DE LA RECHERCHE À L'INDUSTRIE

www.cea.fr

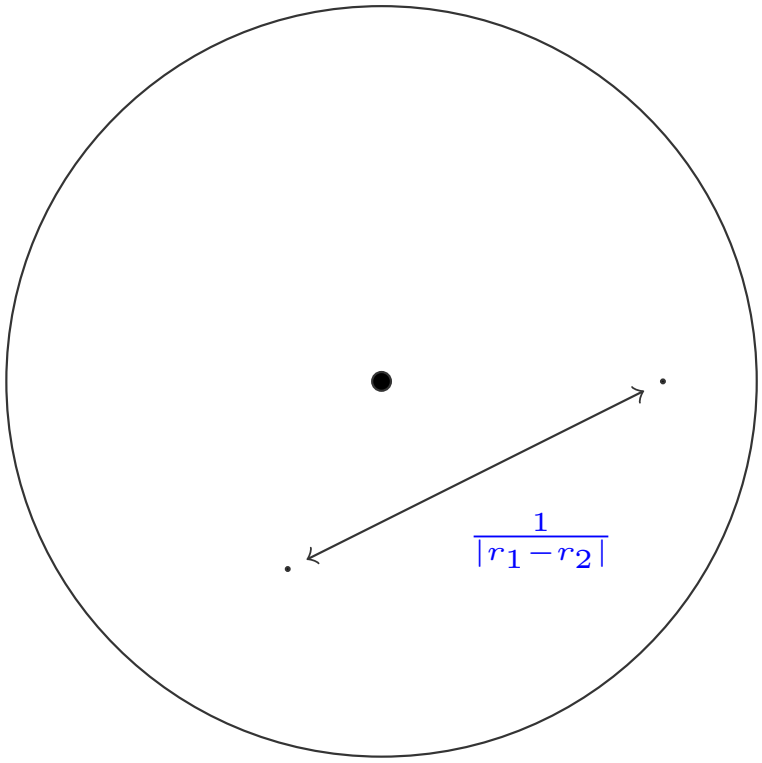
How to compute U in ABINIT with cRPA ?

Bernard Amadon

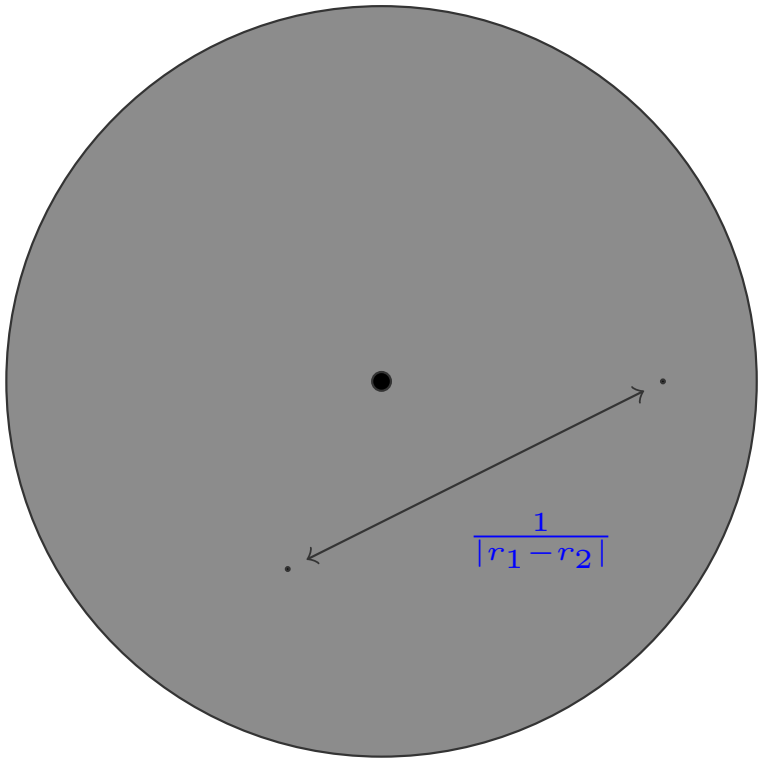
CEA, DAM, DIF, F-91297 Arpajon, France

ABINIT School 2019

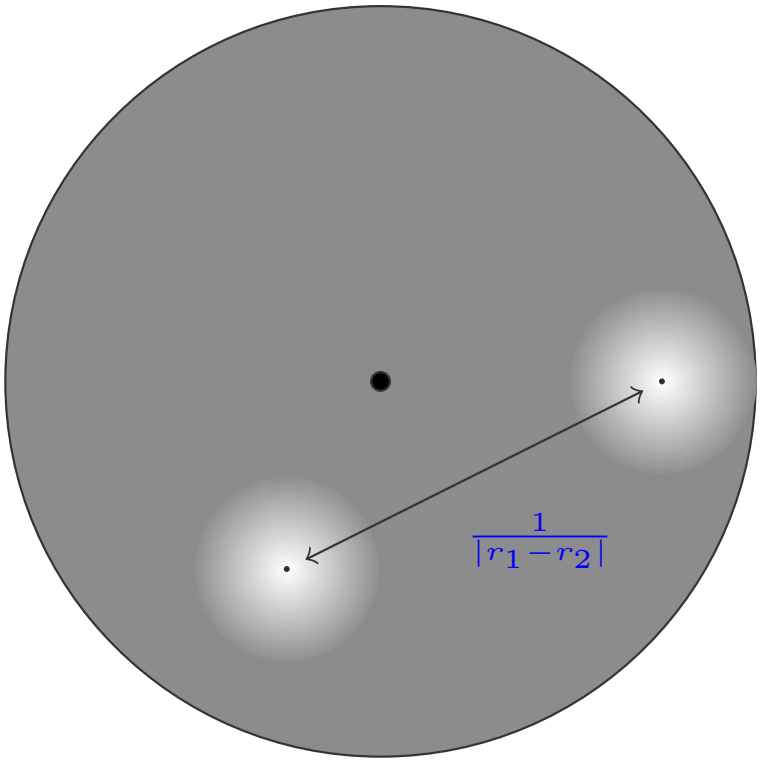
How to compute the effective interaction ?



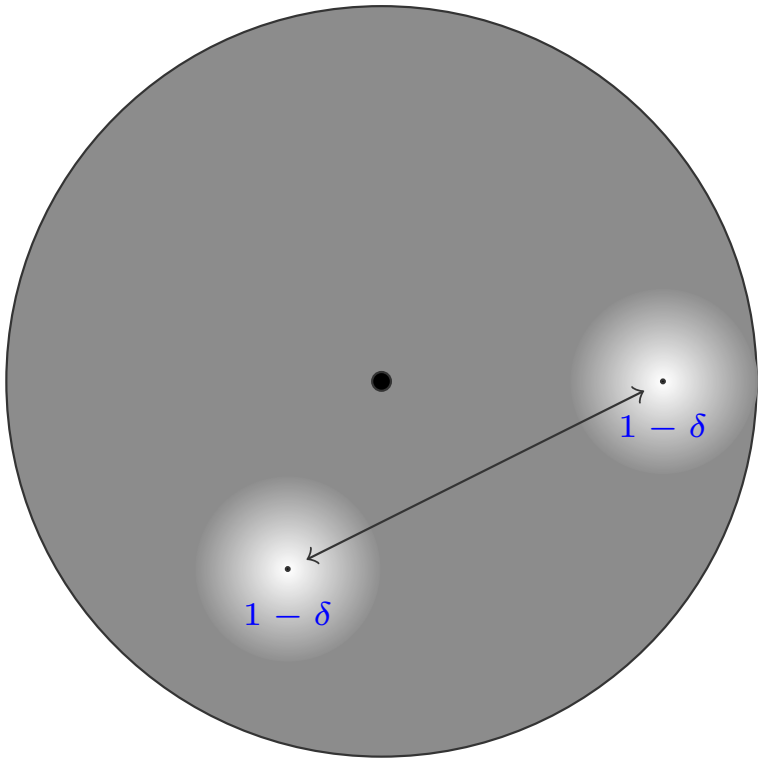
How to compute the effective interaction ?

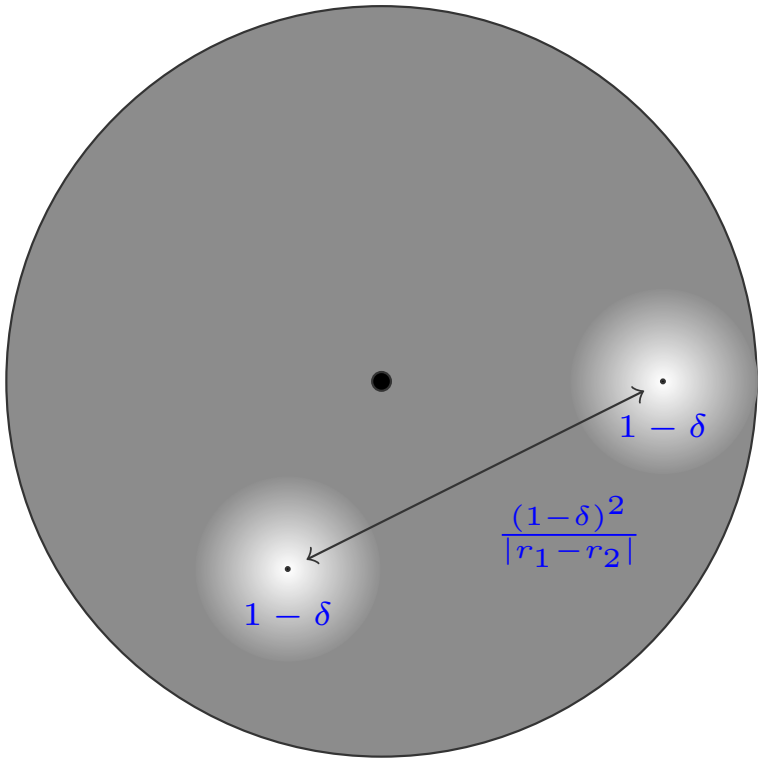


How to compute the effective interaction ?



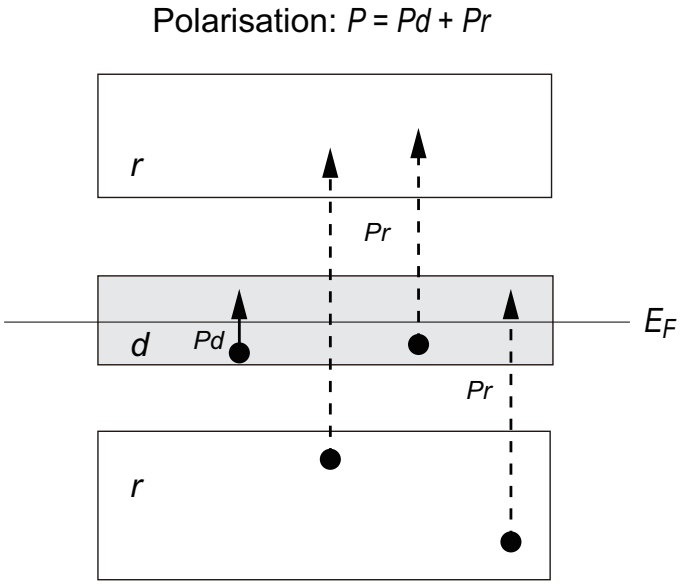
How to compute the effective interaction ?





Screening

The cRPA approach.



- In cRPA, all excitations are taken into account except the one belonging to the correlated subshell.

$$\varepsilon_r(\omega) = 1 - vP_r(\omega).$$

and P_r is the cRPA non interacting polarisability. which describe transitions between occupied and empty states.

Picture from F. Aryasetiawan, The LDA+DMFT approach to strongly correlated materials E. Pavarini, E. Koch, D. Vollhardt, A. Lichtenstein (Eds.), Forschungszentrum Jülich (2011).
F. Aryasetiawan, Imada, Georges, Kotliar, Biermann et Lichtenstein PRB 2004.

The cRPA approach.

We call here χ_0 the non interacting (Kohn-Sham) polarizability of the system. Let's now separate the correlated states (They could be d states but the method is more general and correlated orbitals could gather several orbitals from e.g different atoms) from the rest (r). We thus have:

$$\chi_0 = \chi_0^{\text{correl}} + \chi_0^r$$

thus, we can rewrite the inverse dielectric matrix as:

$$\epsilon^{-1} = \frac{1}{1 - v(\chi_0^{\text{correl}} + \chi_0^r)}$$

We now define the dielectric function due to correlated electrons as

The cRPA approach.

$$\epsilon^{-1}_{\rm correl} \hat{=} \frac{1}{1 - W_r \chi_0^{\rm correl}},$$

the dielectric function of the other electrons as

$$\epsilon^{-1}_{r} \hat{=} \frac{1}{1 - v \chi_0^{r}},$$

and the interaction screened only by the other (r) electrons as:

$$W_r = \frac{v}{1 - v \chi_0^{r}}$$

The cRPA approach.

With these definitions, one shows that

$$\epsilon_{\text{correl}}^{-1}\epsilon_r^{-1} = ... = \frac{1}{1 - v\chi_0^r - v\chi_0^{\text{correl}}} = \frac{1}{1 - v\chi_0} = \epsilon^{-1}$$

Thus, we have

$$W \hat{=} \epsilon^{-1} v = \epsilon_{\text{correl}}^{-1}\epsilon_r^{-1} v$$

We can interpret this result: The fully screened RPA interaction is the combination of two screening processes. First, the bare interaction is screened by non-correlated electrons (r), and it gives rises to a screened interaction W_r. Secondly the screening of this interaction by correlated electrons recovers the fully screened interaction.

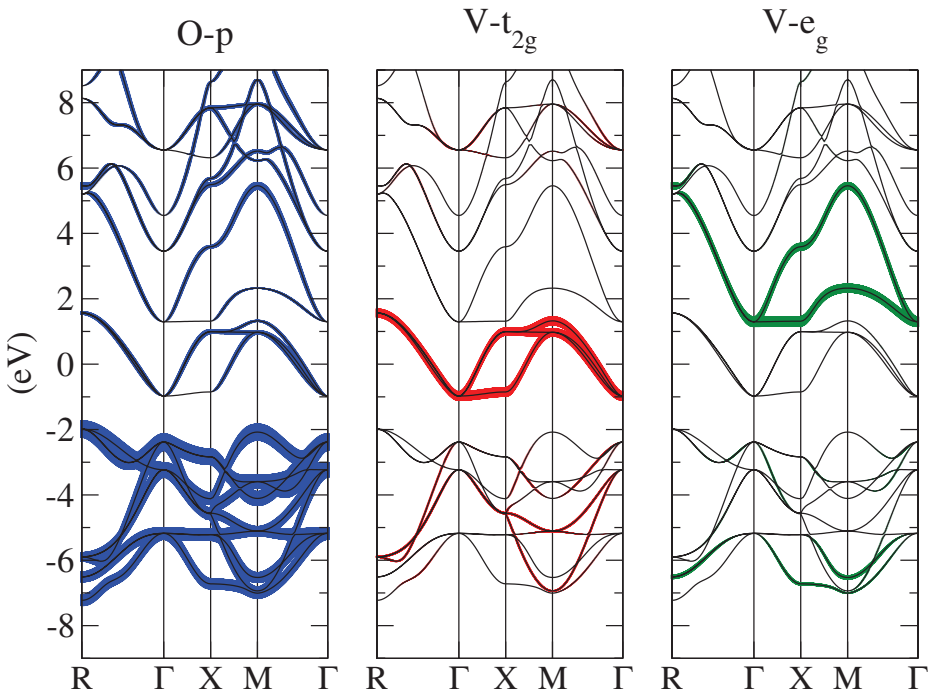
The cRPA approach: key parameters

The definition of correlated orbitals

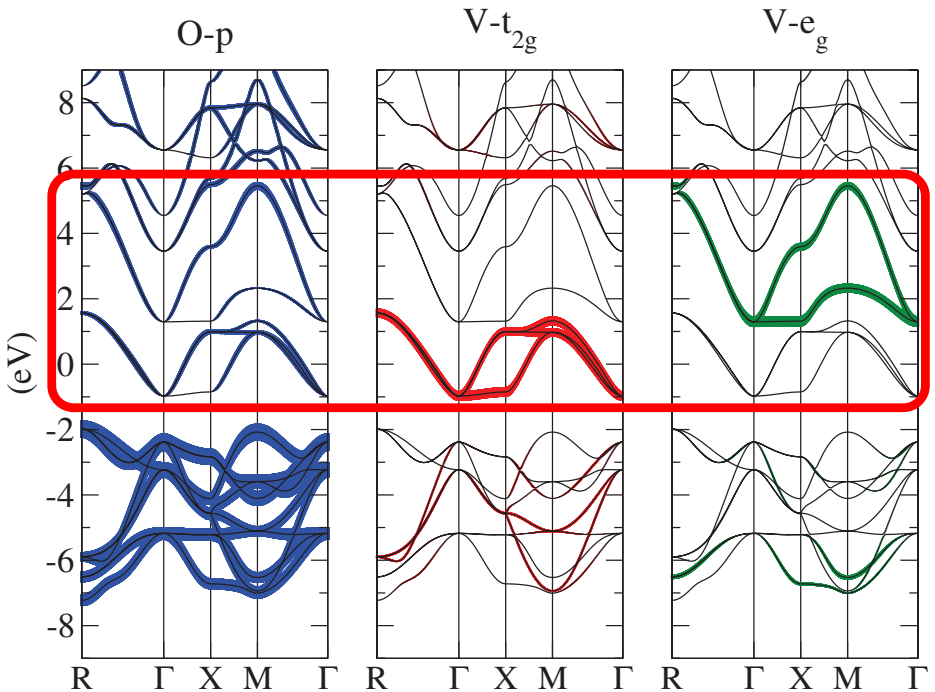
- We use Projected Local Orbitals Wannier functions: effective interaction can thus be used directly in DFT+DMFT calculations.
- Depending on the energy window used in the calculation, several localization of orbitals can be described.

In `ABINIT`, to decide the windows of energy of the Wannier functions, use the keywords `dmftbandi` and `dmftbandf`.

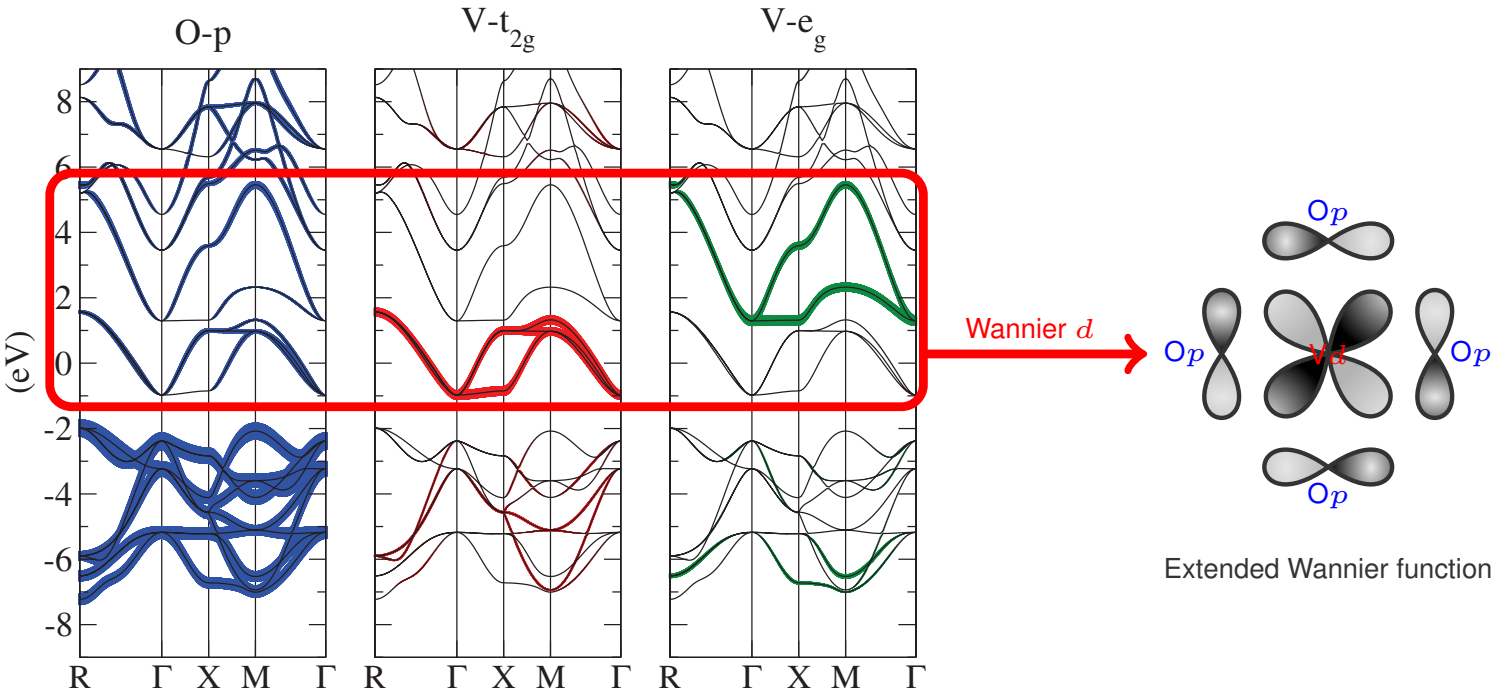
Definition of correlated orbitals: example of $SrVO_3$.



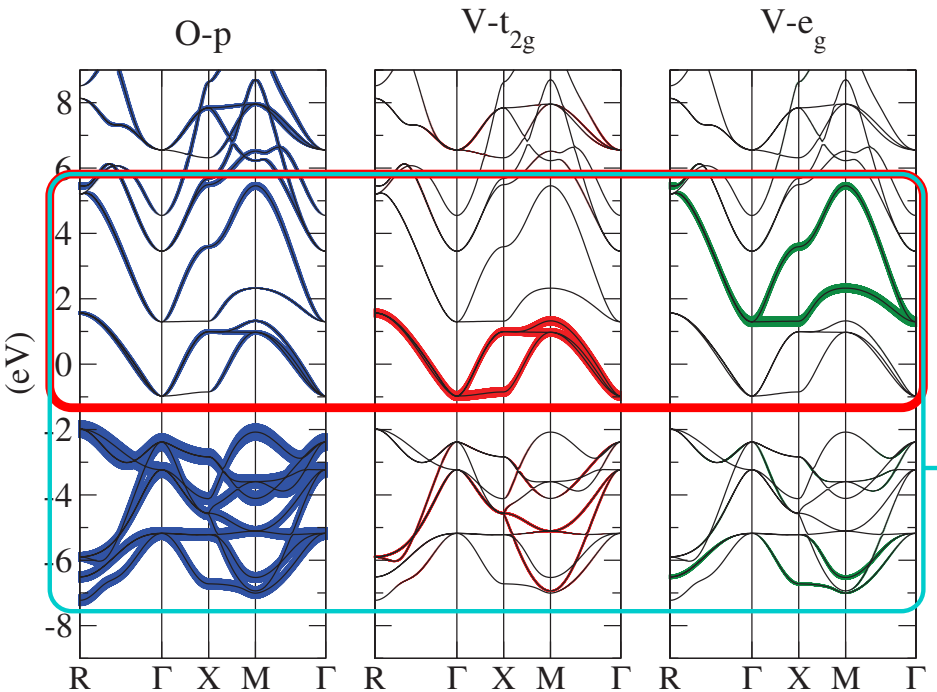
Definition of correlated orbitals: example of $SrVO_3$.



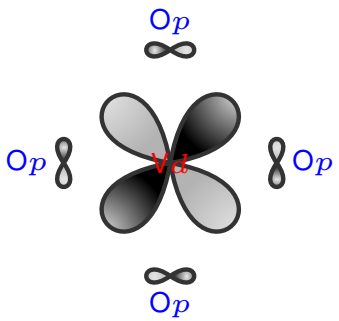
Definition of correlated orbitals: example of $SrVO_3$.



Definition of correlated orbitals: example of $SrVO_3$.

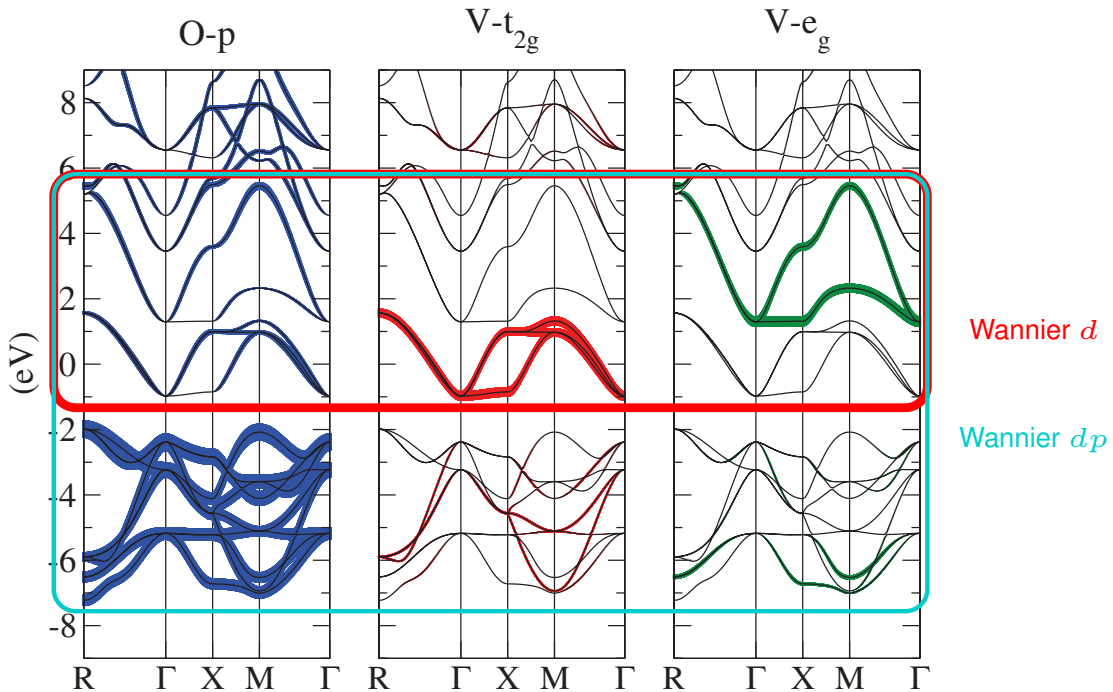


Wannier dp



Localized Wannier function

Definition of correlated orbitals: example of $SrVO_3$.



Bare interaction can be computed as:

$$v = \langle \chi\chi | \frac{1}{r_1 - r_2} | \chi\chi \rangle$$

Wannier function	bare interaction v (eV)
Wannier d	15.3
Wannier dp	19.4

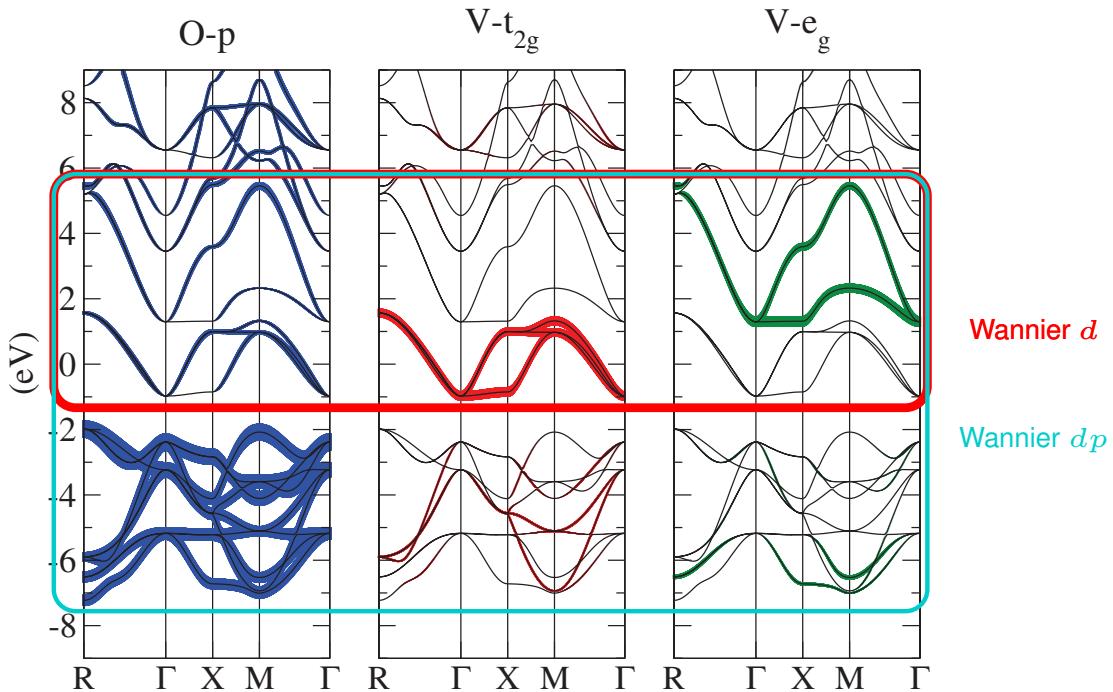
The cRPA approach: key parameters

The definition of screening.

- The core of the cRPA is to suppress the screening corresponding to transitions inside correlated orbitals.

In `ABINIT`, to decide the windows of energy for which the screening is suppressed, use the keywords `ucrpa_bands`.

Definition of correlated orbitals: example of $SrVO_3$.

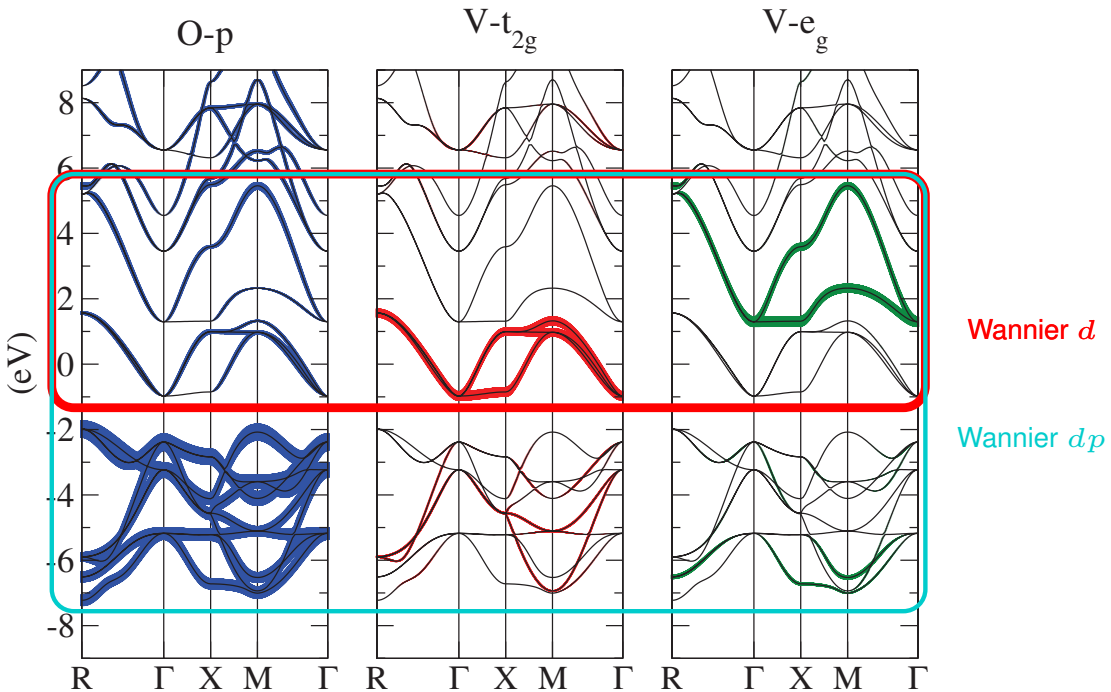


Effective interaction can be computed as:

$$U = \langle \chi\chi | \epsilon^{-1}_{\mathrm{cRPA}} v | \chi\chi \rangle$$

Wannier function	bare interaction v (eV)	effective interaction U (eV)	Name of the model
Wannier d	15.3	2.8	$d-d$
Wannier dp	19.4	10.8	$dp-dp$

Definition of correlated orbitals: example of $SrVO_3$.



Effective interaction can be computed as:

$$U = \langle \chi\chi | \epsilon^{-1}_{\mathrm{cRPA}} v | \chi\chi \rangle$$

Wannier function	bare interaction v (eV)	effective interaction U (eV)	Name of the model
Wannier d	15.3	2.8	$d-d$
Wannier dp	19.4	10.8	$dp-dp$
Wannier dp	19.4	3.4	$d-dp$

Some conventions

$$U_{\rm diag} = \frac{1}{2l+1} \sum_i \langle \chi_i \chi_i | W_r | \chi_i \chi_i \rangle$$

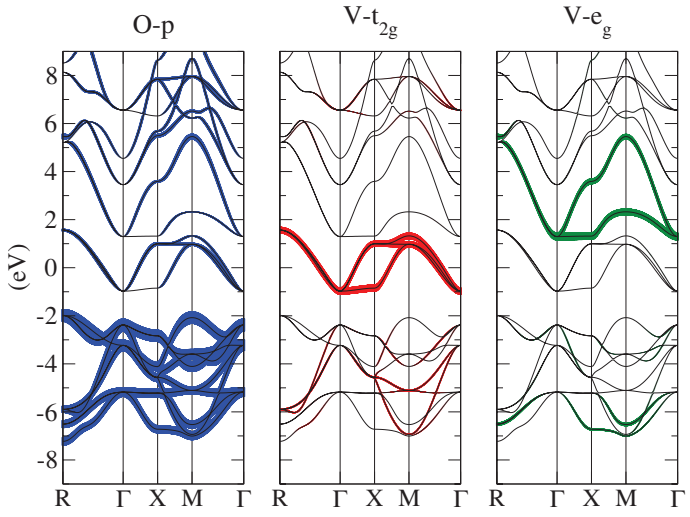
$$U = \frac{1}{(2l+1)^2} \sum_{i,j} \langle \chi_i \chi_j | W_r | \chi_i \chi_j \rangle$$

One has

$$U_{\rm diag} > U$$

In ABINIT, one always uses U as input, whereas in some models, U is defined as $U_{\rm diag}$!

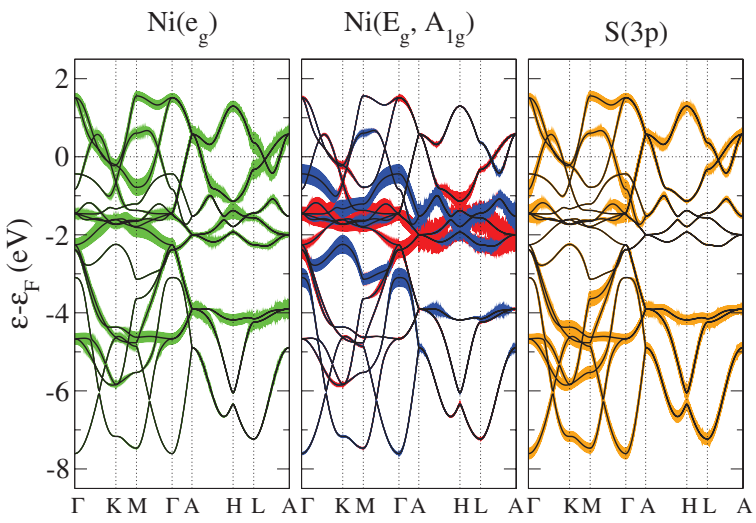
$SrVO_3$



Non entangled bands

From B. Amadon, F. Lechermann et al PRB 2008

NiS



Entangled bands

For non entangled bands (ucrpa=1)

$$\chi_0^{\rm full}(\mathbf{G},\mathbf{G'},\mathbf{q}) = \sum_{\mathbf{k},n,n'} \langle\psi_{n\mathbf{k}}|e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\psi_{n'\mathbf{k}+\mathbf{q}}\rangle \langle\psi_{n'\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G'})\mathbf{r}}|\psi_{n\mathbf{k}}\rangle \frac{f_{n'\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\epsilon_{n'\mathbf{k}+\mathbf{q}}-\epsilon_{n\mathbf{k}}+\omega+i\delta}$$

$$\chi_0^{\rm f}(\mathbf{G},\mathbf{G'},\mathbf{q}) = \sum_{\mathbf{k},n=f,n'=f} \langle\psi_{n\mathbf{k}}|e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\psi_{n'\mathbf{k}+\mathbf{q}}\rangle \langle\psi_{n'\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G'})\mathbf{r}}|\psi_{n\mathbf{k}}\rangle \frac{f_{n'\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\epsilon_{n'\mathbf{k}+\mathbf{q}}-\epsilon_{n\mathbf{k}}+\omega+i\delta}$$

In $\chi_0^{\rm f}(\mathbf{G},\mathbf{G'},\mathbf{q})$ the bands $(n\mathbf{k})$ and $(n'\mathbf{k})$ are f bands, and the transition should be suppressed. Thus

$$\chi_0^{\rm cRPA}(\mathbf{G},\mathbf{G'},\mathbf{q}) = \chi_0^{\rm full}(\mathbf{G},\mathbf{G'},\mathbf{q}) - \chi_0^{\rm f}(\mathbf{G},\mathbf{G'},\mathbf{q})$$

For entangled bands (ucrpa=2)

$$\chi_0^{\rm full}(\mathbf{G},\mathbf{G'},\mathbf{q}) = \sum_{\mathbf{k},n,n'} \langle\psi_{n\mathbf{k}}|e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\psi_{n'\mathbf{k}+\mathbf{q}}\rangle \langle\psi_{n'\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G'})\mathbf{r}}|\psi_{n\mathbf{k}}\rangle \frac{f_{n'\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\epsilon_{n'\mathbf{k}+\mathbf{q}}-\epsilon_{n\mathbf{k}}+\omega+i\delta}$$

$$\chi_0^{\rm f}(\mathbf{G},\mathbf{G'},\mathbf{q}) = \sum_{\mathbf{k},n,n'} \sum_{m_1}|C_{n\mathbf{k}}^{m_1}|^2 \sum_{m_2}|C_{n'\mathbf{k}+\mathbf{q}}^{m_2}|^2 \langle\psi_{n\mathbf{k}}|e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\psi_{n'\mathbf{k}+\mathbf{q}}\rangle \langle\psi_{n'\mathbf{k}+\mathbf{q}}|e^{i(\mathbf{q}+\mathbf{G'})\mathbf{r}}|\psi_{n\mathbf{k}}\rangle \frac{f_{n'\mathbf{k}+\mathbf{q}}-f_{n\mathbf{k}}}{\epsilon_{n'\mathbf{k}+\mathbf{q}}-\epsilon_{n\mathbf{k}}+\omega+i\delta}$$

with $C_{n\mathbf{k}}^{m_1} = \langle\phi_{m_1}|\psi_{n\mathbf{k}}\rangle$. If $\sum_{m_1}|C_{n\mathbf{k}}^{m_1}|^2 = 1$ and $\sum_{m_1}|C_{n'\mathbf{k}}^{m_1}|^2 = 1$: the bands $(n\mathbf{k})$ and $(n'\mathbf{k})$ are f bands, and the transition will be suppressed in $\chi_0^{\rm cRPA}(\mathbf{G},\mathbf{G'},\mathbf{q})$:

$$\chi_0^{\rm cRPA}(\mathbf{G},\mathbf{G'},\mathbf{q}) = \chi_0^{\rm full}(\mathbf{G},\mathbf{G'},\mathbf{q}) - \chi_0^{\rm f}(\mathbf{G},\mathbf{G'},\mathbf{q})$$

Conclusion

- cRPA is a coherent way of computing effective interactions for DMFT
- The same correlated orbitals can be used.
- Care must be taken to estimate the relevant Wannier orbitals and screening.

Implementation in ABINIT is discussed in B. Amadon,T. Applencourt, and F. Bruneval PRB 2014.