An introduction to Dynamical Mean Field Theory (DMFT) and DFT+DMFT

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Contents

In these notes, I present a brief introduction to strong correlations in solid state physics, to Dynamical Mean Field Theory (DMFT) and to the combination of Density Functional Theory (DFT) and DMFT (See also references [1], [2], and [3]).

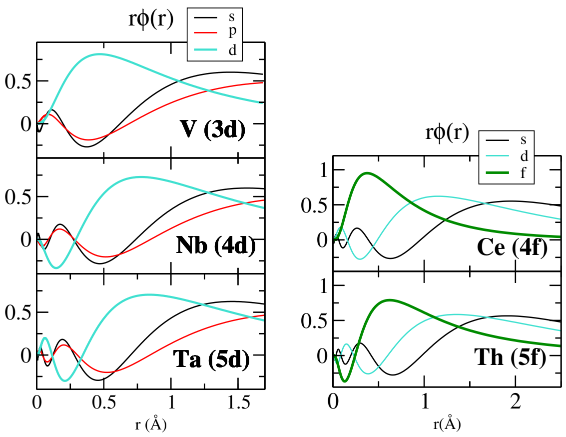


Figure 1: Radial part of valence wavefunctions of some atoms (computed in DFT/LDA).

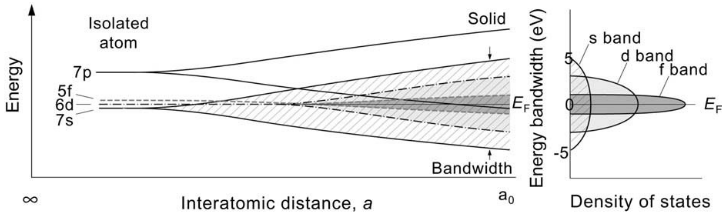


Figure 2: Schematic bandwidth from some orbitals as a function of pressure: the more localized are the orbitals, the smaller is the bandwith.

1 Introduction to strong correlation: localized orbitals

1.1 Atomic orbitals

We first discuss atomic physics, to understand which orbitals are localized and we will see the consequences in the next subsection. Let's analyse the spatial localization of orbitals as a function of their quantum numbers. First, $1s$, $2p$ and $3d$ and $4f$ orbitals are orthogonal to lower orbitals only through the angular part because for their value of l, they are the orbitals with the lowest principal quantum number. As a consequence, the radial part of the wavefunction is not constrained by orthogonality, and can lower its Coulomb interaction with the nucleus by being more localized. Moreover, the angular part has more an more nodal planes has l increases. As a consequence, in particular, $3d$, $4f$ are orbitals that are fairly localized in space (see Fig.1).

1.2 Localization or delocalization of electrons ?

Two consequences arise:

- When a solid is formed from atoms, the overlap of localized orbitals is weaker and thus the bandwidth W is smaller (see Fig. 2).
- The more localized are the orbitals, the stronger the local interactions "U" between electrons are, because electrons are closer to each other.

For the H_2 molecule, this competition leads to a change of the ground state as the interatomic distance increases. In particular, at large distance, the electrons are localized each on its atom to avoid

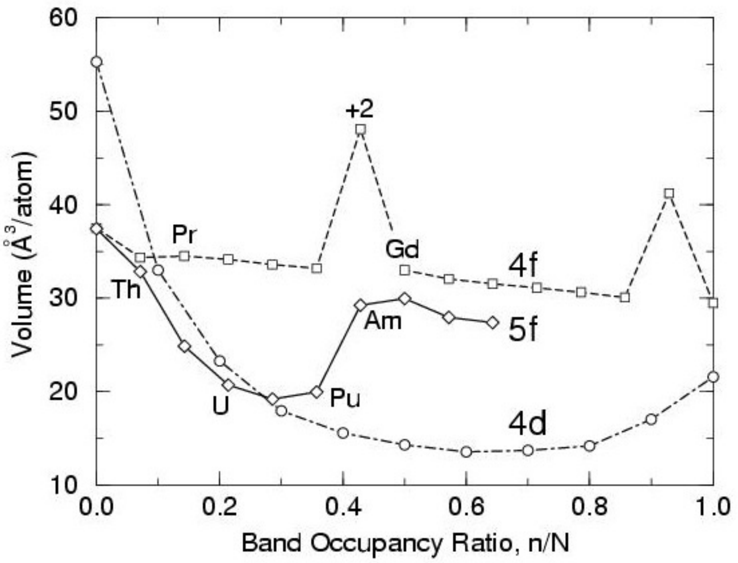


FIG. 2. Atmospheric pressure volumes of the $4d$ transition metals, the rare earths ($4f$), and the actinides ($5f$). The two rare earths with large volumes are divalent.

Figure 3: Evolution of volume of pure elements are a function of volume for some lines of the periodic table (Mac Mahan, Huscroft et al J. Comput.-Aided Mater. Des. 5, 131 (1998))

the Coulomb interaction with the other electrons (here $U > W$) (see also the lectures of Celestino Angeli and Emmanuel Fromager).

Let's see another consequence of this for solids on Fig. 3. It represents the evolution of volume of pure elements are a function of volume for $4d$, $4f$ and $5f$ elements.

- $4d$ orbitals are fairly delocalized, and form bands, thus, as Z increases, electrons fill the $4d$ band, first the bonding states and then antibonding states. As a consequence, the volume decreases and then increases. It thus show than $4d$ electrons are thus delocalized (or less localized than $4f$).
- Lanthanides: $4f$ electrons are localized, there is a negligible overlap between $4f$ orbitals. As a consequence, adding electrons inside the f bands has no effect on the cohesion of the cristal.
- Actinides: The localization appears at the middle of the serie. As Z increases, the $5f$ orbitals are more and more localized because of the attraction with the nucleus. In the middle of the series, the system choose to localize electrons to lower the energy.

2 The Hubbard model

In this section, we will study the Hubbard model, which is appropriate to study the localisation/delocalisation competition.

From the lecture of Emmanuel Fromager on second quantization, one can write the Hamiltonian as

$$H = \sum_{i} \langle i|h|j\rangle c_i^\dagger c_j + \sum_{i,j,k,l} \langle ij|v|kl\rangle c_i^\dagger c_j^\dagger c_k c_l \tag{1}$$

In this equation, i, j, k, l belongs to a complete one particle basis. If (1) the sums in this equation are restricted to only one orbital per atoms, (2) only on site interactions are kept, one can show that one recover the Hubbard model.

Exercice: Show how this expression reduces to the Hubbard model if the preceding conditions are fulfilled.

The Hubbard model writes:

$$H = \sum_i t_{ij} c_i^\dagger c_j + \sum_i \epsilon_0 (n_{i\uparrow} + n_{i\uparrow}) + \sum_i U n_{i\uparrow} n_{i\downarrow} \tag{2}$$

In this equation, as we have only one orbital per site, i, j refers to atomic sites. We will now try to understand two limits of this Hamiltonian.

2.1 Delocalization limit: $U/t << 1$

Let's suppose that we can neglect the interaction term.

$$H = \sum_i t_{ij} c_i^\dagger c_j + \epsilon_0 (n_{i\uparrow} + n_{i\downarrow}) \tag{3}$$

In this case, one can easily solve this non interacting Hamiltonian either by direct diagonalisation or by using Bloch states: We can define Bloch states $|k\rangle$ as

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_i |T_i\rangle \mathrm{e}^{ikT_i} \tag{4}$$

where $|T_i\rangle$ are atomic orbitals: $\langle r|T_i\rangle = \phi(r - T_i)$ on site i. We also have

$$|T_i\rangle = \frac{1}{\sqrt{N}} \sum_k |k\rangle \mathrm{e}^{-ikT_i} \tag{5}$$

We also have the change of basis for creation and annihilation operators:

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k c_k^\dagger \mathrm{e}^{-ikT_i} \tag{6}$$

$$c_i = \frac{1}{\sqrt{N}} \sum_k c_k \mathrm{e}^{ikT_i} \tag{7}$$

As a consequence, one can show (do it in Exercice) that:

$$H = \sum_k \epsilon_k c_k^\dagger c_k \tag{8}$$

with $\epsilon_k = \frac{1}{N} \sum_{ij} t_{ij} \mathrm{e}^{-ik(T_i - T_j)}$

Let now suppose that we are in one dimension, and t_{ij} is non zero only for neighboring atoms, in this case, we have (note that t is negative) the following dispersion relation which gives the energy of levels as a function of the value of k.

$$\epsilon_k = \epsilon_0 + 2t\cos(ka) \tag{9}$$

According to Bloch theorem, k must belong to the first Brillouin Zone $[-\frac{\pi}{a}, \frac{\pi}{a}]$, where a is the distance between atoms. We now suppose that we have one electron per atom, whereas there are two states per atoms. As a consequence, the band is half filled. The system is thus metallic and the Fermi levels is at ϵ_0.

Figure 4: For $U/t >> 1$, the cost of a hopping is $E(|\uparrow\downarrow\rangle) + E(|0\rangle) - 2E(|\uparrow\rangle) = U$

2.2 Localization limit: $U/t >>$

$$H = \sum_i U n_{i\uparrow} n_{i\uparrow} + \sum_i \epsilon_0 (n_{i\uparrow} + n_{i\downarrow}) \tag{10}$$

In this case, the Hamiltonian is a sum of Hamiltonians for independent atoms ! We thus have to solve the atomic problem.

The size of the Hilbert space for this system is four (2^2):

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

Let us now suppose that the system as one electron per atom. From the above energies, one can compute the cost associated to the hopping of one electron from one atom to another atom (see Fig. 4). The cost is U. The order of magnitude of U in a real system is a few eV. As a consequence, at room temperature, electrons will be localized and the system is called a Mott insulator. The insulating character comes from interactions and not from a band structure effect.

One can also compute the photoemission spectra, ie the energy to add $(E(|\uparrow\downarrow\rangle) - E(|\uparrow\rangle) = \epsilon_0 + U)$ or remove $(E(|\uparrow\rangle) - E(|0\rangle) = \epsilon_0)$ an electron. We see that the photoemission spectra (or spectral function) will have two peaks located at ϵ_0 and $\epsilon_0 + U$. The two peaks are separated by U which is thus the photoemission gap. These peaks are called Hubbard bands.

2.3 The Mott transition

From these two limits, one can deduce that as U/t will increase, the systems will change from a metal to a Mott insulator. This is the phenomenon of the Mott transition. But we need an approximation to find the solution for intermediate values of U/t.

3 The Anderson model

We would like to describe correctly the on-site Coulomb interactions which are essential to describe correctly the atomic limit. The first idea of DMFT is to mimic the Hubbard model by a correlated atom with the exact Coulomb interaction, embedded in a bath of uncorrelated orbitals (see Fig. 5). The effect of all the other atoms are gathered in the bath. This is a Anderson model[4] whose Hamiltonian writes:

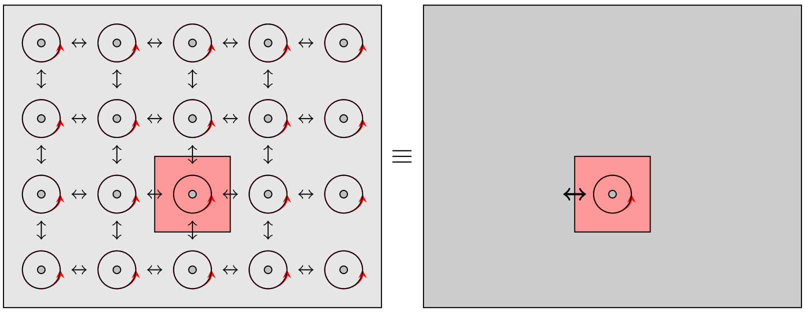
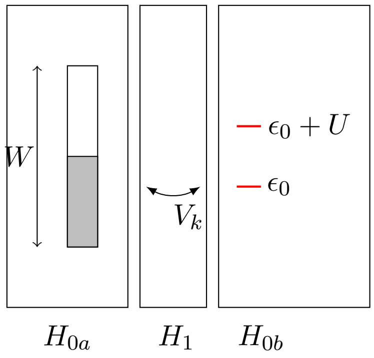


Figure 5: The first DMFT idea: The Hubbard model physics can be mimicked by an Anderson model



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

This is a mean field idea. However, we do not have only one electron in an effective field as in usual static mean field theory, but a whole many body atom whose interactions will be described exactly. Moreover the Anderson model will be defined self-consistently, but we will discuss this in the next section. We just focus in this section on the physics of the Anderson model. Once again, we are going to investigate several limiting cases for this Hamiltonian

3.1 The isolated atom limit: $V_k = 0$

This case is identical to the limit $U/t >> 1$ of the Hubbard model: the correlated atom is insulating.

3.2 The $U = 0$ limit

The hamiltonian writes:

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

This is again a non interacting system which can be solved easily: The atomic level will hybridize with the levels at ω_k, and will acquire a width.

Let's compute the Green's function of this system. We can use the equation of motion of the (non interacting) Green's function presented in the lecture of Fabien Bruneval, we thus have:

$$(\omega I - H) G = I \tag{11}$$

The dimension of these matrices is equal to N+1. It contains the N uncorrelated orbitals ω_k and the correlated orbital ϵ_0. The diagonal elements of H are the energies ω_k and ϵ_0. The only off diagonal terms are the coupling elements of the level at ϵ_0 to the levels at ω_k.

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

$$G = (\omega I - H)^{-1} \tag{12}$$

We can easily inverse this matrix and compute the Green's function of the correlated orbital

Exercice: Use the formula $A^{-1} = \mathrm{Com}(A)^T/\det A$ to compute the correlated level Green's function. We obtain:

$$G(\omega) = \frac{1}{\omega - \epsilon_0 - \sum_k \frac{V_k^2}{\omega - \omega_k}} \tag{13}$$

We now define the Hybridization function $\Delta(\omega)$ as:

$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega - \omega_k} \tag{14}$$

We can now compute the spectral function of this system by computing (see lecture of Xavier Blase):

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im} G^R(\omega + i\delta) \tag{15}$$

We need[1]

$$\Delta(\omega + i\delta) = \sum_k \frac{V_k^2}{\omega - \omega_k} - i\pi \sum_k |V_k|^2 \delta(\omega - \omega_k) \tag{16}$$

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. Interesting, the imaginary part of Δ recovers the Fermi golden rule (width of the level coupled to the continuum is $\pi \sum_k |V_k|^2 \delta(\omega - \omega_k)$).

3.3 The Anderson Molecule

We now simplify the bath by replacing it by a single level. We reproduce here the exemple detailed in Ref. [5].

We suppose that U is infinite so the double occupation of the localized level is impossible. Finally we limit our study to the states with 2 electrons. With these constraints, we have 5 possible states in the Hilbert space: the first is the double occupation of the bath level (this is a state with S=0) and there are four states with one electron in the bath level and one electron in the localized level. Among these four states, there are one triplet (S=1) and one singulet (S=0). If $V = 0$, then the four levels are degenerated. If the hybridization V is non zero, then the two states with $S = 0$ couple (see Fig. 3.3).

As a consequence we have a possible transition between the singlet and the triplet state at very low energy. This phenomenon has the same physical origin as the Kondo effect. It shows that a resonance exists even in a very strongly correlated system (U is large) and this resonance will be at the Fermi

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[1] We use $\lim_{\delta \to 0} \frac{1}{\pi} \frac{\delta}{x^2 + \delta^2} = \delta(x)$.

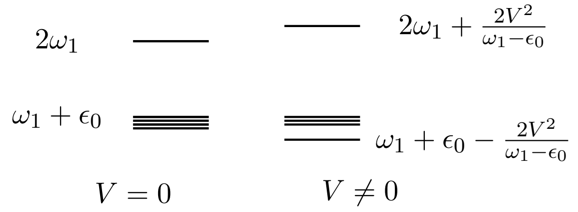

Figure 6: Two electrons levels with $V = 0$ and V small

level. We can define a temperature T^* corresponding to the difference of energy between the singlet and triplet state. Below this temperature, the system will exhibit the resonance, which will fade as temperature increases. Moreover, below this temperature, the magnetic moment of the localized level is completely cancelled by the formation of the singlet state.

Exercice: Compute the stabilization energy indicated in Fig 3.3. To do this, either you compute the eigenfunctions of the spin operators for S=0 and then you diagonalise a matrix of dimension 2 (see Ref.[5]). Or you can use the second quantization and write the variational wave function for the singlet as $|\Psi\rangle = (a_0 + a_1(c^\dagger_{0\uparrow}a_{1\uparrow} + c^\dagger_{0\downarrow}a_{1\downarrow}))|\Phi_0\rangle$ where $\Phi_0\rangle$ is a ground state with the orbital at ω_1 completely filled and solve the Schrödinger equation of our simple model for this variational wave function. It can be generalized to a large number of bath orbitals (see the discussion in Ref. [5]). Compare the stabilization energies in the two cases.

4 Dynamical Mean Field Theory

4.1 The self consistency condition and the DMFT loop

Following the definition of the Green's function on the local orbital basis

$$G_{ij}(t) = -i\langle N|T(c_i^\dagger(t)c_j(0)|N\rangle \tag{17}$$

one can compute the Bloch Green's function

$$G_{\mathbf{k}}(t) = \frac{1}{N}\sum_{ij} \mathrm{e}^{ik(T_i-T_j)} G_{ij}(t) \tag{18}$$

thus, in frequency

$$G_{\mathbf{k}}(\omega) = \frac{1}{N}\sum_{ij} \mathrm{e}^{ik(T_i-T_j)} G_{ij}(\omega) \tag{19}$$

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:

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)} \tag{20}$$

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

$$G_{ii}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} \mathrm{e}^{ik(T_i-T_i)} G_{\mathbf{k}}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}}(\omega) \tag{21}$$

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

$$G_{\text{Anderson}}(\omega) = \frac{1}{\omega - \epsilon_0 - \Delta(\omega) - \Sigma(\omega)} \tag{22}$$

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 [2] : it is the **self-consistency relation** of DMFT. 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:

$$\frac{1}{N}\sum_{k}\frac{1}{\omega-\epsilon_{\mathbf{k}}-\Sigma(\omega)}=\frac{1}{\omega-\epsilon_0-\Delta(\omega)-\Sigma(\omega)} \tag{27}$$

This equation enables us to find $\Delta(\omega)$ as a function of the self energy: $\Delta = \Delta[\Sigma]$ and also $\epsilon_0 = \frac{1}{N}\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}$[3]

Besides, the solution of the Anderson model enables us to have the self energy from the value of ϵ_0 and Δ.[4] 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.

4.2 The Hubbard model in DMFT

The main results for the Hubbard model phase diagram in DMFT (without magnetism and for one electron per atom) are sum up on Figs. 7 and 8. First, the metal insulator is a first order phase transition. Moreover, the paramagnetic insulating phase with a degeneracy of two can be described in contrary to the static mean field approximation which breaks the symmetry and creates magnetism.

Let's describe the evolution of the spectral function. At large value of U, the Hubbard bands are present but still broadened by hybridization. Then, a resonance peak appears at the Fermi level and grows, as U/t decreases. Importantly thus, the metallic phase appears whereas the Hubbard band are still present in the photoemission spectra. Such feature is also not described by the static mean field approximation. Let us finally outline that in DMFT, both the atomic limit ($U/t >> 1$) and the delocalization limit ($U/t << 1$) are exact.

5 DFT+DMFT

The main idea of DFT+DMFT is to use the DFT/LDA Hamiltonian to define the one body term of the Hubbard model and then supplement it by an exact Coulomb interaction for the correlated orbital subset.

However, to apply DMFT ideas to a real system, one need first to define correlated orbitals[7, 8, 9] and a corresponding value of the effective interaction U[10]. This is important but this is not discussed

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[2] Thus we have express also the self energy in the Bloch basis. We start from the expression of the self energy as a sum of local self energies on different sites:

$$\Sigma=\sum_{T_i}|T_i\rangle\Sigma(\omega)\langle T_i| \tag{23}$$

We use then

$$|T_i\rangle=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}|\mathbf{k}\rangle e^{-i\mathbf{k}T_i} \tag{24}$$

Thus by replacing the last equation in Eq. 23, we have (do the derivation in exercice).

$$\Sigma=\sum_{\mathbf{k}}|\mathbf{k}\rangle\Sigma(\omega)\langle\mathbf{k}'| \tag{25}$$

Thus

$$\langle\mathbf{k}|\Sigma|\mathbf{k}\rangle=\Sigma(\omega) \tag{26}$$

Thus for a local self-energy, the self energy in the basis of Bloch states is equal to the local self-energy.

[3] Equivalently, one can say that the non interacting Green's function $\mathcal{G}_0^{-1}=\omega-\epsilon_0-\Delta(\omega)$ can be obtained from the self-energy.

[4] Equivalently, one can obtain the Green's function and the self energy of the Anderson model as a function of the non interacting Green's function

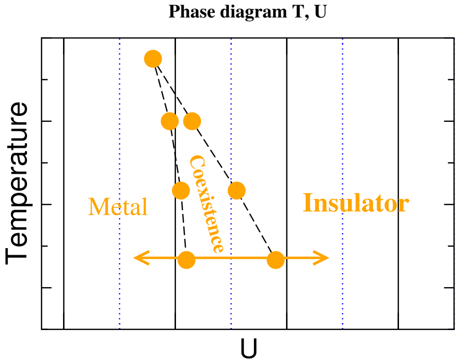

Figure 7: Phase diagram of the Hubbard model in DMFT.

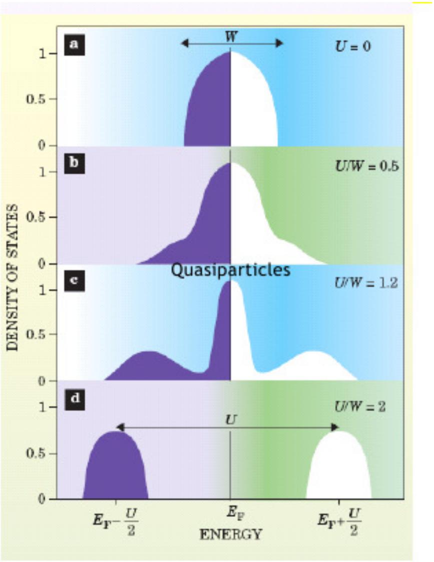

Figure 8: Evolution of the spectral function in the Hubbard model (from Ref[6]).

in these notes. I just outline here that there is no unique way to define correlated orbitals. So several choices have been made in the litterature. It includes atomic orbitals, or wannier orbitals. When the choice of correlated orbitals is done, the effective interaction for these orbitals has to be computed. The most used formalism is the constrained Random Phase Approximation method[10] which considers that the effective interaction between correlated electrons is the bare interaction screened by all the non correlated electrons. It thus requires the calculation of a non interacting polarisability and the inverse dielectric function as presented in the lectures of Fabien Bruneval, and Francesco Sottile.

In a first step, we are going to write the expression of the lattice Green's function for the solid with a local self-energy. The self-energy will later be the DMFT self-energy.

5.1 The lattice Green's function

In comparison to the case of the one band Hubbard model, things are more complicated because

- The number of correlated orbitals is larger (10 for d elements)
- The number of bands in the system is large, and larger that the number of correlated orbitals because some orbitals are not correlated. For example, in Iron, the $3d$ orbitals are correlated but the $4s$ are not. However, $4s$ and $3s$ states are strongly mixed in the DFT/LDA density of states.

We are going to express all quantities (G, Σ) in the Kohn Sham wavefunctions basis because the DFT Hamiltonian has a simple expression in this basis:

$$H_{\text{LDA}} = \sum_{n\mathbf{k}} |\Psi_{\mathbf{k}n}\rangle \epsilon_{n\mathbf{k}} \langle \Psi_{\mathbf{k}n}| \tag{28}$$

The self energy in DMFT is local and is computed in a local basis, thus the self energy operator is a sum of identical self-energies on each correlated sites (m and m' are quantum numbers of the projection of the angular momentum).

$$\Sigma = \sum_{mm'T_i} |\chi_{T_i m}\rangle \Sigma_{m,m'}(\omega) \langle \chi_{T_i m'}| \tag{29}$$

We can define the Bloch transform of the localized functions $\chi_{T_i m}$ as before as

$$|\chi_{T_i m}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} |\chi_{\mathbf{k}m}\rangle \mathrm{e}^{-i\mathbf{k}T_i}. \tag{30}$$

Thus by replacing the last equation in Eq. 29, we have:

$$\Sigma = \sum_{mm'\mathbf{k}} |\chi_{\mathbf{k}m}\rangle \Sigma_{m,m'}(\omega) \langle \chi_{\mathbf{k}m'}|. \tag{31}$$

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

$$\Sigma_{nn'}(\mathbf{k}, \omega) = \sum_{m,m'} \langle \Psi_{\mathbf{k}n} | \chi_{\mathbf{k}m}\rangle \Sigma_{mm'}(\omega) \langle \chi_{\mathbf{k}m'} | \Psi_{\mathbf{k}n'}\rangle \tag{32}$$

In order to avoid a double counting of the correlation for correlated orbitals, the self-energy has to contain a so called "double counting part" which should cancel the DFT/LDA Hartree and exchange correlation potential for the correlated electrons

$$\Sigma = \Sigma_{\text{DMFT}} - \Sigma_{\text{DC}}. \tag{33}$$

The Green's function will obey the usual equation of motion:

$$(\omega I - H - \Sigma)G = I. \tag{34}$$

Thus the Green's function is

$$G_{nn'}(\mathbf{k},\omega) = \left.[\omega I - H(\mathbf{k}) - \Sigma(\mathbf{k},\omega)]^{-1}\right|_{nn'}, \tag{35}$$

where $H(\mathbf{k})$ is a diagonal matrix containing the Kohn Sham eigenvalues and $\Sigma(\mathbf{k},\omega)$ is non diagonal (see above).

The local Green's function is simply:

$$G^{\text{loc}}_{mm'}(\omega) = \sum_{\mathbf{k}} \langle \chi_{\mathbf{k}m} | \Psi_{\mathbf{k}n} \rangle G_{nn'}(\mathbf{k},\omega) \langle \Psi_{\mathbf{k}n'} | \chi_{\mathbf{k}m'} \rangle \tag{36}$$

This equation is the generalisation of Eq. 21.

5.2 The Self-Consistency Condition

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

$$G^{\text{loc}}_{mm'}(\omega) = G^{\text{Anderson}}_{mm'}(\omega) \tag{37}$$

where

$$G^{\text{Anderson}}_{mm'}(\omega) = \left.[\omega I - E_0 - \Delta(\omega) - \Sigma(\omega)]^{-1}\right|_{mm'} \tag{38}$$

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.

5.3 The Anderson impurity model

E_0, Δ and U, J defines the Anderson model. The solution of the Anderson model gives the local self energy, which is used again to compute the lattice Green's function (Eq. 35).

5.4 The DFT loop

The density can be obtained from the full Green's function using:

$$n(\mathbf{r}) = -i \sum_{n,\mathbf{k}} \Psi_{\mathbf{k}n}(\mathbf{r}) G_{nn'}(\mathbf{k}, t-t'=0^-) \Psi_{\mathbf{k}n'}(\mathbf{r}) \tag{39}$$

and is used to reconstruct the Kohn Sham hamiltonian (a functional of the density) and thus the eigenvalues. The scheme is summarized on Fig. 9.

6 Conclusion

In these notes, we have first shown that the Hubbard model is a model for localisation/delocalisation transitions. Then we have presented the mapping to the Anderson model, and finally the DMFT and DFT+DMFT equations. The next lecture shows a more formal derivation based on functionals.

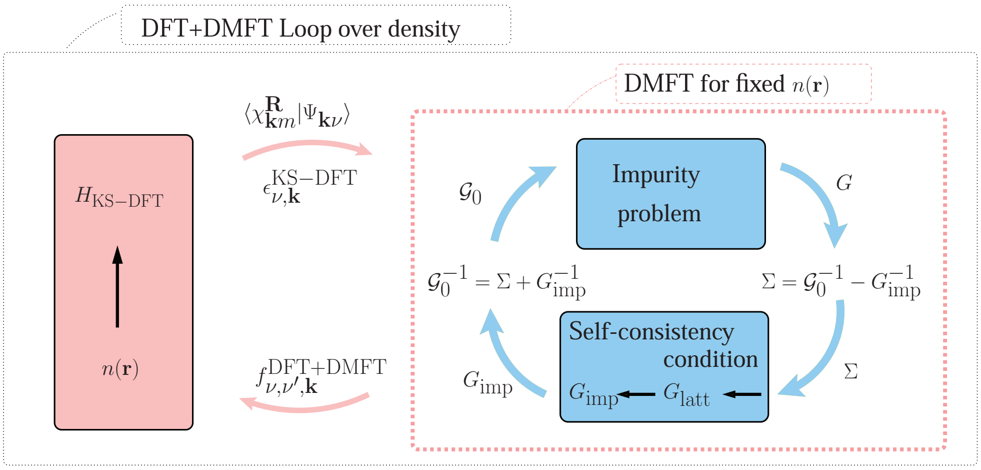

Figure 9: Scheme of the DFT+DMFT loops. $\mathcal{G}_0$ is the non interacting Green's function of the Anderson model and is linked to the hybridization by $\mathcal{G}_0^{-1} = [\omega I - E_0 - \Delta(\omega)]$. The Dyson Equation is $\mathcal{G}_0^{-1} - G^{-1} = \Sigma$. G_{imp} stands for the Anderson impurity Green's function.

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