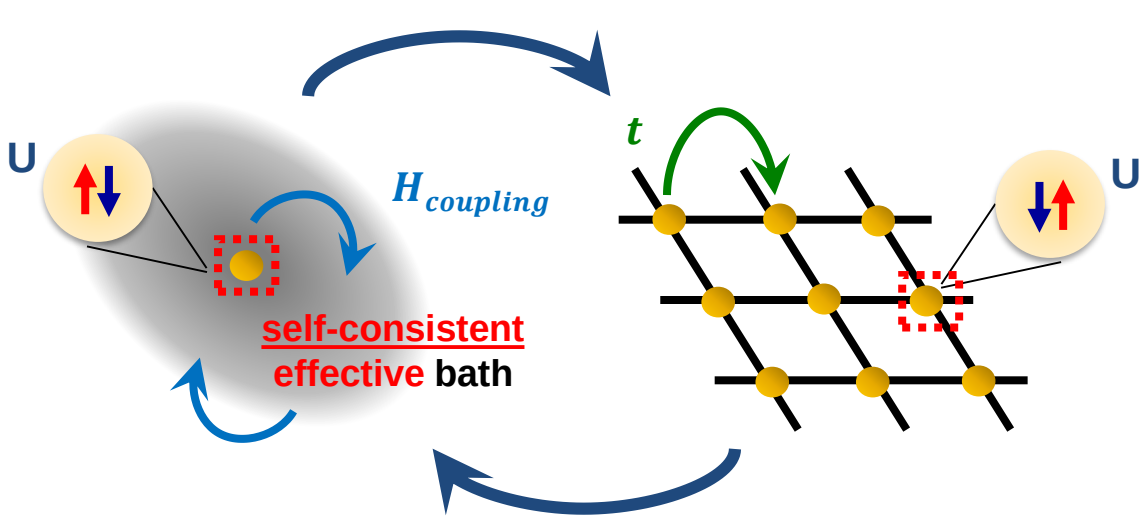
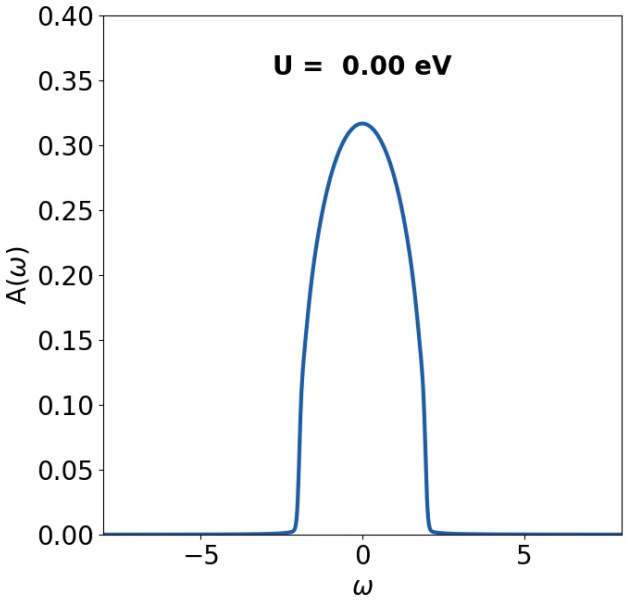
GDR NBODY, Workshop on Model Systems in Quantum Mechanics

Toulouse, January 11th – 12th 2024

An introduction to Dynamical Mean-Field Theory (DMFT)





Cyril Martins

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A brief history about DMFT

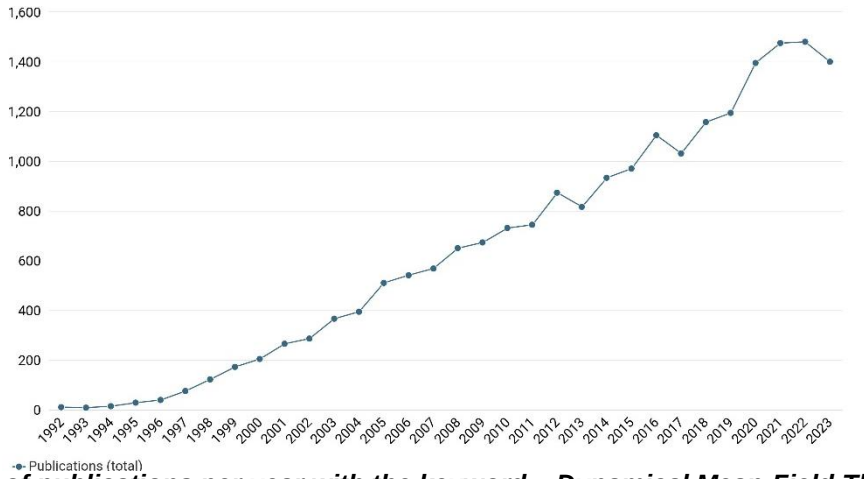
The Dynamical Mean-Field Theory framework was established in the early 1990's.

THE PIONNEER WORKS

1989 : W. Metzner & D. Vollhardt, *Phys. Rev. Lett.* **62**, 324
1991 : V, Janiš, *Z. Physik B - Condensed Matter* **83**, 227–235
1992 : V. Janiš & D. Vollhardt, *Int. J. Mod. Phys. B* **6**, 731
A. Georges & G. Kotliar, Phys. Rev. B **45**, 6479
M. Jarrel, *Phys. Rev. Lett.* **69**, 168

Since then, an increasing interest from the scientific community (condensed matter physics, chemistry, applied mathematics) **:**

~1400 papers in 2023

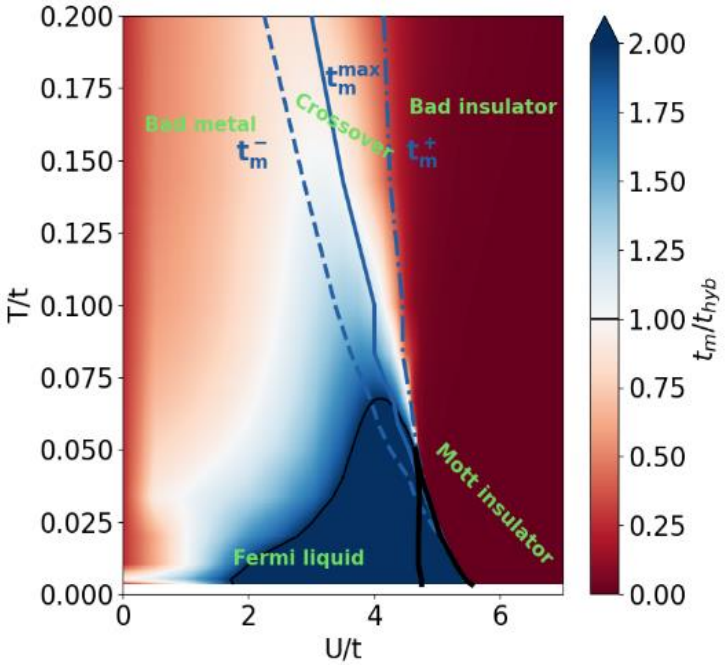


Number of publications per year with the keyword « Dynamical Mean-Field Theory » according to the database Dimensions *(app.dimensions.ai)*

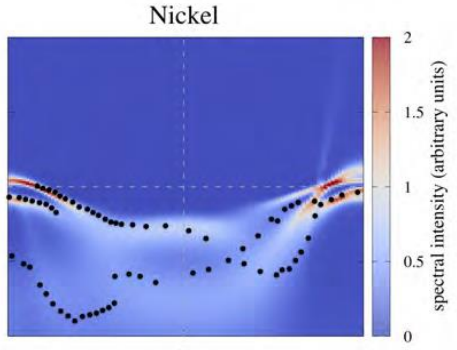
Why such a success ?

DMFT allows to describe the metal/Mott insulating transition

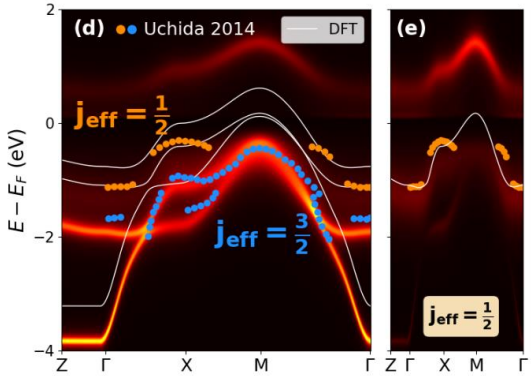
Phase diagram for the half-filled Hubbard model on the Bethe lattice, *using a continuous time Quantum Monte Carlo impurity solver*
Data obtained by L. Gaspard



DMFT can be coupled to DFT to describe « correlated materials »



Calculated and experimental spectral function of nickel
A. Hausoel et al., Nat. Commun. 8, 16062 (2017)



Calculated and experimental spectral function of Ba_2IrO_4
F. Cassol, et al. arxiv:2312.13962

DMFT in a nutshell

WHAT DMFT IS NOT

- **DMFT is not a theory of the many-body ground state** (contrary to the Density Matrix Embedded Theory, DMET)
- **DMFT is not Time Dependent-DFT (TD-DFT) :** TD-DFT focuses on the time-dependent density $n(r,t)$!

DMFT is based on the Green function formalism

(with time-independent – and often translationnaly-invariant – Hamiltonian) **:**

$$G(\boldsymbol{r},t;\boldsymbol{r}',t') = -i\langle\Psi_{GS}|T\left[c(\boldsymbol{r},t)c^{\dagger}(\boldsymbol{r}',t')\right]|\Psi_{GS}\rangle$$

$$G(\boldsymbol{k},t) = -i\langle\Psi_{GS}|T\left[c_{\boldsymbol{k}}(t)c_{\boldsymbol{k}}^{\dagger}(t=\boldsymbol{0})\right]|\Psi_{GS}\rangle$$

In DMFT, the observable of interest is the local spectral function $A(\omega)$

(or the k-resolved spectral function $A(k,\omega)$)

$$A(\omega) = \sum_{\boldsymbol{k}} A(\boldsymbol{k},\omega) = -\frac{1}{\pi}\sum_{\boldsymbol{k}} Im[G(\boldsymbol{k},\omega)]$$

DMFT in a nutshell

WHAT DMFT IS

- **DMFT is a mean-field theory for quantum many-body systems on a lattice.**
- **DMFT was initially designed to address the problem of fermions on a lattice, especially the Hubbard model.**

« Initial » problem	Auxiliary problem	Observable
Ising model	Spins in an *effective* magnetic field h_{eff}^{i}	Local magnetization $\boldsymbol{m_i = \langle S_i \rangle}$
Electrons in a solid (Born-Oppenheimer approximation)	Non-interacting particles in an *effective* local potential $V_{eff}(\boldsymbol{r})$	Local ground-state density $\boldsymbol{n(r)}$
Hubbard model	Atoms coupled to an *effective* bath : **Impurity Anderson model**	Local Green function $\boldsymbol{G_{ii}(t) = -i\langle T[c_i(t)c_i^{\dagger}(t=0)]\rangle}$

Outlines

The single impurity Anderson model

Definition of the model

Impurity Green function, self-energy and hybridization

The physics of the model

Dynamical Mean-Field Theory explained

The DMFT equations

The DMFT self-consistent loop in practice

The metal / Mott insulator transition in DMFT

From models to materials : DMFT and beyond

Describing correlated materials with DFT+DMFT

DFT+DMFT as a first step…

What I will discuss

SCIENTIFIC

ADVISORY

PEDAGOGICAL CONTENT

DISCLAIMER

- I will introduce DMFT formalism on the simplest model (**the one-band Hubbard model at half-filling**) but DMFT can be applied to any fermionic lattice model Hamiltonian at any filling.
- I will use the picture of 2D Hubbard model on a square lattice just to ease the understanding.

USEFUL REVIEWS

- A. Georges, G. Kotliar, W; Krauth & M.J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996)
- "***DMFT at 25 : Infinite Dimensions***", E. Pavarini, E. Koch, D. Vollhardt & A. Lichtenstein (2014)
- "***Dynamical Mean-Field Theory of Correlated Electrons***", E. Pavarini, E. Koch, D. Vollhardt & A. Lichtenstein (2022)

An introduction to
Dynamical Mean-Field Theory (DMFT)

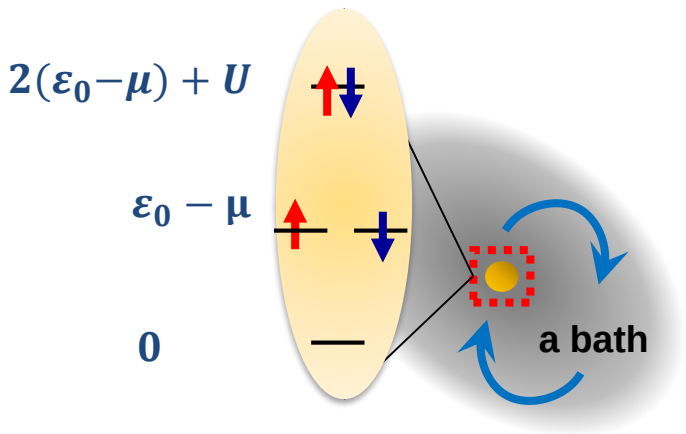
The single impurity Anderson model

Definition of the model

THE SINGLE IMPURITY ANDERSON MODEL

- **Originally introduced by P.W. Anderson in 1961** to explain the formation of local moments in magnetic alloys.
- **A "simplified" model with :**

  a localized, discrete quantum system, **the impurity,**
  coupled to non-interacting states with a continuous spectrum, **the bath**.



$$H_{SIAM} = H_{atom} + H_{bath} + H_{coupling}$$

$$H_{atom} = (\varepsilon_0 - \mu)(n_{d\uparrow} + n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow}$$

$$H_{bath} = \sum_{k,\sigma} \varepsilon_k \, c^{\dagger}_{k\sigma} c_{k\sigma}$$

$$H_{coupling} = \sum_{k,\sigma} V_k \, c^{\dagger}_{k\sigma} d_{\sigma} + V^{*}_{k} \, d^{\dagger}_{\sigma} c_{k\sigma}$$

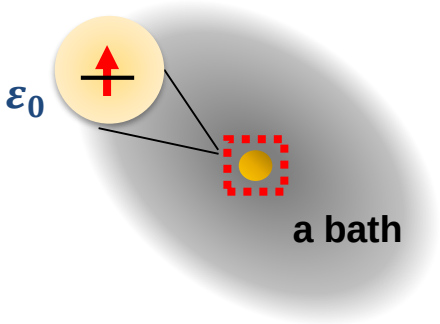
P. W. Anderson, Phys. Rev. 124, 41 (1961)

Impurity Green function, self-energy and hybridization

THE IMPURITY GREEN FUNCTION

- **The impurity Green function $G_{imp}(t,t')$ describes how "evolves" the electron on the impurity site between time t and t' :**

$$| \Psi_0(t') \rangle = G_{imp}(t,t') | \Psi_0(t) \rangle$$



$$H_{atom} = \varepsilon_0 (n_{d\uparrow} + n_{d\downarrow})$$

Without any coupling to the bath and no local interaction, $G_{imp}(t,t')$ is a simple phase shift :

$$G_{imp}(t,t') = \exp\left(-\frac{i(\varepsilon_0 - \mu)}{\hbar}(t-t')\right)$$

$$G_{imp}(\omega) = \frac{1}{\omega + \mu - \varepsilon_0} \quad \text{avec } \omega \equiv \omega + i0^+ \text{ ou } i\omega_n$$

Impurity Green function, self-energy and hybridization

THE IMPURITY GREEN FUNCTION

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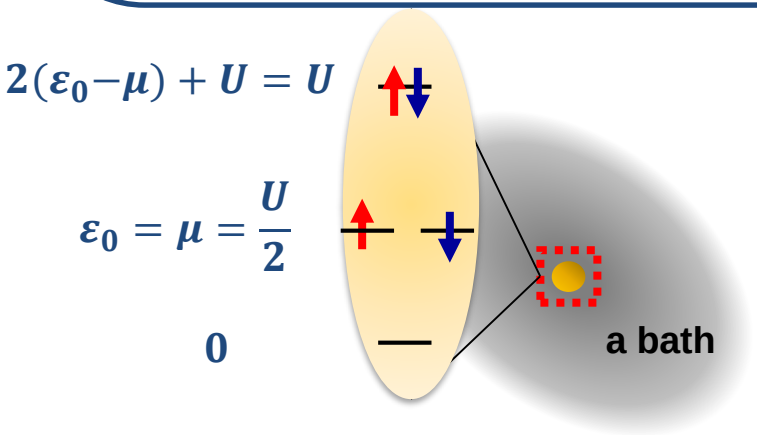
$$| \Psi_0(t') \rangle = G_{imp}(t,t') | \Psi_0(t) \rangle$$

- **The self-energy $\Sigma_{imp}(\omega)$ contains all the "local many-body physics".**



$$H_{atom} = \varepsilon_0(n_{d\uparrow}+n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow}$$

Without any coupling to the bath but local interaction (atomic limit, with $\mu = U/2$) **:**

$$G_{imp}(\omega) = \frac{1}{2}\frac{1}{\omega+\frac{U}{2}} + \frac{1}{2}\frac{1}{\omega-\frac{U}{2}} = \frac{1}{\omega-\Sigma_{at}(\omega)}$$

$$\Sigma_{imp}(\omega) = \Sigma_{at}(\omega) = \frac{U^2}{4\omega} \quad \text{avec } \omega \equiv \omega + i0^+ \text{ ou } i\omega_n$$

Impurity Green function, self-energy and hybridization

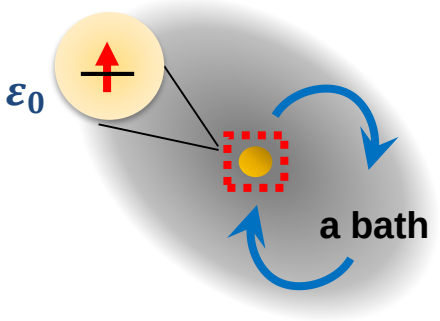
THE IMPURITY GREEN FUNCTION

- The impurity Green function $G_{imp}(t,t')$ describes how "evolves" the electron on the impurity site between time t and t' :

$$| \Psi_0(t') \rangle = G_{imp}(t,t') | \Psi_0(t) \rangle$$

- The self-energy $\Sigma_{imp}(\omega)$ contains all the "local many-body physics".
- The hybridization $\Delta(\omega)$ encodes the possibility to "hop into the bath", propagate and come back" on the impurity site.

$$H_{atom} + H_{bath} + H_{coupling} = (\varepsilon_0 - \mu)(n_{d\uparrow} + n_{d\downarrow}) + \sum_{k,\sigma} \varepsilon_k \, c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{k,\sigma} V_k \, c^{\dagger}_{k\sigma} d_{\sigma} + V_k^{*} \, d^{\dagger}_{\sigma} c_{k\sigma}$$



With a coupling to a bath but no local interaction (independent particle picture) **:**

$$G_{imp}(\omega) = \frac{1}{\omega + \mu - \varepsilon_0 - \Delta\,(\omega)} \qquad \Delta(\omega) = \sum_{k,\sigma} \frac{|V_k|^2}{\omega - \varepsilon_k}$$

avec $\omega \equiv \omega + i0^{+}$ ou $i\omega_n$

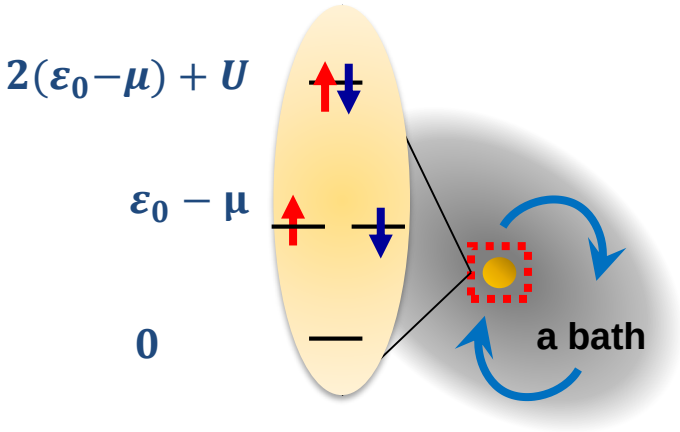
Impurity Green function, self-energy and hybridization

THE IMPURITY GREEN FUNCTION

- The impurity Green function $G_{imp}(t,t')$ describes how "evolves" the electron on the impurity site between time t and t' :

$$G_{imp}(\omega) = \frac{1}{\omega + \mu - \varepsilon_0 - \Delta\,(\omega) - \Sigma_{imp}(\omega)} \quad \text{avec } \omega \equiv \omega + i0^+ \; ou \; i\omega_n$$

- The self-energy $\Sigma_{imp}(\omega) \neq \Sigma_{at}(\omega)$ contains all the "local many-body physics".
- The hybridization $\Delta(\omega)$ encodes the possibility to "hop into the bath", propagate and come back" on the impurity site.



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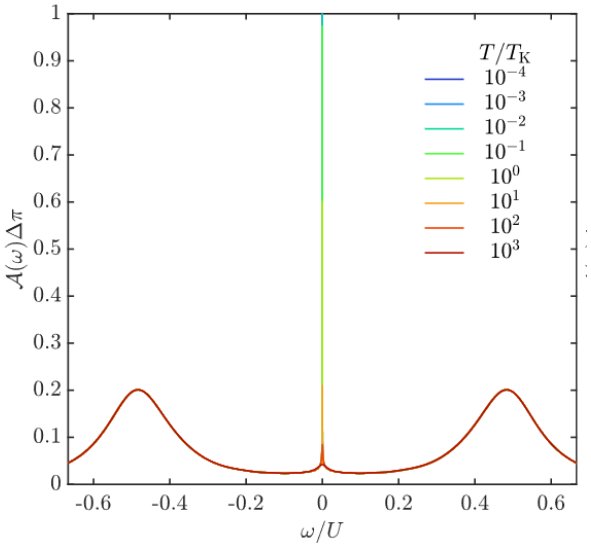
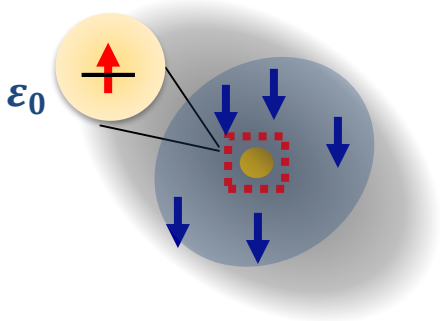
The physics of the model

LOCAL SPECTRAL FUNCTION (ON THE IMPURITY SITE)

- **Two broad peaks in $\pm U/2$:** the hybridization $\Delta(\omega)$ induces a width of the initial "Dirac" peak (at the atomic limit)
- **A sharp peak at $\omega = 0$: Kondo resonance** and **Fermi liquid behavior** of the particles scattered by the singlet ground-state
- This Kondo peak is a **non-perturbative behavior** of the model !



The singlet ground-state is formed by the local moment on the impurity site and a « cloud » of conduction band.



J. Van Delft, The Physics of quantum impurity models in « **Dynamical Mean-Field Theory of Correlated Electrons** *» (2022)*

An introduction to Dynamical Mean-Field Theory (DMFT)

Dynamical Mean-Field Theory explained

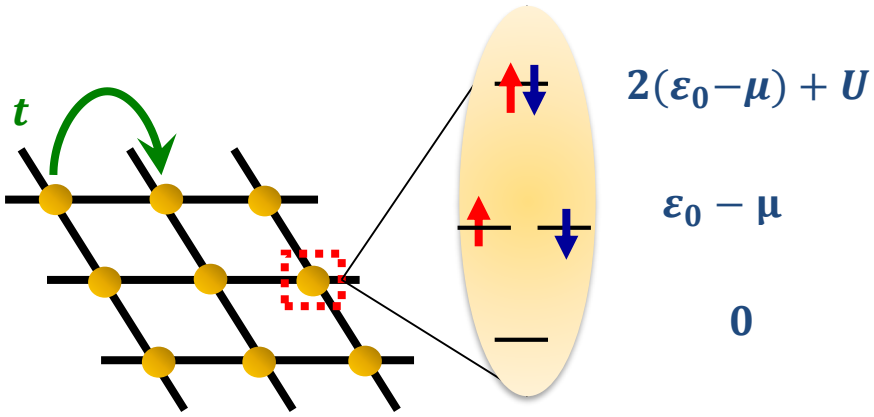
The DMFT equations

The one-band Hubbard model

- **Originally introduced by J. Hubbard in 1964**

$$H = \sum_{i,\sigma} (\varepsilon_0 - \mu)(n_{i\uparrow} + n_{i\downarrow}) - \sum_{\langle i,j\rangle,\sigma} t \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + \sum_{i} U\, n_{i\uparrow} n_{i\downarrow}$$

- **At half-filling,** $\varepsilon_0 = \mu = U/2$



J. Hubbard, Proc Roy Soc Lond A, 276 (1964)

The DMFT equations

The one-band Hubbard model

- **The Green function describes how an electron "propagates" from site i to site j between a time t**

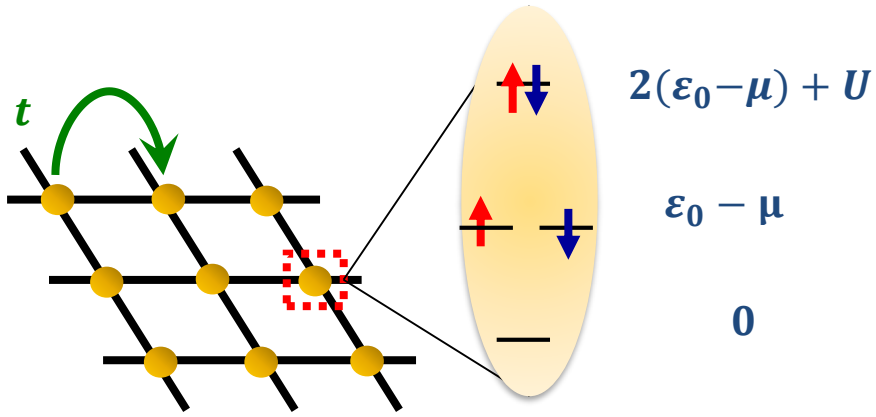
$$G_{ij}(t) = -i\left\langle T\left[c_i(t)c_j^{\dagger}(t=0)\right]\right\rangle$$

- Since the model is translationally-invariant, one rather consider the propagator :

$$G(\boldsymbol{k},\omega) = \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k},\omega)}$$

where $\Sigma(\boldsymbol{k},\omega)$ is the self-energy

!! CAUTION !! The self-energy $\Sigma_{ij}(\omega)$ is non-local.



J. Hubbard, Proc Roy Soc Lond A, 276 (1964)

The DMFT equations

Within DMFT, the « original » one-band Hubbard model is mapped onto an « auxiliary » single-impurity Anderson model.

SELF-CONSISTENT RELATION

The local dynamics of the lattice is the same of the impurity in the effective bath.

$$G_{imp}(\omega) \equiv G_{ii}(\omega) = \sum_k \frac{1}{\omega + \mu - \varepsilon_k - \Sigma(k,\omega)}$$

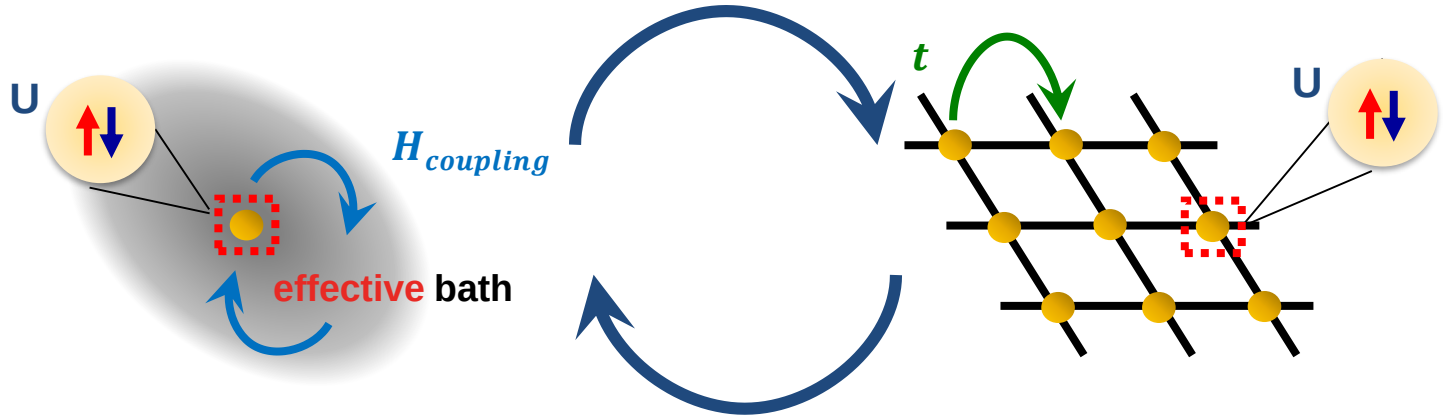
The DMFT equations

DMFT Approximation

The local many-body effects are the same on each site of the lattice.

$$G_{imp}(\omega) = \frac{1}{\omega + \mu - \varepsilon_0 - \Delta(\omega) - \Sigma_{imp}(\omega)}$$

$$\Sigma_{ii}(\omega) \equiv \Sigma_{imp}(\omega) \;\; et \;\; \Sigma_{ij}(\omega) \equiv 0$$



Self-consistent relation

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The DMFT equations

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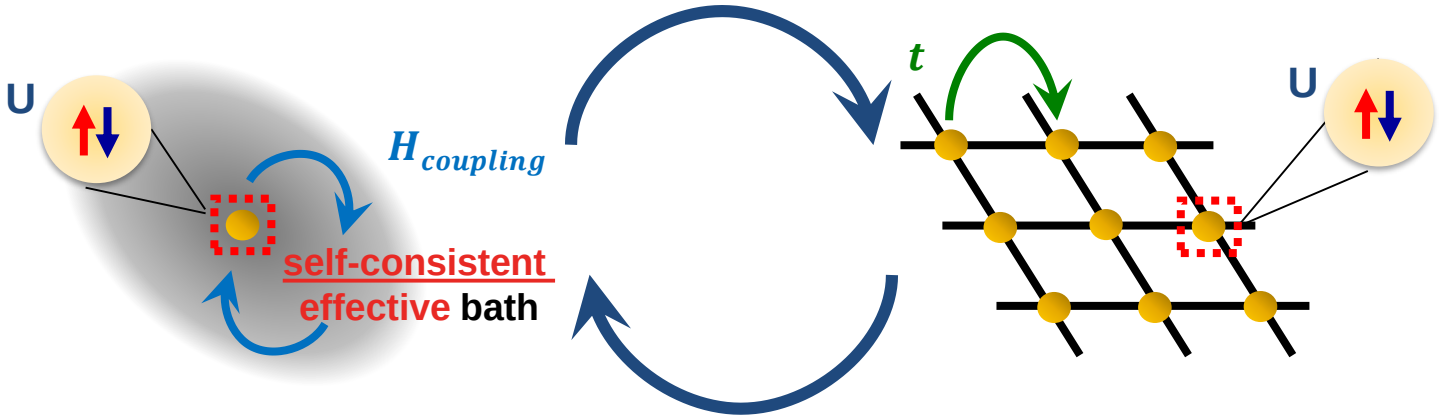

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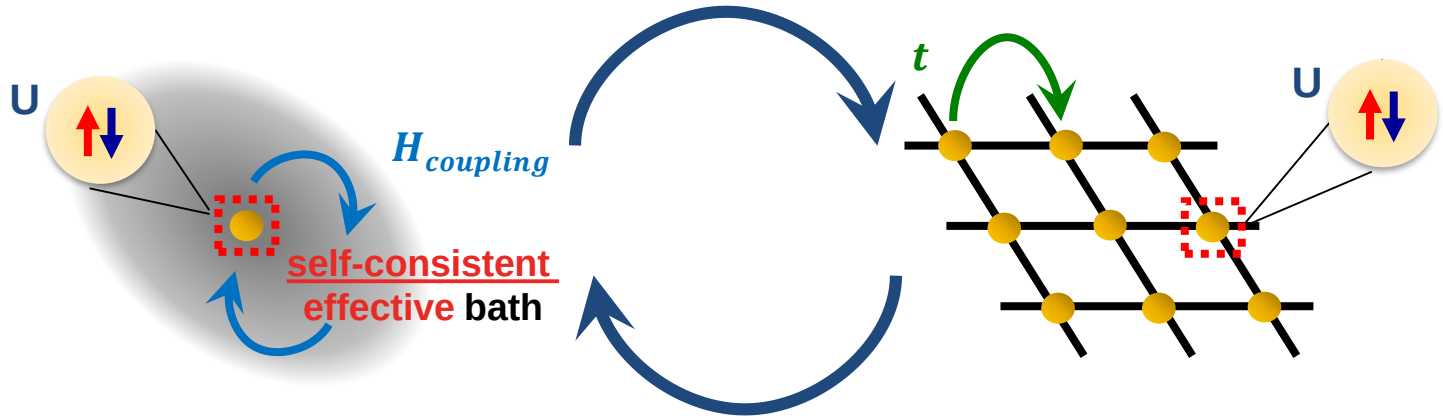
The DMFT equations

THE DMFT EQUATIONS

$$\Sigma_{ii}(\omega) \equiv \Sigma_{imp}(\omega) \; et \; \Sigma_{ij}(\omega) \equiv 0$$



$$G_{imp}(\omega) \equiv G_{ii}\ (\omega)$$

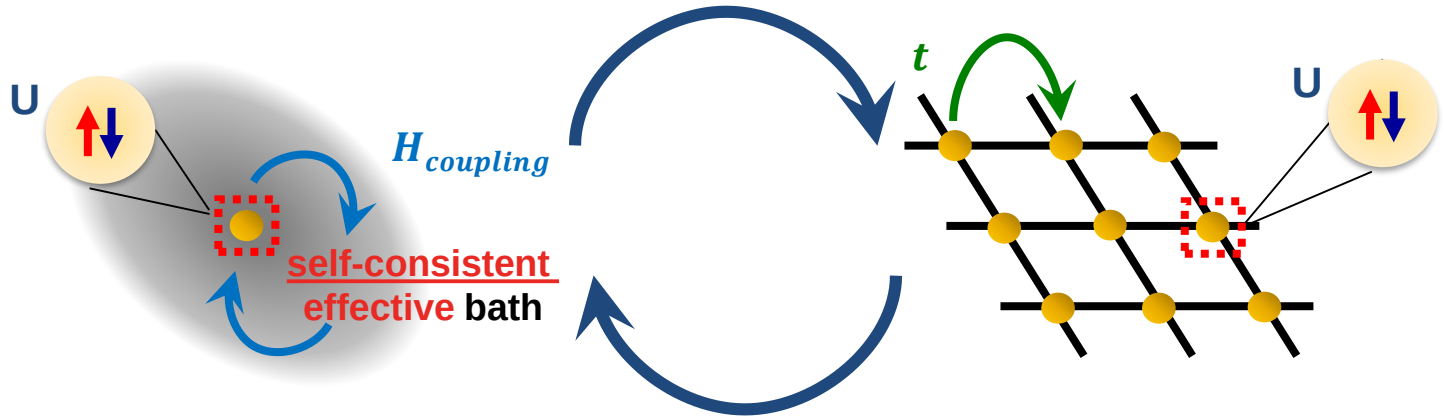
IN DYNAMICAL MEAN-FIELD THEORY

- The self-energy is local : **only local quantum fluctuations are taken into account.**
- The self-energy is momentum-dependent : **the full many-body dynamics of the interacting system is described.**

The DMFT equations

THE DMFT EQUATIONS

$$\Sigma_{ii}(\omega) \equiv \Sigma_{imp}(\omega) \; et \; \Sigma_{ij}(\omega) \equiv 0$$



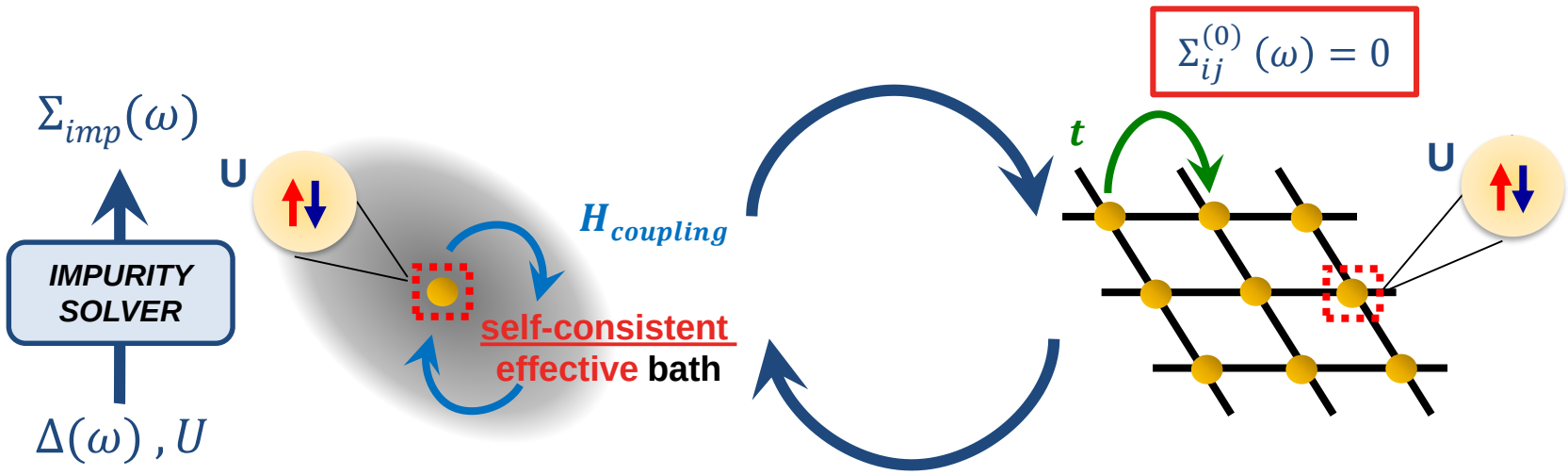
$$G_{imp}(\omega) \equiv G_{ii}\ (\omega)$$

LIMITS IN WHICH DMFT BECOMES EXACT

- **In the non-interacting limit** $(U = 0)$: $\Sigma_{imp}(\omega) = 0$
- **In the atomic limit** $(t = 0)$: $\Sigma_{imp}(\omega) = \Sigma_{atom}(\omega)$ et $\Delta(\omega) = 0$
- **In infinite coordination** (when the connectivity z of the lattice tends to infinity)

The DMFT self-consistent loop in practice

THE DMFT LOOP (FIRST ITERATION)



$$G_{imp(\omega)} = \frac{1}{\omega + \mu - \varepsilon_0 - \Delta^{(1)}(\omega)} = G_{ii(\omega)} = \sum_k \frac{1}{\omega + \mu - \varepsilon_k}$$

In practice, the DMFT loop is solved iteratively

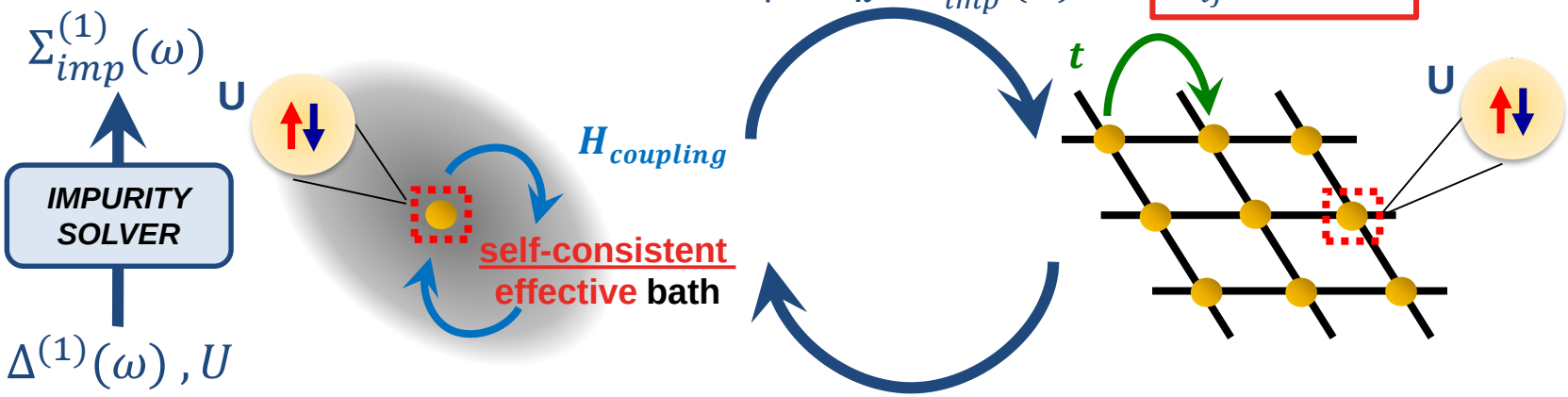
until a criterion of convergence is reached (usually on $G_{imp}(\omega)$**).**

The DMFT self-consistent loop in practice

THE DMFT LOOP (FIRST ITERATION)

$$G(\boldsymbol{k},\omega) = \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma^{(1)}_{imp}(\omega)}$$

$\Sigma^{(0)}_{ij}(\omega) = 0$



$$G_{imp(\omega)} = \frac{1}{\omega + \mu - \varepsilon_0 - \Delta^{(1)}(\omega)} = G_{ii(\omega)} = \sum_{k} \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}}}$$

In practice, the DMFT loop is solved iteratively

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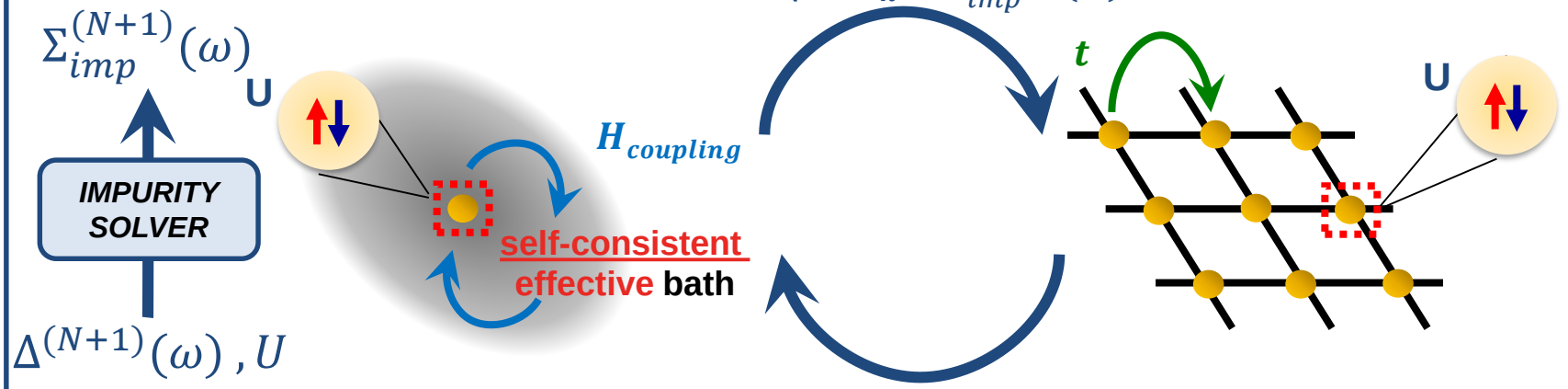
The DMFT self-consistent loop in practice

THE DMFT LOOP (ITERATION N)

$$G(\boldsymbol{k},\omega) = \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma_{imp}^{(N+1)}(\omega)}$$



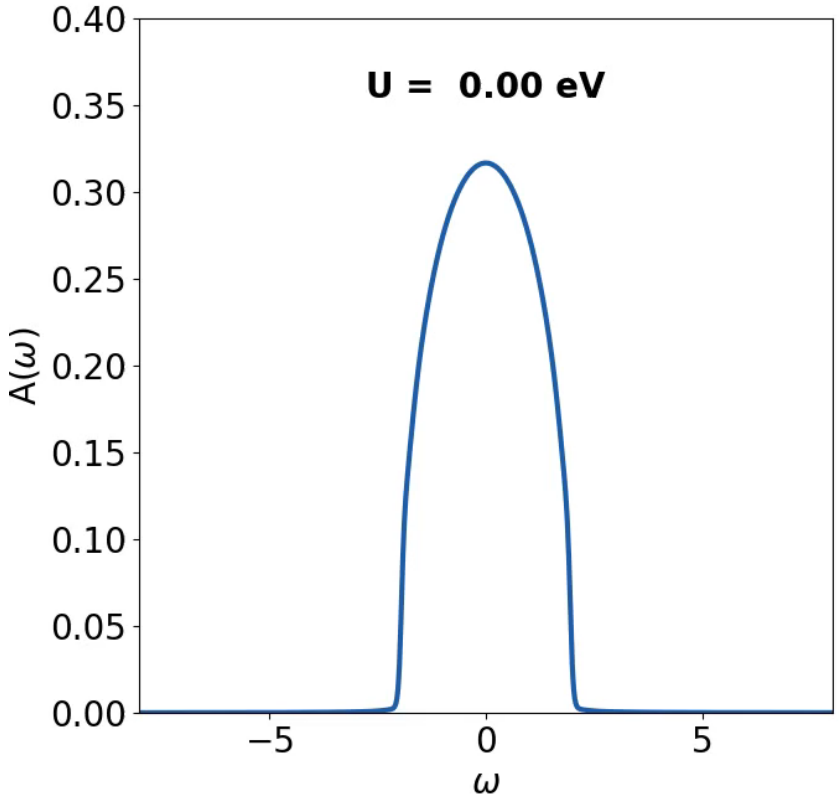
$$G_{imp}(\omega) = \frac{1}{\omega + \mu - \varepsilon_0 - \Delta^{(N+1)}(\omega) - \Sigma_{imp}^{(N)}(\omega)} = G_{ii}(\omega) = \sum_{\boldsymbol{k}} \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma_{imp}^{(N)}(\omega)}$$

- **An impurity solver is a method to solve the single-impurity Anderson model : this is often the most time-consuming part of the loop.**
- **It can be analytical** (Iterated perturbation theory, IPT) **or numerical** (continuous time Quatum Monte-Carlo, CT-QMC).

The metal / Mott insulator in DMFT

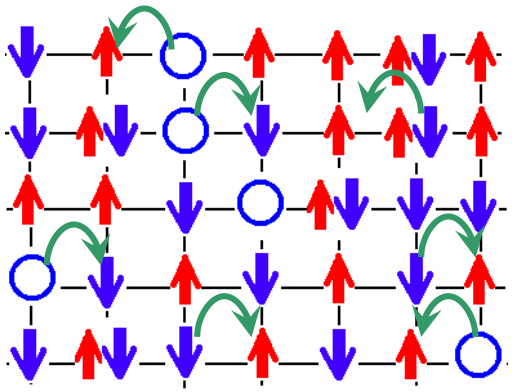
Local spectral function for the half-filled Hubbard model on the Bethe lattice

(impurity solver : Iterated perturbation theory, IPT**)**

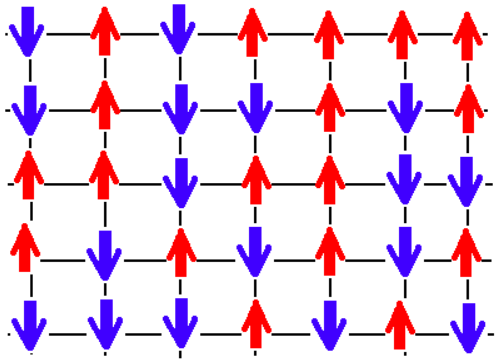


The metal / Mott insulator in DMFT

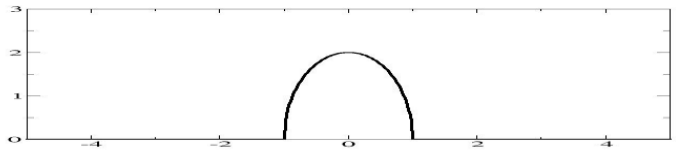
Metallic state (U=0 eV)



Mott insulating state (infinite U)



Metallic state



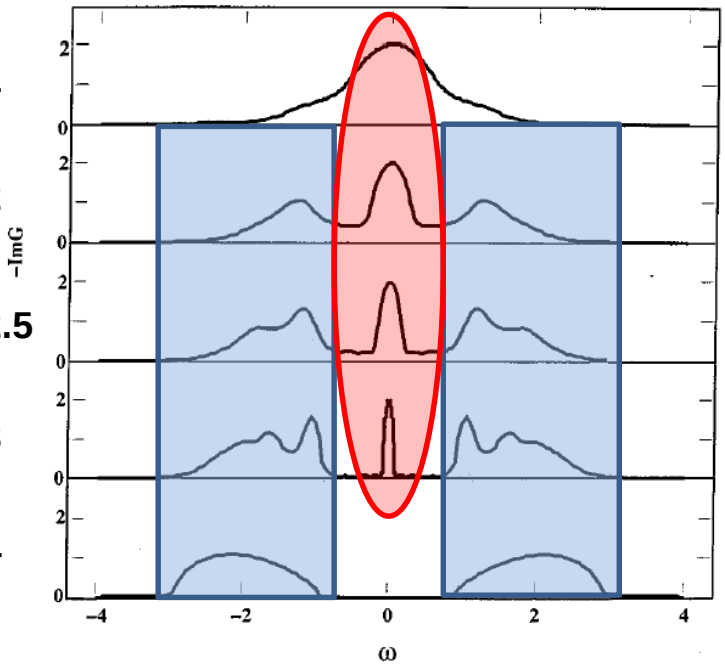
U/t = 1

U/t = 2

U/t = 2.5

U/t = 3

U/t = 4



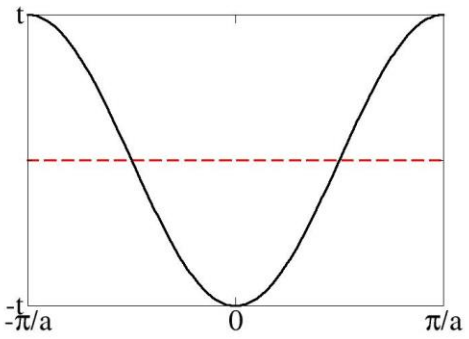
Hubbard bands

A renormalized quasiparticle peak

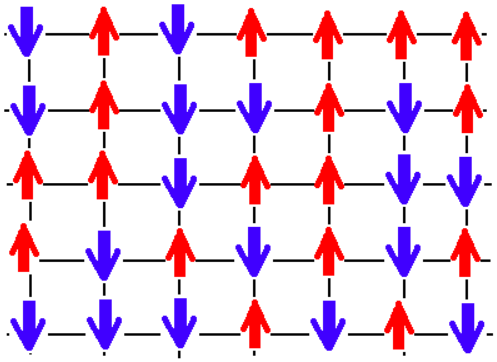
A. Georges & G. Kotliar, Phys Rev B 45, 6479 (1992)

The metal / Mott insulator in DMFT

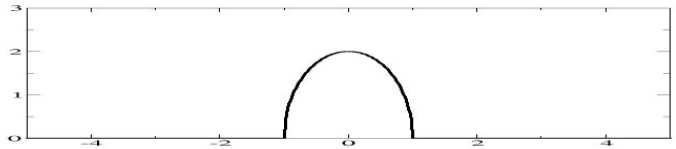
Metallic state (U=0 eV)



Mott insulating state (infinite U)



Metallic state



U/t = 1

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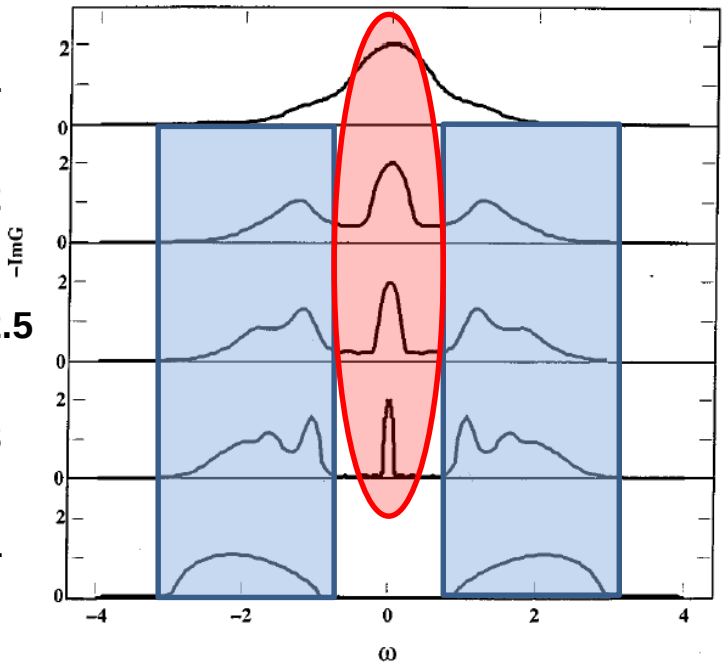
U/t = 4



Hubbard bands

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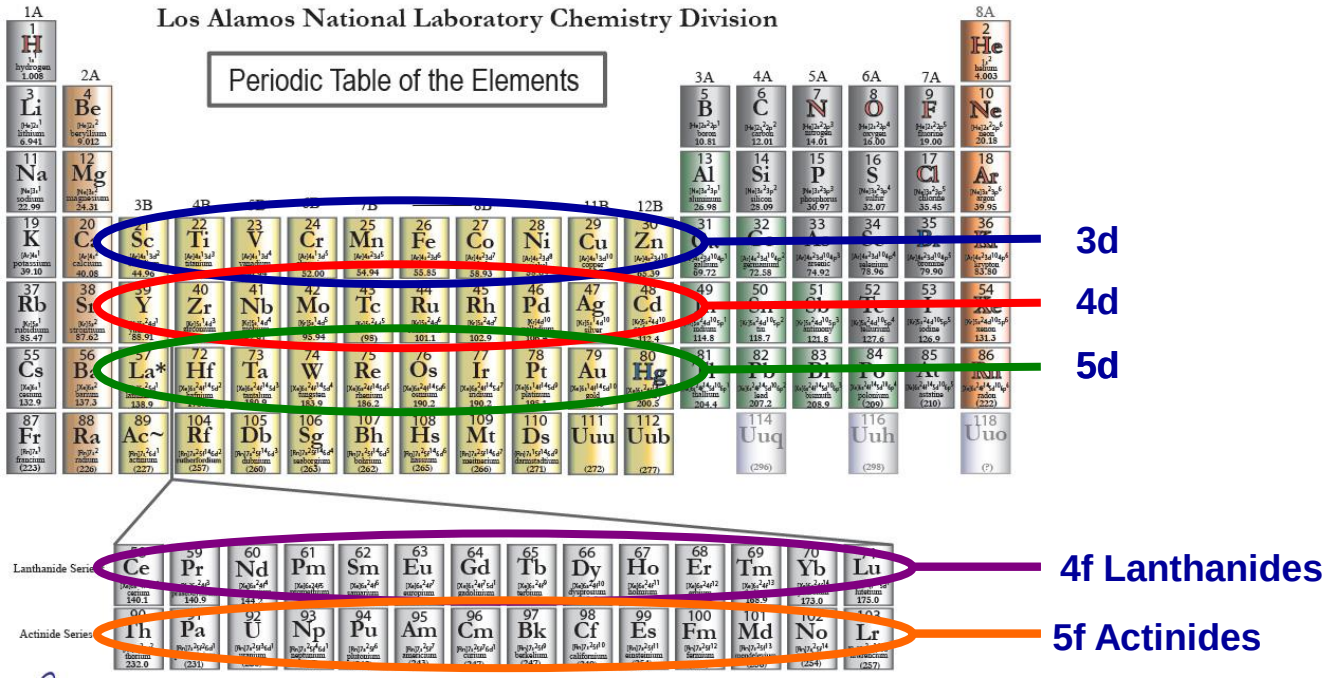
An introduction to

Dynamical Mean-Field Theory (DMFT)

From models to materials :
DMFT and beyond

Describing correlated materials with DFT+DMFT

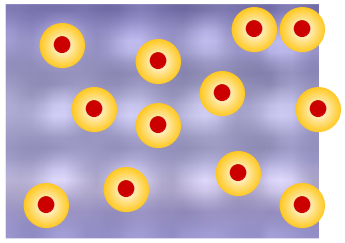


FOR CORRELATED MATERIALS

necessity to consider explicitly the Coulomb interaction between the electrons

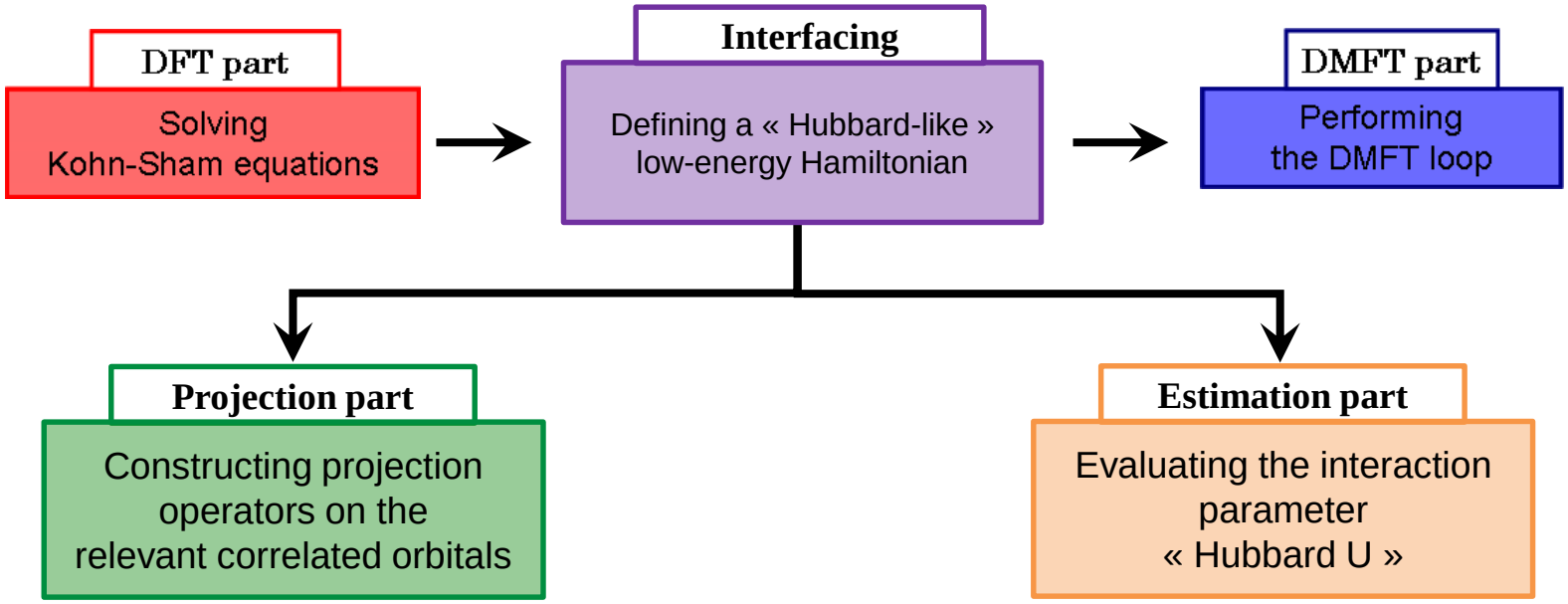
$$H = \sum_{j=1}^{N_e} \left[-\frac{\hbar^2}{2m_0}\nabla^2_{\mathbf{r}_j} + V(\mathbf{r}_j) \right] + \sum_{i<j} \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

One body operator **Two body operator**



Describing correlated materials with DFT+DMFT

PRINCIPLES OF THE DFT+DMFT APPROACH



Wannier orbitals
obtained from the Bloch states
by a projection scheme.
(maximally localized Wannier functions)

N. Marzari et al, Rev. Mod. Phys. 84, 1419 (2012)

U is identified as
the local « partially screened »
Coulomb interaction.
(constrained random-phase approximation)

F. Aryasetiawan et al, Phys Rev B 70, 195104 (2004)

A. I. Lichtenstein & M. I. Katsnelson, Phys Rev B 57, 6884 (1998)
V. I. Anisimov et al, J. Phys. Cond Mat. 9, 7359 (1997)

DFT+DMFT as a first step…

However, « real » material are often far from the « idealized » Hubbard model…

WHAT DMFT CAN ALREADY DO

- **Ordered phase can be captured :** crossover between Mott and Slater insulator
- **DMFT can be performed at finite temperature** (Matsubara formalism)
- **DMFT can be applied to multi-orbital Hubbard model** (correlated materials)

DMFT EXTENSIONS

- **Introducing non-local correlation via a k-depence in the self-energy :** cluster-DMFT, Vertex based extenstions (DΓA, dual methods)
- **Applying the formalism to higher order correlation functions :** Extended-DMFT
- **Applying the formalism for out of equilibrium systems :** out of equilibrium DMFT

Thank you for your attention