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

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Institute for Complex Adaptive Matter



### 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<sub>2</sub>), polymorphism

Introduction

Kohn-Sham-Hubbard "Reference System"

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

**Generic multi-band Hubbard Hamiltonian** 

$$\hat{H} = \sum_{\mathbf{k}} \sum_{ij} \sum_{\alpha\beta} \epsilon_{\mathbf{k},ij}^{\alpha\beta} c_{\mathbf{k}i\alpha}^{\dagger} c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}i \in \text{corr}} \hat{H}_i^{\text{loc}}[\{c_{\mathbf{R}i\alpha}^{\dagger}\}, \{c_{\mathbf{R}i\alpha}\}]$$

$$\epsilon_{\mathbf{k}} = \begin{bmatrix} \mathbf{i} = 0 & \ast & \ast \\ & \ast & & \ast \\ & & \ast & & \ast \\ & & & \ast & & \ast \\ & & & \ast & & \mathbf{i} = 1 \\ & & & \ast & & \mathbf{i} = 2 \end{bmatrix}$$

$$\mathbf{R} = \mathbf{label unit cell}$$

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

$$\alpha, \beta = \mathbf{orbitals in R}, i$$

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

Role RISB mean field theory in context of ab-initio calculations

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.

#### Introduction

Role RISB mean field theory in context of ab-initio calculations

#### What is **RISB/GA** good for?

# **RISB (mean field)** Theory / GA



### Materials Genome Initiative

#### www.whitehouse.gov/mgi

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



The Single-Band Hubbard Model

ive Boson representations Hubbard Hamiltonian ive Boson Mean Field Approximation

#### Quadratic part correlated local orbitals included in H<sup>loc</sup>





R = label site  $\sigma = spin = \uparrow; \downarrow$ U = Hubbard strength  $\epsilon RR' = hopping coefficients$ 

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

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

#### Focus on the local space at given **R**

# **Local Hilbert Space**

$$\begin{array}{rcl} & & \\ & & \\ \hline \mathbf{R} & = & \langle \{ |0, \mathbf{R} \rangle, |\uparrow, \mathbf{R} \rangle, |\downarrow, \mathbf{R} \rangle, |\uparrow\downarrow, \mathbf{R} \rangle, \} \rangle \\ & & = & \langle \{ |0 \rangle, c^{\dagger}_{\mathbf{R}\uparrow} |0 \rangle, c^{\dagger}_{\mathbf{R}\downarrow} |0 \rangle, c^{\dagger}_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} |0 \rangle \} \rangle \end{array}$$

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)

Slave Boson representations Hubbard Hamiltonian

**Defining mapping onto subspace of infinite-dimensional Hilbert space** 



 $\mathcal{H}_{SR}^{\mathbf{R}}$  generated by "artificial" Bosonic and Fermionic degrees of freedom (dimension  $\mathcal{H}_{SB}^{\mathbf{R}} = \infty$ )  $\mathcal{H}_{E}^{\mathbf{R}}$  $\langle \{ |0\rangle, c^{\dagger}_{\mathbf{R}\uparrow} |0\rangle, c^{\dagger}_{\mathbf{R}\downarrow} |0\rangle, c^{\dagger}_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}\downarrow} |0\rangle \} \rangle \equiv \{ |A, \mathbf{R}\rangle \}$  $\{c_{\mathbf{R}\sigma}^{\dagger}, c_{\mathbf{R}\sigma}\}$  $(\Phi_{\mathbf{R}An} \text{ only for } N_A = N_n)$ 

Slave Boson representations Hubbard Hamiltonian

Quadratic part correlated local orbitals included in Hloc



Slave Boson representations Hubbard Hamiltonian

Gutzwiller constraints (introducing definition  $F_a$  matrices)

**Operatorial Gutzwiller Constraints** 

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

 $\Phi^{\dagger}_{\mathbf{R};\mathbf{0},0}|0
angle$  $\begin{pmatrix} \Phi_{\mathbf{R};\uparrow,\uparrow}^{\dagger} f_{\mathbf{R}\uparrow}^{\dagger} | \mathbf{0} \rangle + \Phi_{\mathbf{R};\uparrow,\downarrow}^{\dagger} f_{\mathbf{R}\downarrow}^{\dagger} | \mathbf{0} \rangle \end{pmatrix} / \sqrt{2} \\ \begin{pmatrix} \Phi_{\mathbf{R};\downarrow,\downarrow}^{\dagger} f_{\mathbf{R}\downarrow}^{\dagger} | \mathbf{0} \rangle + \Phi_{\mathbf{R};\downarrow,\uparrow}^{\dagger} f_{\mathbf{R}\uparrow}^{\dagger} | \mathbf{0} \rangle \end{pmatrix} / \sqrt{2} \\ \Phi_{\mathbf{R};\downarrow,\uparrow\downarrow}^{\dagger} f_{\mathbf{R}\downarrow}^{\dagger} f_{\mathbf{R}\downarrow}^{\dagger} | \mathbf{0} \rangle \qquad h_{SB}^{\mathbf{R}}$  $\mathcal{H}_{SB}^{\mathbf{R}}$ 

$$\sum_{An} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}An} = 1$$
$$\sum_{Anm} [F_a^{\dagger} F_b]_{mn} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Am} = f_{\mathbf{R}a}^{\dagger} f_{\mathbf{R}b}$$
$$\left( [F_a]_{nm} \equiv \langle n, \mathbf{R} | f_{\mathbf{R}a} | m, \mathbf{R} \rangle \right)$$

$$|\mathbf{A},\mathbf{R}\rangle \rightarrow |\underline{\mathbf{A}},\mathbf{R}\rangle = \frac{1}{\sqrt{D_{\mathbf{A}}}} \sum_{n} \Phi_{\mathbf{R}\mathbf{A}n}^{\dagger} |n,\mathbf{R}\rangle$$

Slave Boson representations Hubbard Hamiltonian

### **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

$$\hat{H}^{\text{loc}} \equiv \sum_{\mathbf{R}} U c_{\mathbf{R}\uparrow}^{\dagger} c_{\mathbf{R}\uparrow} c_{\mathbf{R}\downarrow}^{\dagger} c_{\mathbf{R}\downarrow} = \sum_{\mathbf{R}} \sum_{AB} [H^{\text{loc}}]_{AB} |A, \mathbf{R}\rangle \langle B, \mathbf{R}|$$
$$\underline{\hat{H}}^{\text{loc}} \equiv \sum_{\mathbf{R}} \sum_{n} U \Phi_{\mathbf{R};\uparrow\downarrow,n}^{\dagger} \Phi_{\mathbf{R};\uparrow\downarrow,n} = \sum_{\mathbf{R}} \sum_{AB} [H^{\text{loc}}]_{AB} \sum_{n} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Bn}$$

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

Slave Boson representations Hubbard Hamiltonian

# **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 <u>Bosonic</u>  $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$  such that:  $\underline{c}_{\mathbf{R}\alpha}^{\dagger} \equiv \sum_{a} \hat{\mathcal{R}}_{\mathbf{R}a\alpha} [\Phi_{\mathbf{R}An}, \Phi_{\mathbf{R}An}^{\dagger}] f_{\mathbf{R}a}^{\dagger}$ .  $\langle \underline{A}, \mathbf{R} | \underline{c}_{\mathbf{R}\alpha}^{\dagger} | \underline{B}, \mathbf{R} \rangle = \langle A, \mathbf{R} | c_{R\alpha}^{\dagger} | B, \mathbf{R} \rangle \quad \forall A, B$ 

Slave Boson representations Hubbard Hamiltonian

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

**Construction of**  $\hat{\mathcal{R}}_{\mathbf{R}a\alpha}$  **such that**  $\langle \underline{A}, \mathbf{R} | \underline{c}_{\mathbf{R}\alpha}^{\dagger} | \underline{B}, \mathbf{R} \rangle = \langle A, \mathbf{R} | c_{\mathbf{R}\alpha}^{\dagger} | B, \mathbf{R} \rangle \quad \forall A, B$ 

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

$$\hat{\mathcal{R}}_{\mathbf{R}a\boldsymbol{\alpha}} = : \left[ r_{\mathbf{R}a\boldsymbol{\alpha}}^{(0)} + [r_{\mathbf{R}a\boldsymbol{\alpha}}^{(2)}]_{An,Bm} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Bm} + \left[ r_{\mathbf{R}a\boldsymbol{\alpha}}^{(4)} \right]_{An,Bm,Cl,Dr} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Bm}^{\dagger} \Phi_{\mathbf{R}Cl} \Phi_{\mathbf{R}Dr} + \ldots \right] :$$

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

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

Slave Boson representations Hubbard Hamiltonian

Alternative 
$$\mathcal{R}_{\mathbf{R}a\alpha}$$
 suitable for MF approximation  
arXiv:1606.09614 (2016)

$$\hat{\mathcal{R}}_{\mathbf{R}a\boldsymbol{\alpha}} \equiv \sum_{ABnmb} \frac{1}{N_A} \sqrt{\frac{D_B}{D_A}} [F_{\boldsymbol{\alpha}}^{\dagger}]_{AB} [F_b^{\dagger}]_{nm}$$

$$: \Phi_{\mathbf{R}An}^{\dagger} \left[ \hat{1} + \left( N_A \sqrt{\frac{D_A}{D_B}} - 1 \right) \sum_{Cl} \Phi_{\mathbf{R}Cl}^{\dagger} \Phi_{\mathbf{R}Cl} \right]$$

$$\left[ \left[ \hat{1} - \hat{\Delta}_p \right]^{\left[-\frac{1}{2}\right]} \bullet \left[ \hat{1} - \hat{\Delta}_h \right]^{\left[-\frac{1}{2}\right]} \right] \Phi_{\mathbf{R}Bm}$$

where:

$$[\hat{\Delta}_{\mathbf{p}}]_{\mathbf{R}ab} \equiv \sum_{Anm} [F_a^{\dagger} F_b]_{mn} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Am}$$

$$[\hat{\Delta}_{h}]_{\mathbf{R}ab} \equiv \sum_{Anm} [F_{b}F_{a}^{\dagger}]_{mn} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Am}$$
$$\left[\hat{1} - \hat{\Delta}\right]^{\left[-\frac{1}{2}\right]} \equiv \sum_{r=0}^{\infty} (-1)^{r} {\binom{1}{2} \choose r} [\hat{\Delta}]^{\left[r\right]}$$

Slave Boson representations Hubbard Hamiltonian

### Summary SB reformulation: quadratic interaction, "renormalized" hopping

# **The Hubbard Hamiltonian**

$$\begin{split} \hat{H} &= \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'} c_{\mathbf{R}\sigma}^{\dagger} c_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} U c_{\mathbf{R}\uparrow}^{\dagger} c_{\mathbf{R}\uparrow} c_{\mathbf{R}\downarrow}^{\dagger} c_{\mathbf{R}\downarrow} \\ \hat{\underline{H}} &= \sum_{\mathbf{R}\mathbf{R}'} \sum_{\sigma} \epsilon_{\mathbf{R}\mathbf{R}'} \underline{C}_{\mathbf{R}\sigma}^{\dagger} \underline{C}_{\mathbf{R}'\sigma} + \sum_{\mathbf{R}} \sum_{n} U \Phi_{\mathbf{R};\uparrow\downarrow,n}^{\dagger} \Phi_{\mathbf{R};\uparrow\downarrow,n} \\ \psi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \\ \psi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \\ \psi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \\ \psi_{\mathbf{R};\downarrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \\ \psi_{\mathbf{R};\downarrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow,n} \Phi_{\mathbf{R};\uparrow\downarrow} \Phi_{\mathbf{R};\uparrow\downarrow} \Phi_{\mathbf{R};\uparrow\downarrow} \Phi_{\mathbf{R};\uparrow\uparrow} \Phi_{\mathbf{R};\uparrow\downarrow} \Phi_{\mathbf{R};\downarrow\uparrow} \Phi_{\mathbf{R};\downarrow\downarrow} \Phi_{\mathbf{R};\downarrow} \Phi_{\mathbf{R};$$

 $|\mathbf{A},\mathbf{R}\rangle \rightarrow |\underline{\mathbf{A}},\mathbf{R}\rangle = \frac{1}{\sqrt{D_{\mathbf{A}}}} \sum_{n} \Phi_{\mathbf{R}\mathbf{A}n}^{\dagger} |n,\mathbf{R}\rangle$ 

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

#### Mean Field theory as a variational approximation

# **The Slave Boson Hubbard Hamiltonian**

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Slave Boson Mean Field Approximation

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

# **The Slave Boson Hubbard Hamiltonian**

Assuming following variational ansatz:

 $|\Psi_{\rm SB}\rangle = |\Psi_0\rangle \otimes |\phi\rangle$ , Constrained Minimization

Show Boson representations Hubbard Hamilton Slave Boson Mean Field Approximation

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

# **The Slave Boson Hubbard Hamiltonian**

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

Assuming following variational ansatz:

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

## **Local interaction:**

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#### **Expectation value Gutzwiller Constraints**

# **The Slave Boson Hubbard Hamiltonian**

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

Assuming following variational ansatz:

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

### **Gutzwiller constraints:**

$$\langle \Psi_{\rm SB} | \sum_{An} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}An} - \hat{1} | \Psi_{\rm SB} \rangle = \operatorname{Tr}[\phi^{\dagger}\phi] - 1 = 0$$
  
$$\langle \Psi_{\rm SB} | \sum_{Anm} [F_a^{\dagger}F_b]_{mn} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Am} - f_{\mathbf{R}a}^{\dagger}f_{\mathbf{R}b} | \Psi_{\rm SB} \rangle = \operatorname{Tr}[\phi^{\dagger}\phi F_a^{\dagger}F_b] - \langle \Psi_0 | f_{\mathbf{R}a}^{\dagger}f_{\mathbf{R}b} | \Psi_0 \rangle = 0$$

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#### **Expectation value <u>Renormalization Operators</u>**

# **The Slave Boson Hubbard Hamiltonian**

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

### Assuming following variational ansatz:

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

### **Renormalization factors:**

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

Slave Boson Mean Field Approximation

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

$$\hat{\mathcal{R}}_{\mathbf{R}a\boldsymbol{\alpha}} \equiv \sum_{ABnmb} \frac{1}{N_A} \sqrt{\frac{D_B}{D_A}} [F_{\boldsymbol{\alpha}}^{\dagger}]_{AB} [F_b^{\dagger}]_{nm}$$

$$: \Phi_{\mathbf{R}An}^{\dagger} \left[ \hat{1} + \left( N_A \sqrt{\frac{D_A}{D_B}} - 1 \right) \sum_{Cl} \Phi_{\mathbf{R}Cl}^{\dagger} \Phi_{\mathbf{R}Cl} \right]$$

$$\left[ \left[ \hat{1} - \hat{\Delta}_p \right]^{\left[-\frac{1}{2}\right]} \bullet \left[ \hat{1} - \hat{\Delta}_h \right]^{\left[-\frac{1}{2}\right]} \right] \Phi_{\mathbf{R}Bm} :$$

where:

$$[\hat{\Delta}_{\mathbf{p}}]_{\mathbf{R}ab} \equiv \sum_{Anm} [F_a^{\dagger}F_b]_{mn} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Am}$$

$$[\hat{\Delta}_{h}]_{\mathbf{R}ab} \equiv \sum_{Anm} [F_{b}F_{a}^{\dagger}]_{mn} \Phi_{\mathbf{R}An}^{\dagger} \Phi_{\mathbf{R}Am}$$
$$\left[\hat{1} - \hat{\Delta}\right]^{\left[-\frac{1}{2}\right]} \equiv \sum_{r=0}^{\infty} (-1)^{r} {\binom{1}{2} \choose r} [\hat{\Delta}]^{\left[r\right]}$$

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### **Mean Field renormalization factors**

$$\mathcal{R}_{a\alpha} \equiv \langle \phi | \, \hat{\mathcal{R}}_{\mathbf{R}a\alpha} \, | \phi \rangle = \sum_{b} \operatorname{Tr}[\phi^{\dagger} F_{\alpha}^{\dagger} \phi F_{b}] \left[ (1 - \Delta_{p}) \Delta_{p} \right]_{ba}^{-\frac{1}{2}}$$
  
where:  $\left[ \Delta_{p} \right]_{ab} = \operatorname{Tr}[\phi^{\dagger} \phi F_{a}^{\dagger} F_{b}]$ 

## **Consequently, in summary:**

$$\langle \Psi_{SB} | \sum_{\mathbf{RR'}} \sum_{\sigma} \epsilon_{\mathbf{RR'}} \underline{c}_{\mathbf{R}\sigma}^{\dagger} \underline{c}_{\mathbf{R'}\sigma} | \Psi_{SB} \rangle = |\mathcal{R}(\phi)|^{2} \langle \Psi_{0} | \sum_{\mathbf{RR'}} \sum_{\sigma} \epsilon_{\mathbf{RR'}} f_{\mathbf{R}\sigma}^{\dagger} f_{\mathbf{R'}\sigma} | \Psi_{0} \rangle$$

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

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

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

Slave Boson representations Hubbard Hamiltoni Slave Boson Mean Field Approximation

**Observation: number of independent SB amplitudes (ignoring symmetry)** 

# Number of independent complex parameters $\phi$ is $2^2 \times 2^2$

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



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#### Quadratic part correlated local orbitals included in Hloc



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

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

### The variational energy

$$\begin{split} \hat{H} &= \sum_{\mathbf{k}} \sum_{\alpha \beta} \boxed{\epsilon_{\mathbf{k},ij}^{\alpha \beta}} c_{\mathbf{k}i\alpha}^{\dagger} c_{\mathbf{k}j\beta} + \sum_{\mathbf{R}i} \boxed{\hat{H}_{\mathbf{R}i}^{\text{loc}}[\{\hat{c}_{\mathbf{R}i\alpha}^{\dagger}\}, \{\hat{c}_{\mathbf{R}i\alpha}\}]} \\ \mathcal{E}[\Psi_{0}, \{\phi_{i}\}] &= \frac{1}{\mathcal{N}} \sum_{\mathbf{k},ij} \sum_{ab} \left[ \mathcal{R}_{i} \epsilon_{\mathbf{k},ij} \mathcal{R}_{j}^{\dagger} \right]_{ab} \langle \Psi_{0} | f_{\mathbf{k}ia}^{\dagger} f_{\mathbf{k}jb} | \Psi_{0} \rangle \\ &+ \sum_{i \in \text{corr}} \text{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} H_{i}^{\text{loc}} \right] \end{split}$$

where

$$\left[\mathcal{R}_{i}\right]_{a\alpha} = \sum_{b} \operatorname{Tr}\left[\phi_{i}^{\dagger} F_{i\alpha}^{\dagger} \phi_{i} F_{ib}\right] \left[\Delta_{pi}(1-\Delta_{pi})\right]_{ba}^{-\frac{1}{2}}$$

to be minimized satisfying the Gutzwiller contraints:

$$\operatorname{Tr}\left[\phi_{i}^{\dagger}\phi_{i}\right] = \langle\Psi_{0}|\Psi_{0}\rangle = 1$$
$$\operatorname{Tr}\left[\phi_{i}^{\dagger}\phi_{i} F_{ia}^{\dagger}F_{ib}\right] = \langle\Psi_{0}|f_{\mathbf{R}ia}^{\dagger}f_{\mathbf{R}ib}|\Psi_{0}\rangle \equiv \Delta_{pi}$$

Functional Formulation Stationarity Equations and Numerical Implementation

### Step 1: promoting $\Delta_p$ , R to independent variables using Lagrange multipliers

# **Functional formulation SB**

$$\begin{split} \mathcal{L}[\Psi_{0}, E; \phi, E^{c}; \mathcal{R}, \mathcal{R}^{\dagger}, \lambda; \mathcal{D}, \mathcal{D}^{\dagger}, \lambda^{c}; \Delta_{p}] &= \\ \frac{1}{\mathcal{N}} \langle \Psi_{0} | \hat{H}_{G}^{qp}[\mathcal{R}, \mathcal{R}^{\dagger}; \lambda] | \Psi_{0} \rangle + E(1 - \langle \Psi_{0} | \Psi_{0} \rangle) + \\ \sum_{i} \operatorname{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} H_{i}^{\text{loc}} + \sum_{a\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} \phi_{i}^{\dagger} F_{i\alpha}^{\dagger} \phi_{i} F_{ia} + \text{H.c.} \right) + \sum_{ab} \left[ \lambda_{i}^{c} \right]_{ab} \phi_{i}^{\dagger} \phi_{i} F_{ia}^{\dagger} F_{ib} \right] + \\ \sum_{i} E_{i}^{c} \left( 1 - \operatorname{Tr} \left[ \phi_{i}^{\dagger} \phi_{i} \right] \right) \\ - \sum_{i} \left[ \sum_{ab} \left( [\lambda_{i}]_{ab} + [\lambda_{i}^{c}]_{ab} \right) [\Delta_{pi}]_{ab} + \sum_{ca\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} [\mathcal{R}_{i}]_{c\alpha} [\Delta_{pi}(1 - \Delta_{pi})]_{c\alpha}^{\frac{1}{2}} + \text{c.c.} \right) \right] \end{split}$$

#### where

$$\hat{H}_{G}^{\mathrm{qp}}[\mathcal{R}, \mathcal{R}^{\dagger}; \lambda] \equiv \sum_{k, ij} \sum_{ab} \left[ \mathcal{R}_{i} \epsilon_{k, ij} \mathcal{R}_{j}^{\dagger} \right]_{ab} f_{kia}^{\dagger} f_{kjb} + \sum_{Ri, ab} \left[ \lambda_{i} \right]_{ab} f_{Ria}^{\dagger} f_{Rib}$$

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

Functional Formulation

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

# **Functional formulation SB**

$$\mathcal{L}[\Psi_{0}, E]; \phi, E^{c}; \mathcal{R}, \mathcal{R}^{\dagger}, \lambda; \mathcal{D}, \mathcal{D}^{\dagger}, \lambda^{c}; \Delta_{p}] = \frac{1}{\mathcal{N}} \langle \Psi_{0} | \hat{H}_{G}^{qp}[\mathcal{R}, \mathcal{R}^{\dagger}; \lambda] | \Psi_{0} \rangle + E(1 - \langle \Psi_{0} | \Psi_{0} \rangle) + \sum_{i} \operatorname{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} H_{i}^{\text{loc}} + \sum_{a\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} \phi_{i}^{\dagger} F_{i\alpha}^{\dagger} \phi_{i} F_{ia} + \text{H.c.} \right) + \sum_{ab} [\lambda_{i}^{c}]_{ab} \phi_{i}^{\dagger} \phi_{i} F_{ia}^{\dagger} F_{ib} \right] + \sum_{i} E_{i}^{c} \left( 1 - \operatorname{Tr} \left[ \phi_{i}^{\dagger} \phi_{i} \right] \right) - \sum_{i} \left[ \sum_{ab} \left( [\lambda_{i}]_{ab} + [\lambda_{i}^{c}]_{ab} \right) [\Delta_{pi}]_{ab} + \sum_{ca\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} [\mathcal{R}_{i}]_{c\alpha} [\Delta_{pi}(1 - \Delta_{pi})]_{c\alpha}^{\frac{1}{2}} + \text{c.c.} \right) \right]$$

#### where

$$\hat{H}_{G}^{qp}[\mathcal{R}, \mathcal{R}^{\dagger}; \lambda] \equiv \sum_{k, ij} \sum_{ab} \left[ \mathcal{R}_{i} \epsilon_{k, ij} \mathcal{R}_{j}^{\dagger} \right]_{ab} f_{kia}^{\dagger} f_{kjb} + \sum_{Ri, ab} \left[ \lambda_{i} \right]_{ab} f_{Ria}^{\dagger} f_{Rib}$$

Functional Formulation

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

# **Functional formulation SB**

$$\begin{split} \mathcal{L}[\phi, E^{c}; \mathcal{R}, \mathcal{R}^{\dagger}, \lambda; \mathcal{D}, \mathcal{D}^{\dagger}, \lambda^{c}; \Delta_{p}] &= \\ \frac{\mathcal{T}}{\mathcal{N}} \sum_{k,\omega} \operatorname{Tr} \log \left( \frac{1}{i\omega - \mathcal{R}\epsilon_{k}\mathcal{R}^{\dagger} - \lambda} \right) e^{i\omega 0^{+}} + \\ \sum_{i} \operatorname{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} H_{i}^{\text{loc}} + \sum_{a\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} \phi_{i}^{\dagger} F_{i\alpha}^{\dagger} \phi_{i} F_{ia} + \text{H.c.} \right) + \sum_{ab} \left[ \lambda_{i}^{c} \right]_{ab} \phi_{i}^{\dagger} \phi_{i} F_{ia}^{\dagger} F_{ib} \right] + \\ \sum_{i} E_{i}^{c} \left( 1 - \operatorname{Tr} \left[ \phi_{i}^{\dagger} \phi_{i} \right] \right) \\ - \sum_{i} \left[ \sum_{ab} \left( [\lambda_{i}]_{ab} + [\lambda_{i}^{c}]_{ab} \right) [\Delta_{pi}]_{ab} + \sum_{ca\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} [\mathcal{R}_{i}]_{c\alpha} [\Delta_{pi}(1 - \Delta_{pi})]_{c\alpha}^{\frac{1}{2}} + \text{c.c.} \right) \right] \end{split}$$

### where

	i=0	*	*	]	1	0	0		0	0	0	1
$\epsilon_{\mathbf{k}} =$	*	i = 1	*	$; \mathcal{R} =$	0	$\mathcal{R}_{i=1}$	0	; $\lambda =$	0	$\lambda_{i=1}$	0	
	*	*	i=2		0	0	$\mathcal{R}_{i=2}$		0	0	$\lambda_{i=2}$	20

#### **Functional Formulation**

tationarity Equations and Numerical Implementation

### Step 3: Re-interpretation $\phi_i$ using Schmidt decomposition

# **Functional formulation SB**

$$\mathcal{L}[\phi, E^{c}; \mathcal{R}, \mathcal{R}^{\dagger}, \lambda; \mathcal{D}, \mathcal{D}^{\dagger}, \lambda^{c}; \Delta_{p}] = \frac{\mathcal{T}}{\mathcal{N}} \sum_{k, \omega} \operatorname{Tr} \log \left( \frac{1}{i\omega - \mathcal{R}\epsilon_{k}\mathcal{R}^{\dagger} - \lambda} \right) e^{i\omega 0^{+}} + \sum_{i} \operatorname{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} H_{i}^{\text{loc}} + \sum_{a\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} \phi_{i}^{\dagger} F_{i\alpha}^{\dagger} \phi_{i} F_{ia} + \text{H.c.} \right) + \sum_{ab} \left[ \lambda_{i}^{c} \right]_{ab} \phi_{i}^{\dagger} \phi_{i} F_{ia}^{\dagger} F_{ib} \right] +$$

$$\sum_{i} E_{i}^{c} \left(1 - \operatorname{Tr}\left[\phi_{i}^{\dagger}\phi_{i}\right]\right)$$
$$-\sum_{i} \left[\sum_{ab} \left(\left[\lambda_{i}\right]_{ab} + \left[\lambda_{i}^{c}\right]_{ab}\right) \left[\Delta_{pi}\right]_{ab} + \sum_{ca\alpha} \left(\left[\mathcal{D}_{i}\right]_{a\alpha} \left[\mathcal{R}_{i}\right]_{c\alpha} \left[\Delta_{pi}(1 - \Delta_{pi})\right]_{c\alpha}^{\frac{1}{2}} + \text{c.c.}\right)\right]$$

### Elements $\phi_i$ can be viewed as coefficients Schmidt decomposition:

$$\begin{split} |\Phi_{i}\rangle &\equiv \sum_{An} e^{i\frac{\pi}{2}N_{n}(N_{n}-1)} \left[\phi_{i}\right]_{An} |A,i\rangle U_{\rm PH}|n,i\rangle \\ |A\rangle &= \left[\hat{c}_{1}^{\dagger}\right]_{\cdots}^{n_{1}} \left[\hat{c}_{M}^{\dagger}\right]^{n_{M}}|0\rangle |n\rangle = \left[\hat{f}_{1}^{\dagger}\right]_{\cdots}^{n_{1}} \left[\hat{f}_{M}^{\dagger}\right]^{n_{M}}|0\rangle \\ \\ \hline \mathbf{Impurity} \mathbf{Bath} \end{split}$$

**Functional Formulation** 

tationarity Equations and Numerical Implementation

#### Step 3: Re-interpretation $\phi_i$ using Schmidt decomposition

# **Functional formulation SB**

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

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

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

#### where

$$\mathcal{H}_{i}^{\text{emb}}[\mathcal{D}_{i}, \mathcal{D}_{i}^{\dagger}; \lambda_{i}^{c}] \equiv \hat{H}_{i}^{\text{loc}}[\{\hat{c}_{i\alpha}^{\dagger}\}, \{\hat{c}_{i\alpha}\}] \\ + \sum_{a\alpha} \left( [\mathcal{D}_{i}]_{a\alpha} \, \hat{c}_{i\alpha}^{\dagger} \hat{f}_{ia} + \text{H.c.} \right) + \sum_{ab} [\lambda_{i}^{c}]_{ab} \hat{f}_{ib} \hat{f}_{ia}^{\dagger}$$

**Functional Formulation** 

**Stationarity Equations and Numerical Implementation** 

### Stationarity equations: $\lambda$ , R, $\Delta_p$ ; $\langle \Phi | \& E^c$ ; $\mathbf{D}, \lambda^c$

# **SB** stationarity equations

$$(\mathcal{R}, \lambda) \longrightarrow \frac{1}{\mathcal{N}} \left[ \sum_{k} \Pi_{i} f\left(\mathcal{R}\epsilon_{k} \mathcal{R}^{\dagger} + \lambda\right) \Pi_{i} \right]_{ba} = [\Delta_{pi}]_{ab}$$

$$(1)$$

$$\frac{1}{\mathcal{N}} \left[ \frac{1}{\mathcal{R}_{i}} \sum_{k} \Pi_{i} \mathcal{R}\epsilon_{k} \mathcal{R}^{\dagger} f\left(\mathcal{R}\epsilon_{k} \mathcal{R}^{\dagger} + \lambda\right) \Pi_{i} \right]_{\alpha a} = \sum_{c} \left[ \mathcal{D}_{i} \right]_{c\alpha} \left[ \Delta_{ip} \left(1 - \Delta_{ip} \right) \right]_{ac}^{\frac{1}{2}}$$

$$(2)$$

$$\left[ \sum_{cb\alpha} \frac{\partial}{\partial d_{is}^{p}} \left[ \Delta_{pi} \left(1 - \Delta_{pi} \right) \right]_{cb}^{\frac{1}{2}} \left[ \mathcal{D}_{i} \right]_{b\alpha} \left[ \mathcal{R}_{i} \right]_{c\alpha} + \text{c.c.} \right] + \left[ l + l^{c} \right]_{is} = 0$$

$$(3)$$

$$\mathcal{H}_{i}^{\text{emb}} \left[ \mathcal{D}_{i}, \mathcal{D}_{i}^{\dagger}; \lambda_{i}^{c} \right] \left| \Phi_{i} \right\rangle = E_{i}^{c} \left| \Phi_{i} \right\rangle$$

$$\left[ \mathcal{F}_{i}^{(1)} \right]_{\alpha a} \equiv \left\langle \Phi_{i} \right| \hat{c}_{i\alpha}^{\dagger} \hat{f}_{ia} \left| \Phi_{i} \right\rangle - \sum_{c} \left[ \Delta_{ip} \left(1 - \Delta_{ip} \right) \right]_{ca}^{\frac{1}{2}} \left[ \mathcal{R}_{i} \right]_{c\alpha} = 0$$

$$\left[ \mathcal{F}_{i}^{(2)} \right]_{ab} \equiv \left\langle \Phi_{i} \right| \hat{f}_{ib}^{\dagger} \hat{f}_{ia}^{\dagger} \left| \Phi_{i} \right\rangle - \left[ \Delta_{pi} \right]_{ab} = 0$$

$$(6)$$

#### where

$$\Delta_{pi} = \sum_{s} d_{is}^{p\ t} h_{is}; \quad \lambda_{i}^{c} = \sum_{s} l_{is}^{c} h_{is}; \quad \lambda_{i} = \sum_{s} l_{is} h_{is}; \quad \mathcal{R}_{i} = \sum_{s} r_{is} h_{is}$$

The correlated orbitals

A+RISB: Solving iteratively Kohn-Sham-Hubbard model mples: low-symmetry systems (UO<sub>2</sub>), polymorphism

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

# **The Projector: Definition of the Correlated Orbitals**

$$\hat{\Xi}(\mathbf{r},\sigma) = \sum_{\sigma'} \sum_{ki,\pi \in P} \xi_{ki,\pi}(\mathbf{r}) \chi_{\sigma'}(\sigma) c_{ki\pi\sigma} + \hat{\Xi}_{\mathcal{Q}}(\mathbf{r},\sigma) \equiv \sum_{i} \hat{\Xi}_{Pi}(\mathbf{r},\sigma) + \hat{\Xi}_{\mathcal{Q}}(\mathbf{r},\sigma)$$
$$\hat{A} = \sum_{\sigma} \int d\mathbf{r} \, \hat{\Xi}^{\dagger}(\mathbf{r},\sigma) A \, \hat{\Xi}(\mathbf{r},\sigma) \equiv \sum_{i} \hat{A}_{i}^{\text{loc}} + \hat{A}^{\text{hop}}$$

#### where

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

$$A = \begin{bmatrix} A^{\text{hop}} & A^{\text{hop}} & A^{\text{hop}} \\ \hline A^{\text{hop}} & A^{\text{hop}} & A^{\text{hop}} \\ \hline A^{\text{hop}} & A^{\text{hop}} & A^{\text{hop}} \end{bmatrix}$$

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

LDA+RISB: Solving iteratively Kohn-Sham-Hubbard model

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

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

$$\begin{split} \Omega_{E^{dc},N}[N^{loc}, V^{dc}; \,\rho(\mathbf{r}), \boldsymbol{J}(\mathbf{r}); \,\Phi, E^{c}, \mathcal{R}, \mathcal{R}^{\dagger}, \lambda, \mu, \mathcal{D}, \mathcal{D}^{\dagger}, \lambda^{c}, \Delta_{p}] &= \\ \mathcal{L}_{\text{KSH}}[\boldsymbol{J}(\mathbf{r}); \,\phi, E^{c}; \,\mathcal{R}, \mathcal{R}^{\dagger}, \lambda; \,\mathcal{D}, \mathcal{D}^{\dagger}, \lambda^{c}; \,\Delta_{p}, \mu] + \\ \int d\mathbf{r} \boldsymbol{J}(\mathbf{r})\rho(\mathbf{r}) + E_{\text{Hxc}}^{\text{LDA}}[\rho(\mathbf{r})] + E_{\text{ion}}[\rho(\mathbf{r})] + E_{\text{ion-ion}} \\ + \sum_{i} \left[ E_{i}^{dc}[N_{i}^{\text{loc}}] - V_{i}^{dc}N_{i}^{\text{loc}} \right] \end{split}$$

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

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

LDA+RISB: Solving iteratively Kohn-Sham-Hubbard model

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

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



Kole KUSB mean field theory in context of absinitio calculations Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism

An example: Orbital Differentiation with Crystal Field Effects in UO<sub>2</sub>

# UO<sub>2</sub> (arXiv:1606.09614 (2016))

# Cubic fluorite structure

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



$$\begin{split} |\Gamma_{6}, 7/2, \pm\rangle &= \sqrt{5/12} |7/2, \pm 7/2\rangle + \sqrt{7/12} |7/2, \pm 1/2\rangle \\ |\Gamma_{7}, 7/2, \pm\rangle &= \mp \sqrt{3/4} |7/2, \pm 5/2\rangle \pm \sqrt{1/4} |7/2, \mp 3/2\rangle \\ |\Gamma_{8}^{(1)}, 7/2, \pm\rangle &= \pm \sqrt{7/12} |7/2, \pm 7/2\rangle \mp \sqrt{5/12} |7/2, \mp 1/2\rangle \\ |\Gamma_{8}^{(2)}, 7/2, \pm\rangle &= \mp \sqrt{1/4} |7/2, \pm 5/2\rangle \mp \sqrt{3/4} |7/2, \mp 3/2\rangle \\ |\Gamma_{7}, 5/2, \pm\rangle &= \sqrt{5/6} |5/2, \pm 3/2\rangle - \sqrt{1/6} |5/2, \mp 5/2\rangle \\ |\Gamma_{8}^{(1)}, 5/2, \pm\rangle &= \sqrt{1/6} |5/2, \pm 3/2\rangle + \sqrt{5/6} |5/2, \mp 5/2\rangle \\ |\Gamma_{8}^{(2)}, 5/2, \pm\rangle &= |5/2, \pm 1/2\rangle , \end{split}$$

Self Energy  $\Sigma(\omega)$  non diagonal (less symmetry  $\rightarrow$  less selection rules)
**Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism** 

#### An example: Orbital Differentiation with Crystal Field Effects in UO<sub>2</sub>

# $UO_2$ (arXiv:1606.09614 (2016))

Eigenvalues of the 5f 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	$\Gamma_8(4)$	$\Gamma_7(2)$	$\Gamma_8(4)$	$\Gamma_7(2)$	$\Gamma_6(2)$
	0	0.92	0.92	0.95	0.95
n	1.92	0.14	0.08	0.06	0.04
w/o CFS		L L	5/2		7/2
Ζ		(	)		0.96
$\overline{n}$		1	1.98		0.16

**Kole RISB mean field theory in context of ab-initio calculation Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism** 

#### An example: Orbital Differentiation with Crystal Field Effects in UO<sub>2</sub>

## $UO_2$ (arXiv:1606.09614 (2016))



**Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism** 

An example: Polymorphism in Strongly Correlated Materials

# **Polymorphism**

Carbon: Graphite, Diamond (different mechanical, optical, electronic properties)

TiO<sub>2</sub>: 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.

Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism

#### An example: Polymorphism in Strongly Correlated Materials

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

			LI	DA				LDA	A+SE	U =	13 J	= 0.9				expe	riment	t		
		g.s. structu	ire g.s.	phase	$V_0$ (Å	$^{3}/f.u.)$	g.s.	struct	ure g	.s. ph	ase $V$	$(Å^3/.$	f.u.)	g.s. st	ructu	e g.s.	phase	$V_0$ (	$A^3/f$ .	u.)
Co	0	Wurtzite	e M	etal	17	.64	R	tocksal	t ]	Insulat	tor	20.48	8	Roo	cksalt	Ins	ulator		19.35	
Co	S	NiAs	M	etal	23	.11		NiAs		Meta	1	25.93	3	N	iAs	N	fetal	1	25.77	
Co	Se	NiAs	M	etal	27	.25		NiAs		Meta	1	30.99	9	N	iAs	N	letal	;	30.27	
$\mathbf{Cr}$	0	Wurtzite	M	etal	17	.64	R	Rocksal	t	Meta	1	18.2'	7	Roo	cksalt			_	18	
Mn	nO	Wurtzite	M	etal	17	.13	R	locksal	t l	Insulat	tor	22.00	6	Roo	cksalt	Ins	ulator	1	21.97	
Fe	0	Zincblend	e M	etal	18	.69	R	locksal	t ]	Insulat	tor	21.2	3	Roo	cksalt	Ins	ulator	2	0.35	
		1 H Hydrogen Name 1008 2 H Lithiam Ber 9 0121 3 Na Sodium 24,305 24,505 Mg Sodium 24,305	3 <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup> <sup>20</sup>	4 Solid L. Gas Unkno	5 wwn	6 Alkali metals	7 Metalloid	8 Othe noni N etais Actir	9 er metals Metals hanoids noids	10 Nonme Haloger	11 tals Noble	e gases	13 5 8 8 8 8 8 8 8 8 9 8 9 10.81 13 13 13 13 13 13 13 13 13 13 13 13 13	14 6 C Carbon 12.011 14 Si Silicon 28.085	15 7 N Nitrogen 14.007 7 9 00.973	16 8 0 0 15.999 16 8 Sulfur 32.06	17 273 9 <sup>2</sup> 7 F Fluorine 18.998 17 <sup>2</sup> 9 Cli Chira 65.45	18 2 He Helium 4.002602 10 Neon 20.1797 18 Argon 39.948	2 K 2 K 2 K 2 K 2 K 2 K 1 M	
		19 <b>4 K</b> Potassium 39.0983 <b>20</b> <b>Ca</b> Calciuu 40.078	221 <sup>8</sup> 2 Scandium 44.955	22 <b>Ti</b> Titanium 47.907	23 28 11 2 .9415	24 28 <b>Cr</b> 13 Chromium 51.9961	25 <sup>2</sup> <b>Mn</b> <sup>13</sup> Manganese 54.938	26 28 Fe 14 Iron 55.845	27 28 Co 15 Cobalt 58.933	28 8 <b>Ni</b> 2 Nickel 58.6934	29 Cu Copper 63.546	<sup>2</sup> / <sub>8</sub> 30 <sup>2</sup> / <sub>8</sub> <sup>18</sup> <b>Zn</b> <sup>18</sup> <sup>2</sup> Zinc 65.38	31 Ga Gallium 69.723	32 8 Ge 4 Germanium 72.63	33 <sup>2</sup> <b>As</b> <sup>18</sup> Arsenic 74.921	34 <sup>2</sup> <b>Se</b> <sup>18</sup> Selenium 78.971	35 <sup>2</sup> <b>Br</b> <sup>18</sup> <sup>7</sup> Bromine 79.904	36 Kr <sup>1</sup> Krypton 83.798	2 K 8 L 8 M 8 N	
	1	5 <b>Rb</b> 18 18 <b>Sr</b> Stronti 87.62	<sup>8</sup> 39 <sup>18</sup> <b>Y</b> 1 <sup>18</sup> 2 <sup>18</sup> Y <sup>1</sup> <sup>10</sup> 2 <sup>10</sup> 2 <sup>10</sup> 2 <sup>10</sup> 1 <sup>10</sup> 2 <sup>10</sup> 2	<sup>40</sup> <b>Zr</b> Zirconium 91.224	41 <b>Nb</b> Niobium 92.90637	42 <sup>8</sup> <b>Mo</b> <sup>18</sup> <sup>13</sup> Molybdenur <sup>1</sup> 95.95	43 <b>Tc</b> 18 13 13 2 (98)	44 8 <b>Ru</b> 15 Ruthenium 1 101.07	45 <b>Rh</b> 18 Rhodium 102.90	46 Pd 18 Palladium 106.42	47 Ag Silver 107.8682	<sup>6</sup> 48 <sup>6</sup> <sup>18</sup> <b>Cd</b> <sup>18</sup> <sup>18</sup> Cadmium <sup>112,414</sup>	49 In Indium 114.818	50 8 <b>Sn</b> 18 Tin 118.710	51 <b>Sb</b> Antimony 121.760 8	52 8 <b>Te</b> 18 18 18 18 18 18 18 18 18 18	53 <sup>8</sup> 18 18 18 18 18 18 18 18 18 18 18 18 18	54 Xe 1 Xenon 131.293	8 K 8 M 8 O	
		55 56 6 Cs 18 Caesium 1 132.90 Barium 137.32	<sup>18</sup> 18 57–71	72 Hf Hafnium 178.49	<sup>2</sup> <sup>2</sup> <sup>3</sup> <sup>3</sup> <sup>3</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup> <sup>1</sup>	74 28 W 18 Tungsten 2 183.84	75 28 <b>Re</b> 18 Rhenium 2 186.207	76 <sup>2</sup> <b>Os</b> <sup>18</sup> <sup>32</sup> <sup>14</sup> <sup>190.23</sup>	77 28 <b>Ir</b> 32 Iridium 2 192.217	78 28 <b>Pt</b> 32 Platinum 1 195.084	79 Au Gold 196.96	<sup>2</sup> <sup>8</sup> <sup>18</sup> <sup>18</sup> <sup>19</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup> <sup>10</sup>	81 <b>TI</b> 33 Thallium 3204.38	82 2 <b>Pb</b> 18 Lead 4 207.2	83 <sup>8</sup> Bi <sup>18</sup> Bismuth <sup>18</sup> 208.98	84 <sup>2</sup> <b>Po</b> <sup>18</sup> Polonium <sup>18</sup> (209)	85 <sup>8</sup> At <sup>18</sup> Astatine <sup>18</sup> (210)	86 <b>Rn</b> <sup>1</sup> Radon (222)	K L M N O P	
		87 2 88 7 Fr 32 Francium 8 (223) 1 8 88 88 88 88 88 88 88 88 88 88 88 88 8	<sup>2</sup> <sup>18</sup> <sup>32</sup> <sup>18</sup> <sup>8</sup> <sup>8</sup> <sup>2</sup> <sup>8</sup> <sup>89</sup> –103	104 Rf Rutherfordiu (267)	<sup>2</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup> <sup>8</sup>	106 2 8 32 Seaborgium 12 (271) 2	107 8 <b>Bh</b> 18 32 Bohrium 13 (272) 2	108 2 Hs 18 Hassium 14 (270) 2	109 28 Mt 32 Metnerium 15 (276) 2	110 28 Ds 32 Darmstadtiu17 (281) 1	111 Rg Roentgeniur (280)	2         112         8           18         Cn         32           32         Cn         32           18         Copernicium 18         32           1         (285)         2	113 <b>Nh</b> Nihonium 1 (284)	114 28 FI 18 FI 322 Flerovium 18 (289) 4	115 28 Mc 32 Moscovium 18 (288) 5	116 28 Lv 322 Livermorium 18 (293) 6	117 28 <b>Ts</b> 18 322 Tennessine 18 (294) 7	118 Og 3 Oganesson 1 (294)	28822288 22288	40

Role RISB mean field theory in context of ab-initio calculation Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism

#### An example: Polymorphism in Strongly Correlated Materials



**Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism** 

#### An example: Polymorphism in Strongly Correlated Materials

# **Energy Profile MnO**



# Thank you for your attention!

Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism

#### An example: The $\gamma$ - $\alpha$ transition of Ce

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



Kohn-Sham-Hubbard "Reference System" Role RISB mean field theory in context of ab-initio calculations Examples: low-symmetry systems (UO<sub>2</sub>), polymorphism

# **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).





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

Fundamental object encoding material structure processed by our symmetryanalysis 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**

```
80
         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
                                           Manual preparation "Atoms" class of MnBi
from numpy.linalg import det
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()
name = material + '.struct'
fullname = path + '/' + material + '/' + name
print fullname
```

write\_struct(name, atoms2=Material, rmt=None, lattice='P', zza=None)



# Example where "Atoms" class is written/read from different structure files



**<u>Detect</u>:** (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, singleparticle 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" ( $2\pi$  rotations not identity for half-integer J).

This enables us to obtain: (I) "symmetry basis" in which the <u>local self-energy</u> and the <u>many-body local density matrix</u> 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  $exp(iL\theta)$ , where L is the orbital angular momentum. If instead both SOC and CFS are important, a rotation within the same space is represented as  $exp(iJ\theta)$ , where J=L+S is the total angular momentum.

• If J is half-integer a rotation of  $2\pi$  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<sub>2</sub> [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.



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

henhans@henhans-Satellite-C55-C: ~ × henhans@henhans-Sat

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

ATOM 2 0 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 Тd Number and name of space group: 225 (F m -3 m) (12:51:05) 0.0u 0.0s 0:00.00 0.0% 0+0k 0+72io 0pf+0w symmetry 2 Atoms found: U O generate atomic configuration for atom 1 : U generate atomic configuration for atom 2 : 0 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/U02/LDA/U02\$ initso\_lapw

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):

```
      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 U02.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 0

      Select atom-numbers (1,2,3) or "ranges of atoms" (1-3,9-12) (without blanks)

      for which you would NOT like to add S0 interaction

      (default none, just press "enter" ): 1
```

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):



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) :

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)

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



😣 🖨 🗊 🛯 😣	upc04:w/test	_UO2/LDA/UO2			
		lanata@rup	c04:w/test_UO2/LDA/	JO2 118x37	
lanata@rupc04:~/m	nt/w/test UO2/	LDA/UO2> ls			
dstart.def	params.dat	U02.in2 ls	U02.kgen	U02.rspdn	UO2.vspdn_st
dstart.error	symmetry.def	U02.in2_st	U02.klist	U02.rspup	U02.vsp_st
GL.INP	U02.bva	U02.in2_sy	U02.nnshells	U02.sigma	WH HS.INP
init_ga_info.h5	UO2.clmsum	U02.inc	U02.outputd	U02.struct	WH_HS.INP_ORIG
init ga.input	U02.dayfile	U02.inc_st	U02.outputkgen	U02.struct_nn	WH N2N.INP
init_ga.slog	U02.in0	UO2.inm	U02.outputnn	U02.struct_orig	WH_SIGMA_STRUCT.INP
input.slog	U02.in0_st	U02.inm_restart_st	U02.outputs	U02.struct_setrmt	WH_SL_VEC.INP
kgen.def	UO2.in0 std	U02.inm st	U02.outputsgroup	U02.struct_sgroup	
:log	U02.in1	U02.ing	U02.outputsgroup1	U02.struct_st	
lstart.def	U02.in1_st	U02.inq_st	U02.outputst	U02.test	
new super.clmsum	U02.in2	U02.inso	U02.rsigma	U02.tmp	
nn.def	U02.in2c	U02.inst	UO2.rsp	UO2.tmpden	

lanata@rupc04:~/mnt/w/test\_U02/LDA/U02> init\_ga.py 📕

#### Running script "init\_ga.py" in folder with completed DFT run

#### 😣 🗖 🗖 lanata@rupc04:...w/test UO2/LDA/UO2

#### lanata@rupc04:...w/test UO2/LDA/UO2 118x37

lanata@rupc04:~/m	nt/w/test_UO2/	LDA/UO2> ls	
dstart.def	params.dat	UO2.in2_ls	U02.kgen
dstart.error	symmetry.def	U02.in2_st	U02.klist
GL.INP	U02.bva	UO2.in2_sy	U02.nnshells
init_ga_info.h5	UO2.clmsum	U02.inc	UO2.outputd
init_ga.input	U02.dayfile	U02.inc_st	U02.outputkgen
init_ga.slog	U02.in0	UO2.inm	UO2.outputnn
input.slog	UO2.in0_st	UO2.inm_restart_st	UO2.outputs
kgen.def	UO2.in0_std	UO2.inm_st	U02.outputsgrou
:log	U02.in1	UO2.inq	U02.outputsgrou
lstart.def	UO2.in1_st	U02.inq_st	UO2.outputst
new_super.clmsum	U02.in2	UO2.inso	UO2.rsigma
nn.def	U02.in2c	U02.inst	UO2.rsp
lanata@rupc04:~/m	nt/w/test UO2/	LDA/UO2> init da.pv	

UO2.rspdn U02.rspup UO2.sigma U02.struct U02.struct\_nn U02.struct\_orig U02.struct setrmt tsgroup U02.struct sgroup tsgroup1 U02.struct st U02.test UO2.tmp

U02.tmpden

U02.vspdn st U02.vsp st WH HS.INP WH HS.INP ORIG WH N2N.INP WH SIGMA STRUCT.INP WH SL VEC.INP

User inputs to initialize the ga job.

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

#### 😣 🖃 🗉 🛛 lanata@rupc04:...w/test\_UO2/LDA/UO2

-

#### lanata@rupc04:...w/test\_UO2/LDA/UO2 118x37

lanata@rupc04:~/m	nt/w/test_UO2/	LDA/UO2> ls			
dstart.def	params.dat	UO2.in2_ls	U02.kgen	UO2.rspdn	UO2.vspdn_st
dstart.error	symmetry.def	U02.in2_st	UO2.klist	UO2.rspup	U02.vsp_st
GL.INP	U02.bva	UO2.in2_sy	UO2.nnshells	UO2.sigma	WH_HS.INP
init_ga_info.h5	UO2.clmsum	UO2.inc	UO2.outputd	U02.struct	WH_HS.INP_ORIG
init_ga.input	UO2.dayfile	UO2.inc_st	U02.outputkgen	UO2.struct_nn	WH_N2N.INP
init_ga.slog	U02.in0	UO2.inm	UO2.outputnn	UO2.struct_orig	WH_SIGMA_STRUCT.IN
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	U02.in1	UO2.inq	UO2.outputsgroup1	UO2.struct_st	
lstart.def	UO2.in1_st	UO2.inq_st	UO2.outputst	UO2.test	
new_super.clmsum	U02.in2	UO2.inso	UO2.rsigma	UO2.tmp	
nn.def	U02.in2c	UO2.inst	UO2.rsp	UO2.tmpden	
lanata@rupc04:~/m	nt/w/test UO2/	LDA/UO2> init da.pv			

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  $URu_2Si_2$ )

#### 😣 🖃 🗉 🛛 lanata@rupc04:...w/test\_UO2/LDA/UO2

2

lanata@rupc04:w	/test UO2/LDA	/UO2 118x37
-----------------	---------------	-------------

lanata@rupc04:~/mr	nt/w/test_U02/I	LDA/UO2> ls							
dstart.def	params.dat	UO2.in2_ls	U02.kgen	UO2.rspdn	UO2.vspdn_st				
dstart.error	symmetry.def	U02.in2_st	U02.klist	UO2.rspup	U02.vsp_st				
GL.INP	U02.bva	UO2.in2_sy	UO2.nnshells	UO2.sigma	WH_HS.INP				
init_ga_info.h5	UO2.clmsum	U02.inc	UO2.outputd	UO2.struct	WH_HS.INP_ORIG				
init_ga.input	UO2.dayfile	U02.inc_st	UO2.outputkgen	UO2.struct_nn	WH_N2N.INP				
init_ga.slog	U02.in0	UO2.inm	U02.outputnn	UO2.struct_orig	WH_SIGMA_STRUCT.INP				
input.slog	UO2.in0_st	U02.inm_restart_st	U02.outputs	UO2.struct_setrmt	WH_SL_VEC.INP				
kgen.def	UO2.in0_std	UO2.inm_st	UO2.outputsgroup	UO2.struct_sgroup					
:log	U02.in1	U02.inq	UO2.outputsgroup1	UO2.struct_st					
lstart.def	UO2.in1_st	U02.inq_st	UO2.outputst	U02.test					
new_super.clmsum	U02.in2	UO2.inso	UO2.rsigma	UO2.tmp					
nn.def	UO2.in2c	U02.inst	UO2.rsp	UO2.tmpden					
lanata@rupc04:~/mr	nt/w/test_U02/	LDA/UO2> init_ga.py							
User inputs to in	nitialize the g	ga job.							
Do you want to BF Pick one from [y	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)

#### 😰 🗐 🗉 🛛 lanata@rupc04:...w/test\_UO2/LDA/UO2

#### lanata@rupc04:...w/test\_UO2/LDA/UO2 118x37

lanata@rupc04:~/m	nt/w/test_U02/	LDA/UO2> ls			
dstart.def	params.dat	UO2.in2_ls	U02.kgen	UO2.rspdn	UO2.vspdn_st
dstart.error	symmetry.def	U02.in2_st	U02.klist	UO2.rspup	UO2.vsp_st
GL.INP	U02.bva	UO2.in2_sy	U02.nnshells	UO2.sigma	WH_HS.INP
init_ga_info.h5	UO2.clmsum	U02.inc	U02.outputd	U02.struct	WH_HS.INP_ORIG
init_ga.input	UO2.dayfile	U02.inc_st	U02.outputkgen	UO2.struct_nn	WH_N2N.INP
init_ga.slog	U02.in0	UO2.inm	U02.outputnn	UO2.struct_orig	WH_SIGMA_STRUCT.INP
input.slog	UO2.in0_st	UO2.inm_restart_st	U02.outputs	UO2.struct_setrmt	WH_SL_VEC.INP
kgen.def	UO2.in0_std	UO2.inm_st	UO2.outputsgroup	UO2.struct_sgroup	
:log	U02.in1	UO2.inq	UO2.outputsgroup1	UO2.struct_st	
lstart.def	UO2.in1_st	U02.inq_st	U02.outputst	U02.test	
new_super.clmsum	U02.in2	UO2.inso	UO2.rsigma	UO2.tmp	
nn.def	UO2.in2c	U02.inst	UO2.rsp	UO2.tmpden	
lanata@rupc04:~/m User inputs to i	nt/w/test_UO2/ nitialize the REAK SPIN-SYMM	'LDA/UO2> init_ga.py ga job. IETRV2			
Pick one from [y	, n]n				
Do you want to C Pick one from [y	OMPLETELY BREA , n]n	K ORBITAL-SYMMETRY?			
Symmetrically-eq (note: '0 0 0 1 Accept? Pick one from [y	uivalent atom l' means 1-3 a , n]y	indices: 0 1 1 nd 4-5 are two inequ	ivalent atoms).		

atom 0 U

**F**.

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

#### 😣 🖻 🗉 lanata@rupc04:...w/test\_UO2/LDA/UO2

[S, p, d, †]...†

#### lanata@rupc04:...w/test\_UO2/LDA/UO2 118x37

lanata@rupc04:~/m	nt/w/test_UO2/	LDA/UO2> ls			
dstart.def dstart.error GL.INP	params.dat symmetry.def U02.bva	U02.in2_ls U02.in2_st U02.in2_sy	UO2.kgen UO2.klist UO2.nnshells	UO2.rspdn UO2.rspup UO2.sigma	U02.vspdn_st U02.vsp_st WH_HS.INP
init_ga_info.h5 init_ga.input init_ga.slog input.slog kgen.def :log lstart.def new_super.clmsum nn.def	U02.clmsum U02.dayfile U02.in0 U02.in0_st U02.in0_std U02.in1 U02.in1_st U02.in2 U02.in2c	U02.inc U02.inc_st U02.inm U02.inm_restart_st U02.inm_st U02.inq U02.inq_st U02.inso U02.inst	U02.outputd U02.outputkgen U02.outputnn U02.outputs U02.outputsgroup U02.outputsgroup1 U02.outputst U02.rsigma U02.rsp	U02.struct U02.struct_nn U02.struct_orig U02.struct_setrmt U02.struct_sgroup U02.struct_st U02.test U02.tmp U02.tmp U02.tmpden	WH_HS.INP_ORIG WH_N2N.INP WH_SIGMA_STRUCT.INP WH_SL_VEC.INP
lanata@rupc04:~/m	nt/w/test_U02/	LDA/U02> init_ga.py			
User inputs to i	nitialize the	ga job.			
Do you want to B Pick one from [y	REAK SPIN-SYMM , n]n	ETRY?			
Do you want to C Pick one from [y	OMPLETELY BREA , n]n	K ORBITAL-SYMMETRY?			
Symmetrically-eq (note: '0 0 0 1 Accept? Pick one from [y	uivalent atom 1' means 1-3 a , n]y	indices: 0 1 1 nd 4-5 are two inequ	ivalent atoms).		
atom 0 U					
Is this atom cor Pick one from [y	related? , n]y				
Enter correlated Pick one or comb	shells? inations separ	ated by blank space	U atom has	s f correlated e	lectrons

#### 😣 😑 🗉 🛛 lanata@rupc04:...w/test\_UO2/LDA/UO2

```
-----
                                        lanata@rupc04:...w/test UO2/LDA/UO2 118x37
                               UO2.inm
init ga.slog
                 U02.in0
                                                  U02.outputnn
                                                                    U02.struct orig
                                                                                       WH SIGMA STRUCT.INP
input.slog
                 U02.in0 st
                              U02.inm restart st U02.outputs
                                                                     U02.struct setrmt
                                                                                       WH SL VEC.INP
kgen.def
                 U02.in0 std
                              UO2.inm st
                                                  U02.outputsgroup
                                                                    U02.struct sgroup
:log
                 U02.in1
                              U02.ing
                                                  U02.outputsgroup1 U02.struct st
lstart.def
                                                  U02.outputst
                 U02.in1 st
                               U02.ing st
                                                                     U02.test
new super.clmsum U02.in2
                               U02.inso
                                                  U02.rsigma
                                                                    UO2.tmp
nn.def
                 U02.in2c
                               U02.inst
                                                  UO2.rsp
                                                                     U02.tmpden
lanata@rupc04:~/mnt/w/test U02/LDA/U02> 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?
                                                               SOC and CFS not negligible: System
Pick one or combinations separated by blank space
from [s, p, d, f]...f
                                                               not spin rotationally-invariant.
Do you want to take into account the SPIN-ORBIT interaction?
                                                               Discrete group with rotations
Pick one from [y, n]...y
                                                               generated by J=L+S
Do you want to take into account the CRYSTAL FIELD effect?
Pick one from [y, n]...y
```

😣 🗆 💷 lanata@rupc04:w/te	st_UO2/LDA/UO2		
	lanata@rup	c04:w/test_UO2/LDA/L	UO2 118x37
nn.def U02.in2c lanata@rupc04:~/mnt/w/test_U0	U02.inst D2/LDA/U02> init_ga.py	UO2.rsp	U02.tmpden
User inputs to initialize th	e ga job.		
Do you want to BREAK SPIN-SY Pick one from [y, n]n	MMETRY?		
Do you want to COMPLETELY BR Pick one from [y, n]n	EAK ORBITAL-SYMMETRY?		
Symmetrically-equivalent ato (note: '0 0 0 1 1' means 1-3 Accept? Pick one from [y, n]y	m indices: 0 l l and 4-5 are two inequ	uivalent atoms).	
atom 0 U			
Is this atom correlated? Pick one from [y, n]y			
Enter correlated shells? Pick one or combinations sep from [s, p, d, f]f	arated by blank space		
Do you want to take into acc Pick one from [y, n]y	ount the SPIN-ORBIT in	teraction?	
Do you want to take into acc Pick one from [y, n]y	ount the CRYSTAL FIELD	) effect?	
atom 1 0	Code asking	user if atom w	rith label "1" (which is O) is

correlated or not (it's not)

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

😣 🔵 💷 lanata@rupc04:w/test_UO2/LDA/UO2		
	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	with symmetry and	'elatea alysis
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 interact Pick one from [y, n]y	tion?	
Do you want to take into account the CRYSTAL FIELD effect Pick one from [y, n]y	ct?	
atom 1 0		
Is this atom correlated? Pick one from [y, n]n		
<pre>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</pre>	We choose Slater parametrization interaction (consequently values will be asked)	n local of U,J
#### Ianata@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 0
```

```
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 V2A0.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

## ermined.) calculations

We generally choose standard

(quadratic) double counting in all of our

# Other questions not related with symmetry analysis

#### 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 0 Other questions not related Is this atom correlated? with symmetry analysis 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 V2A0.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 Question specific for GA/RISB solver (keep same Vdc/n0 at each charge iteration, n0 to be provided.) (precision requested for self-energy self 1: Standard double counting potential (n0 self-consistently determined.) consistency, which is formulated as a root 0: No double counting. Please select LDC: problem) 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

#### 🔕 🖃 🗉 🛛 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 V2A0.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

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

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

#### 😣 🖃 🗉 🛛 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 V2A0.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, \backslash\}
(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

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

#### Other questions not related with symmetry analysis

#### 😣 🗖 🔲 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

Pick one from [5, 0, 1, 2, 3]...5

3: Exact diagonalization (ZHEEVX, selective lowest two eigen-vectors) in LAPACK 5: PRIMME (Recommended for large dimension.) Please select LEIGV: 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.

# Other questions not related with symmetry analysis



```
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, \backslash\}
                                                                      Other questions not related
(recommend 1.e-5 or smaller)...5.e-6
                                                                        with symmetry analysis
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
                                                        Relevant valence range of U atom.
       3: Exact diagonalization (ZHEEVX,
          selective lowest two eigen-vectors) in LAPACK
                                                        Embedding problem computationally
       5: PRIMME (Recommended for large dimension.)
Please select LEIGV:
                                                        challenging when CFS and SOC both non-
Pick one from [5, 0, 1, 2, 3]...5
                                                        negligible. Valence truncation necessary
INFORMATION FOR f ELECTRONS OF U :
Please provide interaction parameters U,J
                                                        with Lanczos (and fortunately licit for this
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
                                                        system).
Please provide guess n0 for valence
(0 < n0 < 4 overwritten by GL NELF1.INP): 2.1
```

😣 🗇 💷 lanata@rupc04:w/test_UO2/LDA/UO2	
anata@rupc04:w/test_UO2/LDA/U	O2 118x37
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Initialization completed. Corresponding information
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Please run ga init dmft.pv with parameters given in init ga.slog	
The default dist cut for extracting a centered cluster	processed information)
for symmetry evaluation = 3.9044007499	dumped in file
Molecule extracted 0_8 U_13 :	
atom x y z distance	"init ga.slog".
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lanata@rupc04:~/mnt/w/test\_U02/LDA/U02> less init\_ga.slog

Lemma (calculated by our symmetry code)

dumped in file

"init ga.slog".

#### 😣 亘 🔲 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] Initialization completed. 2.69011757e+00 0.00000000e+00]] 2.69011757e+00 ['U', 'O', 'O'] Symbols: Corresponding information Scaled positions: [[ 0. Θ. Θ. given (and part of the 0.75 0.75 0.75] 0.25 0.25 0.25] processed information) 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 enerav Θ [[1200000000000 Θ [340000000000000000 0 0 00000 Θ 01 03 40000000 Θ 0 0 Block structure of self energy of *f* electrons of U 5 Θ Θ Θ 6 0 8 Θ Θ Θ Θ Θ atom in symmetry basis accordingly to Shur 0 0 0 ΘΘ 05 -6 Θ Θ

Please run ga\_init\_dmft.py with the following parameters. init ga.slog lines 1-36/54 76%

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## **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  $\alpha$ -Ce.

## Hands-on Session: α-Ce

#### **Folder structure:**

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	drwxrwxr-x 3 winterschool winterschool 4.0K Jan 4 20:40 LDA_SB_sol		
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	-rw-rw-r 1 winterschool winterschool 375 Jan 4 20:56 README_LDA -rw-rw-r 1 winterschool winterschool 2 5K Jan 4 20:57 README LDA SR		
	drwxrwxr-x 2 winterschool winterschool 4.0K Jan 4 00:14 scripts		
	drwxrwxr-x 2 winterschool winterschool 4.0K Jan 3 22:45 solutions		
	winterschool@winterschool-virtualBox:~/winterschool/Ce\$		
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## 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.ht ml#ce-with-spin-orbit-interaction for details

# Hands-on Session: α-Fe

#### **Folder structure:**

🐕 ubuntu [孰行中] - Oracle VM VirtualBox	
檔案 機器 檢視 輸入 装置 說明	
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drwxrwxr-x 2 winterschool winterschool 4.0K Jan 7 04:55 scripts	
winterschool@winterschool-VirtualBox:~/winterschool/FeS	S
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## Hands-on Session: a-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.ht ml#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/PhysR evLett.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:**

$$|\Gamma; \mathbf{R}, i\rangle = \left(c_{\mathbf{R}i1}^{\dagger}\right)^{n_{1}} \dots \left(c_{\mathbf{R}iM}^{\dagger}\right)^{n_{M}} |0\rangle$$

$$|n; \mathbf{R}, i\rangle = \left(f_{\mathbf{R}i1}^{\dagger}\right)^{n_{1}'} \dots \left(f_{\mathbf{R}iM}^{\dagger}\right)^{n_{M}'} |0\rangle \quad \left(\langle \Psi_{0} | f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} | \Psi_{0} \rangle \equiv n_{iab}^{0} = \delta_{ab} n_{ibb}^{0}\right)$$

Calculations considerably simplified by the following assumptions:

# **Gutzwiller Approximation:**

 $|\Psi_G\rangle$  can be dealt only numerically unless in the limit of  $\infty$ -coordination lattices (as in DMFT)

## **Gutzwiller constraints:**

 $\begin{aligned} \left| \left\langle \Psi_{0} \right| \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} \left| \Psi_{0} \right\rangle \\ = \left\langle \Psi_{0} \right| \Psi_{0} \right\rangle = 1 \\ \left\langle \Psi_{0} \right| \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} \left| \Psi_{0} \right\rangle \\ = \left\langle \Psi_{0} \right| f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} \left| \Psi_{0} \right\rangle \quad (\forall a, b) \end{aligned}$ 

("slightly" reduce variational freedom) Considerable simplification of the calculations

# **Gutzwiller constraints:**

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

#### Key consequence:

$$\begin{split} \langle \Psi_{0} | \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ia} | \Psi_{0} \rangle &= \langle \Psi_{0} | \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} | \Psi_{0} \rangle \langle \Psi_{0} | f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ia} | \Psi_{0} \rangle \\ &+ \langle \Psi_{0} | \left[ \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} \right] \left( f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ia} \right) | \Psi_{0} \rangle_{2\text{-legs contracted}} \end{split}$$

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

### Local operators:

$$\begin{split} \langle \Psi_{G} | \, \hat{\mathcal{O}}_{\mathbf{R}i} [c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}^{\dagger}] | \Psi_{G} \rangle &\equiv \langle \Psi_{0} | \, \mathcal{P}^{\dagger} \, \hat{\mathcal{O}}_{\mathbf{R}i} [c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}^{\dagger}] \, \mathcal{P} | \Psi_{0} \rangle \\ &= \langle \Psi_{0} | \, \left[ \prod_{\mathbf{R}', i' \neq \mathbf{R}, i} \mathcal{P}_{\mathbf{R}'i'}^{\dagger} \mathcal{P}_{\mathbf{R}'i'} \right] \, \mathcal{P}_{\mathbf{R}i}^{\dagger} \, \hat{\mathcal{O}}_{\mathbf{R}i} [c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}^{\dagger}] \, \mathcal{P}_{\mathbf{R}i} \, | \Psi_{0} \rangle \\ &= \langle \Psi_{0} | \, \mathcal{P}_{\mathbf{R}i}^{\dagger} \, \hat{\mathcal{O}}_{\mathbf{R}i} [c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}^{\dagger}] \, \mathcal{P}_{\mathbf{R}i} \, | \Psi_{0} \rangle \\ &+ \langle \Psi_{0} | \, \left[ \prod_{\mathbf{R}', i' \neq \mathbf{R}', i} \mathcal{P}_{\mathbf{R}'i'}^{\dagger} \mathcal{P}_{\mathbf{R}'i'} \right] \, \left( \mathcal{P}_{\mathbf{R}i}^{\dagger} \, \hat{\mathcal{O}}_{\mathbf{R}i} [c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}^{\dagger}] \, \mathcal{P}_{\mathbf{R}i} \right) \, | \Psi_{0} \rangle_{2\text{-legs}} \\ &+ \langle \Psi_{0} | \, \left[ \prod_{\mathbf{R}', i' \neq \mathbf{R}', i} \mathcal{P}_{\mathbf{R}'i'}^{\dagger} \mathcal{P}_{\mathbf{R}'i'} \right] \, \left( \mathcal{P}_{\mathbf{R}i}^{\dagger} \, \hat{\mathcal{O}}_{\mathbf{R}i} [c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}^{\dagger}] \, \mathcal{P}_{\mathbf{R}i} \right) \, | \Psi_{0} \rangle_{(N \geq 4)\text{-legs}} \end{split}$$

# Local operators:

$$\langle \Psi_{0} | \mathcal{P}^{\dagger} \hat{\mathcal{O}}_{\mathbf{R}i}[c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}] \mathcal{P} | \Psi_{0} \rangle = \left| \langle \Psi_{0} | \mathcal{P}_{\mathbf{R}i}^{\dagger} \hat{\mathcal{O}}_{\mathbf{R}i}[c_{\mathbf{R}i\alpha}^{\dagger}, c_{\mathbf{R}i\alpha}] \mathcal{P}_{\mathbf{R}i} | \Psi_{0} \rangle \right|$$

Inter-site single-particle quadratic operators:

$$\begin{aligned} \left\langle \Psi_{0} \right| \mathcal{P}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} c_{\mathbf{R}'j\beta} \mathcal{P} \left| \Psi_{0} \right\rangle \\ &= \left\langle \Psi_{0} \right| \left[ \mathcal{P}_{\mathbf{R}i}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} \mathcal{P}_{\mathbf{R}i} \right] \left[ \mathcal{P}_{\mathbf{R}'j}^{\dagger} c_{\mathbf{R}'j\beta} \mathcal{P}_{\mathbf{R}'j} \right] \left| \Psi_{0} \right\rangle \end{aligned}$$

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:*

$$\begin{split} \langle \Psi_{0} | \mathcal{P}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} c_{\mathbf{R}'j\beta} \mathcal{P} | \Psi_{0} \rangle &= \langle \Psi_{0} | \left[ \mathcal{P}_{\mathbf{R}i}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} \mathcal{P}_{\mathbf{R}i} \right] \left[ \mathcal{P}_{\mathbf{R}'j}^{\dagger} c_{\mathbf{R}'j\beta} \mathcal{P}_{\mathbf{R}'j} \right] | \Psi_{0} \rangle \\ &= \langle \Psi_{0} | \left[ \mathcal{P}_{\mathbf{R}i}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} \mathcal{P}_{\mathbf{R}i} \right] \left[ \mathcal{P}_{\mathbf{R}'j}^{\dagger} c_{\mathbf{R}'j\beta} \mathcal{P}_{\mathbf{R}'j} \right] | \Psi_{0} \rangle_{1\text{-leg}} \\ &\equiv \sum_{ab} \langle \Psi_{0} | \left( \left[ \mathcal{R}_{i} \right]_{a\alpha} f_{\mathbf{R}ia}^{\dagger} \right) \left( \left[ \mathcal{R}_{j} \right]_{b\beta}^{*} f_{\mathbf{R}'jb} \right) | \Psi_{0} \rangle \end{split}$$

Original ladder operators effectively transform as

$$c^{\dagger}_{\mathbf{R}i\alpha} \rightarrow \sum_{a} \left[ \mathcal{R}_{i} \right]_{a\alpha} f^{\dagger}_{\mathbf{R}ia}$$

under the action of the Gutzwiller projector, where:

$$\begin{bmatrix} \mathcal{R}_{i} \end{bmatrix}_{a\alpha} = \left[ \langle \Psi_{0} | \mathcal{P}_{\mathbf{R}i}^{\dagger} [c_{\mathbf{R}i\alpha}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia} | \Psi_{0} \rangle \right] / \langle \Psi_{0} | f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ia} | \Psi_{0} \rangle$$
$$\mathcal{P}_{\mathbf{R}i} = \sum_{\Gamma n} \lambda_{i,\Gamma n} | \Gamma; \mathbf{R}, i \rangle \langle n; \mathbf{R}, i |$$

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

$$\begin{split} \boxed{\left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} \middle| \Psi_{0} \right\rangle} &= \operatorname{Tr} \left[ P_{i}^{0} \lambda_{i}^{\dagger} \lambda_{i} \right] = 1 \\ \boxed{\left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} \middle| \Psi_{0} \right\rangle} &= \operatorname{Tr} \left[ P_{i}^{0} \lambda_{i}^{\dagger} \lambda_{i} F_{ia}^{\dagger} F_{ib} \right] = \left\langle \Psi_{0} \middle| f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} \middle| \Psi_{0} \right\rangle \equiv n_{iab}^{0} \delta_{ab} \\ \boxed{\left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia} \middle| \Psi_{0} \right\rangle} &= \operatorname{Tr} \left[ P_{i}^{0} \lambda_{i}^{\dagger} F_{i\alpha}^{\dagger} \lambda_{i} F_{ia} \right] \\ \boxed{\left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} \hat{\mathcal{O}}_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} \middle| \Psi_{0} \right\rangle} &= \operatorname{Tr} \left[ P_{i}^{0} \lambda_{i}^{\dagger} O \lambda_{i} \right] \\ \mathcal{P}_{\mathbf{R}i} &\equiv \sum_{\Gamma_{n}} \lambda_{i,\Gamma_{n}} \middle| \Gamma; \mathbf{R}, i \rangle \langle n; \mathbf{R}, i \middle| \\ \left| \Gamma; R, i \right\rangle &\equiv \left[ c_{Ri1}^{\dagger} \right]_{\cdots}^{n_{1}} \left[ c_{RiM}^{\dagger} \right]^{n_{M}} \left| 0 \right\rangle; \quad \left| n; R, i \right\rangle \equiv \left[ f_{Ri1}^{\dagger} \right]_{\cdots}^{n_{1}} \left[ f_{RiM}^{\dagger} \right]^{n_{M}} \left| 0 \right\rangle \end{split}$$

$$[\Gamma; R, i\rangle \equiv [C_{Ri1}] \cdots [C_{RiM}] \quad |0\rangle; \quad |n; R, i\rangle \equiv [f_{Ri1}] \cdots [f_{RiM}]$$

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

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

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

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

$$\begin{split} \boxed{\left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} \middle| \Psi_{0} \right\rangle} &= \operatorname{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} \right] = 1 \\ \hline \left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} \middle| \Psi_{0} \right\rangle} &= \operatorname{Tr} \left[ \phi_{i}^{\dagger} \phi_{i} F_{ia}^{\dagger} F_{ib} \right] = \left\langle \Psi_{0} \middle| f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ib} \middle| \Psi_{0} \right\rangle \equiv n_{iab}^{0} \delta_{ab} \\ \hline \left[ \left[ \mathcal{R}_{i} \right]_{a\alpha} \right] &\equiv \left[ \left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} c_{\mathbf{R}i\alpha}^{\dagger} \mathcal{P}_{\mathbf{R}i} f_{\mathbf{R}ia} \middle| \Psi_{0} \right\rangle \right] / \left\langle \Psi_{0} \middle| f_{\mathbf{R}ia}^{\dagger} f_{\mathbf{R}ia} \middle| \Psi_{0} \right\rangle \\ &= \operatorname{Tr} \left[ \phi_{i}^{\dagger} F_{i\alpha}^{\dagger} \phi_{i} F_{ia} \right] / \sqrt{n_{iaa}^{0} \left( 1 - n_{iaa}^{0} \right)} \\ \hline \left[ \left\langle \Psi_{0} \middle| \mathcal{P}_{\mathbf{R}i}^{\dagger} \hat{\mathcal{O}}_{\mathbf{R}i} \mathcal{P}_{\mathbf{R}i} \middle| \Psi_{0} \right\rangle \right] &= \operatorname{Tr} \left[ \phi_{i} \phi_{i}^{\dagger} O \right] \\ \hline \mathcal{P}_{\mathbf{R}i} &\equiv \sum_{\Gamma n} \lambda_{i,\Gamma n} \left| \Gamma; \mathbf{R}, i \right\rangle \langle n; \mathbf{R}, i \right| \\ \left[ P_{i}^{0} \right]_{nn'} &\equiv \left\langle \Psi_{0} \middle| n', Ri \right\rangle \langle n, Ri \middle| \Psi_{0} \right\rangle \delta_{nn'} \\ \left[ F_{ib} \right]_{nn'} &= \left\langle \Gamma, Ri \middle| c_{Rib} \middle| \Gamma', Ri \right\rangle = \left\langle n, Ri \middle| f_{Rib} \middle| n', Ri \right\rangle \\ \left[ O \right]_{\Gamma\Gamma'} &= \left\langle \Gamma, Ri \middle| \hat{\mathcal{O}}_{\mathbf{R}i} \middle| \Gamma', Ri \right\rangle \\ \left[ \phi_{i} \right] &= \lambda_{i} \sqrt{P_{i}^{0}} \end{split}$$



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

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thlee@	thlee@zakynthos UO2]\$ python \${WIEN_GUTZ_ROOT}/tools/Gutzwiller/init_mott.py ********* Impurity 0 ********** Sigma structure:															
Sigma	struct	ure:														
Index	0	1	2	3	4	5	б	7	8	9	10	11	12	13		
0	1	2	0	0	0	0	0	0	0	0	0	0	O	0		
1	3	4	0	0	0	0	0	0	0	0	0	0	0	0		
2	Θ	Θ	1	2	0	0	Θ	0	Θ	Θ	0	0	Θ	0		
3	0	Θ	3	4	0	0	0	0	0	0	0	0	0	0		
4	0	0	0	0	5	б	0	0	0	0	0	0	0	0		
5	0	0	0	0	7	8	0	0	0	0	0	0	0	0		
б	0	0	0	0	0	0	5	б	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	Θ	0	0	0	0	0	0	0	Θ	0	0	9	0		
13	0	Θ	0	0	0	0	Θ	0	0	Θ	0	0	Θ	9		
Please	provi	de th	e ind	ices	of or	bital	s to	be Mo	tt lo	cali	zed					
(e.g.,	02)	: 4 6	8 10													

hen	hans@h	enhans	s-Satel	lite-C5	5-C: ~	×t	hlee@z	akynth	ios:~/c	ygutz/	UO2/L	DA_SB.	×	thlee	@zakynthos:~/cygutz/UO	2/LDA_SB	×	henhans@henhans-Satellite-C55-C: ~/cyg ×
[thlee@: *******	zakynt *** I	hos U mpuri	02]\$ ty 0	pytho	on \${W	IEN_C	UTZ_R	00Т}/	tools	/Gut	zwill	er/in	it_mo	ott.py	1			
Sigma s	struct	ure:																
index	0	1	2	3	4	5	б	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	Θ	1	2	0	Θ	0	0	0	0	0	0	0	0				
3	0	0	3	4	0	0	0	0	0	0	0	0	0	0				
4	Θ	Θ	0	Θ	5	6	0	0	0	0	0	0	0	0				
5	0	Θ	0	0	7	8	0	0	0	0	0	0	0	0				
б	0	0	0	0	0	Θ	5	б	Θ	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	Θ	Θ	0	0	0	Θ	0	0	7	8	0	0	0	0				
10	0	Θ	0	0	0	Θ	0	0	Θ	Θ	5	б	0	0				
11	0	Θ	0	0	0	Θ	0	0	Θ	Θ	7	8	0	0				
12	0	0	0	0	0	0	0	0	Θ	0	0	0	9	0				
13	0	0	0	0	0	0	0	0	0	0	0	0	0	9				
Please	provi	de th	e ind	lices	of or	bital	.s to	be Mo	tt lo	cali	zed							
	02)	· 4 6	8 10															

You selected [4 6 8 10] to be Mott localized, right? (y/n):y

hen	hans@h	nenhan	s-Satell	lite-C5	5-C: ~	× tl	hlee@;	zakyntł	nos:~/c	ygutz/	UO2/L	DA_SB	×	thlee@zak	ynthos:~/cygu	Jtz/UO2/LD	A_SB ×	henhans@henhans-Satellite	-C55-C: ~/cyg ×
[thlee@ ******	zakynt *** I	hos l mpuri	JO2]\$ Lty 0	pytho	on \${W	IIEN_G	UTZ_F	ROOT}/	tools	/Gut:	zwill	er/in	it_mo	ott.py					
Sigma	struct	ure:																	
index	0	1	2	3	4	5	б	7	8	9	10	11	12	13					
0	1	2	0	0	0	0	0	0	0	0	O	O	0	0					
1	3	4	0	0	Θ	0	Θ	0	Θ	Θ	0	0	0	0					
2	0	Θ	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	Θ	Θ	0	5	б	0	0	Θ	0	0	Θ	0	0					
5	0	Θ	0	0	7	8	0	0	0	Θ	0	0	0	0					
б	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	Θ					
8	0	Θ	0	0	0	0	Θ	0	5	6	0	0	0	Θ					
9	0	Θ	0	0	0	0	0	0	7	8	0	0	0	0					
10	0	Θ	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	9					
Please	provi	de tr	ne ind	lices	of or	bital	s to	be Mo	ott lo	cali	zed								
(e.g.,	02)	: 4 6	5 8 10	)															
You se	lected	[4 6	8 10	n to	De Mo	ott lo	caliz	ed, r	tght?	-(y/i	n):y								
Please	ρΓονί	de th	ne tot	at nu	Imber	OT MO	ττ ια	caliz	ed el	ectro	ons (j	per u	nit c	ett): 2					

hei	nhans@h	enhans	s-Satel	lite-C5	5-C: ~	×t	hlee@z	akynth	nos:~/c	ygutz/	UO2/LI	DA_SB	×	thle	e@zakynthos:~/cygutz/UO2/LDA_SB ×	henhans@henhans-Satellite-C55-C: ~/cyg ×
thlee(	zakynt *** I	hos U mpuri	02]\$ ty 0	pytho	on \${k	VIEN_G	UTZ_R	00Т}/	tools	s/Gutz	zwille	er/in	it_mo	ott.p	у	
Sigma	struct	ure:														
ndex	0	1	2	3	4	5	б	7	8	9	10	11	12	13		
0	1	2	0	0	0	Θ	0	0	O	0	0	0	O	0	1	
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	Θ	0	0	Θ	0	Θ	0	)	
4	0	0	0	0	5	б	0	0	0	0	0	0	Θ	0	)	
5	0	0	Θ	0	7	8	0	Θ	0	0	Θ	0	Θ	0	)	
б	0	0	0	0	0	0	5	б	0	0	Θ	0	Θ	0	)	
7	0	0	Θ	0	0	0	7	8	0	0	0	0	Θ	0	)	
8	0	0	0	0	0	0	0	0	5	б	Θ	0	Θ	0	)	
9	0	0	Θ	0	0	0	0	0	7	8	0	0	0	0	)	
10	0	0	Θ	0	0	0	0	Θ	0	Θ	5	б	Θ	0	)	
11	0	0	0	0	0	0	0	0	0	0	7	8	0	0	)	
12	0	0	Θ	0	0	0	0	Θ	0	0	0	0	9	0	)	
13	0	0	0	0	0	0	0	Θ	0	0	0	0	0	9		
Please	provi	de th	e ind	dices	of or	bital	s to	be Mo	ott lo	caliz	zed					
(e.g.,	02)	: 4 6	8 10	0												

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

hen	hans@h	nenhan	ns-Satel	lite-C55	-C: ~	×t	hlee@z	zakynth	os:~/c	ygutz/	JO2/L	DA_SB	×	thlee	@zakynthos:~/cygutz/UO2/LDA_SB >	henhans@henhans-Satellite-C55-C: ~/cyg ×
(e.g., You se Please Total	02) lected provi 2elec	: 4 ( [ [4 ( .de th :trons	6 8 10 6 8 10 he tot s will	) )] to tal nu L be M	be Mo mber ott l	ott lo of Mo .ocali	ocaliz ott lo .zed,	ed, r ocaliz right	ight: ed el ? (y/	? (y/r .ectro (n):y	n):y ons (p	oer u	nit c	ell):	2	
k SLIU ndev		1	2	2	А	5	6	7	0	9	10	11	10	12		
IUEX	0	1	2	2	4	د	0	'	0	,	10	11	12	12		
0	1	2	0	0	0	0	Θ	0	0	0	0	0	0	0		
1	3	4	0	0	0	0	0	0	0	0	0	0	0	0		
2	0	Θ	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	Θ	0	0	0	0	0	0		
5	0	0	0	0	б	7	0	Θ	0	0	0	0	0	0		
б	0	0	0	0	0	0	5	0	0	0	0	0	0	0		
7	0	Θ	0	0	Θ	0	б	7	0	0	0	0	0	0		
8	0	0	0	0	0	0	0	Θ	5	0	0	0	0	0		
9	0	0	0	0	0	0	0	0	б	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	Θ	0	0	0	0	0	0	0	0	0	0	8	0		
13	0	0	0	0	Θ	0	0	0	0	0	0	0	Θ	8		
Lambda	struc	:ture	:													
ndex	0	1	2	3	4	5	6	7	8	9	10	11	12	13		
•	1	2	0		0	0	0	0	0	0	0	•	0	0		
1	2	2	0	0	0	0	0	0	0	0	0	0	0	0		
2	د ۵	4	1	2	0	0	0	0	0	0	0	0 0	0	0		
2	0	0 0	יד א	4	0	0 0	0	0	٥	0 0	0 0	٥ ٥	0 0	0 0		
4	õ	õ	0	•	5	õ	õ	0	õ	õ	õ	õ	0	õ		
5	õ	õ	õ	õ	0	6	õ	õ	õ	õ	õ	õ	õ	õ		
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	б	0	0	0	0		
10	0	Θ	0	0	Θ	0	0	0	0	0	5	0	Θ	0		
11	0	Θ	0	0	Θ	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@	zakynt	hos l	UO2]\$	pytho	n \${W	IEN_C	UTZ_R	OOT}/	ga_ru	un_dmf	t.py					

# Initialization UO<sub>2</sub>: LDA + RISB Mott (DOS Band Structure)

#### **Initialization UO<sub>2</sub> : LDA + RISB Mott (DOS Band Structure)**

henhans@henhans-Satel... × henhans@henhans-Satel
henhans@henha	× henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×
UO2.nmat_only	-> Ce_SCF/UO2.nmat_	_only					
U02.vsp -> Ce	_SCF/U02.vsp						
UO2.vspup ->	Ce_SCF/U02.vspup						
UU2.VSpan ->	SCE/UD2 r2v						
U02.r2vdn ->	Ce_SCF/U02.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.INF	P O					
WH_N2N_TNP ->	Ce_SCF/WH_NSN_TNP	r					
WH RLNEF.INP	-> Ce SCF/WH RLNEF.]	INP					
WH_SIGMA_STRU	CT.INP -> Ce_SCF/WH	_SIGMA_STRUCT.INP					
WH_SIGMA_STRU	CT_L.INP -> Ce_SCF/W	WH_SIGMA_STRUCT_L.I	NP				
WH_SIGMA_STRU	CT_R.INP -> Ce_SCF/W	WH_SIGMA_STRUCT_R.I	NP				
WH_SL_VEC.INF	<pre>&gt; Ce_SCF/WH_SL_VEG</pre>	C.INP					
WH_ELU.OUI ->	Ce_SCF/WH_EL0.001	онт					
GL. TNP -> Ce	SCE/GL. INP	501					
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						
GUIZ4.INP ->	Ce_SCF/GUIZ4.INP						
GL LOG.OUT ->	Ce SCF/GL LOG.OUT						
GL_NELF1.OUT	-> Ce_SCF/GL_NELF1.0	оит					
GLPJC_1.OUT ·	> Ce_SCF/GLPJC_1.0UT	Г					
FROZEN.INP ->	Ce_SCF/FROZEN.INP						
glog.h5 -> Ce	_SCF/glog.h5						
init_ga_info.	h5 -> Ce_SCF/init_ga	a_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/U02/LDA\_SB\_Mott\_k2000/U02\$ sed -i 's/.\*LSCF.\*/LSCF = 2/' GL.INP && sed -i 's/.\*LSCF.\*/&\nLEFERMI = 1/' GL.INP && sed -i 's/.\*LSCF.\*/&\nLEFERMI = 1/' GL.INP

nenhans@henha × henhans@	nenha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×	henhans@henha ×
U02.vsp -> Ce_SCF/U02.vs	P						
U02.vspup -> Ce_SCF/U02.	vspup						
U02.vspdn -> Ce_SCF/U02.	vspdn						
U02.r2v -> Ce_SCF/U02.r2	v .						
U02.r2vdn -> Ce_SCF/U02.	r2vdn						
params.dat -> Ce_SCF/par	ams.dat						
EFLDA.INP -> Ce_SCF/EFLL							
WH HS I TNP -> Ce_SCF/WH_F							
WH HS R. INP -> Ce SCF/W	HS R. INP						
WH N2N.INP -> Ce SCF/WH	N2N.INP						
WH RLNEF.INP -> Ce SCF/W	H RLNEF.I	NP					
WH_SIGMA_STRUCT.INP -> 0	e_SCF/WH_	SIGMA_STRUCT.INP					
WH_SIGMA_STRUCT_L.INP ->	Ce_SCF/W	H_SIGMA_STRUCT_L.	INP				
WH_SIGMA_STRUCT_R.INP ->	Ce_SCF/W	H_SIGMA_STRUCT_R.1	INP				
WH_SL_VEC.INP -> Ce_SCF/	WH_SL_VEC	.INP					
WH_EL0.OUT -> Ce_SCF/WH_	EL0.OUT						
WH_RLNEF.OUT -> Ce_SCF/W	H_RLNEF.0	UT					
GL.INP -> Ce_SCF/GL.INP		ND					
GL_NELFI.INP -> Ce_SCF/C	L_NELFI.I	NP					
$CIIT71$ INP -> Ce_SCE/CIIT7	1_0.1NF						
GUT72.INP -> Ce SCF/GUT7	2. TNP						
GUTZ3.INP -> Ce SCF/GUTZ	3.INP						
GUTZ4.INP -> Ce SCF/GUTZ	4.INP						
GUTZ5.INP -> Ce_SCF/GUTZ	5.INP						
GL_LOG.OUT -> Ce_SCF/GL_	LOG.OUT						
GL_NELF1.OUT -> Ce_SCF/C	L_NELF1.0	UT					
GLPJC_1.OUT -> Ce_SCF/GL	PJC_1.OUT						
FROZEN.INP -> Ce_SCF/FRC	ZEN.INP						
glog.h5 -> Ce_SCF/glog.h	5	ter br					
init_ga_info.h5 -> Ce_SC	F/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/U02/LDA\_SB\_Mott\_k2000/U02\$ 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/U02/LDA\_SB\_Mott\_k2000/U02\$ cp WH\_EL0.OUT WH\_EL0.INP && cp EFLDA.OUT EFLDA.INP

henhans@henha... × henhans@henha

henhans@henha... × henhans@henha