha... × henhans@henha... × henhans@henha... × henhans@henha... × henhans@henha... × henhans@henha... × henhans@henha... × henhans@henha... ×

```
   UO2.vsp -> Ce_SCF/UO2.vsp
   UO2.vspup -> Ce_SCF/UO2.vspup
   UO2.vspdn -> Ce_SCF/UO2.vspdn
   UO2.r2v -> Ce_SCF/UO2.r2v
   UO2.r2vdn -> Ce_SCF/UO2.r2vdn
   params.dat -> Ce_SCF/params.dat
   EFLDA.INP -> Ce_SCF/EFLDA.INP
   EFLDA.OUT -> Ce_SCF/EFLDA.OUT
   WH_HS.INP -> Ce_SCF/WH_HS.INP
   WH_HS_L.INP -> Ce_SCF/WH_HS_L.INP
   WH_HS_R.INP -> Ce_SCF/WH_HS_R.INP
   WH_N2N.INP -> Ce_SCF/WH_N2N.INP
   WH_RLNEF.INP -> Ce_SCF/WH_RLNEF.INP
   WH_SIGMA_STRUCT.INP -> Ce_SCF/WH_SIGMA_STRUCT.INP
   WH_SIGMA_STRUCT_L.INP -> Ce_SCF/WH_SIGMA_STRUCT_L.INP
   WH_SIGMA_STRUCT_R.INP -> Ce_SCF/WH_SIGMA_STRUCT_R.INP
   WH_SL_VEC.INP -> Ce_SCF/WH_SL_VEC.INP
   WH_EL0.OUT -> Ce_SCF/WH_EL0.OUT
   WH_RLNEF.OUT -> Ce_SCF/WH_RLNEF.OUT
   GL.INP -> Ce_SCF/GL.INP
   GL_NELF1.INP -> Ce_SCF/GL_NELF1.INP
   GMPI_0.INP -> Ce_SCF/GMPI_0.INP
   GUTZ1.INP -> Ce_SCF/GUTZ1.INP
   GUTZ2.INP -> Ce_SCF/GUTZ2.INP
   GUTZ3.INP -> Ce_SCF/GUTZ3.INP
   GUTZ4.INP -> Ce_SCF/GUTZ4.INP
   GUTZ5.INP -> Ce_SCF/GUTZ5.INP
   GL_LOG.OUT -> Ce_SCF/GL_LOG.OUT
   GL_NELF1.OUT -> Ce_SCF/GL_NELF1.OUT
   GLPJC_1.OUT -> Ce_SCF/GLPJC_1.OUT
   FROZEN.INP -> Ce_SCF/FROZEN.INP
   glog.h5 -> Ce_SCF/glog.h5
   init_ga_info.h5 -> Ce_SCF/init_ga_info.h5

broyden files deleted, clm*, dmat*, vorb*, vresp*, eece*, scf, struct and input files saved under Ce_SCF/init_ga_info

henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ sed -i 's/.*LSCF.*/LSCF = 2/' GL.INP && sed -i 's/.*LSCF.*/&\nLEL0 = 1/' GL
.INP && sed -i 's/.*LSCF.*/&\nLEFERMI = 1/' GL.INP
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ cp WH_EL0.OUT WH_EL0.INP && cp EFLDA.OUT EFLDA.INP
```

Initialization UO_2 : LDA + RISB Mott (DOS Band Structure)

henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... ×

```
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ cp band_kpts/UO2.klist .
```

Initialization UO_2 : LDA + RISB Mott (DOS Band Structure)

henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... × | henhans@henha... ×

```
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ cp band_kpts/UO2.klist .
henhans@henhans-Satellite-C55-C:~/cygutz/UO2/LDA_SB_Mott_k2000/UO2$ ${WIEN_GUTZ_ROOT}/ga_run_dmft.py -s lapw1 -e CyGutz
```