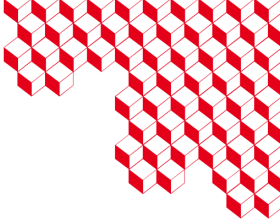
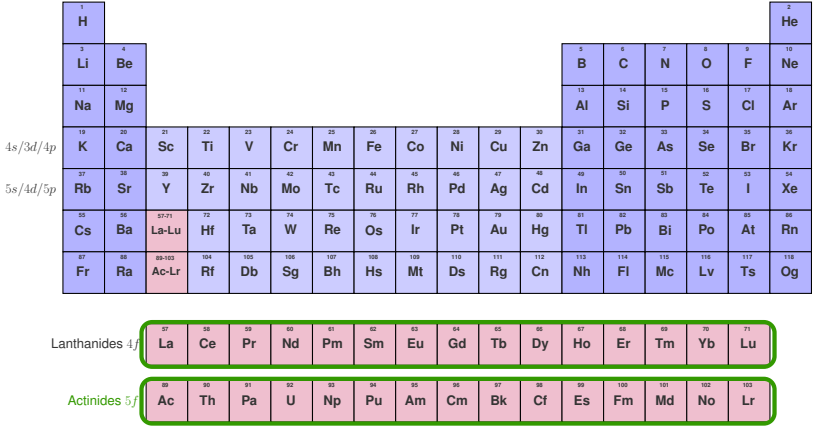


DMFT for f electron systems

Bernard Amadon
CEA, DAM, DIF
Université Paris-Saclay, CEA, LMCE
Bruyères-le-Châtel, France

THE PERIODIC TABLE



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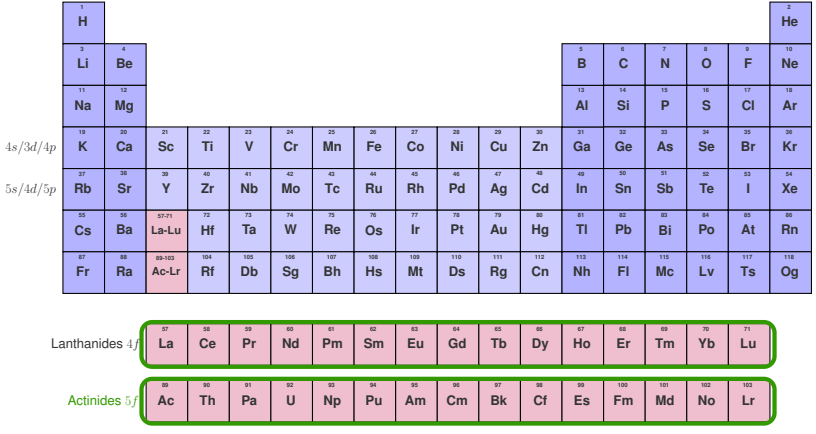

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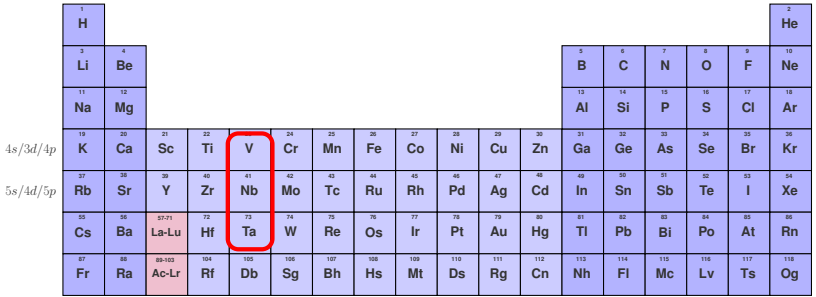
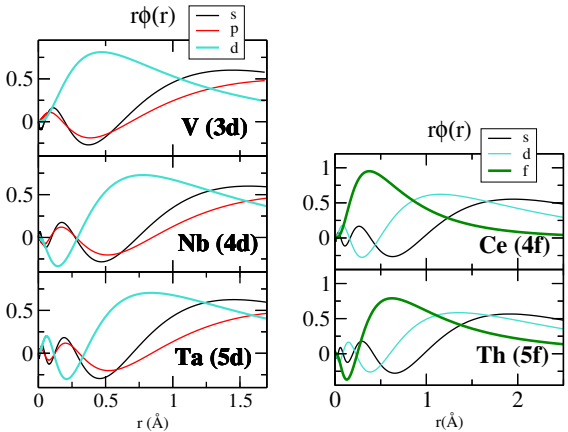


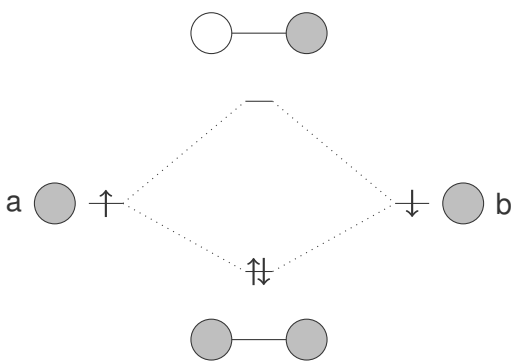
Localization of $3d$, $4f$ and $5f$ orbitals.



- $\Psi_{nlm}(\mathbf{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)$
- For $1s, 2p, 3d, 4f$, R has no node, their maxima are thus closer to the nucleus
- $3d$ and $4f$ orbitals are more localized.

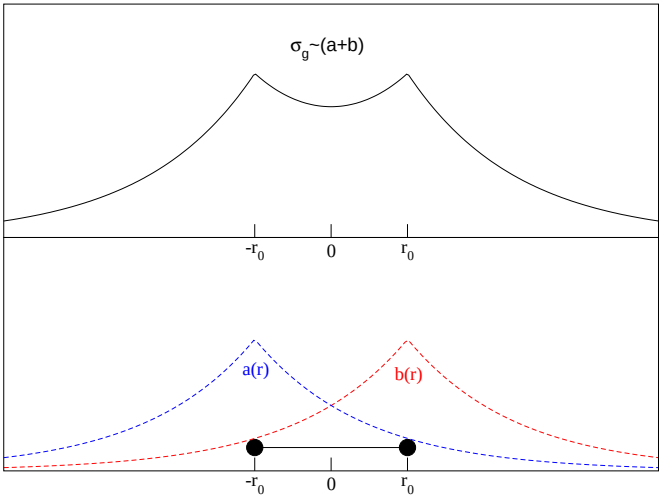
Hydrogen Molecule

antibonding state $\sigma_u = \frac{a-b}{\sqrt{2}}$



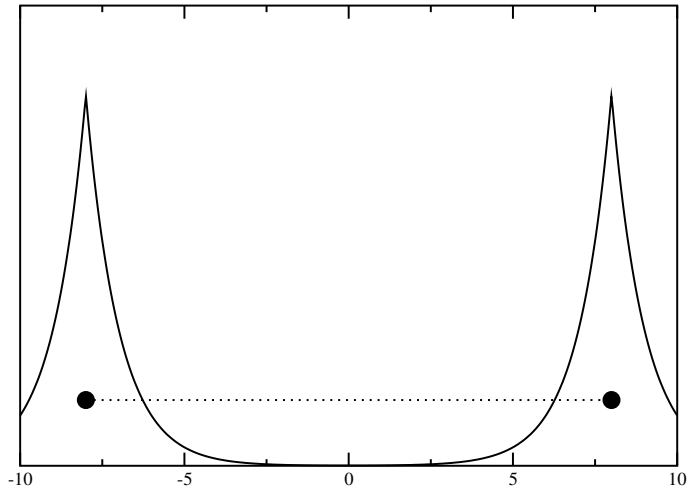
bonding state $\sigma_g = \frac{a+b}{\sqrt{2}}$

Hydrogen molecule: molecular orbital.

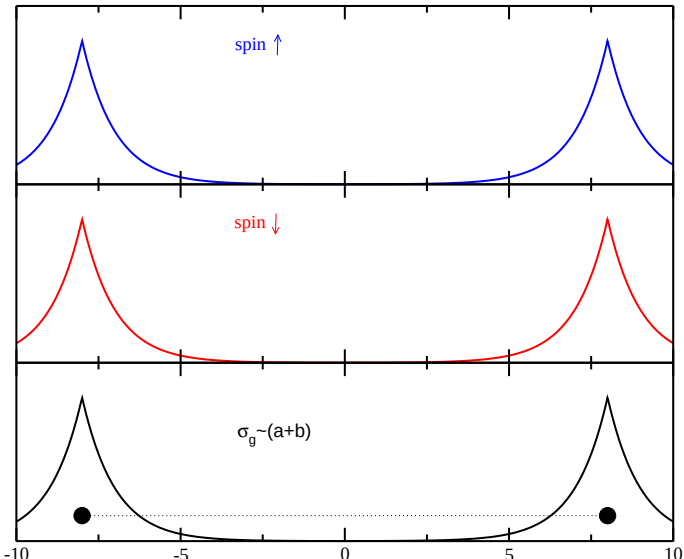


$$\sigma_g = \frac{a+b}{\sqrt{2}}$$

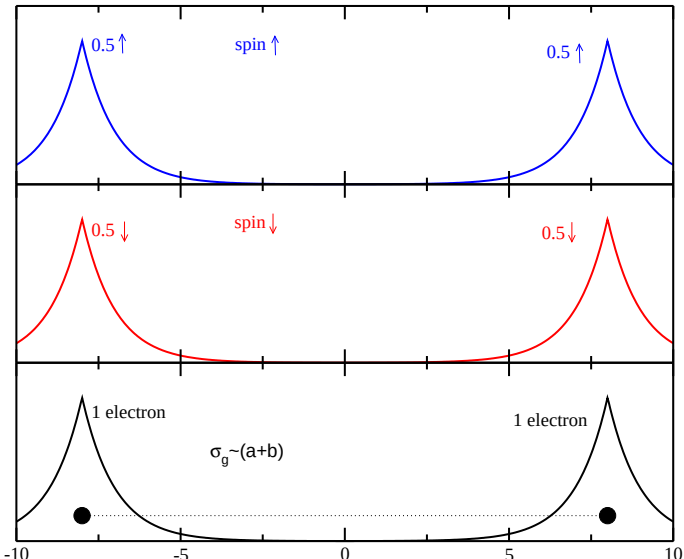
Hydrogen molecule: stretched.



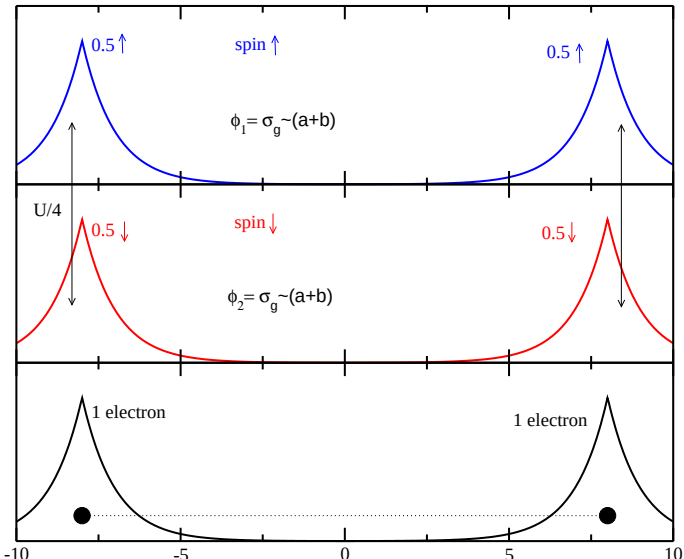
Hydrogen molecule: same orbital for both spins !



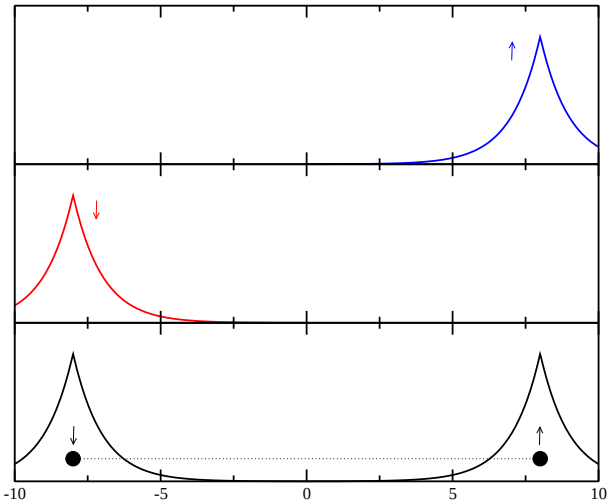
Hydrogen molecule: same orbital for both spins !



Hydrogen molecule: dissociation limit is bad



A solution: break symmetry

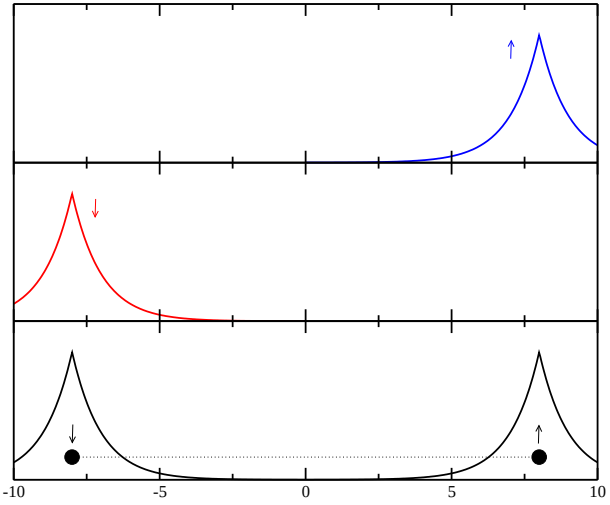


no more artificial delocalization, no more interaction

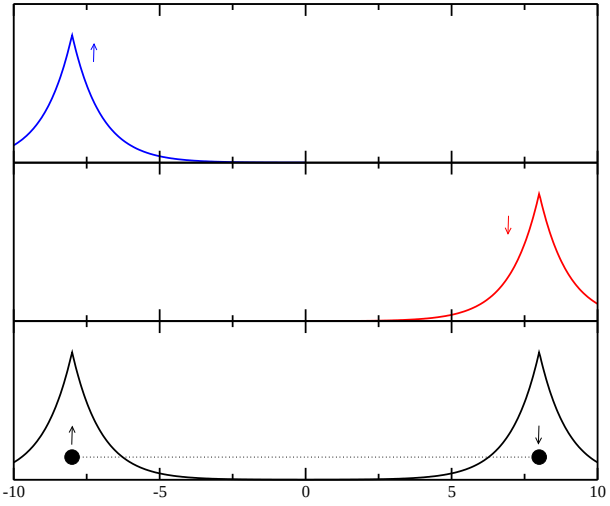
But

- Symmetry breaking. An artificial magnetism is induced.
- A static theory, which overestimates localization.

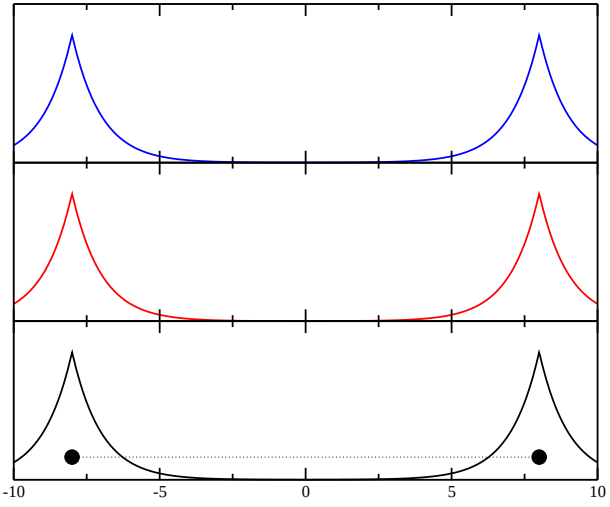
Solution 1: localization: lowers interaction



Solution 2: localization: lowers interaction



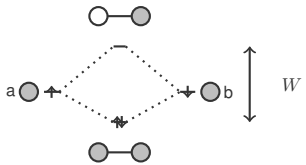
Solution 3: delocalization: lowers kinetic energy



The exact solution

$$|\Psi\rangle = c_1|1 : \text{localized} \uparrow\downarrow\rangle + c_2|2 : \text{localized} \downarrow\uparrow\rangle + c_3|3 : \text{delocalized}\rangle$$

- This mixing of configuration correctly describes the system (magnetism, structural properties).
  - $c_1 = c_2$: no ordered magnetism.
  - c_3 increases if distance between atoms lowers.
- Localized state increases if $U/W > 1$.



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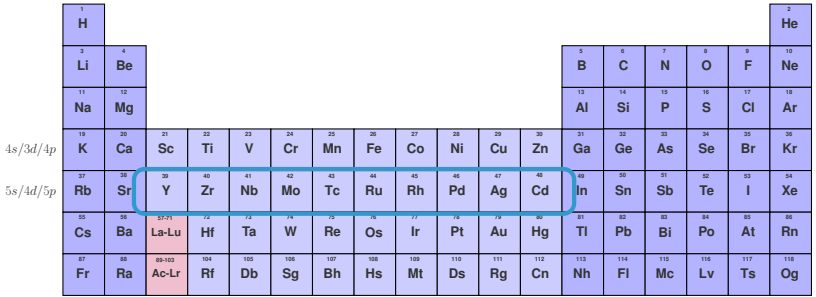
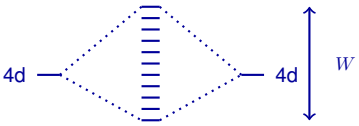
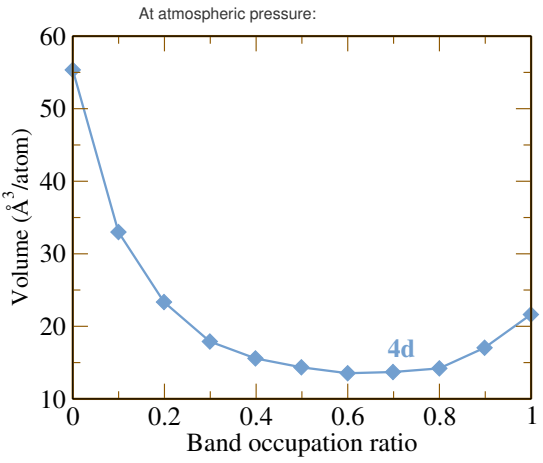


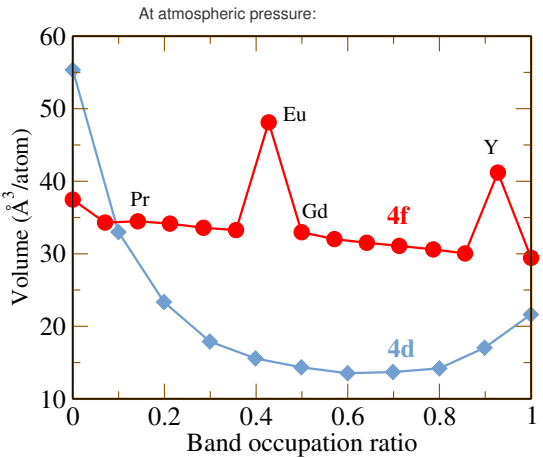
Localization in f electrons systems





[Mac Mahan, et al J. Comp.-Aid. Mater. Des. 5, 131 (1998)]

Localization in f electrons systems



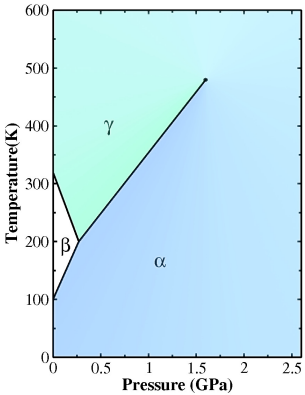
[Mac Mahan, et al J. Comp.-Aid. Mater. Des. 5, 131 (1998)]

Isostructural transition in Cerium

Isostructural transition $\frac{V_\gamma - V_\alpha}{V_\gamma} = 15\%$, ends at a critical point

Electronic configuration $4f^1$.

- α phase: Pauli paramagnetism
  - $\Rightarrow$ α phase: f e^- more delocalized.
- γ phase: Curie Paramagnetism
  - $\Rightarrow$ γ phase: f e^- is localized



[Johansson, B. Phil. Mag. **30**, 469 (1974)]

Transition in lanthanides.

We now discuss the equation of states of lanthanides as a function of pressure.

- At low pressure, compact structures.
- Under pressure, more distorted structure
  - f electrons participate to the bonding

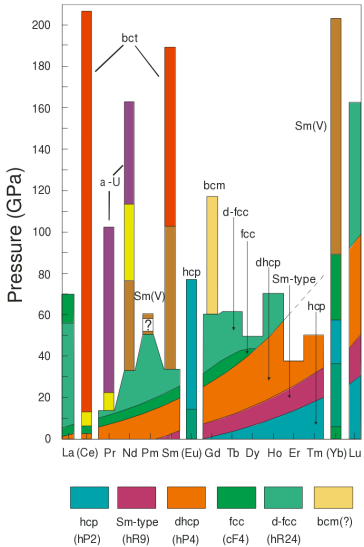


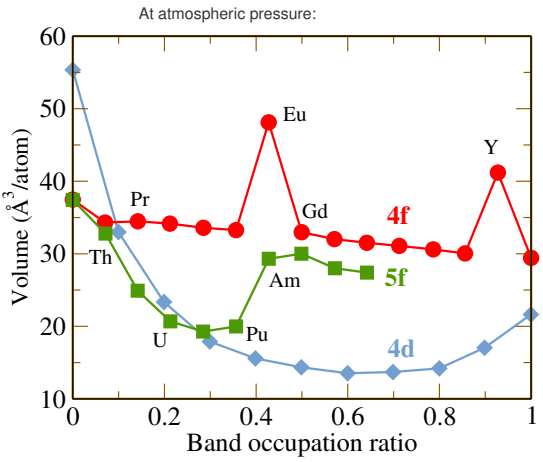
Figure from [Schiwek, (2002)]

Localization in f electrons systems

$4d$ element: filling of the $4d$ band (Bonding states and antibonding): $4d$ electrons are **delocalized**.

Lanthanides: $4f$ electrons **localized**, negligible overlap between $4f$ orbitals .

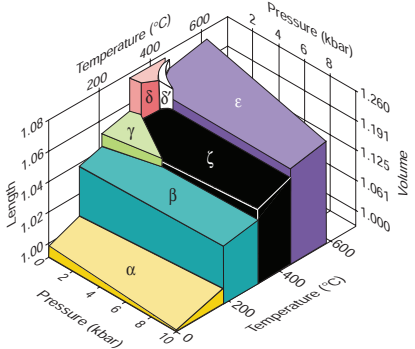
Actinides: intermediate case of localization.



[Mac Mahan, et al J. Comp.-Aid. Mater. Des. 5, 131 (1998)]

PLUTONIUM: A LARGE NUMBER OF PHASES.

- Many phases
- Some phases with delocalized electrons (low volume) and phases with localized electrons (large volume).



From Kevin T. Moore and Gerrit van der Laan Rev. Mod. Phys. 81, 235 (2009)

THE EXACT HAMILTONIAN

The exact hamiltonien is:

$$H = \sum_{i=1}^{N} [-\frac{1}{2}\nabla_{\mathbf{r}_i}^2 + V_{\text{ext}}(\mathbf{r}_i)] + \frac{1}{2}\sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

It can be exactly rewritten in second quantization as:

$$H = \sum_{i,j} \langle i|h|j\rangle c_i^\dagger c_j + \sum_{i,j,k,l} \langle ij|v|kl\rangle c_i^\dagger c_j^\dagger c_k c_l$$

If interactions are purely local (as in lanthanides), one can write a simplified Hamiltonian as:

$$H = \underbrace{\sum_{\mathbf{R},\mathbf{R}'} t_{\mathbf{R},\mathbf{R}'} c_{\mathbf{R}}^\dagger c_{\mathbf{R}'}}_{\text{one electron term : delocalization}} + \underbrace{\sum_{\mathbf{R}} U \hat{n}_{\mathbf{R}\uparrow} \hat{n}_{\mathbf{R}\downarrow}}_{\text{interaction term : localization}}$$

Now, we have a parameter to describe the Coulomb interaction which is called U.

Competition between delocalization and localization

The Hubbard model: Competition between localization and delocalization

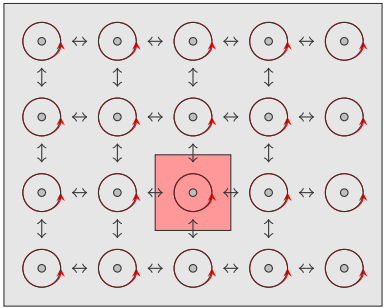
$$H = \underbrace{\sum_{\mathbf{R},\mathbf{R}'} t_{\mathbf{R},\mathbf{R}'} c^{\dagger}_{\mathbf{R}} c_{\mathbf{R}'}}_{\text{one electron term : delocalization}} + \underbrace{\sum_{\mathbf{R}} U \hat{n}_{\mathbf{R}\uparrow} \hat{n}_{\mathbf{R}\downarrow}}_{\text{interaction term : localization}}$$

U is the energy repulsion of two electrons on the same site.

- For large value of the interaction U, electrons are localized
- For low value of the interaction U, electrons are delocalized

Dynamical Mean Field Theory

The Hubbard model physics can be mimicked by an Anderson model + Self-consistency



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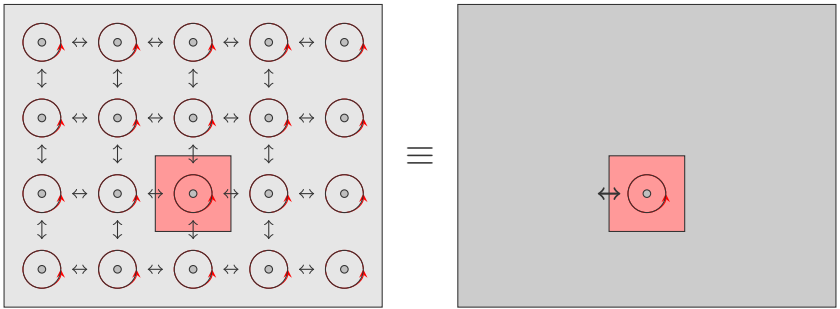

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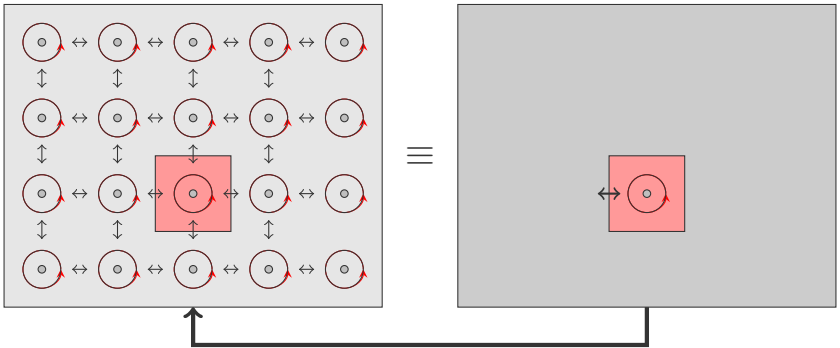
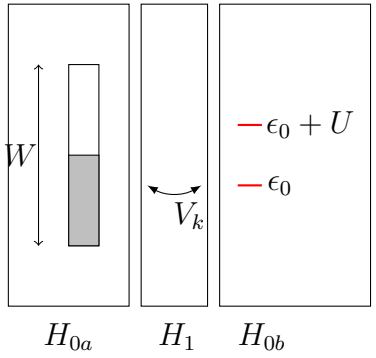


W. Metzner and D. Vollhardt Phys. Rev. Lett. 62 (3) 324 (1989)
A. Georges and G.Kotliar Phys. Rev. B 45 (12) 6479 (1992)
Antoine Georges, Gabriel Kotliar, Werner Krauth, and Marcelo J. Rozenberg Rev. Mod. Phys. 68, 13 (1996)

Anderson Hamiltonian in the DMFT



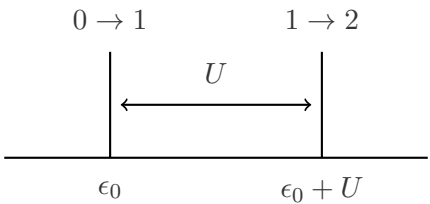
$$H_{\text{Anderson}} = \underbrace{\sum \omega_k a^+_{k,\sigma} a_{k\sigma}}_{H_{0a}} + \underbrace{\sum_{k,\sigma} V_k (a^+_{k,\sigma} c_\sigma + c^+_\sigma a_{k,\sigma})}_{H_1} + \underbrace{\epsilon_0 (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow}_{H_{0b}} \quad (1)$$

Anderson Hamiltonian with $V_k = 0$: Hubbard bands

The isolated atom limit: $V_k = 0$

$$H = Un_\uparrow n_\uparrow + \epsilon_0(n_\uparrow + n_\downarrow) = Un_\uparrow n_\uparrow + \epsilon_0(n_\uparrow + n_\downarrow)$$

- 0 electron: $|0\rangle$:$E = 0$
- 1 electron: $|\uparrow\rangle$ and $|\downarrow\rangle$: $E = \epsilon_0$
- 2 electrons: $|\uparrow\downarrow\rangle$: $E = 2\epsilon_0 + U$



Anderson Hamiltonian with $U = 0$.

The hamiltonian writes:

$$H_{\text{Anderson}} = \sum \omega_k a^+_{k,\sigma} a_{k\sigma} + \sum_{k,\sigma} V_k (a^+_{k,\sigma} c_\sigma + c^+_\sigma a_{k,\sigma}) + \epsilon_0 (n_\uparrow + n_\downarrow)$$

H is:

$$\begin{pmatrix} \epsilon_0 & V_1 & ... & V_k & ... & V_N \\ V_1 & \omega_1 & 0 & 0 & 0 & 0 \\ .... & 0 & ..... & 0 & 0 & 0 \\ V_k & 0 & 0 & \omega_k & 0 & 0 \\ ... & 0 & 0 & 0 & ..... & 0 \\ V_N & 0 & 0 & 0 & 0 & \omega_N \end{pmatrix}$$

This hamiltonian contains the hybridization of a single level ϵ_0 to other levels. The level with move and will be broadened by hybridization on other levels.

$$(\omega I - H)G = I \tag{2}$$

Anderson Hamiltonian with $U = 0$.

H is:

$$\begin{pmatrix} \epsilon_0 & V_1 & ... & V_k & ... & V_N \\ V_1 & \omega_1 & 0 & 0 & 0 & 0 \\ .... & 0 & ..... & 0 & 0 & 0 \\ V_k & 0 & 0 & \omega_k & 0 & 0 \\ ... & 0 & 0 & 0 & ..... & 0 \\ V_N & 0 & 0 & 0 & 0 & \omega_N \end{pmatrix}$$

$$G = (\omega I - H)^{-1} \tag{3}$$

We can easily inverse this matrix and compute the Green's function of the correlated orbital (Using $A^{-1} = \mathrm{Com}(A)^T / \mathrm{det}A$ to inverse $I - H$). We obtain:

$$G(\omega) = \frac{1}{\omega - \epsilon_0 - \Delta(\omega)} \quad \text{with} \quad \Delta(\omega) = \sum_k \frac{V_k^2}{\omega - \omega_k} \tag{4}$$

Where $\Delta(\omega)$ is called the hybridization function.

Anderson Hamiltonian with $U = 0$.

We can now compute the spectral function of this system by computing:

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}G^R(\omega + i\delta) \tag{5}$$

We need

$$\Delta(\omega + i\delta) = \sum_k \frac{V_k^2}{\omega - \omega_k} - i\pi \sum_k |V_k|^2 \delta(\omega - \omega_k) \tag{6}$$

If $\Delta = 0$, then the spectral function has a peak at ϵ_0. Using the last two equations, the peak at ϵ_0 in the spectral function will be shifted by the real part of Δ and will be broadened by the imaginary part of Δ. Interestingly, the imaginary part of Δ recovers the Fermi golden rule (width of the level coupled to the continuum is $\pi \sum_k |V_k|^2 \delta(\omega - \omega_k)$).

Anderson Hamiltonian: one orbital for the bath.

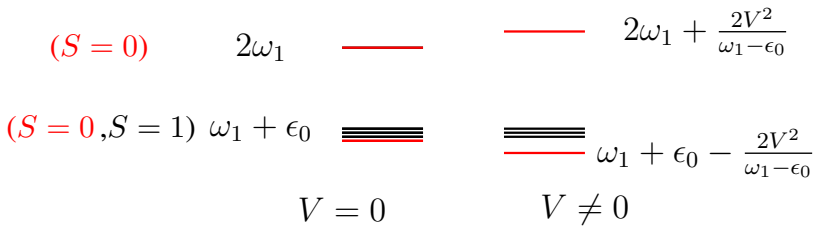
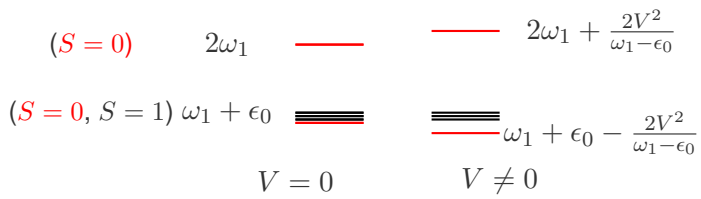


FIGURE: Two electrons levels with $V = 0$ and V small

What is it ?

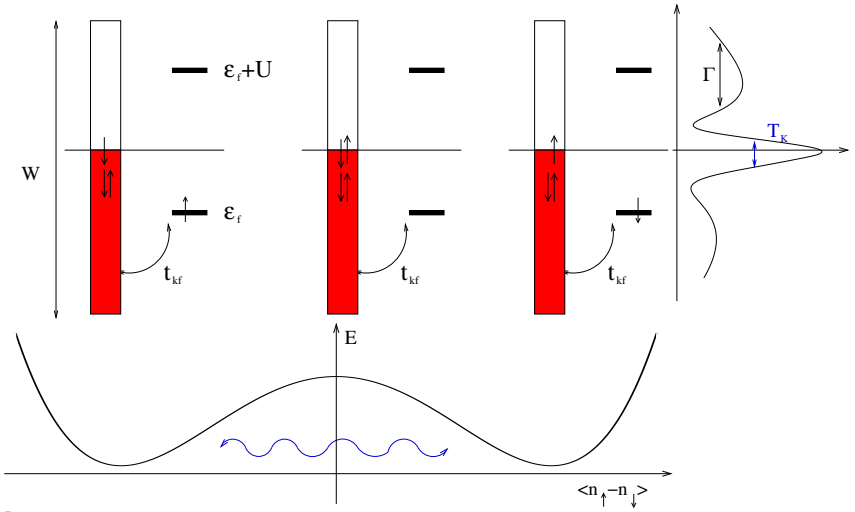
The Anderson model: W→0 limit: (molecule)



Two orbitals l and f coupled with $V << (\epsilon_l - \epsilon_f)$
The f orbital is correlated ($U >>$) $\rightarrow$ double occupancy is forbidden
$V = 0 \Rightarrow$ 4 states with one electron in each orbitals: 1 singlet and one triplet
one excited state singlet with 2 electrons in l
$V \neq 0 \Rightarrow$ coupling between singlets: stabilization $\leftrightarrow$ Temperature T^*
$T << T^*$ Spin excitations at low energy.
Charge excitation $f \rightarrow l$.
$T >> T^*$ Singlet and triplet equally populated.
Magnetic moment starts to appear.

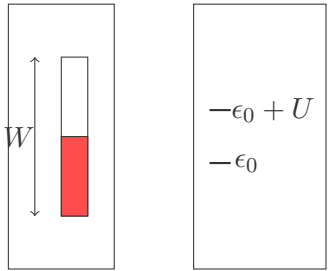
cf Fulde *Electron Correlations in Molecules and Solids*

The Anderson model: general case



[cf L. Kouwenhoven et L. Glazman, Physics World Jan 2001 p33]

The Anderson Hamiltonian (solved by CTQMC)



E Gull, AJ Millis, AI Lichtenstein, AN Rubtsov, M Troyer, P Werner Reviews of Modern Physics 83 (2), 349 (2011)

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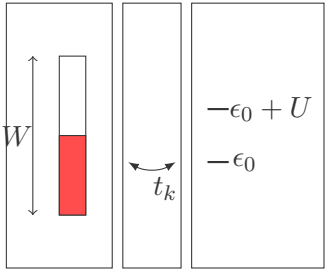

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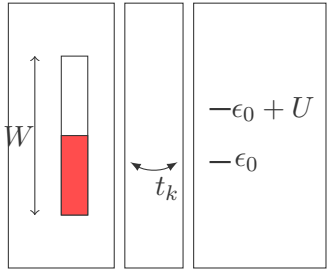

$$H_{\text{Anderson}} = \underbrace{\sum \omega_k a^+_{k,\sigma} a_{k\sigma}}_{H_{0a}} + \underbrace{\sum_{k,\sigma} t_{kf} a^+_{k,\sigma} f_\sigma}_{H_1} + \underbrace{\sum_\sigma \epsilon_f f^+_\sigma f_\sigma + U n_{f\uparrow} n_{f\downarrow}}_{H_{0b}}$$

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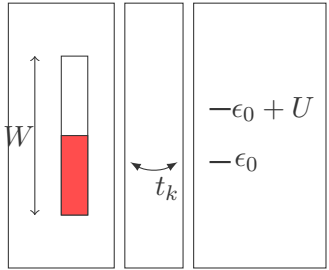

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Continuous Time Quantum Monte Carlo: Expansion as a function of H_1

[P. Werner, A. Comanac, L. de medici, M. Troyer and A. J. Millis Phys. Rev. Lett. 97, 076405 (2006)] E Gull, AJ Millis, AI Lichtenstein, AN Rubtsov, M Troyer, P Werner Reviews of Modern Physics 83 (2), 349 (2011)

The self consistency condition and the DMFT loop

Using the equation of Motion of the Green's function $(\omega - H - \Sigma)G = 1$, the lattice Green's function for the Hubbard model is written:

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)}$$

where the self energy is unknown. The local Green's function of the lattice is

$$G_{ii}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} \mathrm{e}^{ik(T_i - T_i)} G_{\mathbf{k}}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}}(\omega)$$

The self consistency condition and the DMFT loop

Besides, the Green's function for the Anderson impurity model is

$$G_{\text{Anderson}}(\omega) = \frac{1}{\omega - \epsilon_0 - \Delta(\omega) - \Sigma(\omega)}$$

The DMFT idea is to identify the local Green's function of the Hubbard model with the Green's function of Anderson model and the self energy of the Hubbard model to be equal to the self energy of the Anderson model it is the **self-consistency relation** of DMFT.

The self consistency condition and the DMFT loop

This implies in particular that the local one particle excitations of the Hubbard model will be the same as the one particle excitations of the Anderson model. This writes:

$$\frac{1}{N}\sum_{k}\frac{1}{\omega-\epsilon_{\mathbf{k}}-\Sigma(\omega)}=\frac{1}{\omega-\epsilon_0-\Delta(\omega)-\Sigma(\omega)}$$

This equation enables us to find $\Delta(\omega)$ as a function of the self energy: $\Delta=\Delta[\Sigma]$ and also $\epsilon_0=\frac{1}{N}\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}$[1]
Besides, the solution of the Anderson model enables us to have the self energy from the value of ϵ_0 and Δ. So this creates a system of two equations that can be solved self-consistently. These two equations constitute the DMFT self-consistent loop that can be solved by iteration.

Phase diagram of Hubbard model in DMFT

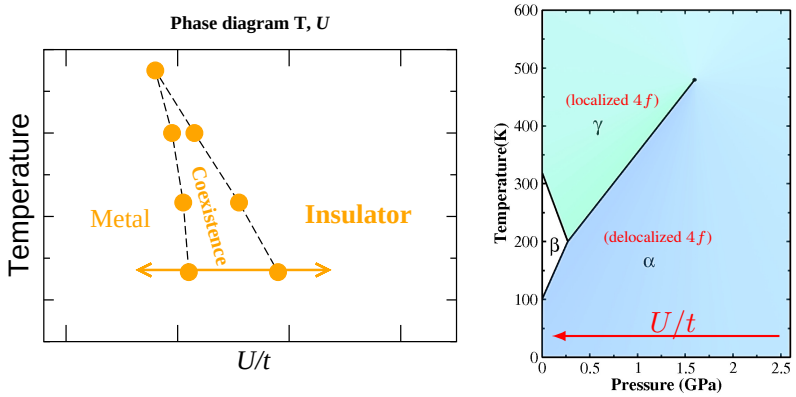
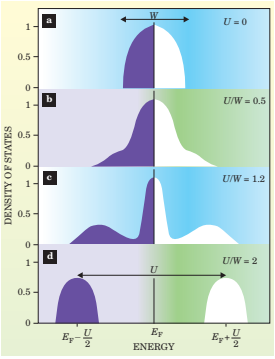
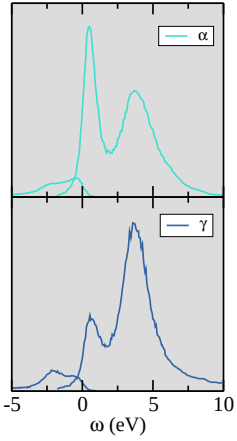


FIGURE: Phase diagram of the Hubbard model in DMFT compared to phase diagram of Cerium.

Spectral function of Hubbard model in DMFT

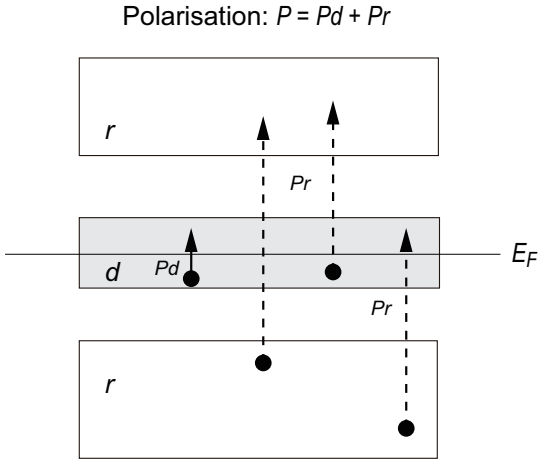




[G.Kotliar *et al* Phys. Today, AIP, 57, 53-59 (2004)]

[E. Weschke, *et al* Phys. Rev. B 44, 8304 (1991)
M. Grioni, *et al* Phys. Rev. B 55, 2056 (1997)]

Calculation of effective interactions with cRPA



$$\epsilon_r^{-1} \hat{=} \frac{1}{1 - vP_r}$$

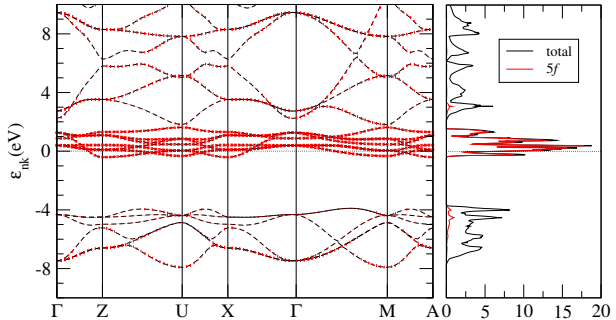
$$W_r = \epsilon_r^{-1} v = \frac{v}{1 - vP_r}$$

$$U_{1234}(w) = \langle w_1 w_2 | W_r(w) | w_3 w_4 \rangle$$

F Aryasetiawan, M Imada, A Georges, G Kotliar, S Biermann, AI Lichtenstein PRB 2004

Effective interactions in UO_2

model	v	U
$f-f$	16.0	3.4
$fp-fp$	17.1	6.2



Bare interaction for $SrVO_3$ is 19.1 eV, for cerium 24 eV and for UO_2 16.1 eV (Amadon et al 2014). It highlights the large localization of orbitals in lanthanides and the fact that interaction in actinides is lower.

DFT+DMFT

Can be formulated using the basis of DFT Kohn Sham function $\Psi_{\mathbf{k}\nu}$ and correlated orbitals $\chi_{\mathbf{T}_i m}$.

$$H_{\mathrm{LDA}} = \sum_{n\mathbf{k}} |\Psi_{\mathbf{k}\nu}\rangle \epsilon_{n\mathbf{k}} \langle \Psi_{\mathbf{k}\nu}|$$

$$\Sigma = \sum_{mm'\mathbf{T}_i} |\chi_{\mathbf{T}_i m}\rangle \Sigma_{m,m'}(\omega) \langle \chi_{\mathbf{T}_i m'}|$$

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

$$\Sigma = \sum_{mm'\mathbf{k}} |\chi_{\mathbf{k}m}\rangle \Sigma_{m,m'}(\omega) \langle \chi_{\mathbf{k}m'}|.$$

It can be expressed in the Kohn Sham basis directly using the fact that $\langle \Psi_{\mathbf{k}\nu}|\chi_{\mathbf{k}'m}\rangle$ is zero if $\mathbf{k}$ and $\mathbf{k}'$ are different,

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

DFT+DMFT

$$\Sigma = \Sigma_{\mathrm{DMFT}} - \Sigma_{\mathrm{DC}}.$$

$$(\omega I - H - \Sigma)G = I.$$

$$G_{nn'}(\mathbf{k},\omega) = \left[\omega I - H(\mathbf{k}) - \Sigma(\mathbf{k},\omega)\right]^{-1}\big|_{nn'},$$

The local Green's function is simply:

$$G^{\mathrm{loc}}_{mm'}(\omega) = \sum_{\mathbf{k}} \langle \chi_{\mathbf{k}m} | \Psi_{\mathbf{k}\nu} \rangle G_{nn'}(\mathbf{k},\omega) \langle \Psi_{\mathbf{k}\nu'} | \chi_{\mathbf{k}m'} \rangle$$

This equation is the generalisation of Eq. 7.

DFT+DMFT

The DMFT self-consistency relation equals the local Green's function and the Green's function of the Anderson model:

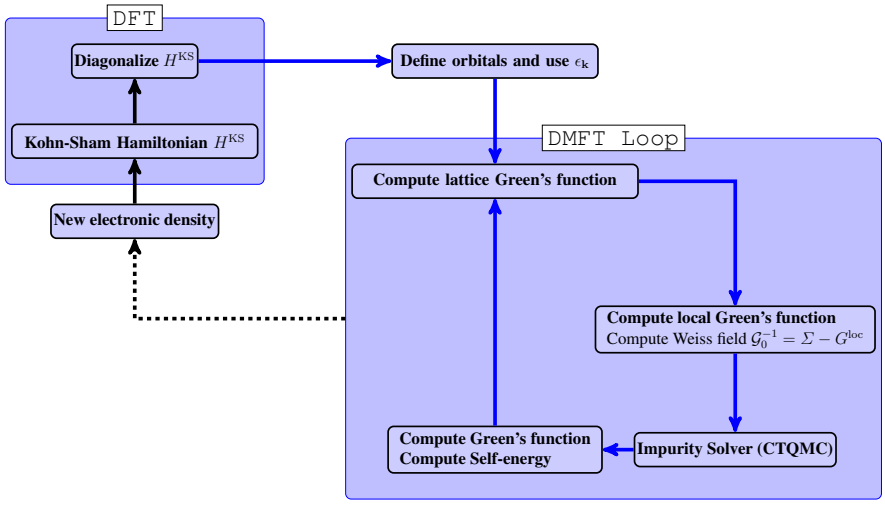
$$G^{\mathrm{loc}}_{mm'}(\omega) = G^{\mathrm{Anderson}}_{mm'}(\omega) \tag{7}$$

where

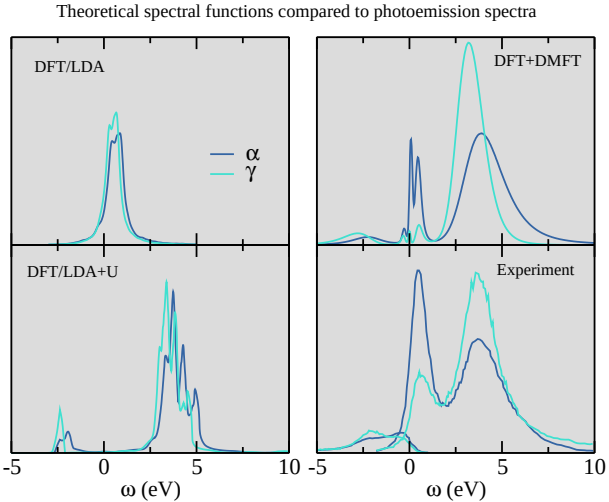
$$G^{\mathrm{Anderson}}_{mm'}(\omega) = \left[\omega I - E_0 - \Delta(\omega) - \Sigma(\omega)\right]^{-1}\Big|_{mm'} \tag{8}$$

E_0 is a diagonal matrix with the levels of correlated orbitals in the (multiorbital) Anderson model, Σ and Δ are the self-energy and hybridization matrices in the correlated orbital basis. E_0 and Δ are obtained from the self-consistency condition.

DFT+DMFT

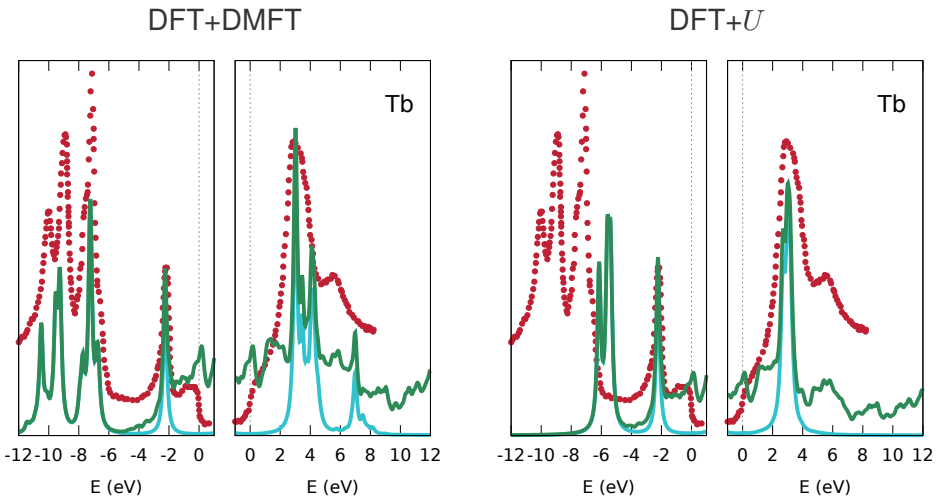

DFT
Diagonalize H^{KS}
Kohn-Sham Hamiltonian H^{KS}
New electronic density
Define orbitals and use $\epsilon_{\mathbf{k}}$
DMFT Loop
Compute lattice Green's function
Compute local Green's function
Compute Weiss field $\mathcal{G}_0^{-1} = \Sigma - G^{\mathrm{loc}}$
Impurity Solver (CTQMC)
Compute Green's function
Compute Self-energy

Spectral functions of cerium



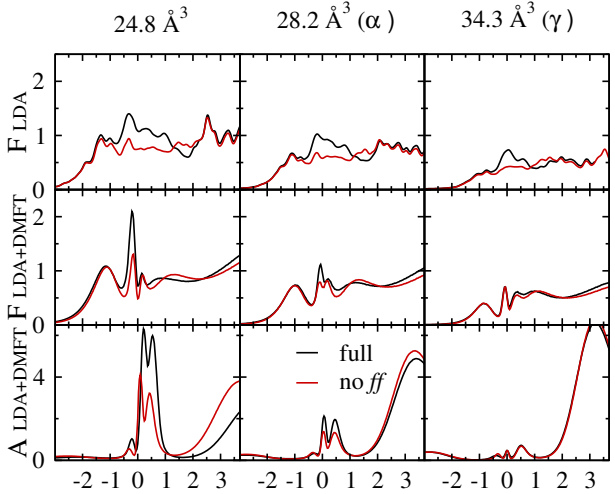
Amadon et al PRB 2015

Spectral functions of Tb



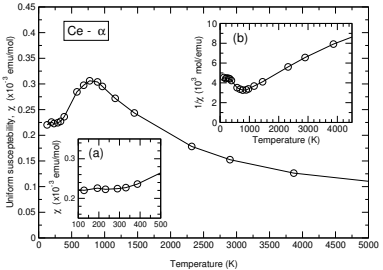
L. M. Locht et al, Phys. Rev. B 94, 085137 (2016)

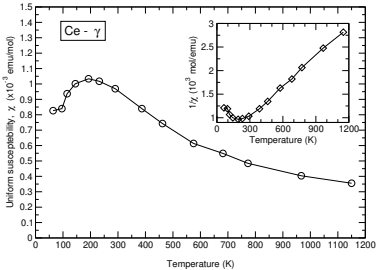
Relative role of ff and fd hoppings



B. Amadon and A. Gerossier, Phys. Rev. B 91, 161103 (2015)

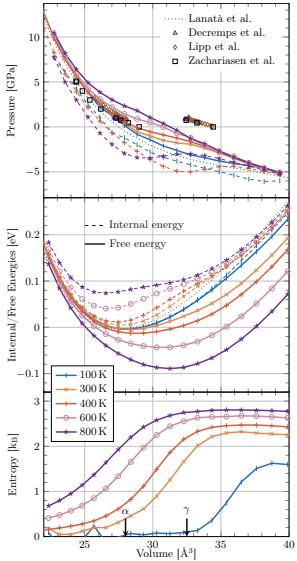
Magnetic susceptibility





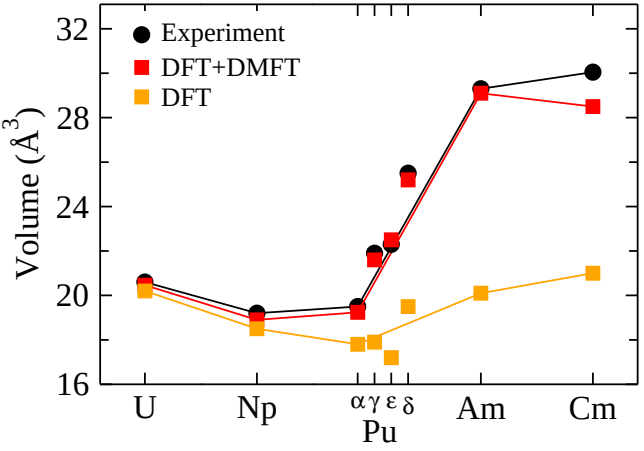
S. V. Streltsov, E. Gull, A. O. Shorikov, M. Troyer, V. I. Anisimov, and P. Werner, Phys. Rev. B 85, 195109 (2012)

Cerium phase transition in DMFT



J. Bieder and B. Amadon PRB 2014
see also K. Haule and T. Birol, Phys. Rev. Lett. 115, 256402 (2015).

Actinides in DMFT

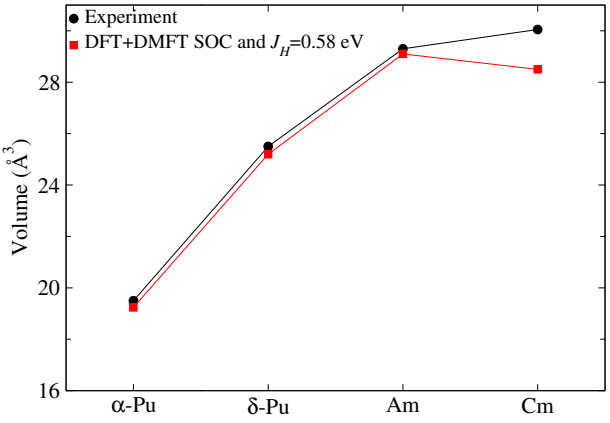


B. Amadon PRB (2016)

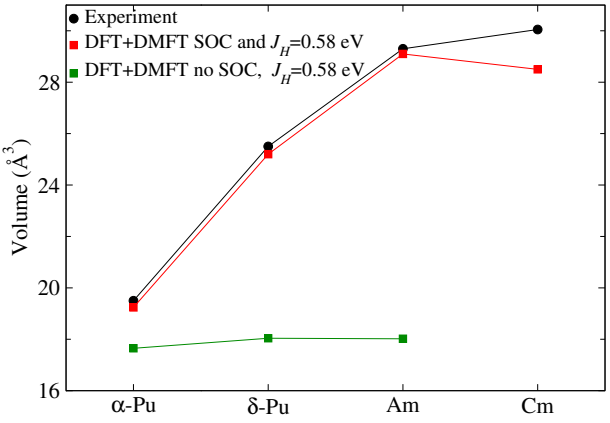
Electronic origin of the transition ?

Role of SOC and J_{H} ?

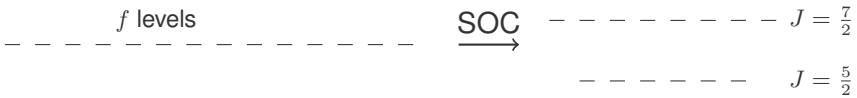
Role of spin-orbit coupling



Spin-orbit coupling is mandatory !

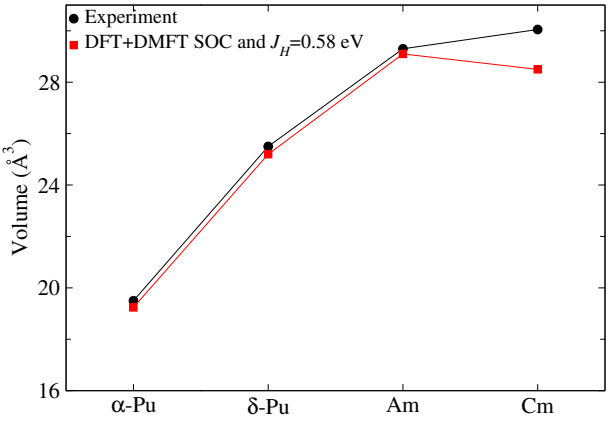


Effect of SOC on f levels.

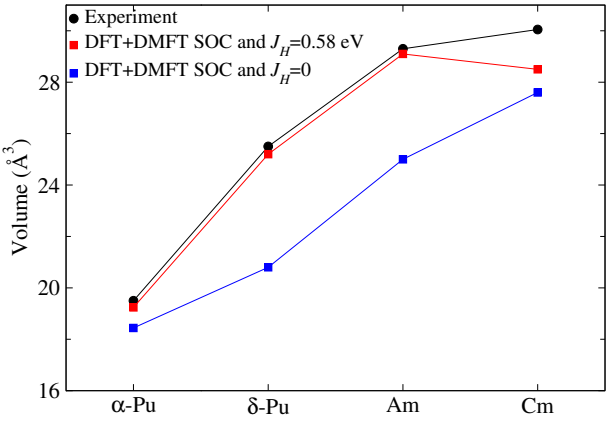


- As in multibands Hubbard models, degeneracy is reduced, thus correlations are enhanced.

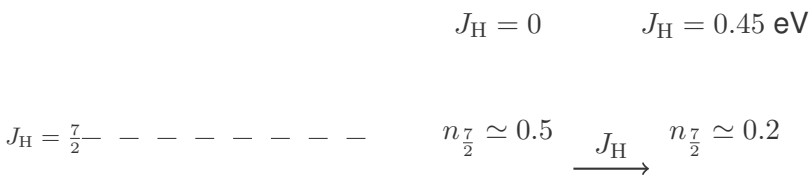
Hund's Exchange is important



Hund's exchange is important



Role of J_{H} in δ Plutonium



- Hund's coupling J_{H} increases the polarization of $\frac{5}{2}$ orbitals.
- why ?

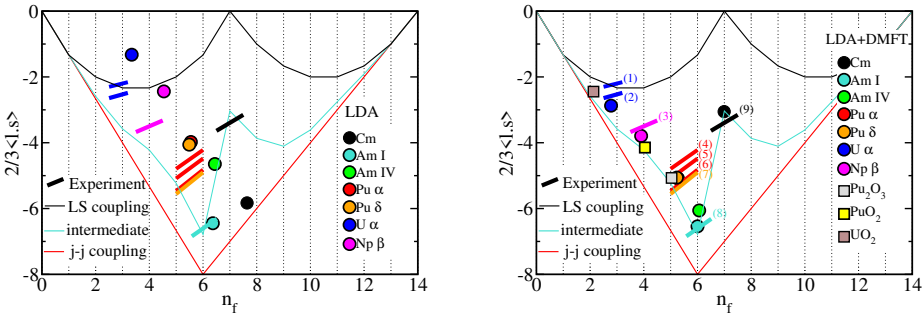
J_{H} enhances the polarization of J=5/2 orbitals.

$$E = U_{\frac{5}{2}\frac{5}{2}} \qquad E = U_{\frac{5}{2}\frac{7}{2}} + \lambda_{\mathrm{SOC}}$$

$U_{\frac{5}{2}\frac{7}{2}} > U_{\frac{5}{2}\frac{5}{2}} \Rightarrow$ The occupations of $\frac{7}{2}$ states is reduced not only by SOC but also by Hund's interaction.

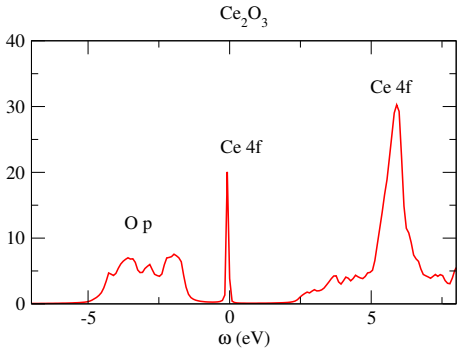
For interactions, see also J.-P. Julien, J.-X. Zhu, and R. C. Albers, Phys. Rev. B 77, 195123 (2008)

Actinides in DMFT



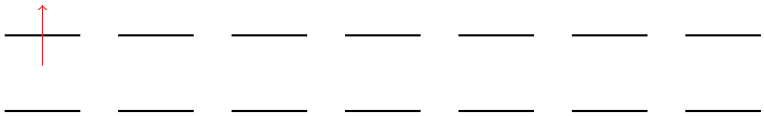
J. H. Shim, K. Haule, and G. Kotliar, EPL (Europhysics Letters) 85, 17007 (2009)

Spectral function in Ce_2O_3



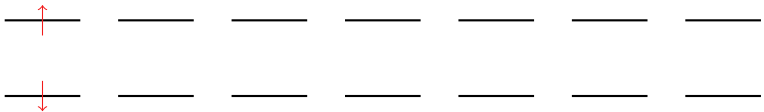
B. Amadon JPCM (2012)

DFT+DMFT can describe paramagnetic insulators



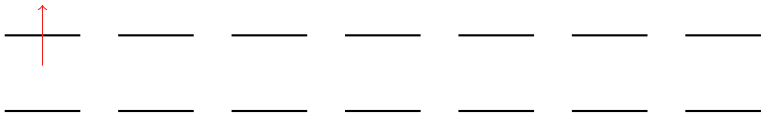
DFT+U: a configuration

DFT+DMFT can describe paramagnetic insulators



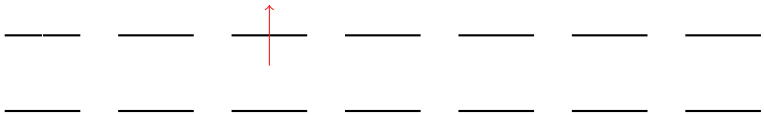
DFT+U: an instable configuration

DFT+DMFT can describe paramagnetic insulators



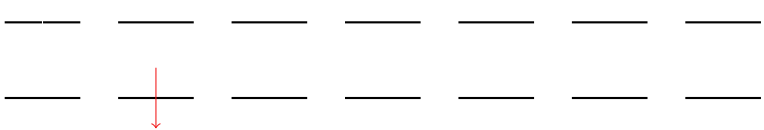
DFT+U: a configuration

DFT+DMFT can describe paramagnetic insulators



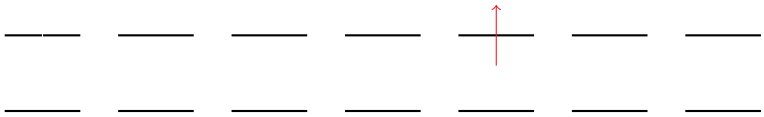
DFT+U: another configuration

DFT+DMFT can describe paramagnetic insulators



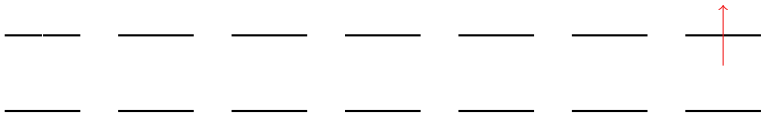
DFT+U: another configuration

DFT+DMFT can describe paramagnetic insulators



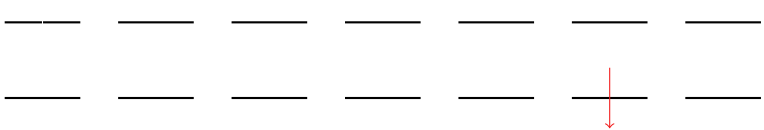
DFT+U: another configuration

DFT+DMFT can describe paramagnetic insulators



DFT+U: another configuration

DFT+DMFT can describe paramagnetic insulators



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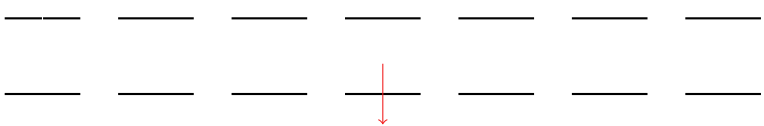

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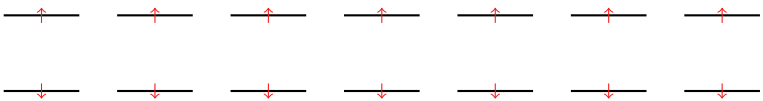
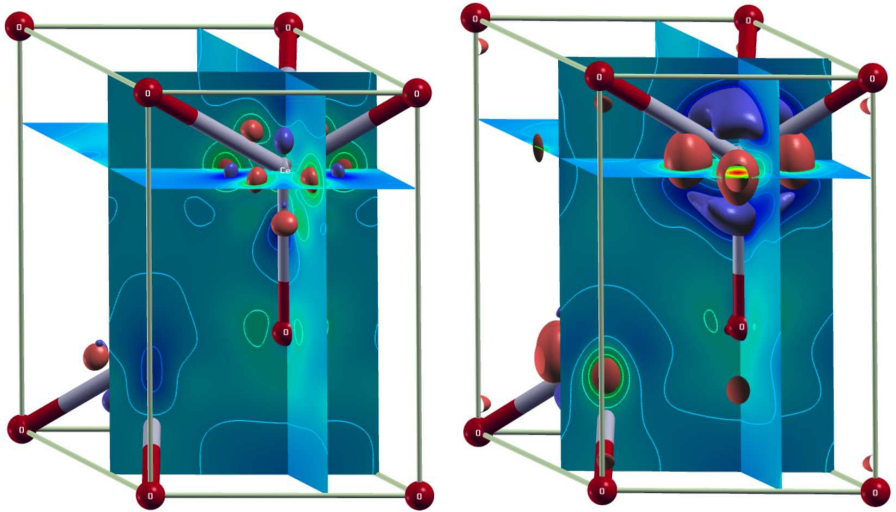


DFT+DMFT: More physical description

DFT+DMFT: Better description of magnetism

Electronic density in Ce_2O_3



B. Amadon JPCM (2012)

- f-electron systems exhibit significant orbital localization for lanthanides and comparatively lesser localization for actinides.
- As a consequence electrons are sensible to electronic interaction and somewhat less to crystal field in comparison to d elements.
- Spin orbit coupling is important for these heavy elements.
- Because of the competition of interaction and hybridization, phases transitions can appear as a function of pressure or temperature.