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Dynamical Mean Field Theory using Projected Local Orbital Wannier functions

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References about Wannier functions in DMFT and ABINIT

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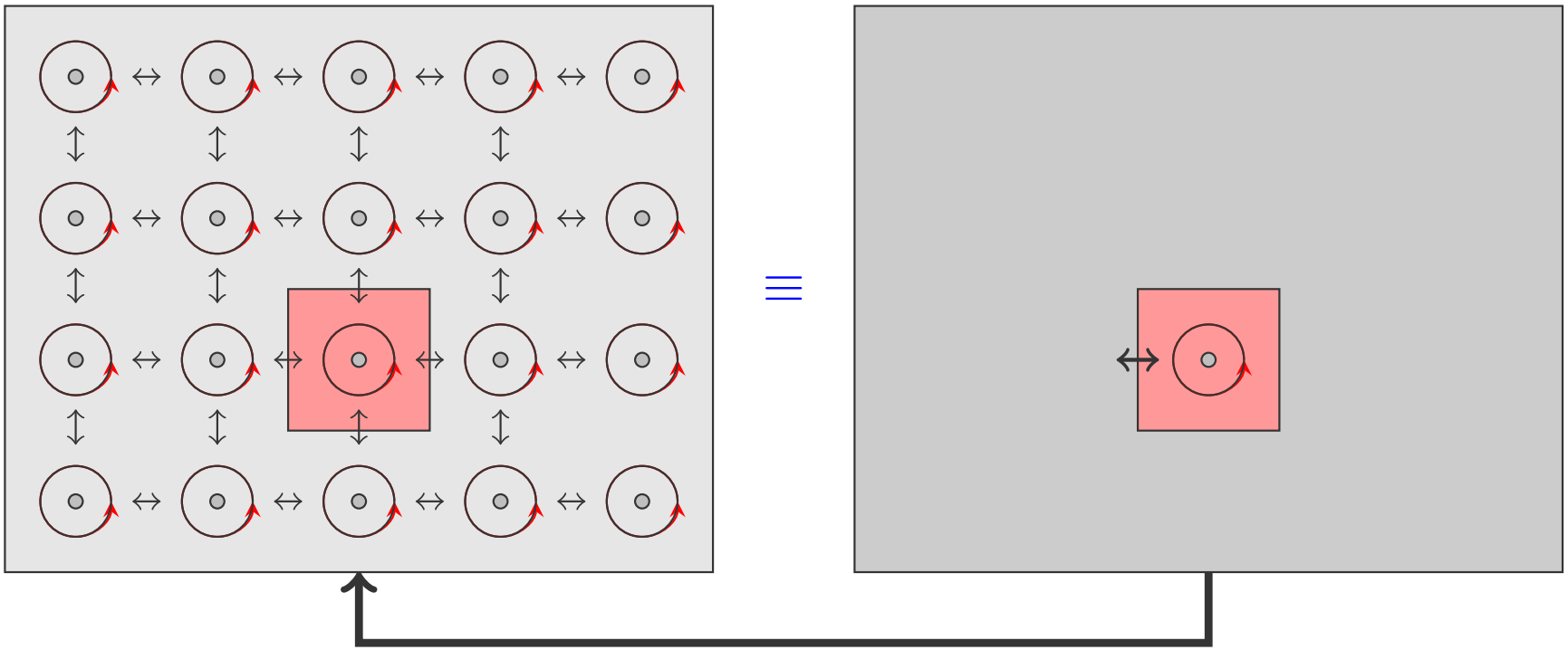
The DMFT Loop



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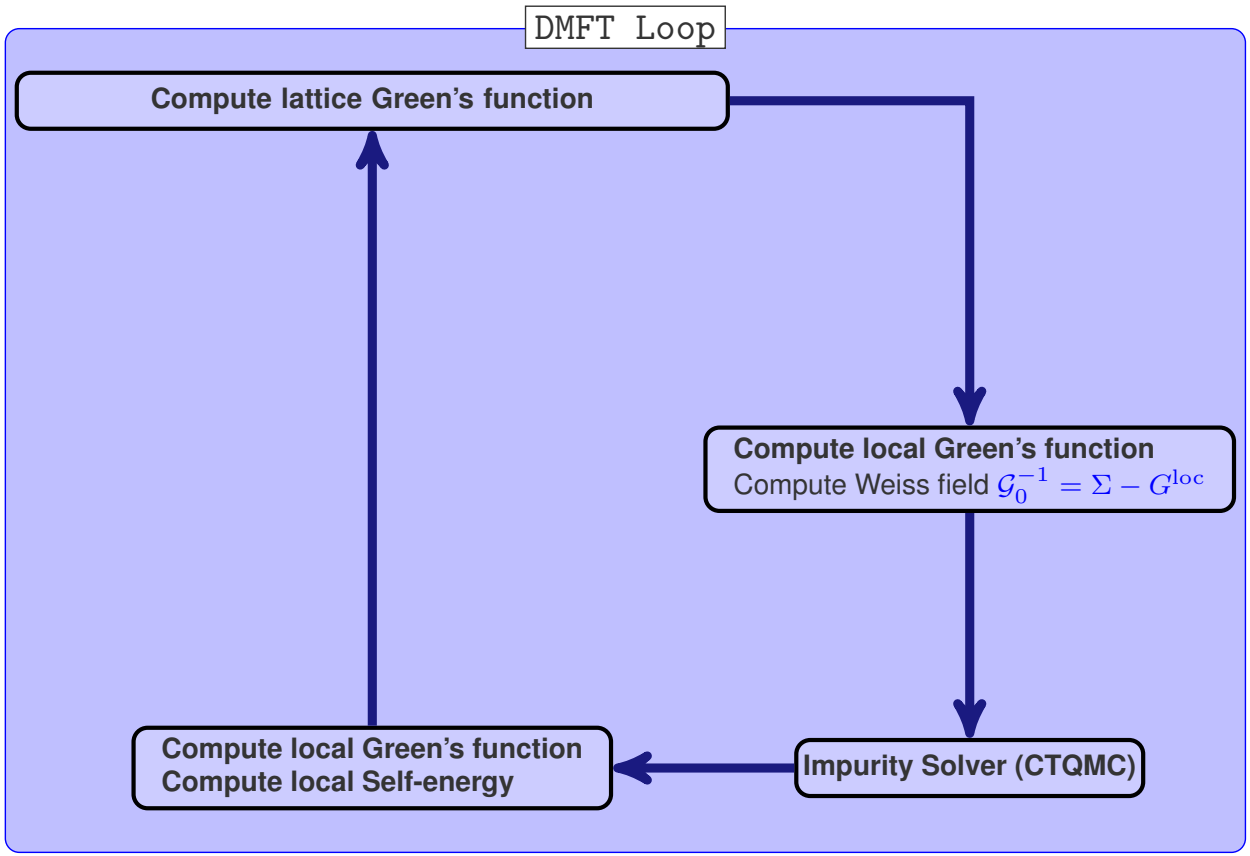

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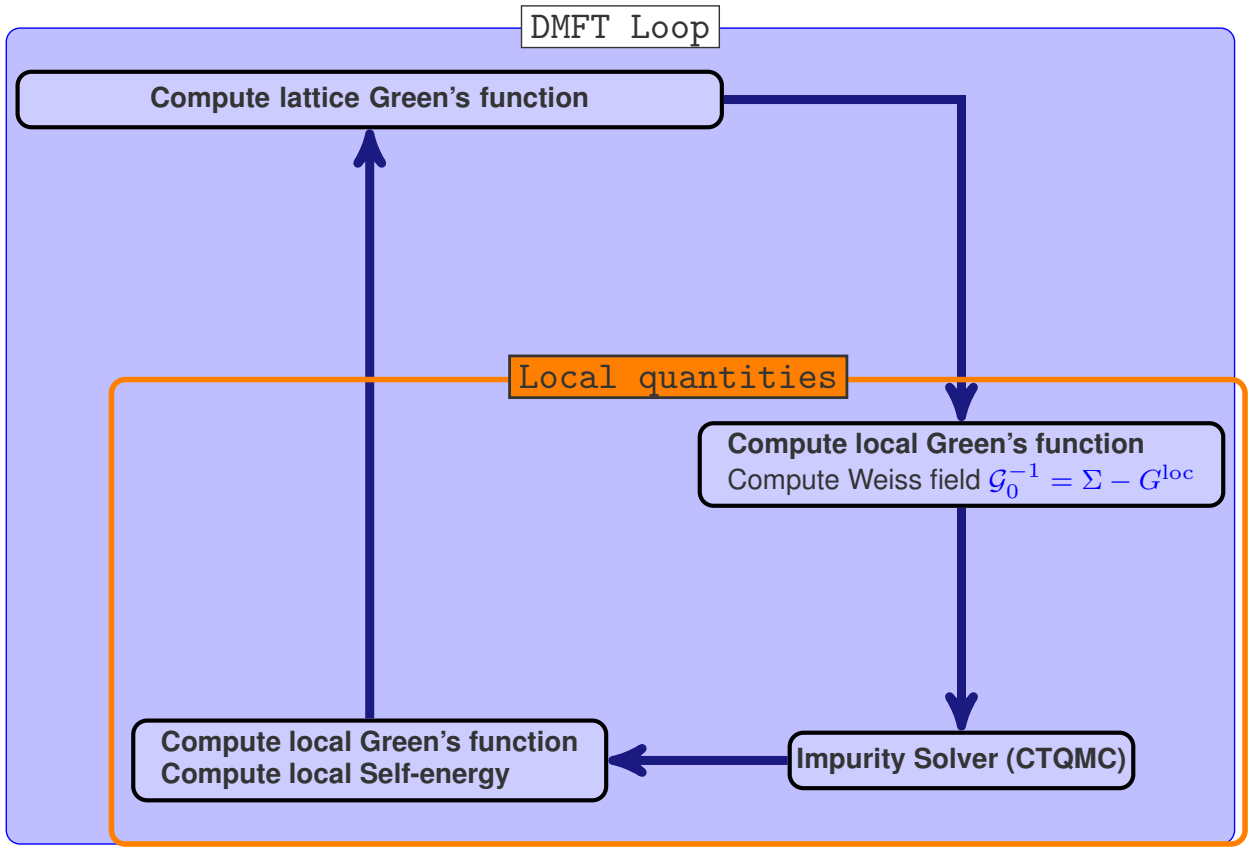


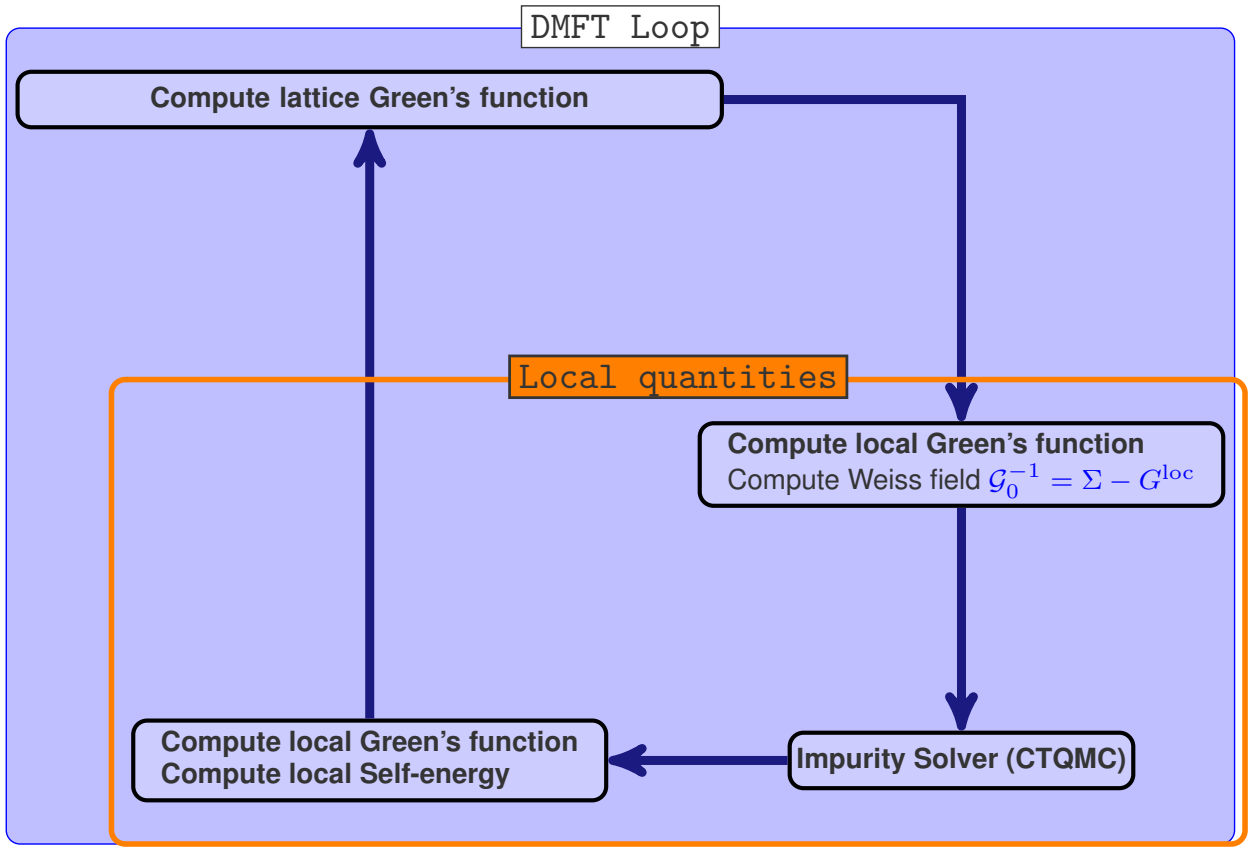
Reminder about Hubbard model

- Local quantities are expressed in a basis of correlated orbitals.

$$\widehat{\Sigma}(i\omega_n) = \sum_{\mathbf{T}} |\chi_{\mathbf{T}}\rangle \Sigma(i\omega_n) \langle \chi_{\mathbf{T}}|$$

where $\chi_{\mathbf{T}}$ is the unique orbital on the atom at $\mathbf{T}$ and $\mathbf{T}$ are the lattice vectors.

The DMFT Loop



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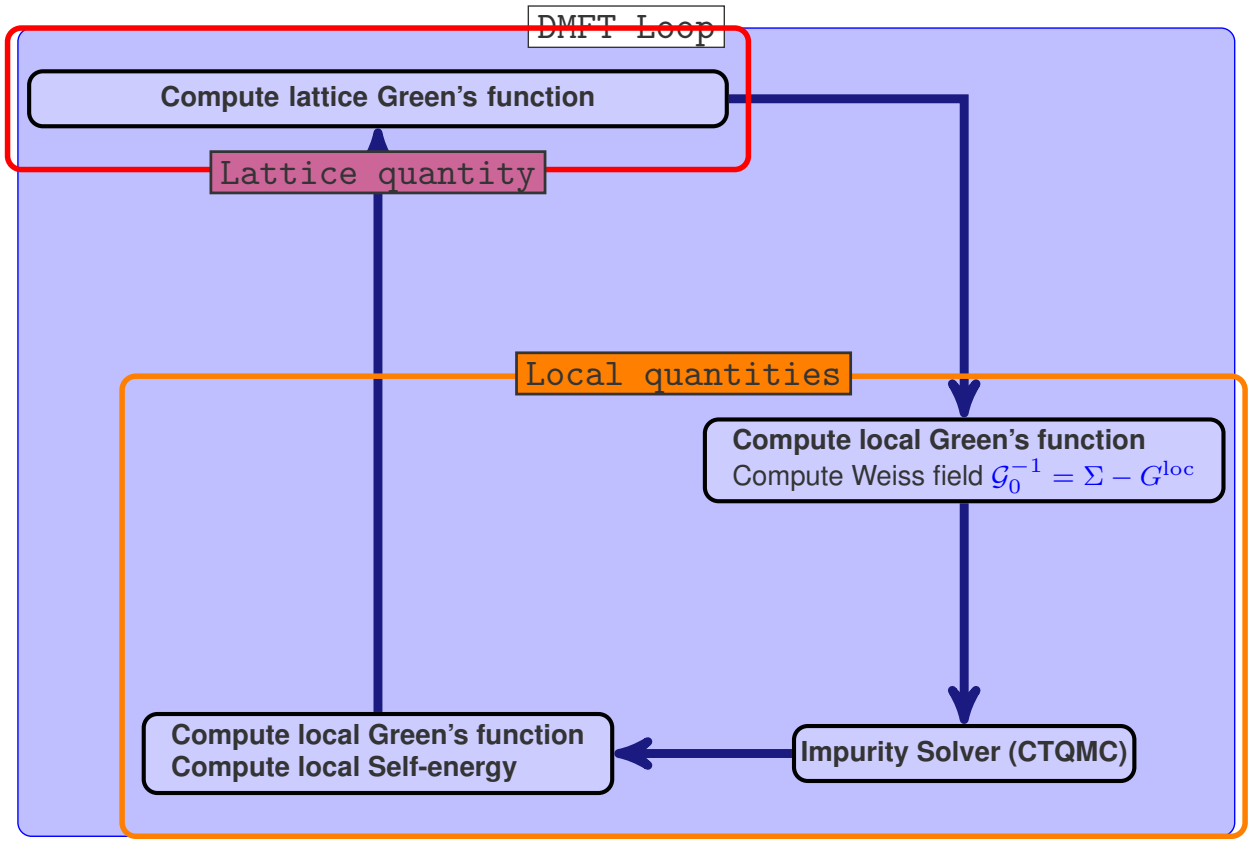


Reminder about Hubbard model

- Lattice Green's functions are expressed in Bloch eigenvectors of the non interacting Hamiltonian ($\epsilon_{\mathbf{k}} = \frac{1}{N}\sum_{ij} t_{ij} \mathrm{e}^{-i\mathbf{k}(\mathbf{T}_i - \mathbf{T}_j)}$)

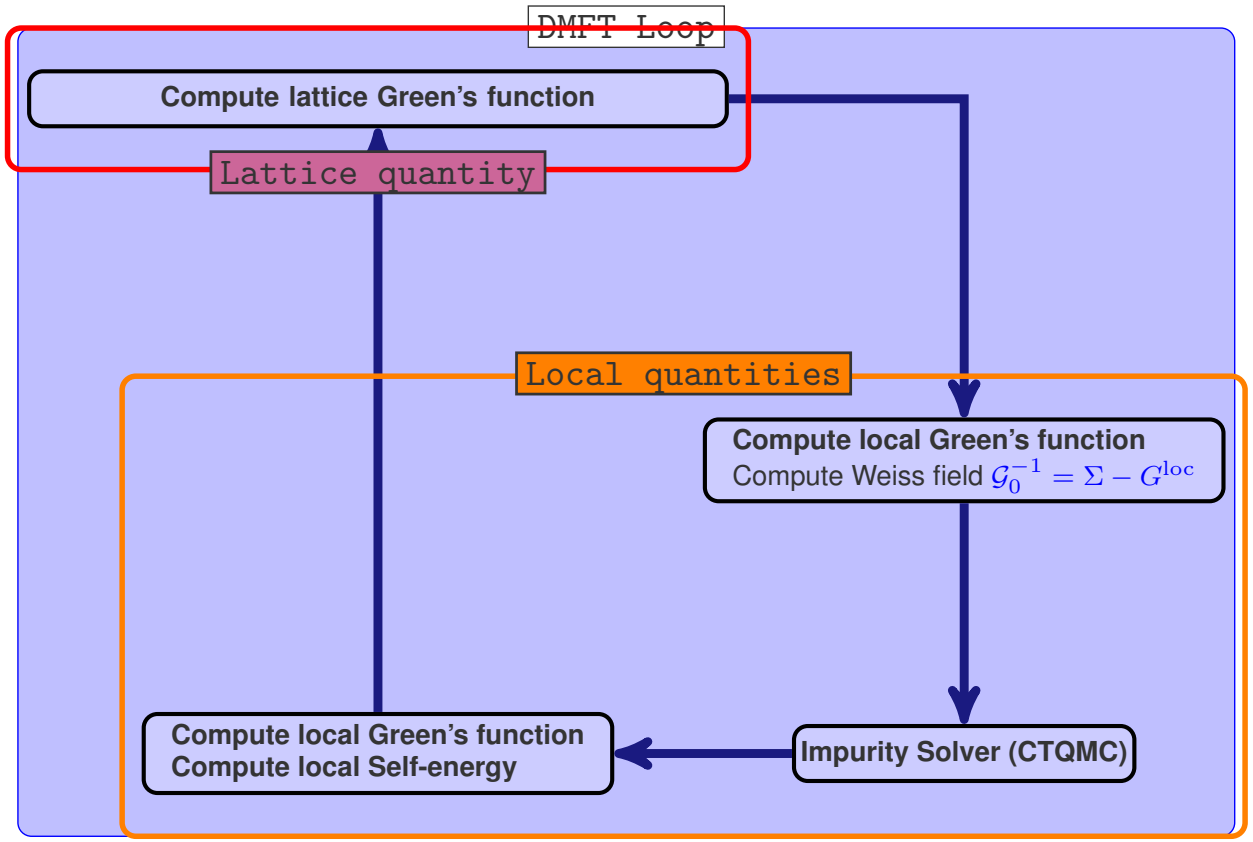
$$\widehat{H}_0 = |\chi_{\mathbf{k}}\rangle \epsilon_{\mathbf{k}} \langle \chi_{\mathbf{k}}|$$

with

$$|\chi_{\mathbf{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{T}} |\chi_{\mathbf{T}}\rangle \mathrm{e}^{i\mathbf{k}\mathbf{T}}$$

where $\mathbf{T}$ are lattice vectors.

The DMFT Loop



Reminder about Hubbard model: from local to lattice

- Transforming $\widehat{\Sigma}$ in the Bloch basis:

$$\Sigma_{\mathbf{k}}(i\omega_n) = \langle \chi_{\mathbf{k}} | \widehat{\Sigma}(i\omega_n) | \chi_{\mathbf{k}} \rangle = \langle \chi_{\mathbf{k}} \left[\sum_{\mathbf{T}} |\chi_{\mathbf{T}}\rangle \Sigma(i\omega_n) \langle \chi_{\mathbf{T}}| \right] \chi_{\mathbf{k}} \rangle = ... = \Sigma(i\omega_n),$$

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one can compute the lattice Green's function as:

$$G^{-1}_{\mathbf{k}}(i\omega_n) = G^{-1}_{\mathbf{k}\mathrm{U}=0}(i\omega_n) - \Sigma_{\mathbf{k}}(i\omega_n) = (i\omega_n - \epsilon_{\mathbf{k}}) - \Sigma(i\omega_n)$$

$$\Rightarrow \quad G_{\mathbf{k}}(i\omega_n) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)} \qquad \text{(cf lecture of David Sénéchal)}$$

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$$\widehat{G}(i\omega_n) = \sum_{\mathbf{k}} |\chi_{\mathbf{k}}\rangle G_{\mathbf{k}}(i\omega_n) \langle \chi_{\mathbf{k}}|,$$

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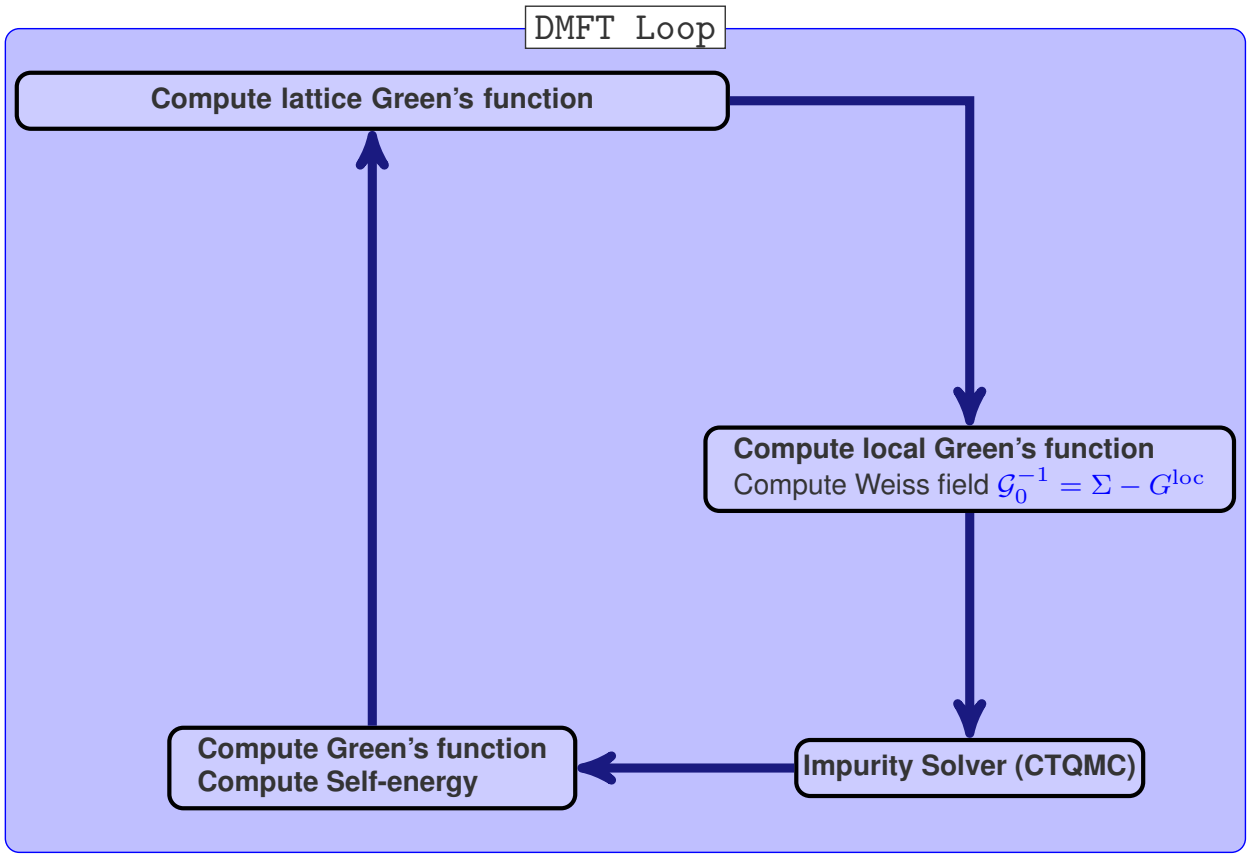
- Using the operator expression of the lattice Green's function

$$\widehat{G}(i\omega_n) = \sum_{\mathbf{k}} |\chi_{\mathbf{k}}\rangle G_{\mathbf{k}}(i\omega_n) \langle \chi_{\mathbf{k}}|,$$

  one can write the local Green's function as:

$$G(i\omega_n) = \sum_{\mathbf{k}} \langle \chi_{\mathbf{T}} | \chi_{\mathbf{k}} \rangle G_{\mathbf{k}}(i\omega_n) \langle \chi_{\mathbf{k}} | \chi_{\mathbf{T}} \rangle = \sum_{\mathbf{k}} G_{\mathbf{k}}(i\omega_n)$$

The DMFT Loop



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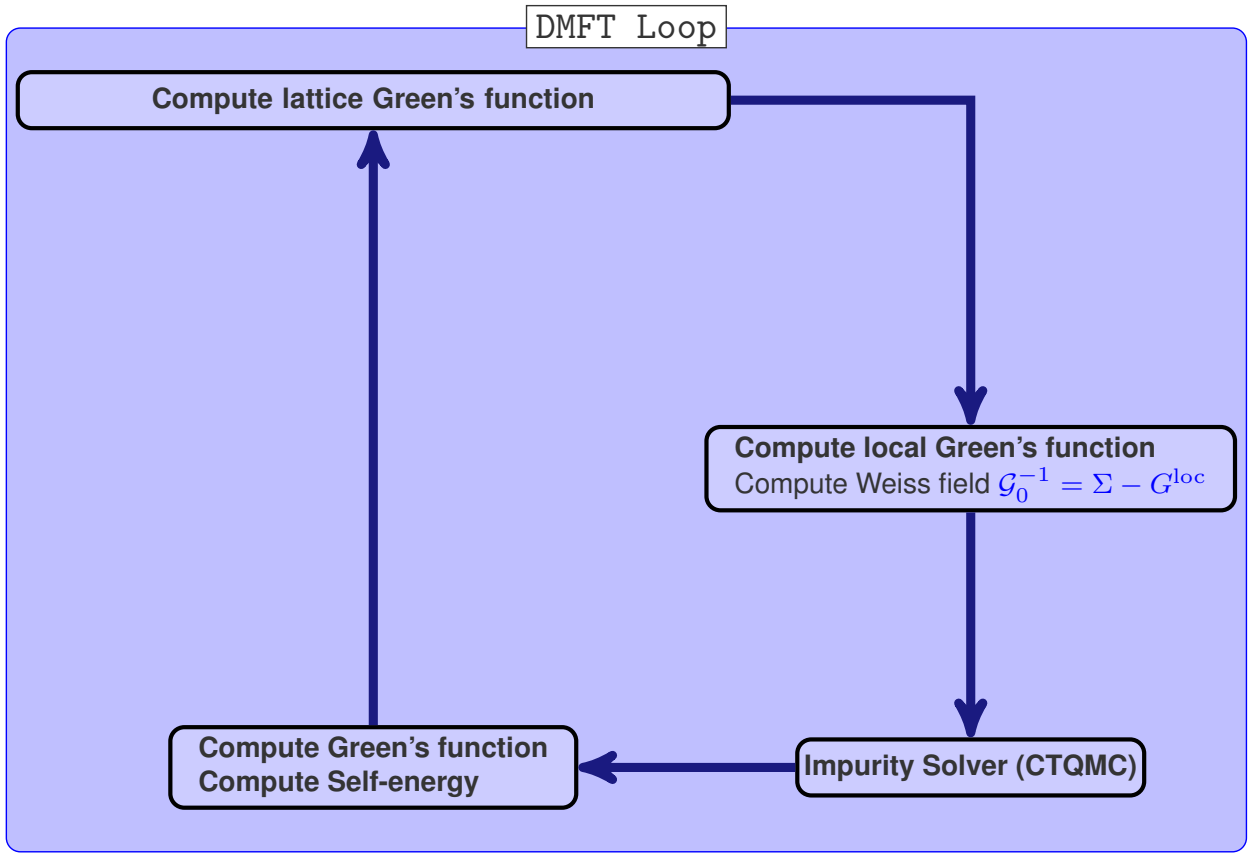
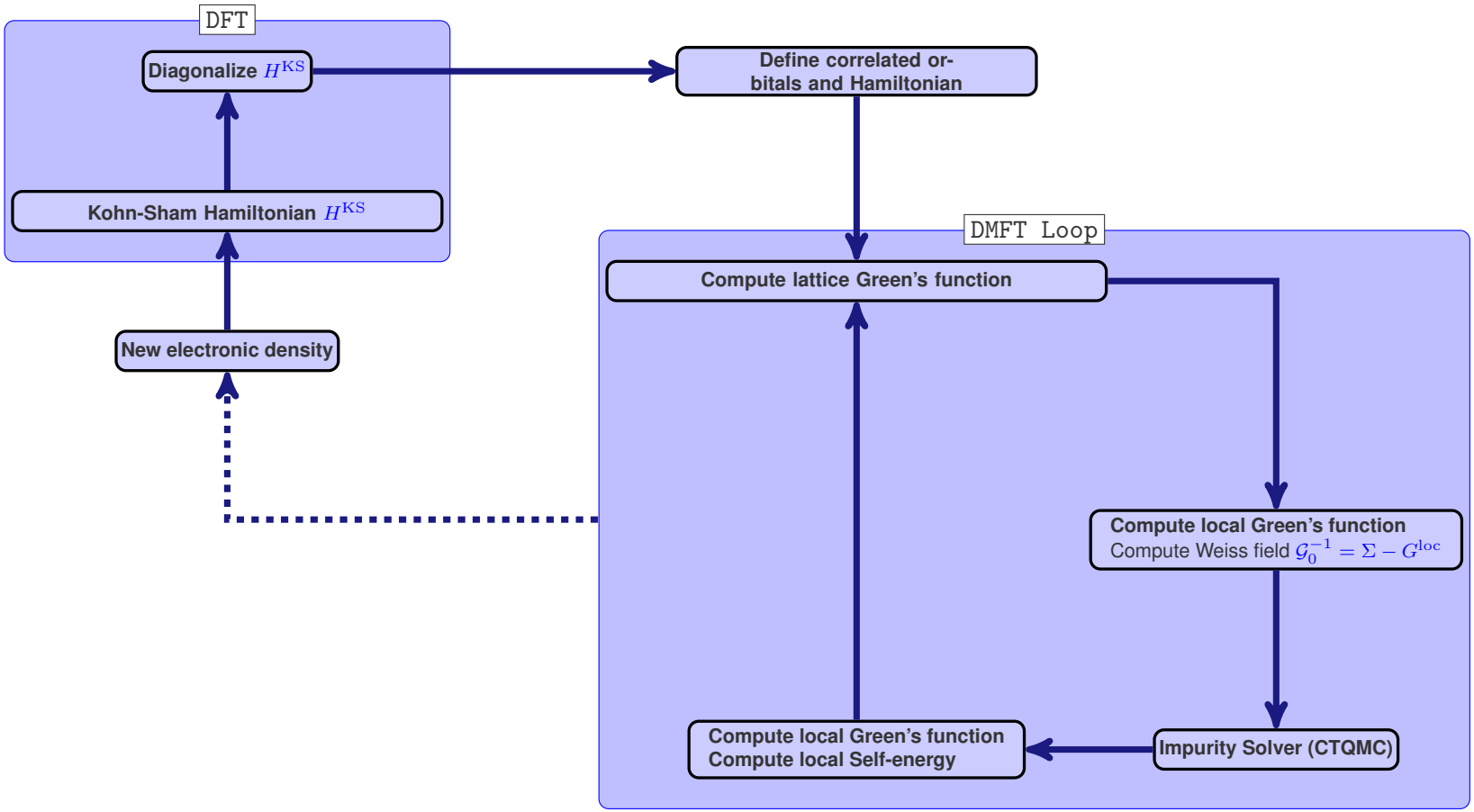


How to apply such idea for a real solid, with both **strongly interacting orbitals**, and **weakly interacting orbitals**

DFT+DMFT scheme



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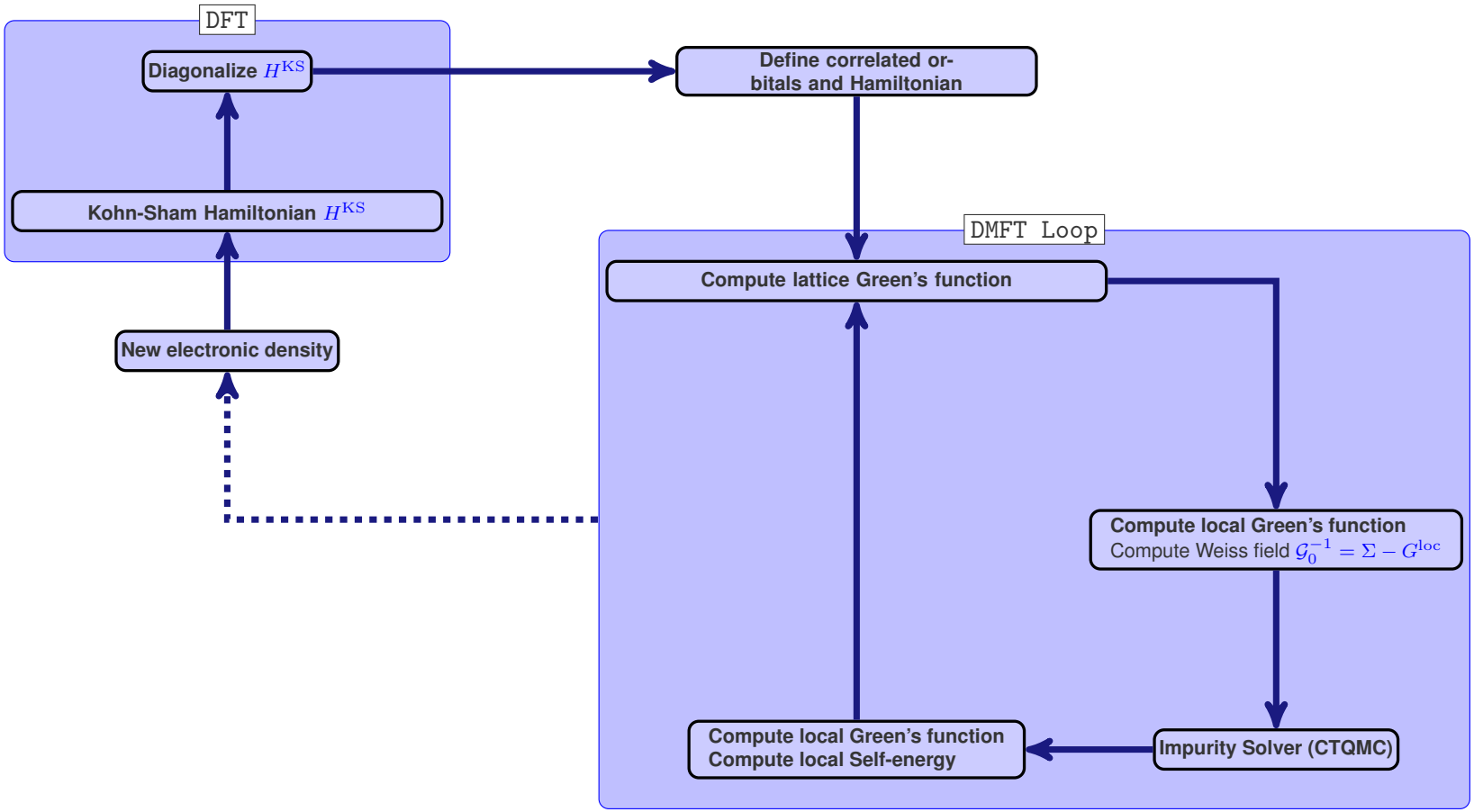
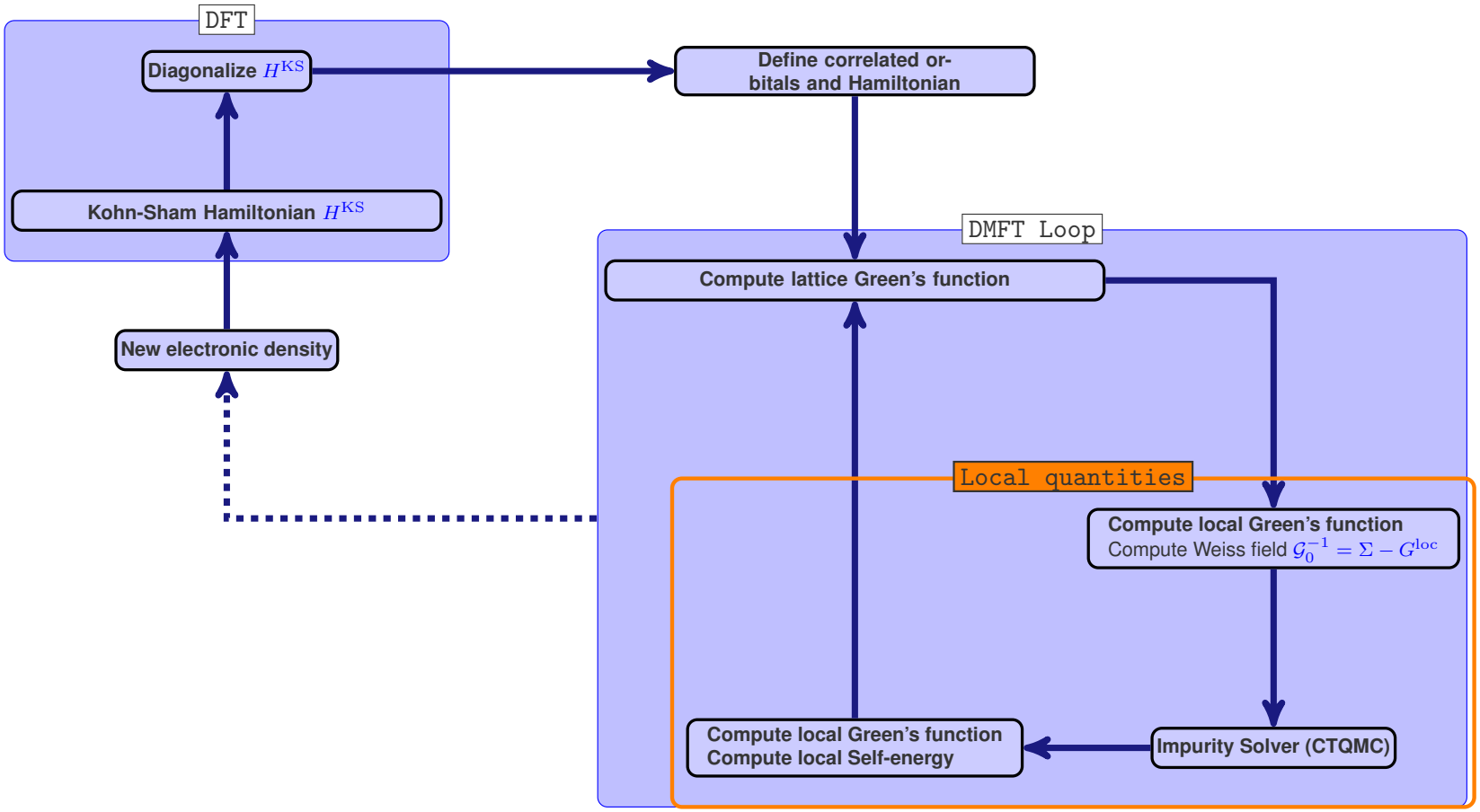


More generally, DFT+DMFT can be expressed as functional of the local Green's function and the electronic density $\Rightarrow$ Internal and free energies can be computed.

DFT+DMFT scheme



Correlated orbitals: what are they

For d orbitals (l=2), $m \in \{-2, -1, 0, 1, 2\}$, a correlated atomic orbital writes:

$$\chi_m(\mathbf{r}) = \langle \mathbf{r} | \chi_m \rangle = R(r) Y_m(\theta, \phi)$$

- The angular part $Y_m(\theta, \phi)$ is well defined.
- The radial part $R(r)$ is not defined in a solid.

In a first step, let's assume that we have found a good choice for $R(r)$ and thus $|\chi_m\rangle$ is defined.

In a real system in DFT+DMFT

- Local Quantity are expressed in a basis of correlated orbitals.

$$\widehat{\Sigma}(i\omega_n) = \sum_{m,m',\mathbf{T}} |\chi_{\mathbf{T}m}\rangle \Sigma_{m,m'}(i\omega_n) \langle \chi_{\mathbf{T}m'}|$$

where $m, m' \in -l, ..., l$ and $\chi_{\mathbf{T}m}$ is an orbital whose angular part is Y_{lm}. Note that $\Sigma_{m,m'}$ can be a matrix and have non diagonal elements.

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[for Hubbard model

$$\widehat{\Sigma}(i\omega_n) = \sum_{\mathbf{T}} |\chi_{\mathbf{T}}\rangle \Sigma(i\omega_n) \langle \chi_{\mathbf{T}}|$$

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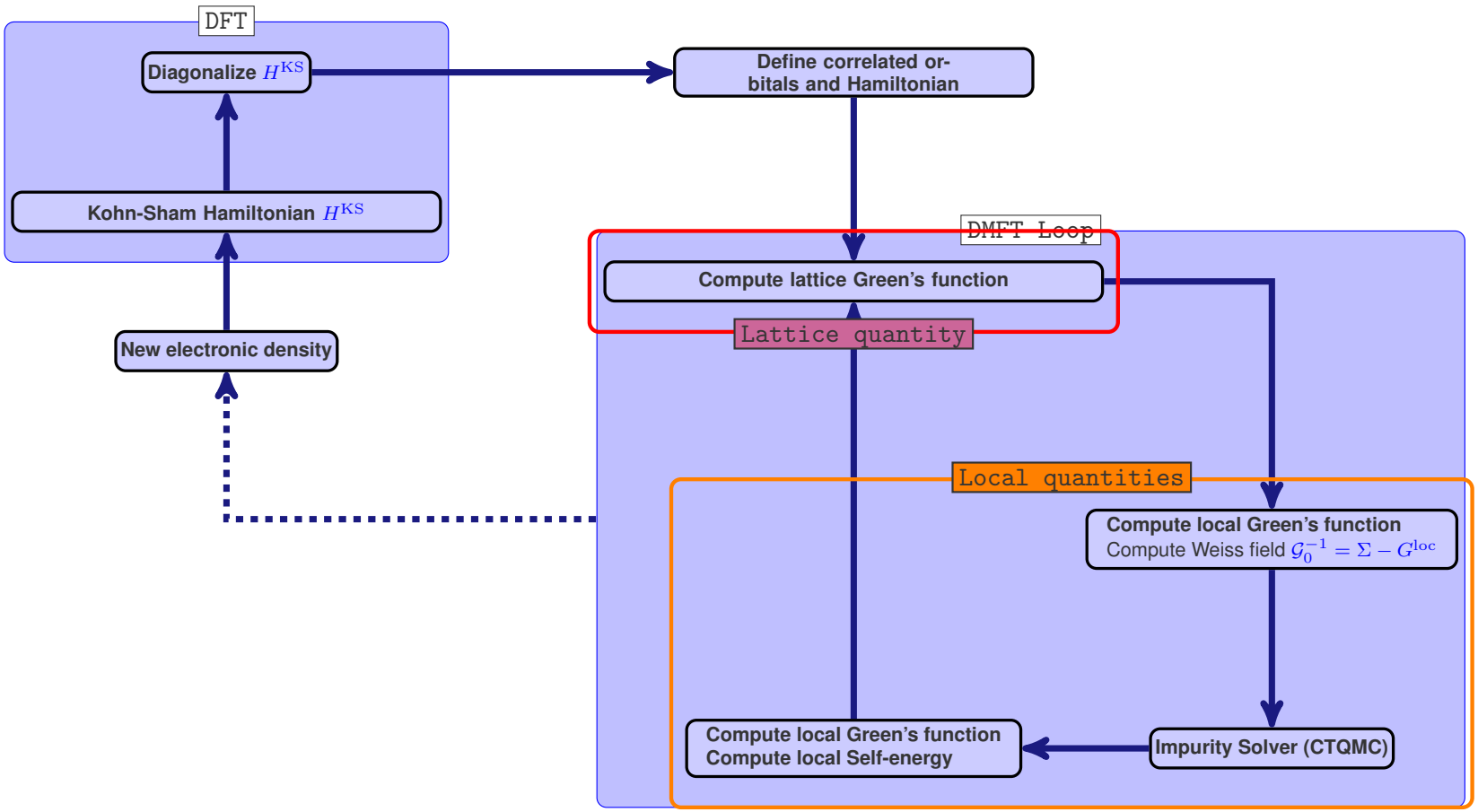

In a real system in DFT+DMFT

- DFT Hamiltonian and thus lattice Green's functions are more easily expressed in Bloch eigenvectors of the DFT Kohn Sham Hamiltonian.

$$\widehat{H}_{\mathrm{KS}} = |\Psi_{\mathbf{k}\nu}\rangle \epsilon_{\mathbf{k}\nu} \langle \Psi_{\mathbf{k}\nu}|$$

Where $\Psi_{\mathbf{k}\nu}$ are one electron Kohn Sham wave function for the k-point $\mathbf{k}$ and band number ν.
$\Psi_{\mathbf{k}\nu}$ contains both correlated atomic orbitals and other non correlated orbitals.
(Reminder: in the Hubbard model, the analogue of $\Psi_{\mathbf{k}\nu}$ was just the Bloch transform of atomic orbitals.)

In a real system in DFT+DMFT

- Local quantities such as $\widehat{\Sigma}$ can be computed in the Bloch basis:

$$\Sigma_{\nu\nu'\mathbf{k}}(i\omega_n) = \langle\Psi_{\mathbf{k}\nu}|\widehat{\Sigma}(i\omega_n)|\Psi_{\mathbf{k}\nu'}\rangle = \sum_{m,m',\mathbf{T}} \langle\Psi_{\mathbf{k}\nu}|\chi_{\mathbf{T}m}\rangle\Sigma_{mm'}(i\omega_n)\langle\chi_{\mathbf{T}m'}|\Psi_{\mathbf{k}\nu'}\rangle$$

Using $|\chi_{\mathbf{T}m}\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}|\chi_{\mathbf{k}m}\rangle \mathrm{e}^{-i\mathbf{k}\mathbf{T}}$, one arrive to

$$\Sigma_{\nu\nu'\mathbf{k}}(i\omega_n) = \sum_{m,m'} \langle\Psi_{\mathbf{k}\nu}|\chi_{\mathbf{k}m}\rangle\Sigma_{mm'}(i\omega_n)\langle\chi_{\mathbf{k}m'}|\Psi_{\mathbf{k}\nu'}\rangle$$

Note that now, the self-energy is a $\mathbf{k}$ dependent quantity, because of weight of orbitals over Kohn Sham states depends on the k-point.

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- From the Self energy, the full lattice Green's function in the Kohn Sham basis

$$G^{-1}(i\omega_n) = G^{-1}_{\mathrm{KS}}(i\omega_n) - \Delta\Sigma(i\omega_n) = (i\omega_n - H_{\mathrm{KS}})\mathcal{I} - \Delta\Sigma(i\omega_n)$$

$$G_{\nu\nu'\mathbf{k}}(i\omega_n) = [i\omega_n - \epsilon_{\mathbf{k}\nu} - \Delta\Sigma_{\nu\nu'\mathbf{k}}(i\omega_n)]^{-1}_{\nu\nu'\mathbf{k}}$$

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In a real system in DFT+DMFT

- Using the operator expression of the lattice Green's function

$$\widehat{G}(i\omega_n) = \sum_{\nu\nu'\mathbf{k}} |\Psi_{\mathbf{k}\nu}\rangle G_{\nu\nu'\mathbf{k}}(i\omega_n) \langle\Psi_{\mathbf{k}\nu'}|$$

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- One can write the local Green's function as:

$$G_{mm'}(i\omega_n) = \sum_{\nu\nu'\mathbf{k}} \langle\chi_{\mathbf{T}m}|\Psi_{\mathbf{k}\nu}\rangle G_{\nu\nu'\mathbf{k}}(i\omega_n) \langle\Psi_{\mathbf{k}\nu'}|\chi_{\mathbf{T}m'}\rangle$$

for Hubbard model $G(i\omega_n) = \sum_{\mathbf{k}} G_{\mathbf{k}}(i\omega_n)$

Projectors

Projectors are the key quantity of the interface between DFT and DMFT:

$$\langle \chi_{\mathbf{k}m} | \Psi_{\mathbf{k}\nu} \rangle$$

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- If $|\chi_{\mathbf{k}m}\rangle$ is an atomic orbital, it can be decomposed exactly on all KS eigenstates as:

  $$|\chi_{\mathbf{k}m}\rangle = \sum_{\nu} \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m} \rangle | \Psi_{\mathbf{k}\nu} \rangle$$

  A calculation not feasable because it requires the complete basis set of KS eigenstates.

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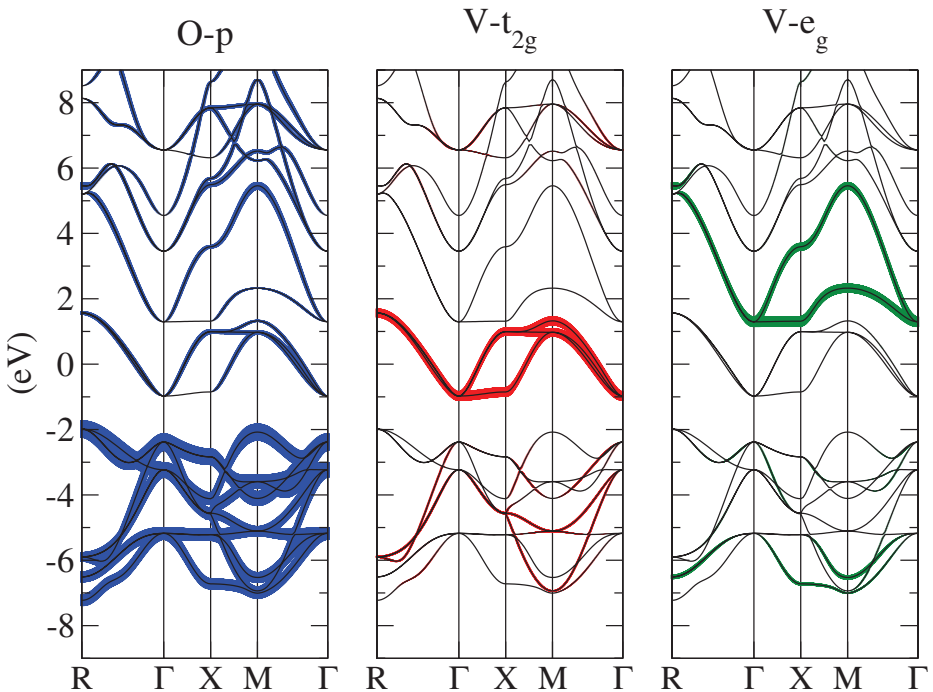
  A calculation not feasable because it requires the complete basis set of KS eigenstates.
- We need to restrict the sum over KS states belonging to a window $\mathcal{W}$ and built new functions $|\tilde{\chi}_{\mathbf{k}m}\rangle$:

  $$|\tilde{\chi}_{\mathbf{k}m}\rangle = \sum_{\nu \in \mathcal{W}} \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m} \rangle | \Psi_{\mathbf{k}\nu} \rangle$$

Definition of correlated orbitals: example of $SrVO_3$.



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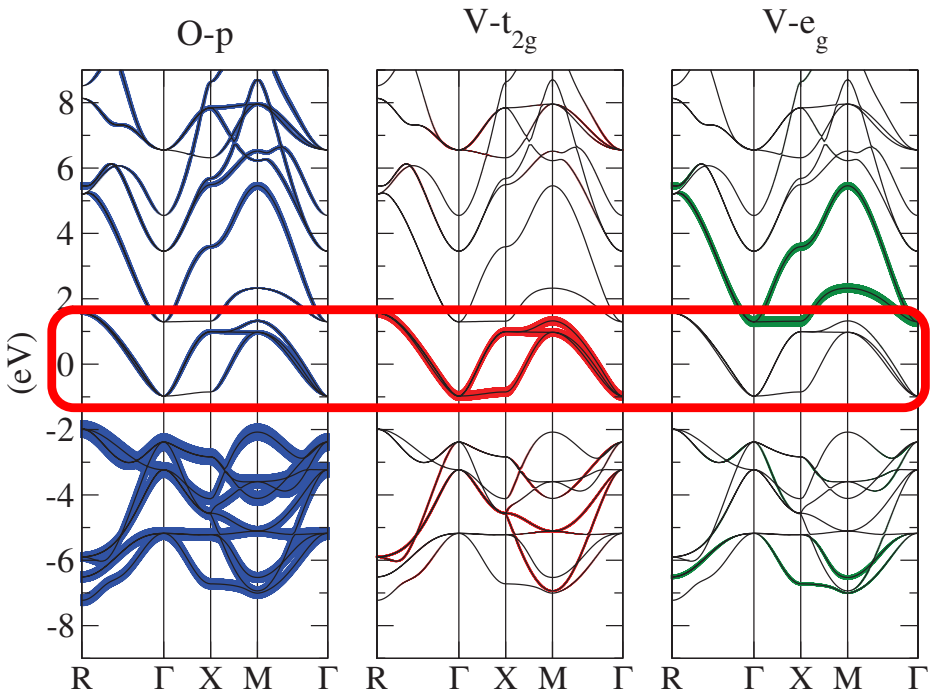


Projectors

Projectors are the key quantity of the interface between DFT and DMFT:

$$\langle \chi_{\mathbf{k}m} | \Psi_{\mathbf{k}\nu} \rangle$$

- If $|\chi_{\mathbf{k}m}\rangle$ is an atomic orbital, it can be decomposed exactly on all KS bands as:

  $$|\chi_{\mathbf{k}m}\rangle = \sum_{\nu} \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m} \rangle | \Psi_{\mathbf{k}\nu} \rangle$$

  A calculation not feasable because it requires a complete basis set of Kohn Sham states.
- We need to restrict the sum over KS states belonging to a window $\mathcal{W}$ and built new functions $|\tilde{\chi}_{\mathbf{k}m}\rangle$:

  $$|\tilde{\chi}_{\mathbf{k}m}\rangle = \sum_{\nu \in \mathcal{W}} \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m} \rangle | \Psi_{\mathbf{k}\nu} \rangle$$

  because of the truncation, the projection matrix is not longer unitary, and the new functions are not normalized (and not Wannier functions)

  $$\langle \tilde{\chi}_{\mathbf{k}m'} | \tilde{\chi}_{\mathbf{k}m} \rangle = \sum_{\nu \in \mathcal{W}} \langle \chi_{\mathbf{k}m'} | \Psi_{\mathbf{k}\nu} \rangle \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m} \rangle \neq \delta_{mm'}$$

  After a proper orthonormalization, new functions $|w_{\mathbf{k}m}\rangle$ can be obtained that are unitarily related to KS wave functions.

Projectors orthonormalization

We define the overlap matrix by:

$$O_{m,m'}(\mathbf{k}) = \langle \tilde{\chi}_{\mathbf{k}m} | \tilde{\chi}_{\mathbf{k}m'} \rangle = \sum_{\nu} \langle \chi_{\mathbf{k}m} | \Psi_{\mathbf{k}\nu} \rangle \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m'} \rangle$$

$$|w_{\mathbf{k}m}\rangle = \sum_{m'} \left\{ [O(\mathbf{k})]^{-1/2} \right\}_{m,m'} |\tilde{\chi}_{\mathbf{k}m'}\rangle$$

In order for the correlated orbitals to be orthogonal on a given site, on need to define the overlap matrix as:

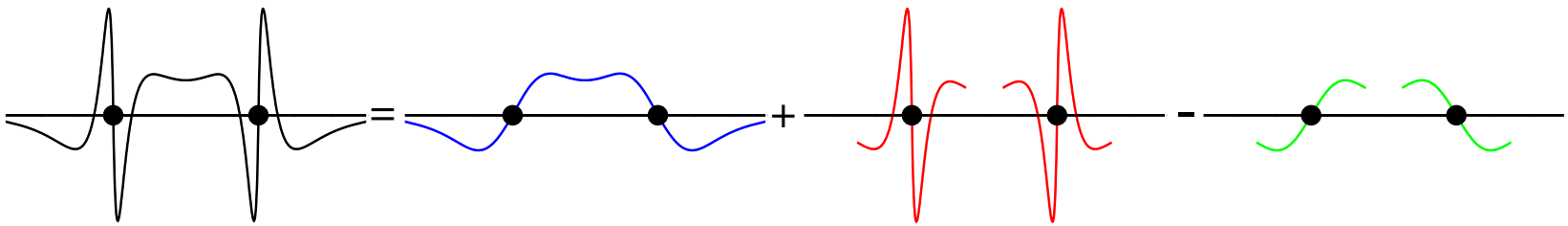
$$O_{m,m'} = \sum_{\mathbf{k}} \langle \tilde{\chi}_{\mathbf{k}m} | \tilde{\chi}_{\mathbf{k}m'} \rangle = \sum_{\nu\mathbf{k}} \langle \chi_{\mathbf{k}m} | \Psi_{\mathbf{k}\nu} \rangle \langle \Psi_{\mathbf{k}\nu} | \chi_{\mathbf{k}m'} \rangle$$

(Do the proof as an exercice)

Expression of a Kohn Sham function of Cl_2 in PAW

$$|\Psi_{\mathbf{k}\nu}\rangle = \underbrace{|\widetilde{\Psi}_{\mathbf{k}\nu}\rangle}_{\text{On plane waves}} + \underbrace{\sum_i |\varphi_i\rangle\langle\widetilde{p}_i|\widetilde{\Psi}_{\mathbf{k}\nu}\rangle - \sum_i |\widetilde{\varphi}_i\rangle\langle\widetilde{p}_i|\widetilde{\Psi}_{\mathbf{k}\nu}\rangle}_{\text{On a local radial grid}}$$

Blöchl PRB 1994



[Developed in ABINIT by the CEA group]

[M. Torrent, F. Jollet, F. Bottin, G. Zérah, X. Gonze Comp. Mat. Science 42 (2), 337-351 (2008)]

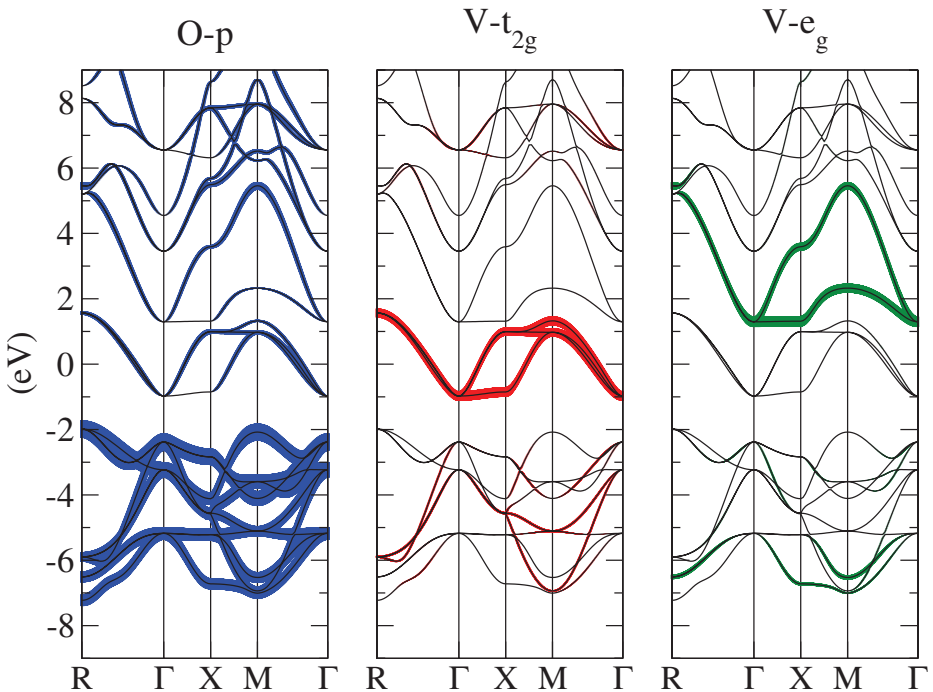
A grid devoted to local properties : well adapted to correlated systems and to compute:

- DFT+U density matrix.
- Projected Wannier orbitals.

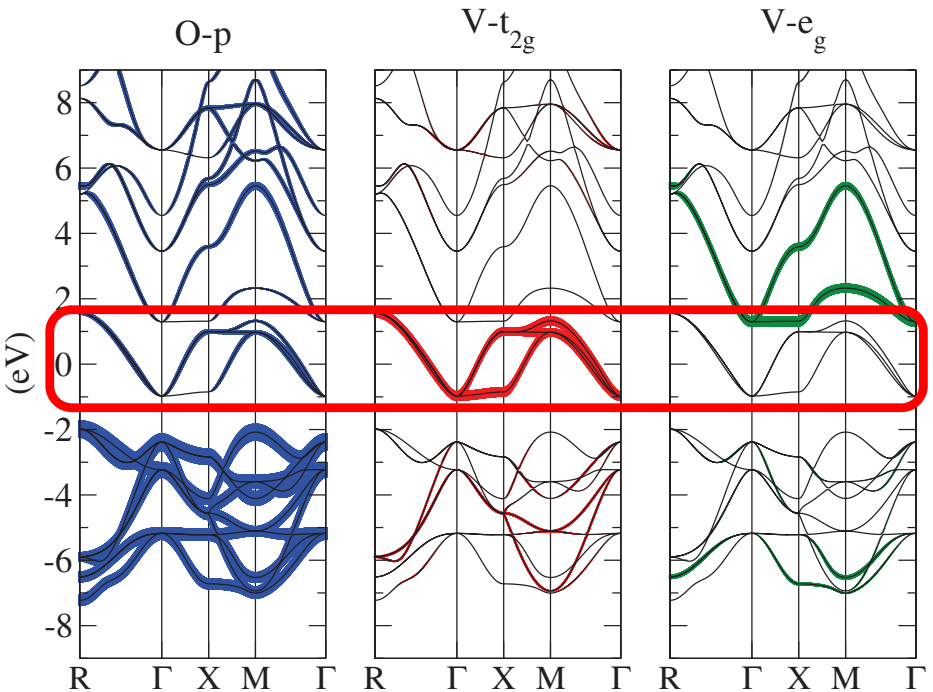
Projectors are the key quantity of the interface between DFT and DMFT:

$$\langle\chi_{\mathbf{k}m}|\Psi_{\mathbf{k}\nu}\rangle = \sum_i \langle\chi_{\mathbf{k}m}|\varphi_i\rangle\langle\widetilde{p}_i|\widetilde{\Psi}_{\mathbf{k}\nu}\rangle$$

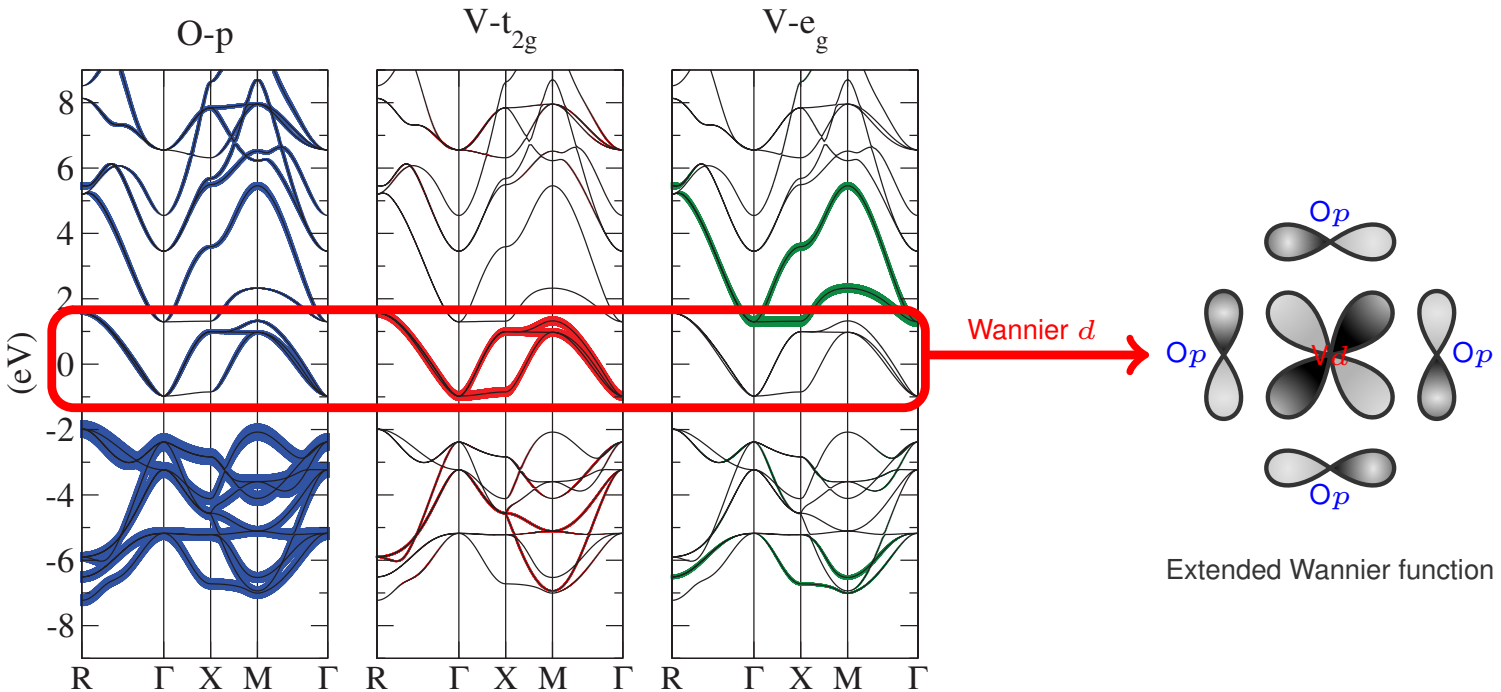
Definition of correlated orbitals: example of $SrVO_3$.



Definition of correlated orbitals: example of $SrVO_3$.

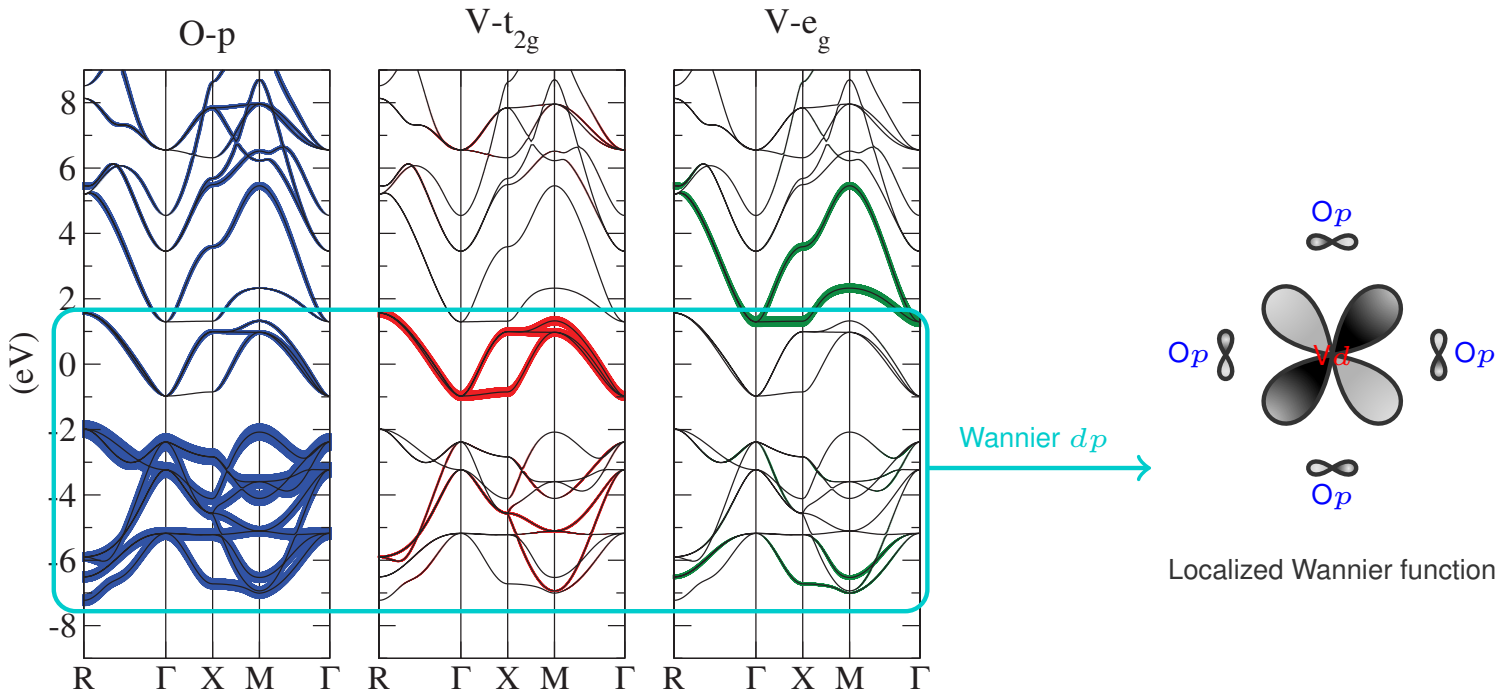


Definition of correlated orbitals: example of $SrVO_3$.



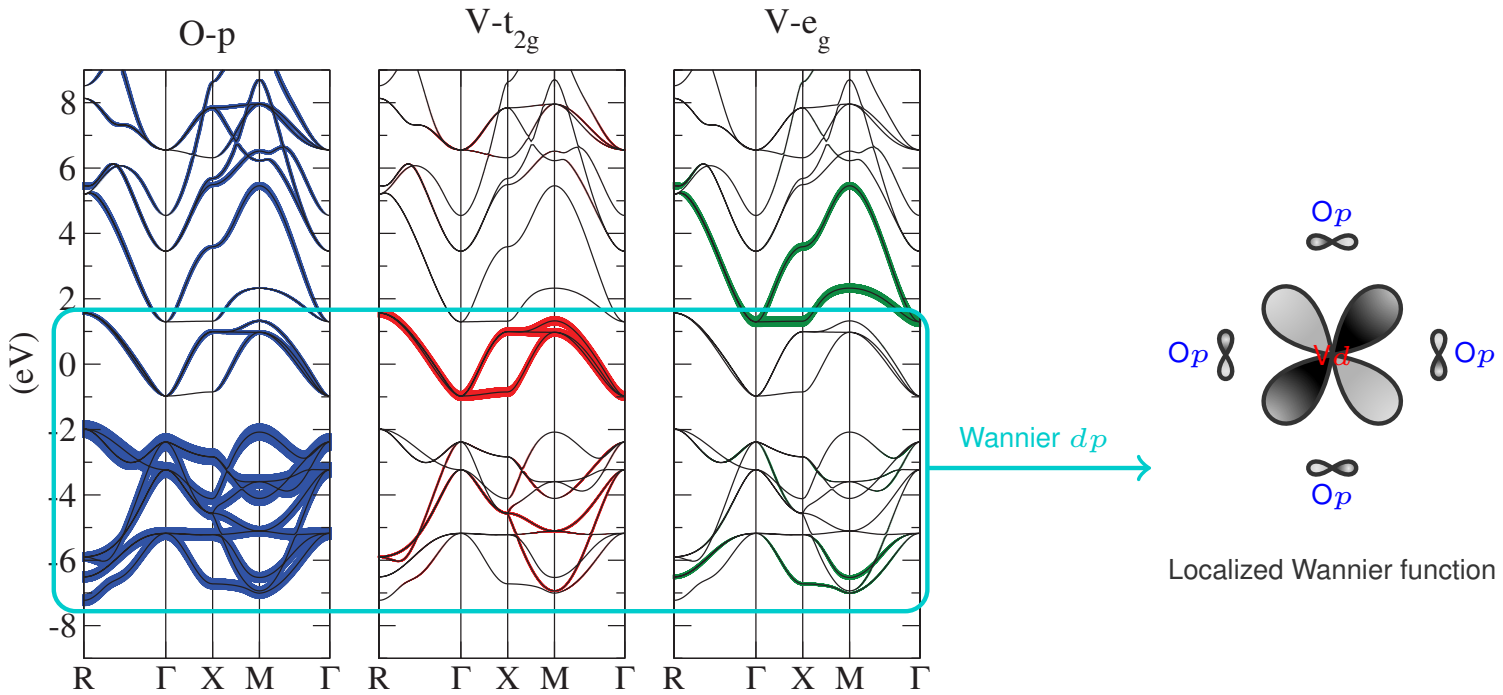
Wannier orbitals are made from Vdt_{2g} bands so, they are not pure dt_{2g} orbitals because of the hybridization

Definition of correlated orbitals: example of $SrVO_3$.



Wannier orbitals are made from Vdt_{2g} bands and O p bands so, they are closer to dt_{2g} orbitals because more t_{2g} character is taken into account.

Definition of correlated orbitals: example of $SrVO_3$.

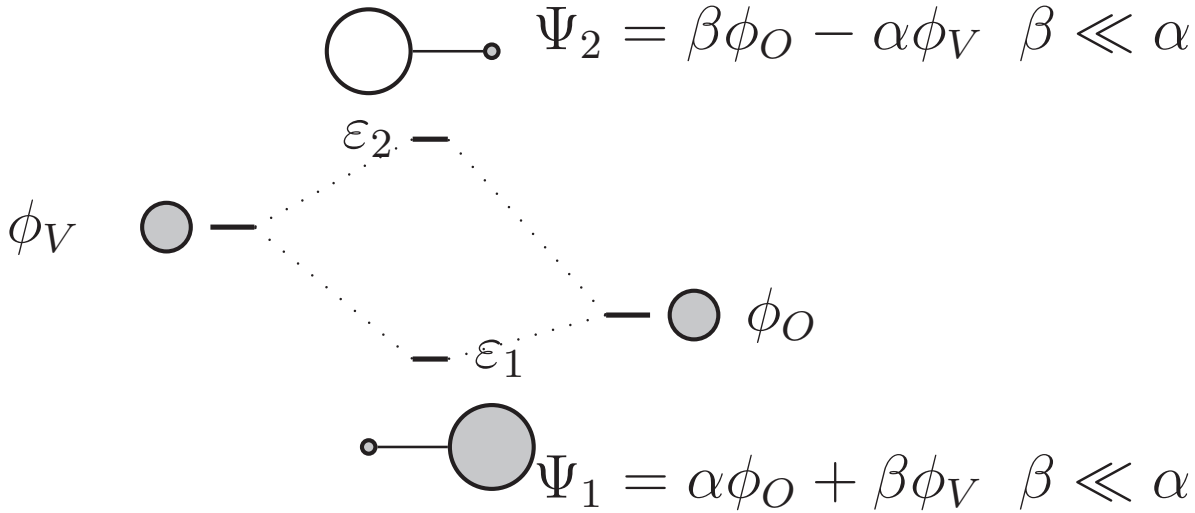


For $SrVO_3$, these Wannier functions are similar to Maximally localized one.

B. Amadon, F. Lechermann, A. Georges, F. Jollet, T. Wehling and A. I. Lichtenstein Phys. Rev. B 77, 205112 (2008)

Implemented in `ABINIT`

An oversimplified derivation

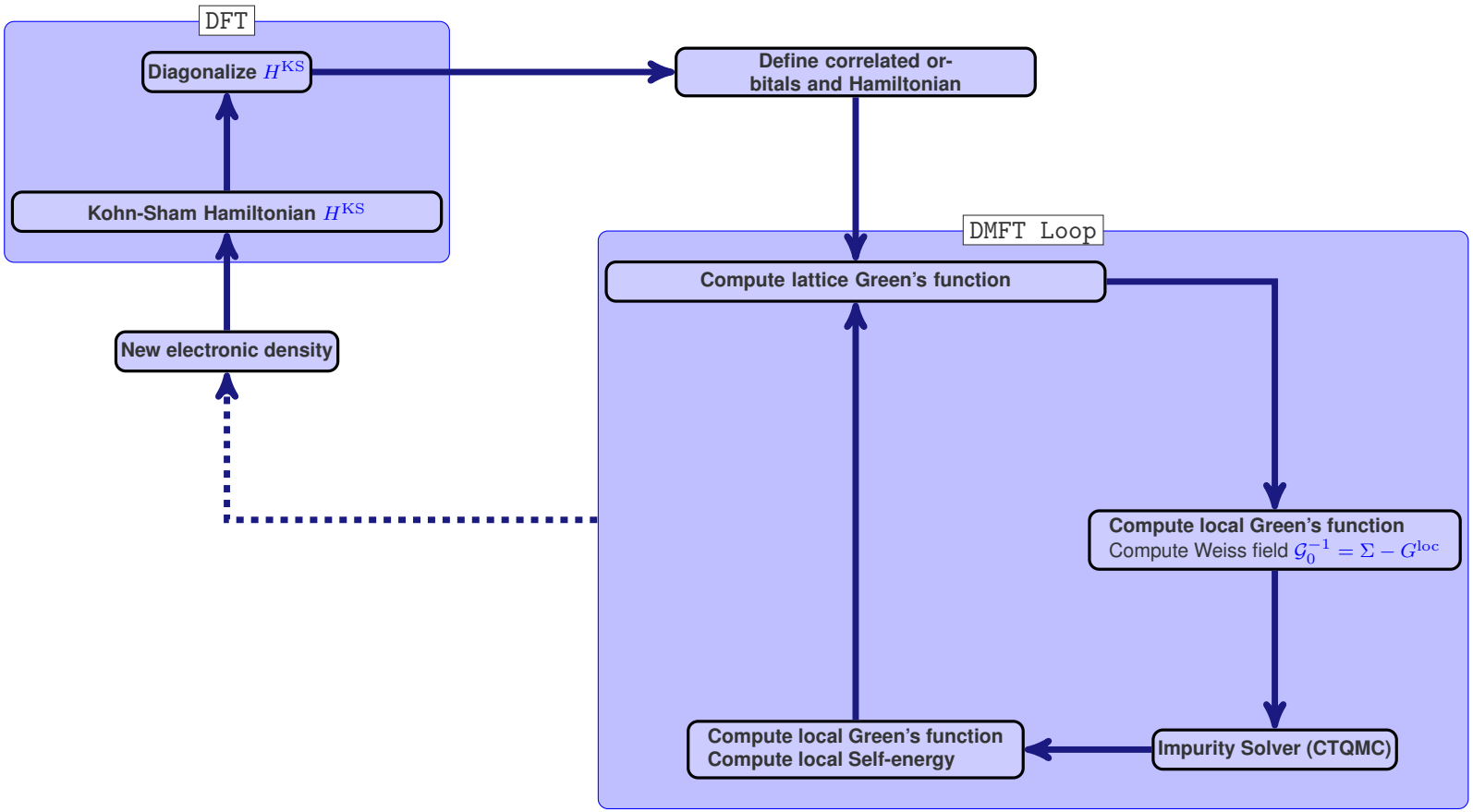


Two windows of energy are possible to compute

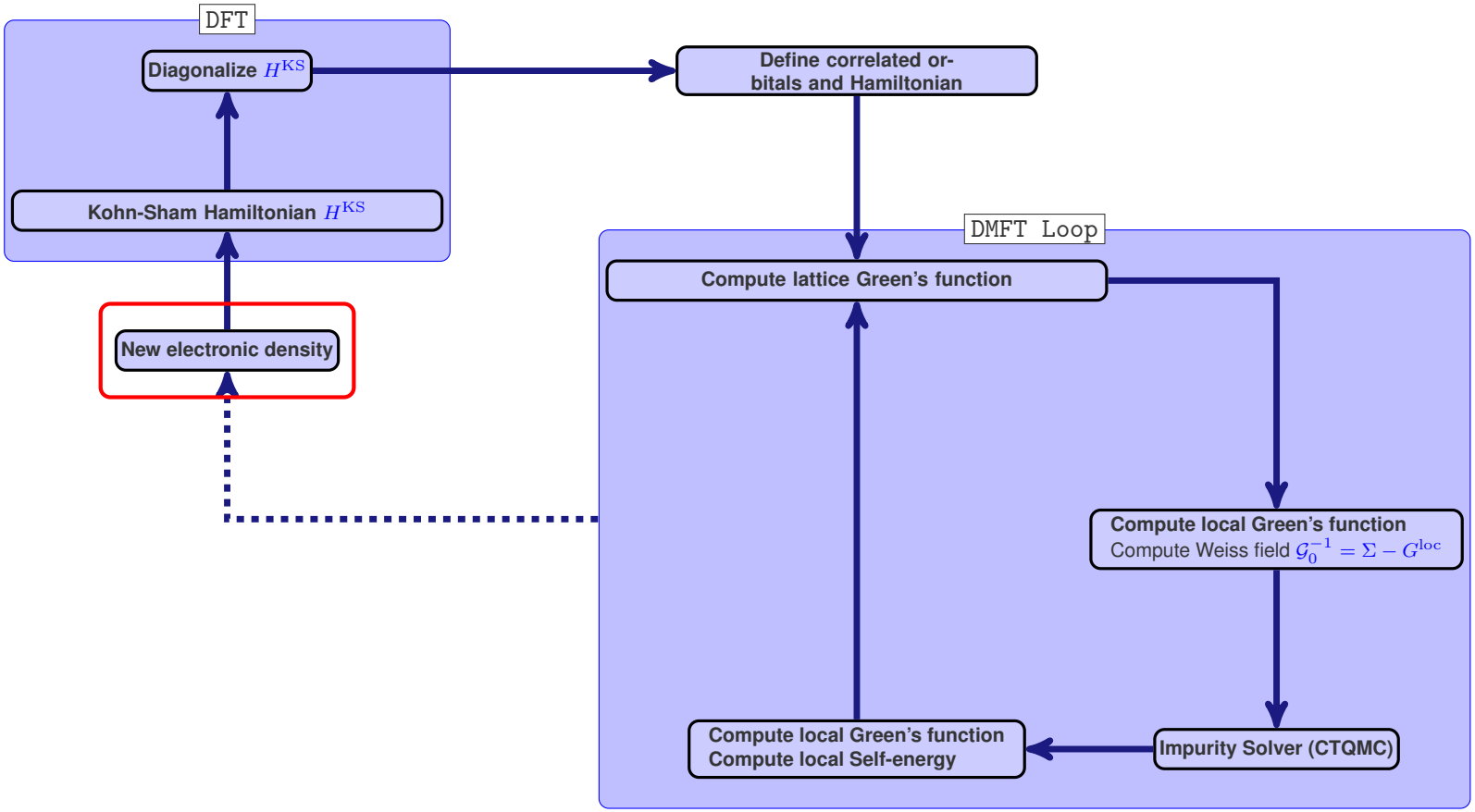
$$|\widetilde{\chi}\rangle = \sum_{i \in \mathcal{W}} \langle \Psi_i | \phi_V \rangle |\Psi_i\rangle$$

- If $\mathcal{W} = \{\varepsilon_2\}$, the correlated wavefunction is $|\widetilde{\chi}\rangle = |\Psi_2\rangle = \beta|\phi_O\rangle - \alpha|\phi_V\rangle$. No renormalization is necessary thus $|w\rangle = |\widetilde{\chi}\rangle$. It contains an Oxygen contribution
- If $\mathcal{W} = \{\varepsilon_1, \varepsilon_2\}$, the correlated wavefunction is $|\widetilde{\chi}\rangle = \sum_i \langle \Psi_i | \phi_V \rangle |\Psi_i\rangle = |\phi_V\rangle$ and is much more localized.

The DFT+DMFT scheme



The DFT+DMFT scheme



From the Green's function in the Kohn Sham basis, new occupations can be constructed and the full DFT+DMFT loop be performed.

$$n(\mathbf{r}) = \sum_{\mathbf{k}\nu} f_{\mathbf{k}\nu\nu'} \Psi_{\mathbf{k}\nu} \Psi_{\mathbf{k}\nu'}$$

Conclusion

- Wannier functions can be conveniently used in the context of DFT+DMFT calculations
- Projected Local Orbital Wannier functions are easy to construct, especially for entangled cases.
- According to the definition of Wannier functions, effective interactions U can be computed.

DE LA RECHERCHE À L'INDUSTRIE

www.cea.fr

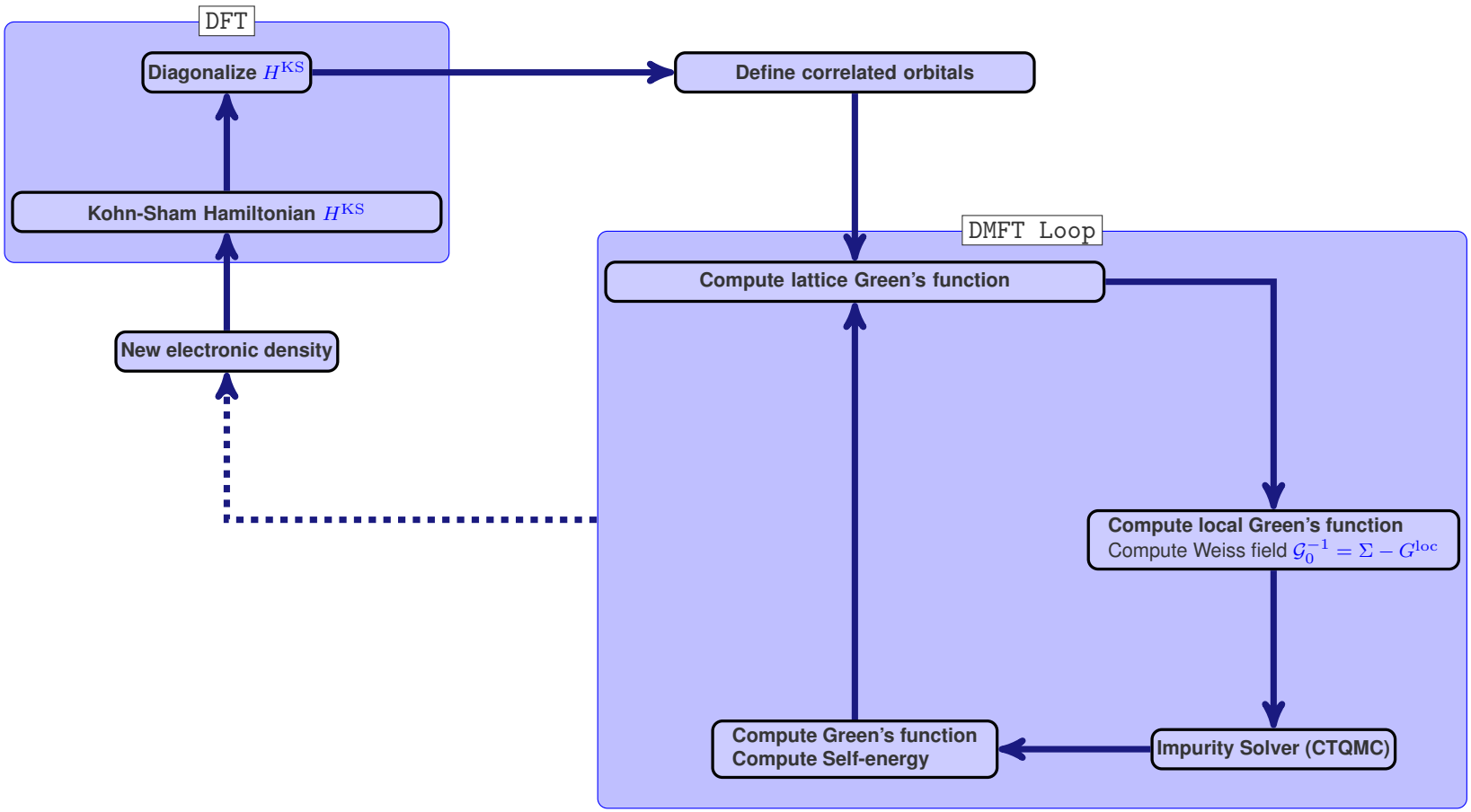
The constrained Random Phase approximation: How to compute effective interactions ?

Bernard Amadon

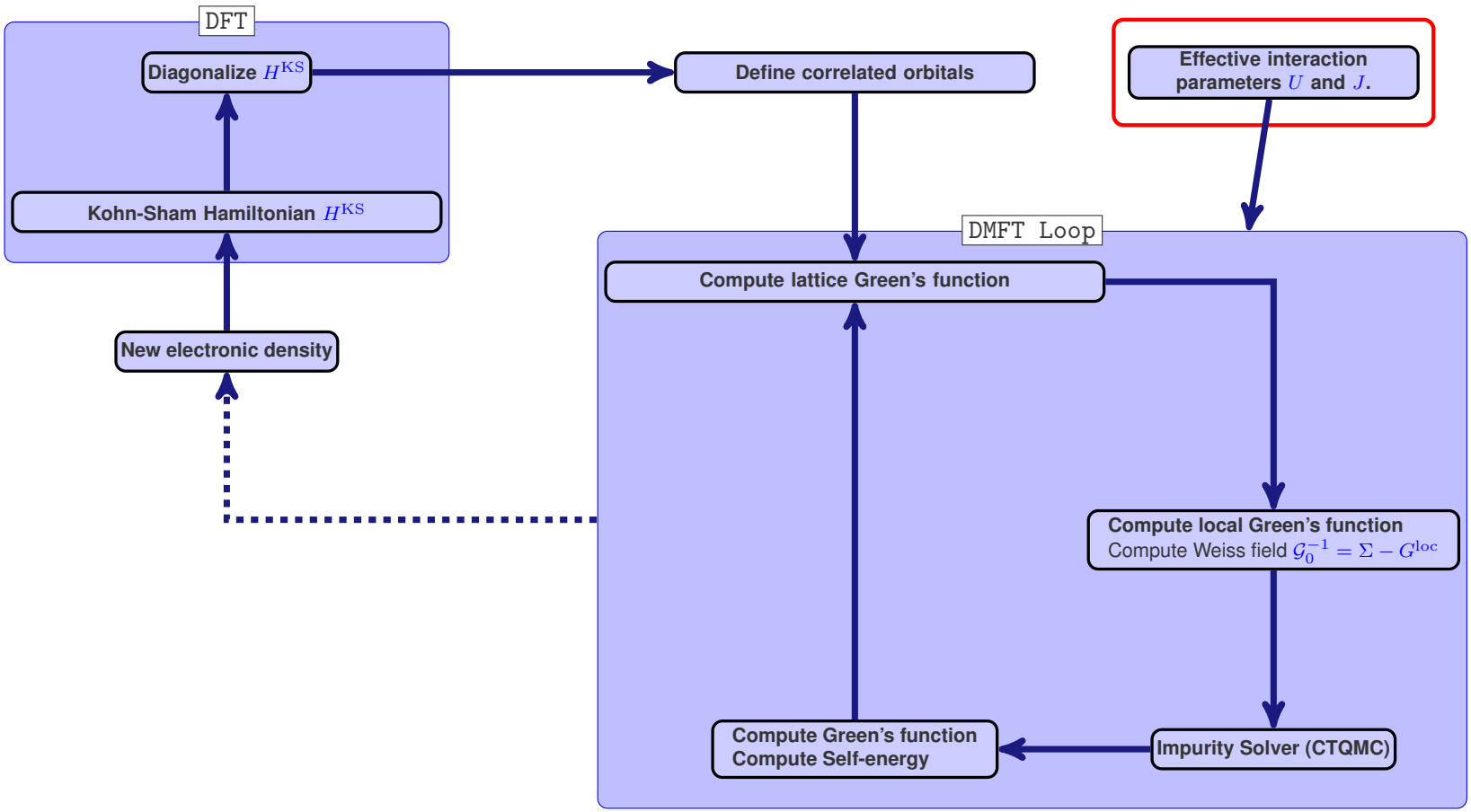
CEA, DAM, DIF, F-91297 Arpajon, France

International Summer School on Computational Quantum Material 2018

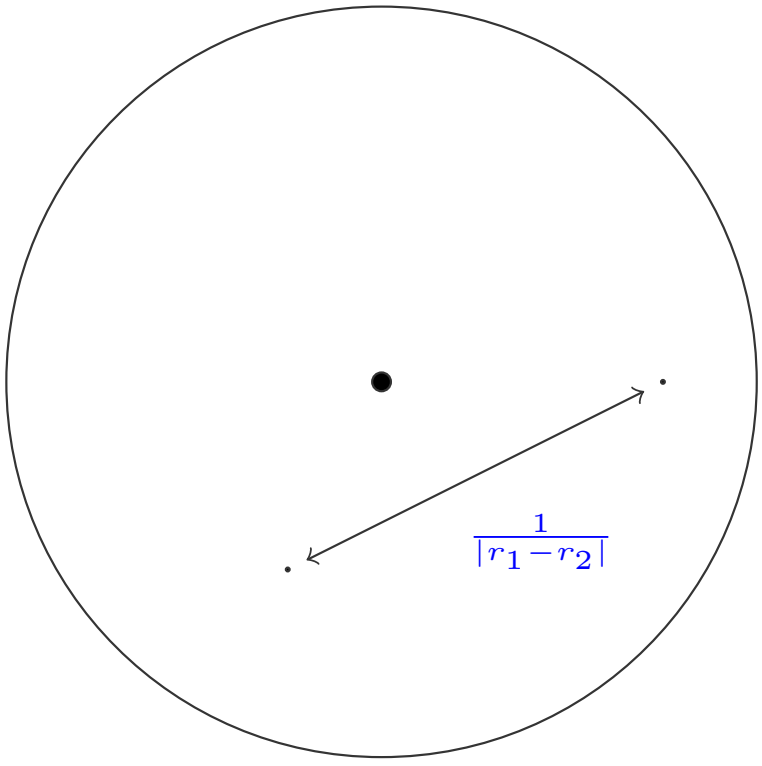
DFT+DMFT scheme



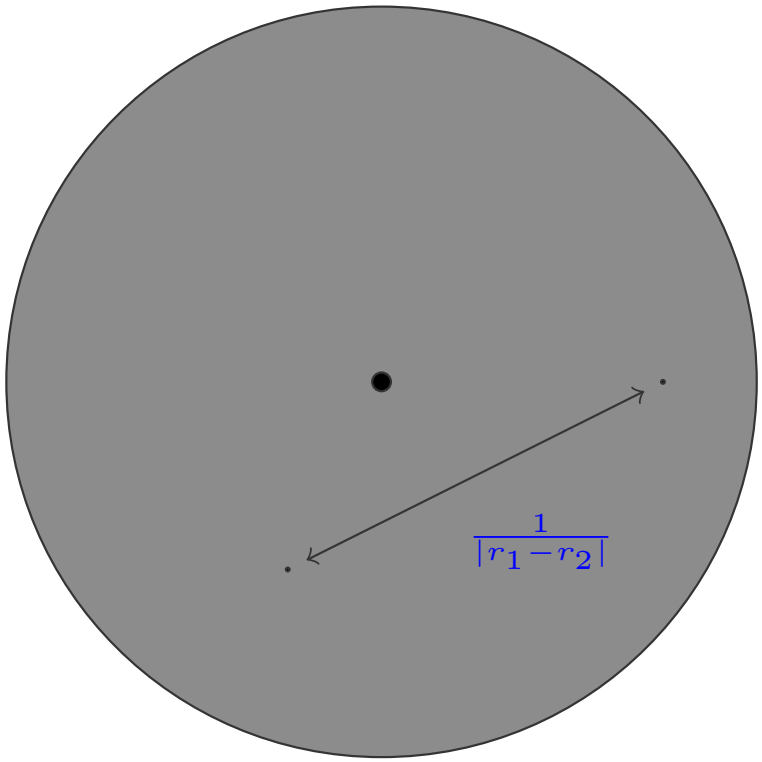
DFT+DMFT scheme



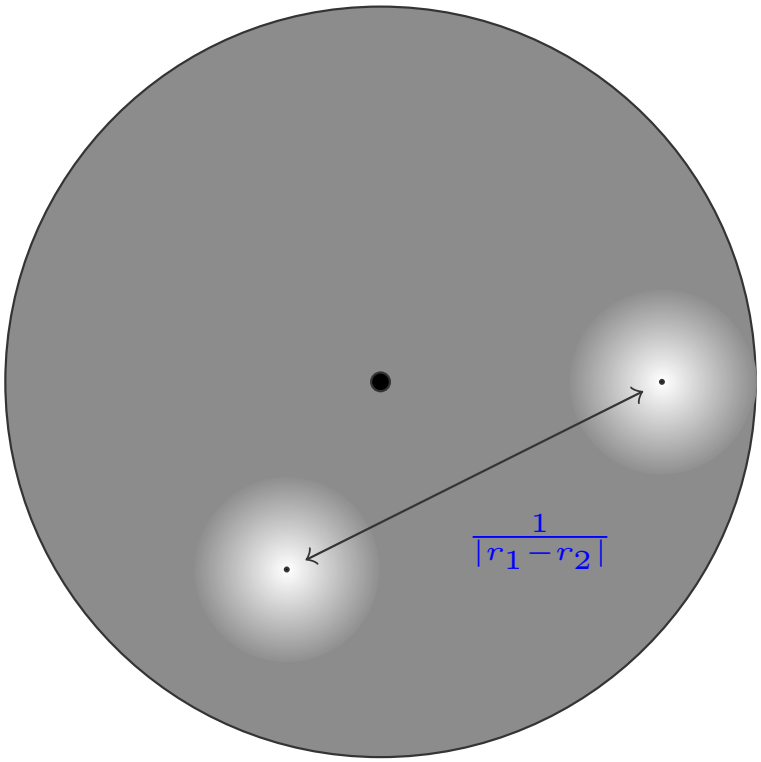
How to compute the effective interaction ?



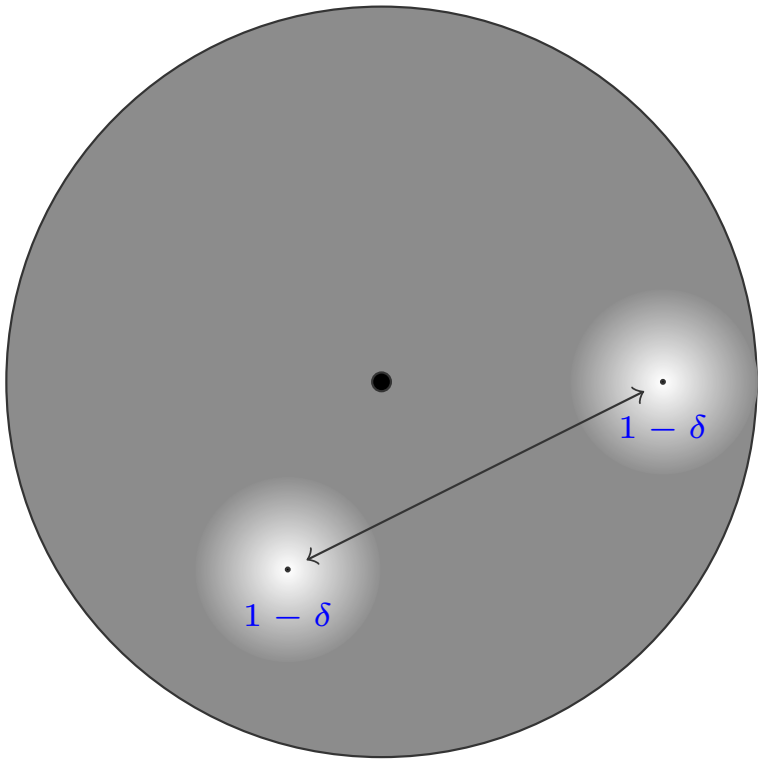
How to compute the effective interaction ?

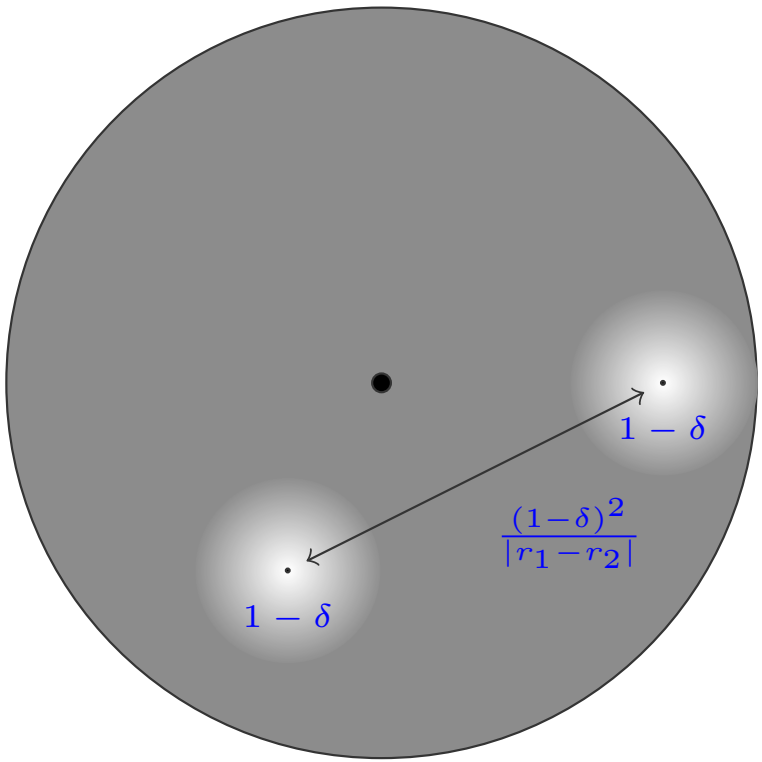


How to compute the effective interaction ?



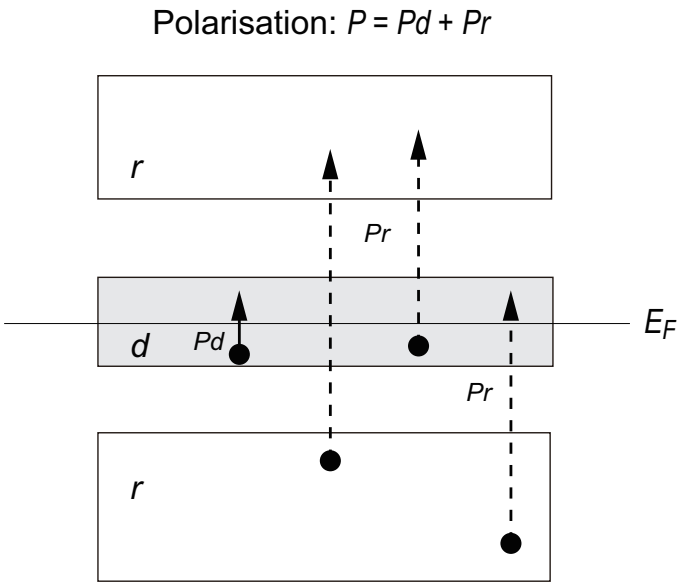
How to compute the effective interaction ?





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 (see lectures of F. Bruneval and A.M. Tremblay) 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.

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

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

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

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.

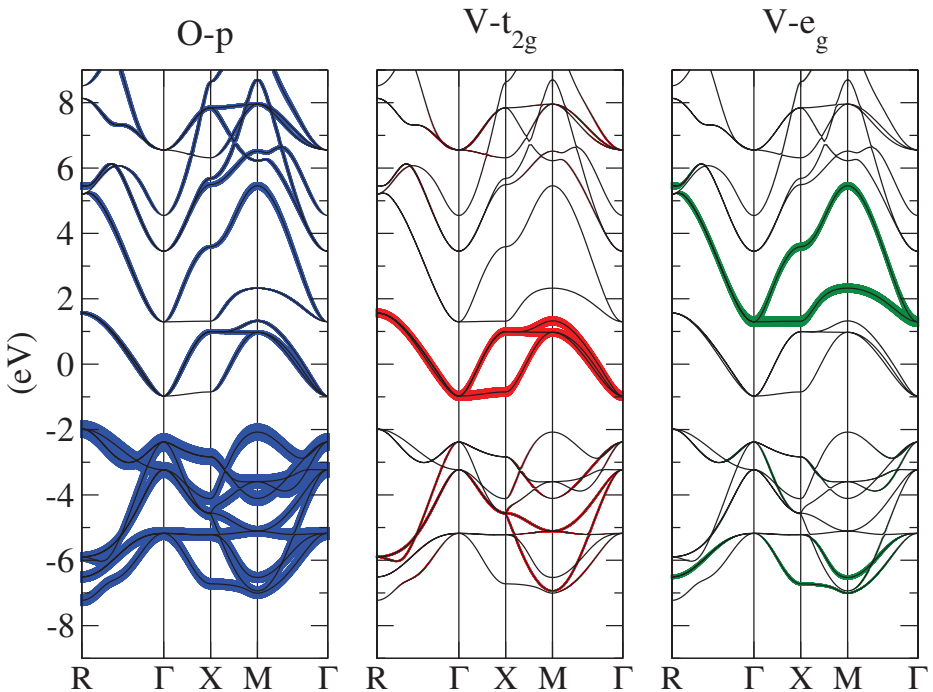
The cRPA approach: key parameters

The definition of correlated orbitals

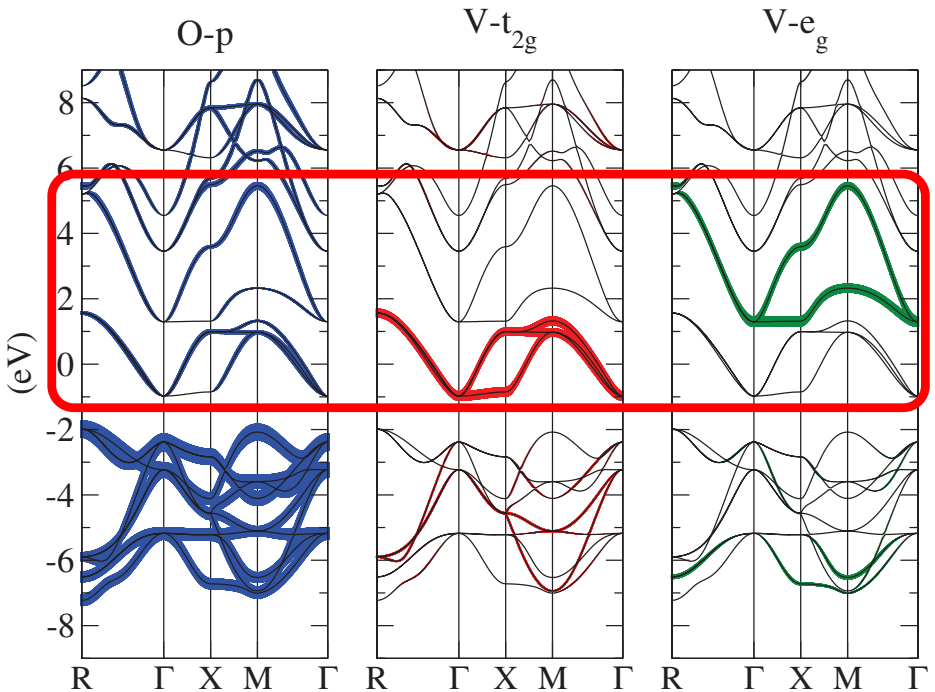
- We use Projected Local Orbitals Wannier functions: effective interaction can thus be used directly in DFT+DMFT calculations.
- Depending on the energy window used in the calculation, several localization of orbitals can be described.

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

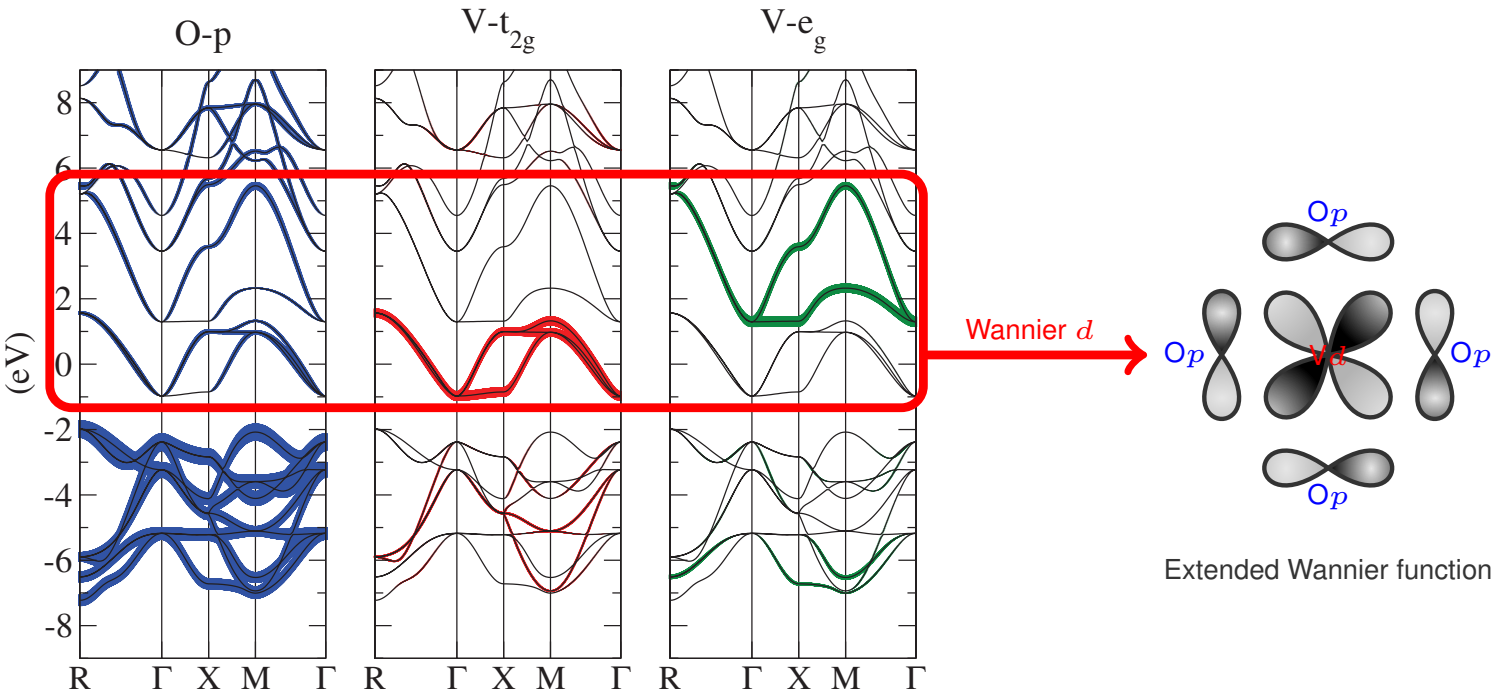
Definition of correlated orbitals: example of $SrVO_3$.



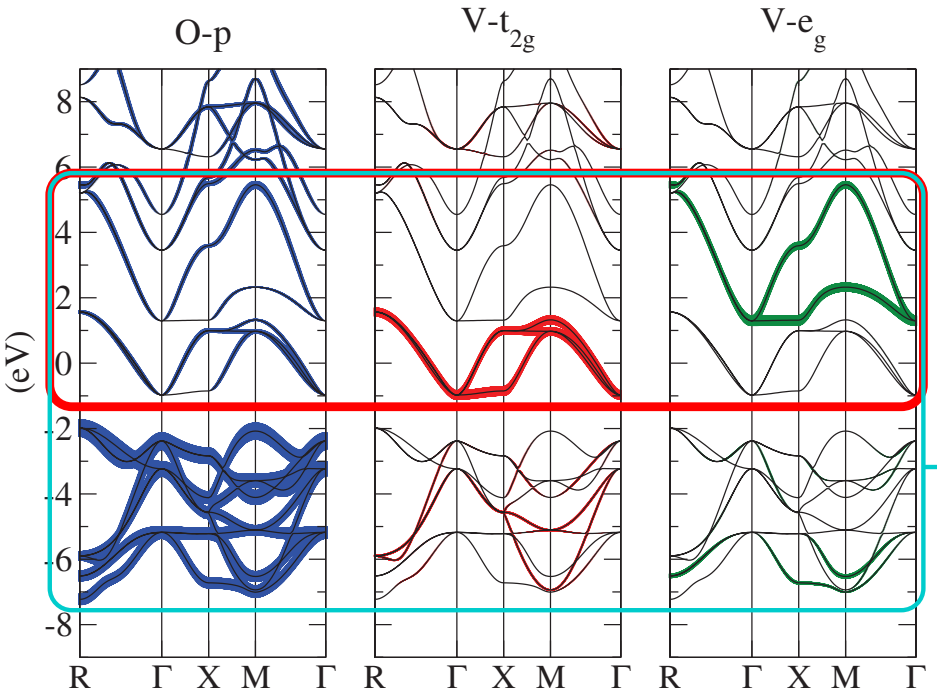
Definition of correlated orbitals: example of $SrVO_3$.



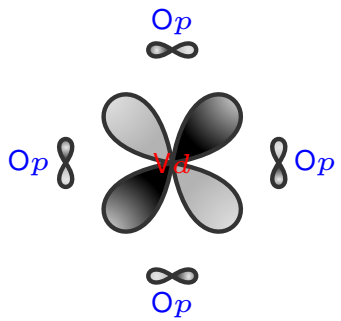
Definition of correlated orbitals: example of $SrVO_3$.



Definition of correlated orbitals: example of $SrVO_3$.

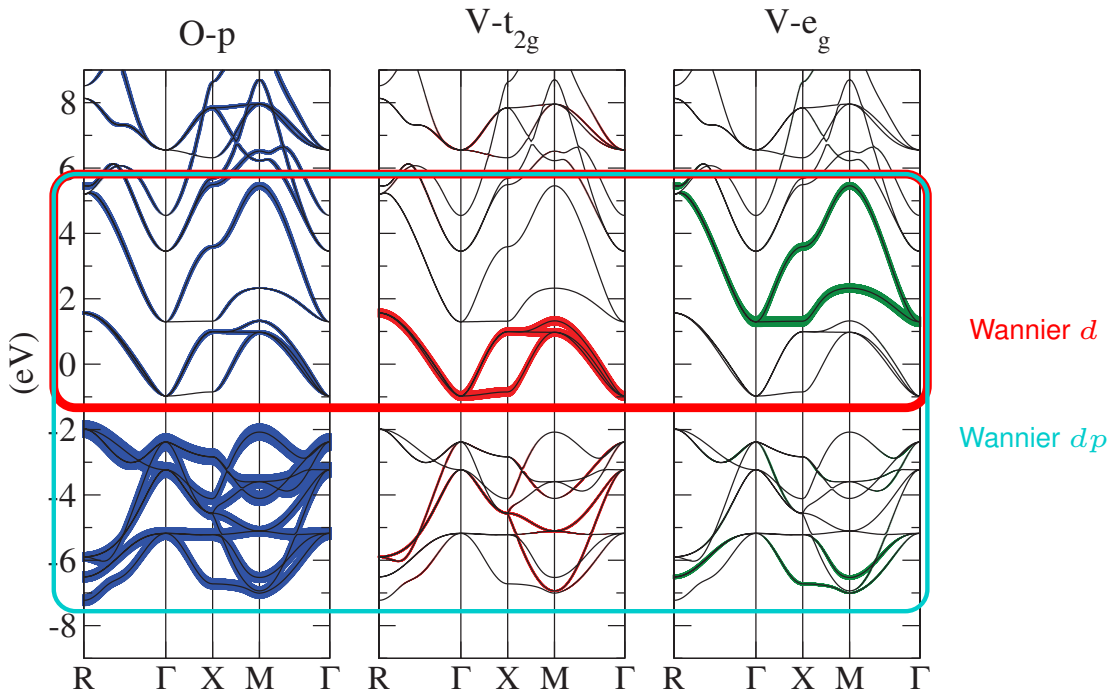


Wannier dp



Localized Wannier function

Definition of correlated orbitals: example of $SrVO_3$.



Bare interaction can be computed as:

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

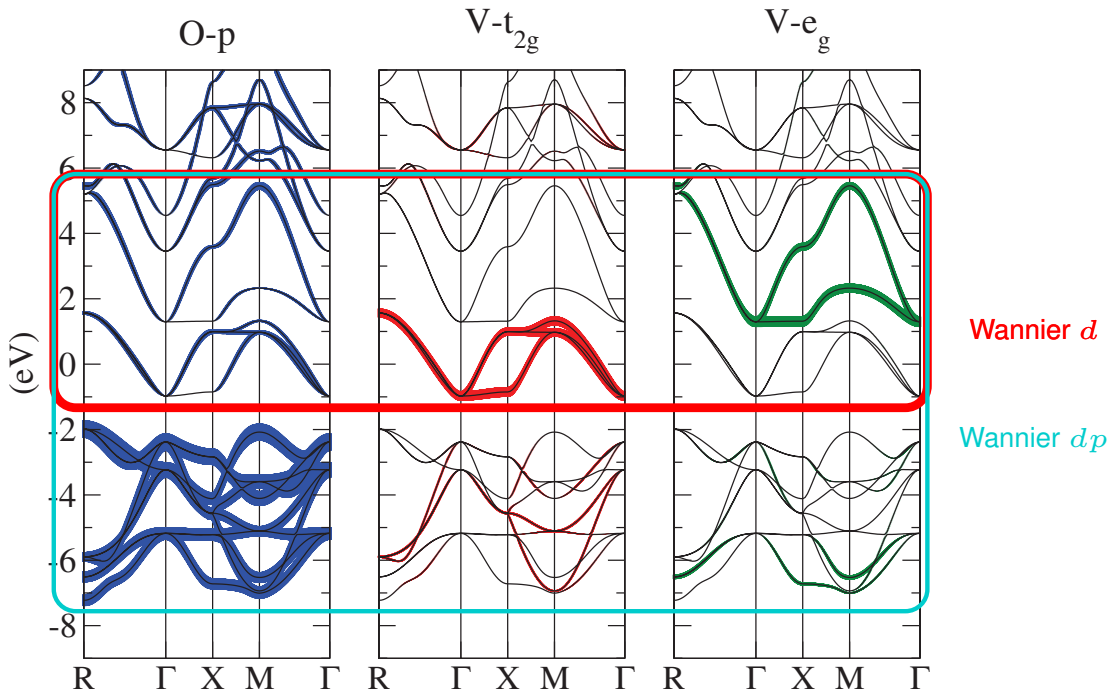
Wannier function	bare interaction v (eV)
Wannier d	15.3
Wannier dp	19.4

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.

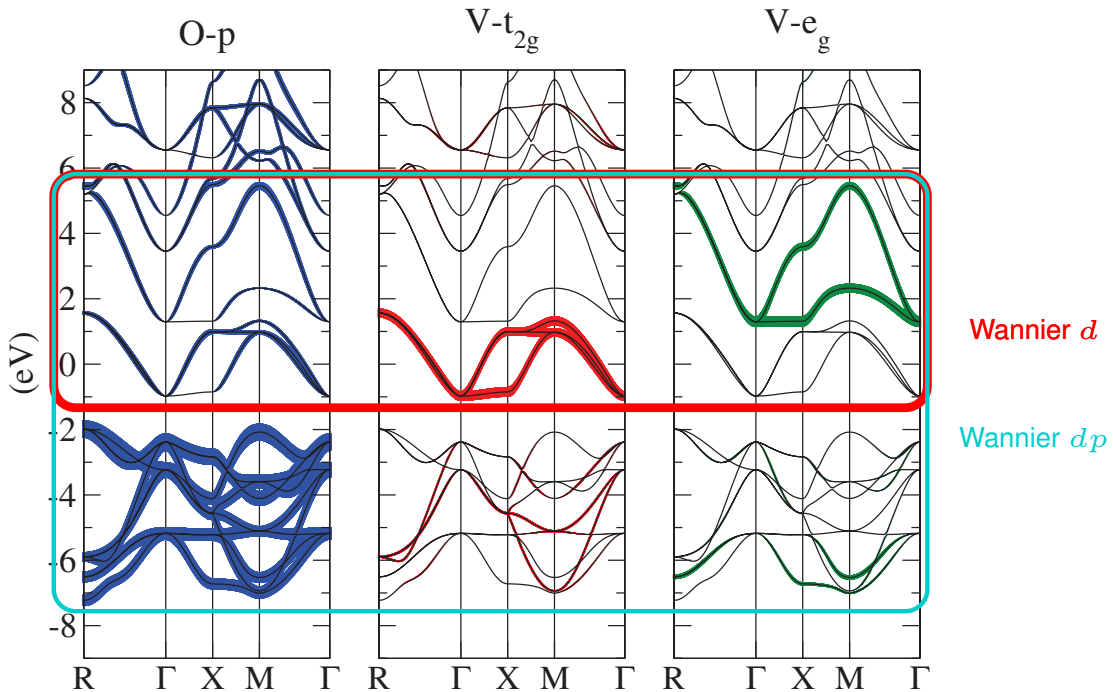
In `ABINIT`, to decide the windows of energy for which the screening is suppressed, use the keywords `ucrpa_bands`.



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	$dp-dp$



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

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

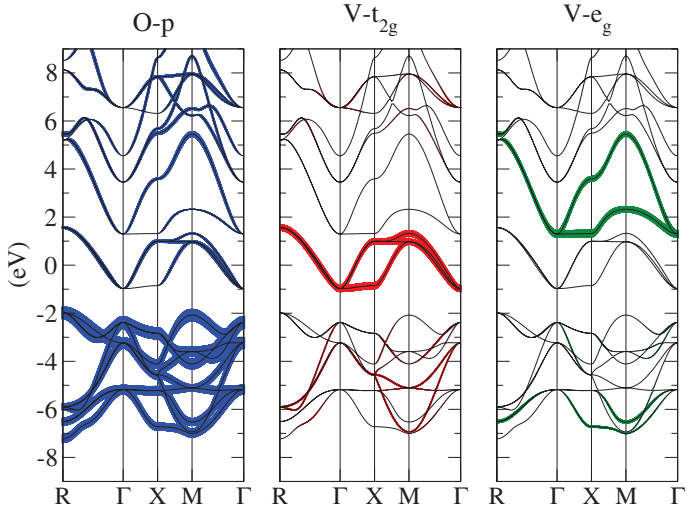
$$U = \frac{1}{(2l+1)^2} \sum_{i,j} \langle \chi_i \chi_j | W_r | \chi_i \chi_j \rangle$$

One has

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

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

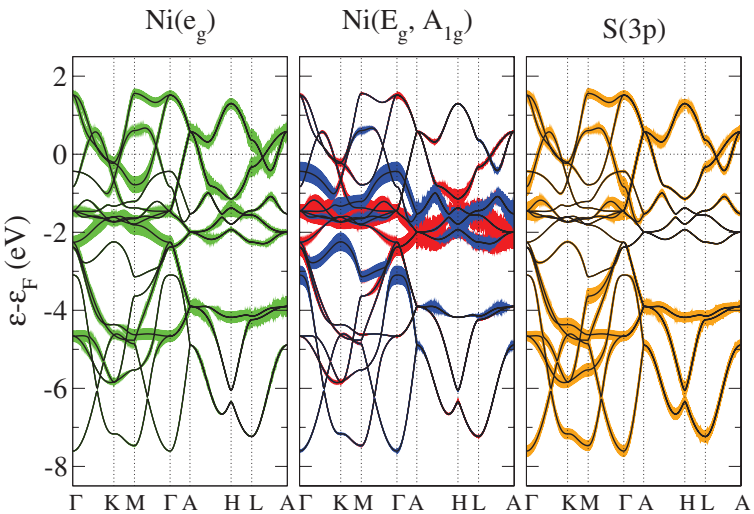
$SrVO_3$



Non entangled bands

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

NiS



Entangled bands

For non entangled bands (ucrpa=1)

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

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

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

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

For entangled bands (ucrpa=2)

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

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

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 $\chi_0^{\text{cRPA}}(\mathbf{G},\mathbf{G}',\mathbf{q})$:

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

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.