Calculation of U for systems with several strongly correlated orbitals

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1. cRPA calculation

$\Rightarrow$ Which orbital is correlated ? (d in TM and f in lanthanides/actinides)

Constrained Random Phase Approximation [1]

Three steps :

- Define the correlated orbital : PLO-Wannier
- Constrained Screening : ϵ
- Calculation of $U = \langle w_1 w_2 | \epsilon^{-1} v | w_3 w_4 \rangle$

Goal of the work

- Extension of the scheme to several orbitals [2] (e.g. U^{ff}, U^{dd}, U^{df})
- Interfacing cRPA routines [3] with PLO-Wannier

1. F. Aryasetiawan *et al.*, Phys. Rev. B **70**, 195104 (2004)
2. P. Seth *et al.*, Phys. Rev. Lett. **119**, 056401 (2017)
3. B. Amadon *et al.*, Phys. Rev. B **89**, 125110 (2014)

2. Wannier functions

Model choice for Ce in ABINIT and single orbital cRPA

```
usepawu 1
lpawu 3
usedmft2 1
dmftbandi2 1
dmftbandf2 20
```

Model choice for Ce in ABINIT with PLO-Wannier [4] and 1 orbital

```
plowan_natom 1
plowan_iatom 1
plowan_bandi 1
plowan_bandf 20
plowan_nbl 1
plowan_lcalc 3
plowan_projcalc 7
plowan_realspace 1
plowan_nt 1
plowan_it 0 0 0
```

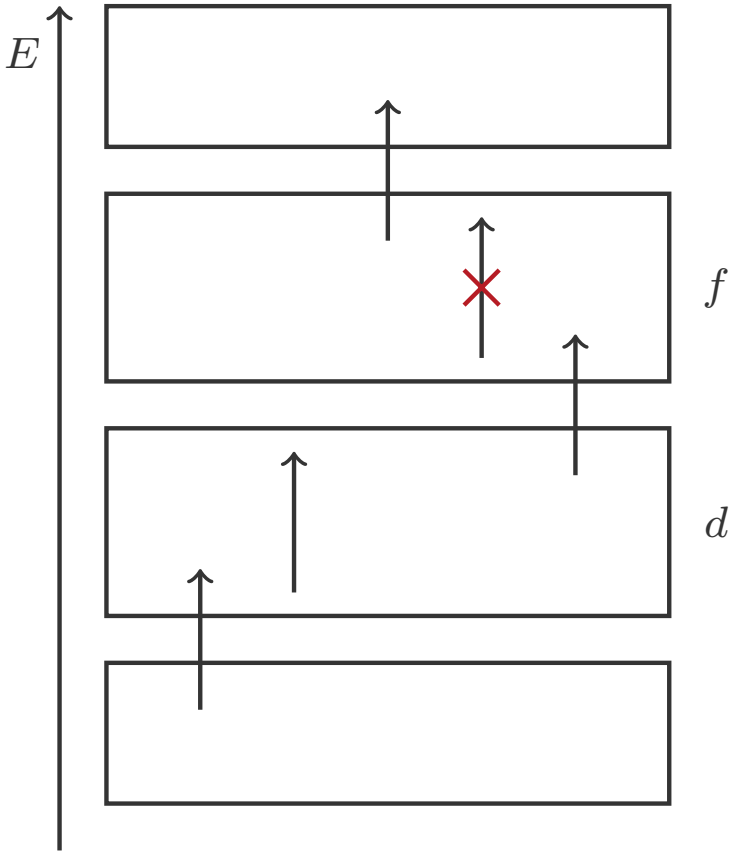
Model choice for Ce in ABINIT using PLO-Wannier and several orbitals cRPA

```
plowan_natom 1
plowan_iatom 1
plowan_bandi 1
plowan_bandf 20
plowan_nbl 2
plowan_lcalc 2 3
plowan_projcalc 5 7
plowan_realspace 1
plowan_nt 1
plowan_it 0 0 0
```

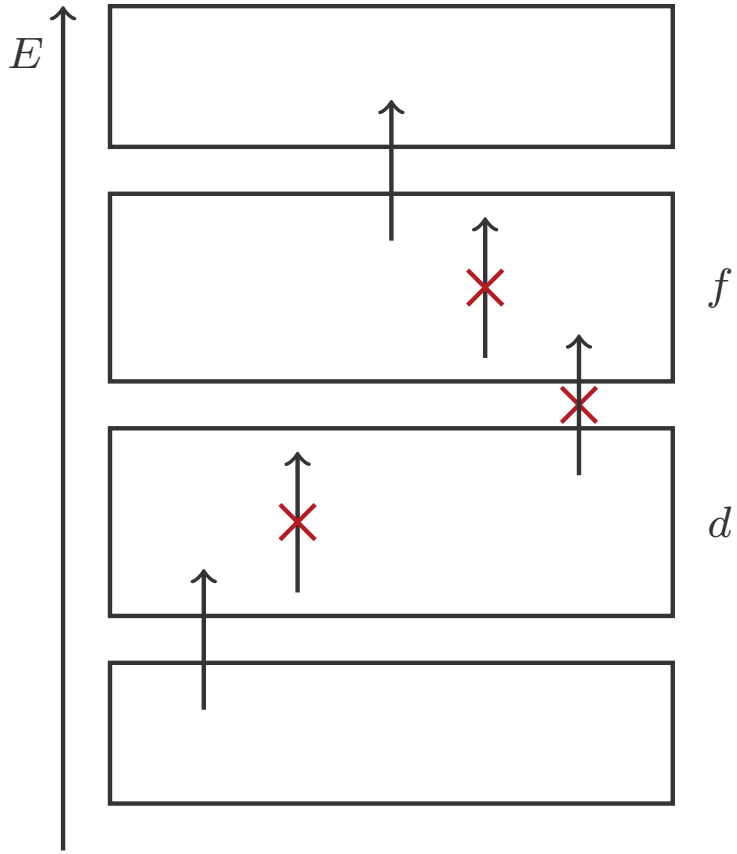
4. PLO-Wannier implementation by A. Gerossier, see B. Amadon *et al.*, Phys. Rev. B **91**, 161103 (2015)

3. Constrained screening

One orbital cRPA



Several orbitals cRPA



Removed transitions in Ce with f orbital VS. f and d orbitals

4. The interaction matrix

Definition of the interaction matrix

One orbital model : $[U]_{m_1,m_2,m_1,m_2} = \langle w_{m_1}^{\mathbf{R}_1 l_1} w_{m_2}^{\mathbf{R}_1 l_1} | W^r(\mathbf{r},\mathbf{r}',\omega) | w_{m_1}^{\mathbf{R}_1 l_1} w_{m_2}^{\mathbf{R}_1 l_1} \rangle$

Several orbital model : $[U]_{m_1,m_2,m_1,m_2} = \langle w_{m_1}^{\mathbf{R}_1 l_1} w_{m_2}^{\mathbf{R}_2 l_2} | W^r(\mathbf{r},\mathbf{r}',\omega) | w_{m_1}^{\mathbf{R}_1 l_1} w_{m_2}^{\mathbf{R}_2 l_2} \rangle$

$$U = \frac{1}{(2l_1+1)(2l_2+1)} \sum_{m_1=-l_1}^{l_1} \sum_{m_2=-l_2}^{l_2} U_{m_1,m_2,m_1,m_2}$$

One orbital cRPA

- $l_1 = l_2 \Rightarrow$ only one U is calculated
- in Ce $\Rightarrow U^{ff}$

Several orbital cRPA

- $l_1 \neq l_2 \Rightarrow$ one U per combination
- in Ce $\Rightarrow U^{ff}, U^{fd}, U^{dd}$

5. Conclusion

Results :

- Implementation has been done
- Results for one orbital calculation are recovered

Short term goal :

- Calculate U between any couple of orbitals in a system [5]
- Test the importance of inter-orbital interaction

In the future

Implementation of DFT+U and DFT+DMFT with several orbitals

5. P. Seth *et al.*, Phys. Rev. Lett. **119**, 056401 (2017)