

LISA DMFT for the Hubbard model

1. Green's functions framework

Nice review : <https://arxiv.org/pdf/1303.1438.pdf>

1.1. Spectral function

The *one-particle spectral function* $A(\vec{k}, \omega)$, or spectral density, is what is observed in one-electron removal and addition (in ARPES for a 2D single-band system, $I(\vec{k}_{\parallel}, \epsilon = \hbar \omega) \propto |\text{matrix elem}|^2 f^{\text{FD}}(\epsilon) A(\vec{k}, \omega)$), and what we're interested at the end of the day. Defined as

$$A(\vec{k}, \omega) = \begin{cases} \sum_{\alpha} |\langle \Psi_{\text{GS}}^{(N)} | c_{\vec{k}} | \Psi_{\alpha}^{(N+1)} \rangle|^2 \delta(\omega - \epsilon_{\alpha}) & \text{if } \omega > 0 \text{ (inverse PE)} \\ \sum_{\beta} |\langle \Psi_{\text{GS}}^{(N)} | c_{\vec{k}}^{\dagger} | \Psi_{\beta}^{(N-1)} \rangle|^2 \delta(\omega + \epsilon_{\beta}) & \text{if } \omega < 0 \text{ (photoemission)} \end{cases} \quad (1)$$

($\hbar = 1$ from now) where $\{|\Psi_{\alpha}^{(N+1)}\rangle\}_{\alpha}$ is an eigenbasis of the $N+1$ -electrons system, of energies $\mathcal{E}_{\alpha}^{(N+1)}$:

$$\mathbf{H}^{(N+1)} |\Psi_{\alpha}^{(N+1)}\rangle = \mathcal{E}_{\alpha}^{(N+1)} |\Psi_{\alpha}^{(N+1)}\rangle$$

and where $\{|\Psi_{\beta}^{(N-1)}\rangle\}_{\beta}$ is an eigenbasis of the $N-1$ -electrons system, of energies $\mathcal{E}_{\beta}^{(N-1)}$; and where

$$\begin{aligned} -\epsilon_{\alpha} &= \mathcal{E}_0^{(N)} - \mathcal{E}_{\alpha}^{(N+1)} + \mu \simeq \mathcal{E}_0^{(N+1)} - \mathcal{E}_{\alpha}^{(N+1)} \\ -\epsilon_{\beta} &= \mathcal{E}_0^{(N)} - \mathcal{E}_{\beta}^{(N-1)} - \mu \simeq \mathcal{E}_0^{(N-1)} - \mathcal{E}_{\beta}^{(N-1)} \end{aligned}$$

are excitation energies under a chemical potential μ , the real hamiltonian describing the system being

$$\mathbf{H}_{\text{GC}} = \mathbf{H} - \mu \mathbf{N} \quad (2)$$

The spectral function verifies

$$1 = \int_{-\infty}^{+\infty} d\omega A(\vec{k}, \omega) \quad \text{and} \quad \langle n_{\vec{k}} \rangle = \int_{-\infty}^{\mu} d\omega A(\vec{k}, \omega) \quad (3)$$

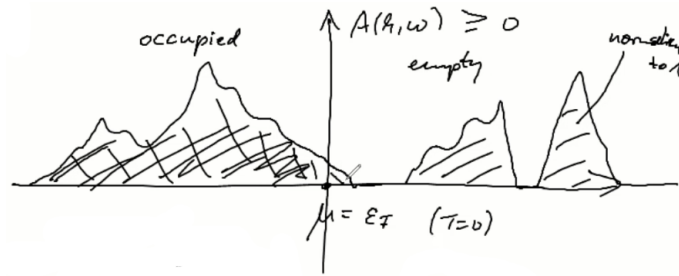


Figure 1. Illustration of a spectral function $A(\vec{k}, \omega)$ at a given \vec{k} , as function of ω .

For the **non-interacting electron gas** of dispersion $\epsilon(\vec{k})$, the N -electrons and $N+1$ -electrons eigenbasis are simple Slater determinants indexed by $\{\vec{k}_1, \dots, \vec{k}_N, (\vec{k}_{N+1} = \vec{k})\}$, $\Psi_{\text{GS}}^{(N)}$ is a Fermi sea so $\vec{k}_1, \dots, \vec{k}_N$ are fixed in the sum ($|\Psi_{\alpha}^{(N+1)}\rangle$ must be $c_{\vec{k}}^{\dagger} |\Psi_{\text{GS}}^{(N)}\rangle$), $\epsilon_{\alpha} = \epsilon(\vec{k}) - \mu$, and are simply left with

$$A_0(\vec{k}, \omega) = \delta(\omega + \mu - \epsilon(\vec{k})) \quad (4)$$

The k -summed spectral function $A_0(\omega) = \int d\vec{k} A_0(\vec{k}, \omega) = \int d\vec{k} \delta(\omega - (\epsilon(\vec{k}) - \mu))$ is the *density of states* relative to the Fermi energy μ .

1.2. Green's function

The spectral function is related to the *zero-temperature*¹ *Green's function / response function* $G(t)$, which characterizes the fate of an electron injected into the system, and which is defined, for $t > 0$, by

$$\begin{aligned} G_{\ell,m}(t) &= -i \left\langle \begin{array}{c} \text{additional electron} \\ \text{in state } \ell \text{ at time } t \end{array} \middle| \begin{array}{c} \text{additional electron in} \\ \text{state } m, \text{ evolved during } t \end{array} \right\rangle \\ &= -i (\mathbf{c}_\ell^\dagger | \text{GS}(t) \rangle)^\dagger \mathbf{U}(t) (\mathbf{c}_m^\dagger | \text{GS}(0) \rangle) \\ &= -i \langle \text{GS} | \underbrace{\mathbf{U}^{-1}(t) \mathbf{c}_\ell \mathbf{U}(t)}_{= \mathbf{c}_\ell(t) \text{ in Heis. pic.}} \mathbf{c}_m^\dagger | \text{GS} \rangle \end{aligned} \quad (5)$$

where $\mathbf{U}(t)$ is the evolution operator under the hamiltonian $\mathbf{H}_{\text{GC}} = \mathbf{H} - \mu \mathbf{N}$ ($\mathbf{U}(t) = e^{-i\mathbf{H}_{\text{GC}} t}$ for time indep.)². For arbitrary t , we define

$$\boxed{G_{\ell,m}(t) = -i \langle \text{GS} | \mathbf{T} \mathbf{c}_\ell(t) \mathbf{c}_m^\dagger(0) | \text{GS} \rangle} \quad \text{with} \quad \mathbf{T} \mathbf{c}(t) \mathbf{c}^\dagger(0) = \begin{cases} \mathbf{c}(t) \mathbf{c}^\dagger(0) & \text{if } t > 0 \\ \mathbf{c}^\dagger(t) \mathbf{c}(0) & \text{if } t < 0 \end{cases} \quad (6)$$

In the position basis, $G(\vec{r}, t, \vec{r}', t') = -i \langle \text{GS} | \mathbf{T} \Psi(\vec{r}, t) \Psi^\dagger(\vec{r}', t') | \text{GS} \rangle$, and for an homogeneous system, its spatial Fourier transform is

$$G(\vec{k}, t) = -i \langle \text{GS} | \mathbf{T} \mathbf{c}_{\vec{k}}(t) \mathbf{c}_{\vec{k}}^\dagger(0) | \text{GS} \rangle$$

By inserting closure relations for α (for $t > 0$) and β basis (for $t < 0$), we get

$$i G(\vec{k}, t) = \begin{cases} + \sum_\alpha e^{+i(\mathcal{E}_0^{(N)} - \mathcal{E}_\alpha^{(N+1)} + \mu)t} |\langle \Psi_{\text{GS}}^{(N)} | \mathbf{c}_{\vec{k}} | \Psi_\alpha^{(N+1)} \rangle|^2 & \text{for } t > 0 \\ - \sum_\beta e^{-i(\mathcal{E}_0^{(N)} - \mathcal{E}_\beta^{(N-1)} - \mu)t} |\langle \Psi_{\text{GS}}^{(N)} | \mathbf{c}_{\vec{k}}^\dagger | \Psi_\beta^{(N-1)} \rangle|^2 & \text{for } t < 0 \end{cases} \quad (7)$$

Now, using the fact that $1_{t>0} = -\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} \frac{e^{i\omega t}}{\omega + i0^+}$, we get that its time Fourier transform verifies

$$\boxed{G(\vec{k}, \omega) = \int_{-\infty}^{+\infty} d\omega' \frac{A(\vec{k}, \omega')}{\omega - \omega' + i0^+ \text{sgn } \omega'}} \quad (8)$$

Using that $\lim_{\eta \rightarrow 0^+} \frac{1}{x + i\eta} = \text{pp}\left(\frac{1}{x}\right) + i\pi \delta(x)$, we can get the reciprocal relation

$$\boxed{A(\vec{k}, \omega) = -\frac{1}{\pi} \Im(G(\vec{k}, \omega))} \quad (9)$$

Thus, if we know the Green's function, we know the spectrum. If we separate Green's functions in term of bands ν and spin projections σ , we have more generally

$$A(\vec{k}, \omega) = -\frac{1}{\pi} \Im \left(\sum_{\nu, \sigma} G_{\nu\sigma}(\vec{k}, \omega) \right)$$

For the non-interacting electron gas, the Green's function is, using (4),

$$G_0(\vec{k}, \omega) = \frac{1}{\omega - \epsilon(\vec{k}) + \mu + i0^+ \text{sgn}(\epsilon(\vec{k}) - \mu)} \quad (10)$$

1.3. Green's function in Wannier basis

If we write $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_{\text{int}}$ with \mathbf{H}_0 separable, and define the Bloch wave-functions by

$$\mathbf{H}_0 |\varphi_{\nu\vec{k}}\rangle = \epsilon_\nu(\vec{k}) |\varphi_{\nu\vec{k}}\rangle$$

1. Because we're looking at $|\Psi_{\text{GS}}\rangle$.

2. Note that if $\mathbf{c}(t) = \mathbf{U}^{-1}(t) \mathbf{c} \mathbf{U}(t)$, then $\mathbf{c}(t)^\dagger = \mathbf{U}(t)^\dagger \mathbf{c}^\dagger \mathbf{U}^{-1}(t)^\dagger = \mathbf{U}^{-1}(t) \mathbf{c}^\dagger \mathbf{U}(t) = \mathbf{c}^\dagger(t)$ as expected.

the Wannier function for band ν and atomic site \vec{R} is defined by

$$\mathcal{W}_{\vec{R},\nu}(\vec{r}) = \int \frac{d\vec{k}}{V_0} \varphi_{\nu\vec{k}}(\vec{r}) e^{-i\vec{k}\cdot\vec{R}} \quad (11)$$

which verifies $\mathcal{W}_{\vec{0},\nu}(\vec{r} - \vec{R}) = \mathcal{W}_{\vec{R},\nu}(\vec{r})$ and form a basis. We then write

$$\Psi_{\sigma}^{\dagger}(\vec{r}, t) = \sum_{\vec{R},\nu} \mathcal{W}_{\vec{R},\nu\sigma}(\vec{r})^* c_{\vec{R},\nu\sigma}^{\dagger} \quad (12)$$

\uparrow creates a Wannier state at site \vec{R}

Now

$$G(\vec{r}, t, \vec{r}', t') = \sum_{\vec{R},\nu} \sum_{\vec{R}',\nu'} \mathcal{W}_{\vec{R},\nu}(\vec{r}) \mathcal{W}_{\vec{R}',\nu'}(\vec{r}') G_{\nu\nu'}^{\mathcal{W}}(\vec{R}, \vec{R}', t)$$

with $G_{\nu\nu'}^{\mathcal{W}}(\vec{R}, \vec{R}', t) = -i \langle \text{GS} | \mathbf{T} c_{\vec{R},\nu}(t) c_{\vec{R}',\nu'}^{\dagger}(0) | \text{GS} \rangle$ the Green's function in Wannier basis, which is more usefull because it depends only on lattice sites \rightarrow allows to map to the Hubbard model.

Then the spatial Fourier transform of the Green's function is much simpler :

$$G(\vec{k}, t) = \sum_{\vec{R}} G^{\mathcal{W}}(\vec{R}, t) e^{i\vec{k}\cdot\vec{R}} \longleftrightarrow G^{\mathcal{W}}(\vec{R}, t) = \int \frac{d\vec{k}}{V_0} G(\vec{k}, t) e^{-i\vec{k}\cdot\vec{R}} \quad (13)$$

1.4. Green's functions at finite temperature, Matsubara time

To define a Green's function at finite $\beta = 1/T$, we could simply take a thermal average :

$$G_{\beta}(\vec{k}, t) = \frac{1}{Z} \text{tr}(e^{-\beta \mathbf{H}_{\text{GC}}} \mathbf{T} c_{\vec{k}}(t) c_{\vec{k}}^{\dagger}(0)) \quad \text{with} \quad Z(\beta) = \text{tr}(e^{-\beta \mathbf{H}_{\text{GC}}})$$

But from time evolution $c(t) = e^{-i\mathbf{H}_{\text{GC}}t} c e^{i\mathbf{H}_{\text{GC}}t}$, we would then get a nasty $e^{-(\beta+it)\mathbf{H}_{\text{GC}}}$ which destroys the nice analytical properties of the Green's function and generates numerical instability because of large oscillation. So let's go fully on the imaginary axis and "take t imaginary" \rightarrow for any operator O , define³

$$O(\tau) := e^{\mathbf{H}_{\text{GC}}\tau} O e^{-\mathbf{H}_{\text{GC}}\tau} \quad (14)$$

where τ is called the *Matsubara time*, and then define the Green's function in Matsubara space :

$$G_{\beta}(\vec{k}, \tau) := \frac{1}{Z} \text{tr}(e^{-\beta \mathbf{H}_{\text{GC}}} \mathbf{T} c_{\vec{k}}(\tau) c_{\vec{k}}^{\dagger}(0)) \quad (15)$$

(we suppose time-homogeneity, else τ, τ'). It is anti-periodic with period β : $G(\tau + \beta) = -G(\tau)$, and the minus sign stems from the fermionic $c c^{\dagger} = c^{\dagger} c$. For bosons, it would be β -periodic. Anyway, we can restrict to the $[0, \beta]$ interval and expand as a Fourier series

$$G_{\beta}(\vec{k}, \tau) =: \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\omega_n\tau} G_{\beta}(\vec{k}, i\omega_n) \quad \text{where} \quad \omega_n = \frac{2n+1}{\beta} \pi \quad (16)$$

are *Matsubara frequencies* (odd multiples of π/β only for fermions). We'll work mostly with this transform of Green's function, denoted $G(i\omega_n)$, which we can compute as $G(i\omega_n) = \int_0^{\beta} d\tau G(\tau) e^{i\omega_n\tau}$.

The behavior at $\tau \rightarrow 0$ is singular : there is a $\tau = 0$ jump $G(\tau \rightarrow 0^+) - G(\tau \rightarrow 0^-) = -1$.

³. Warning : $O(\tau)^{\dagger} = O(-\tau) \neq O^{\dagger}(\tau)$!

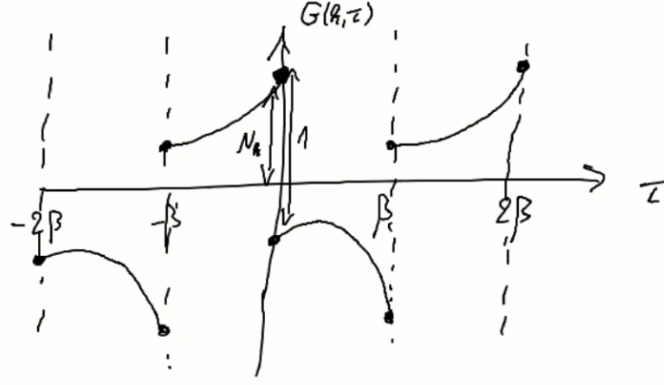


Figure 2. Rough picture of Green's function in Matsubara space.

To compute an observable O from Green's function in Matsubara space :

$$\langle O \rangle_\beta = \frac{1}{Z(\beta)} \text{tr}(e^{-\beta H_{\text{GC}}} O) = \sum_{\vec{k}} O_{\vec{k}} G_\beta(\vec{k}, \tau=0^-)$$

with $O_{\vec{k}} = ???$. In particular, the momentum distribution is given by $N_{\vec{k}} = G(\vec{k}, \tau=0^-)$. But what we're really interested in is the spectral function. As for the $T=0$ case, we inject the closure relations for $N+1$ particles eigenstates (indexed by α) against what was the ground state $|\Psi_{\text{GS}}^{(N)}\rangle$, and now is the thermal mixture of N particles states (indexed by γ) :

$$G_\beta(\vec{k}, i\omega_n) = \frac{1}{Z(\beta)} \sum_{\alpha, \gamma} |\langle \Psi_\gamma^{(N)} | c_{\vec{k}} | \Psi_\alpha^{(N+1)} \rangle|^2 \frac{e^{-\beta \mathcal{E}_\gamma^{(N)}} + e^{-\beta \mathcal{E}_\alpha^{(N+1)}}}{i\omega_n + \mathcal{E}_\gamma^{(N)} - \mathcal{E}_\alpha^{(N+1)}} \quad (17)$$

[todo : pourquoi pas de $N-1$? comment ça se prouve ? ne devrait-on pas prendre une closure relation sur tous les états avec un nombre quelconque de nombre de particule ? pourquoi $e^{\dots} + e^{\dots}$ et pas \times ?]

and define a finite-temperature spectral function

$$A_\beta(\vec{k}, \omega) = \frac{1}{Z(\beta)} \sum_{\alpha, \gamma} |\langle \Psi_\gamma^{(N)} | c_{\vec{k}} | \Psi_\alpha^{(N+1)} \rangle|^2 (e^{-\beta \mathcal{E}_\gamma^{(N)}} + e^{-\beta \mathcal{E}_\alpha^{(N+1)}}) \delta(\omega + \mathcal{E}_\gamma^{(N)} - \mathcal{E}_\alpha^{(N+1)}) \quad (18)$$

which has the same interpretation as the $T=0$ spectral function ($\int d\omega A(\vec{k}, \omega, \beta) = 1 \dots$) and verifies

$$G_\beta(\vec{k}, i\omega_n) = \int_{-\infty}^{+\infty} d\omega' \frac{A_\beta(\vec{k}, \omega')}{i\omega_n - \omega'} \quad (19)$$

[pas de $i0^+$ comme avant ?] Then, for the non-interacting electron gas, the Green's function is, using (4),

$$G_{0,\beta}(\vec{k}, i\omega_n) = \frac{1}{\omega - \epsilon(\vec{k}) + \mu} \quad (20)$$

Also, from (19), we show⁴ that

$$G_\beta(\vec{k}, \tau) = - \int_{-\infty}^{+\infty} d\omega A_\beta(\vec{k}, \omega) \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} \quad (21)$$

which has to be inverted to get $A_\beta(\vec{k}, \omega)$. However, this is unfortunately an ill-defined problem (which can be understood by the fact that the $e^{-\tau\omega}$ makes $A(\omega)$ contribute very little to the integral, so $A(\omega)$ for $\omega\tau \gg 1$ can't be recovered from $G(\tau)$). We have to resort to exotic and approximate inversion methods.

4. $G(\tau) \stackrel{(16)}{=} \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} G(i\omega_n) \stackrel{(19)}{=} \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \int d\omega \frac{A(\omega)}{i\omega_n - \omega} = \int d\omega A(\omega) \underbrace{\frac{1}{\beta} \sum_n \frac{e^{-i\omega_n \tau}}{i\omega_n - \omega}}_{= -\frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}}} \text{ with } \omega_n = \frac{\pi}{\beta} (2n+1)$

c.f. the table at https://en.wikipedia.org/wiki/Matsubara_frequency#Green's_function_related.

[dont we compute $G(i\omega_n)$ and not $G(\tau)$, so it is (19) which need to be inversed, not (21) ?]

The second reason for using Matsubara time is that we'll use Quantum Monte Carlo to solve the problem.

2. The Hubbard model

Single-orbital nearest-neighbor Hubbard model on a lattice $\{i\}$:

$$\mathbf{H} = \underbrace{-t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})}_{\text{hopping / tight-binding / Bloch hybridization}} + \underbrace{U \sum_i n_{i\uparrow} n_{i\downarrow}}_{\text{Coulomb repulsion / double occ. cost}}$$

2.1. Limits

The $t \gg U$ limit leads to full delocalization and **non-interacting** electrons, that is a **band** $\epsilon(\vec{k})$ which is computed by the usual tight-binding methods. \rightarrow non-interacting electron gas $A_0(\vec{k}, \omega) = \delta(\omega - \epsilon(\vec{k}))$.

The $U \gg t$ limit leads to a sum of isolated sites $\mathbf{H}_{\text{GC}}^{(1)} = U n_{i\uparrow} n_{i\downarrow} - \mu (n_{i\uparrow} + n_{i\downarrow})$. The possible states are

state	n	ϵ	ϵ_{GC}
$ \emptyset\rangle$	0	0	0
$\frac{1}{\sqrt{2}}(\uparrow\rangle + \downarrow\rangle)$	1	0	$-\mu$
\dots	1	0	$-\mu$
$ \uparrow\downarrow\rangle$	2	U	$U - 2\mu$

By imposing the condition $\langle n_{i\uparrow} + n_{i\downarrow} \rangle_{\text{GC}} = 1$, we get $\mu = U/2$, and then the spectral function reads

$$A_\sigma(\omega) = \frac{1}{2} \delta\left(\omega - \frac{U}{2}\right) + \frac{1}{2} \delta\left(\omega + \frac{U}{2}\right)$$

This is the *atomic limit*. The Green's function is then computed with (8) :

$$G(\omega) = \frac{1}{2} \frac{1}{\omega - \frac{U}{2} + i0^+} + \frac{1}{2} \frac{1}{\omega + \frac{U}{2} - i0^+} \quad (22)$$

2.2. Self-energy

A quantity easier to handle than Green's functions is the *self-energy*, which is the difference of the inverses of the interacting G and non-interacting $G_0 = G|_{U=0}$ Green's functions :

$$\Sigma := G_0^{-1} - G^{-1} \quad (23)$$

(defined on whatever basis we want), which encodes all 1-body interactions properties. Because the non-interacting problem has a known solution in term of a band $\epsilon(\vec{k})$, G_0 is known (10). In general, $\Sigma \in \mathbb{C}$.

In the atomic limit (22),

$$\Sigma \underset{U \gg t}{=} \left(\frac{U}{2}\right)^2 \frac{1}{\omega + i0^+}$$

In general, the self-energy is temperature-dependant, and going far beyond just putting Fermi-Dirac thermal distributions : the consequences of interactions depends on the temperature (e.g. phase transitions).

Moreover, in the site / Wannier basis, $\Sigma_{ij} = \Sigma_{\vec{R}_i, \vec{R}_j}$ has no reason to be diagonal, *even if the coulombic interactions are purely local* ($U \sum_i n_{i\uparrow} n_{i\downarrow}$, i.e. does not involve $n_i n_j$ terms⁵). This means that the effects of the interaction (encoded in Σ_{ij}) are non-local even if the interaction is local \Rightarrow *non-local correlations*.

⁵ If interactions would be non-local too, i.e. the *exchange interaction*, this would be also included in non-diagonal self-energies of course. But here in the Hubbard model there is no exchange interaction.

In Matsubara time, $\Sigma(\vec{k}, i\omega_n) := G_0(\vec{k}, i\omega_n)^{-1} - G(\vec{k}, i\omega_n)^{-1}$. Using that $G_0(\vec{k}, i\omega_n)^{-1} = \omega - \epsilon(\vec{k}) + \mu$ (20), the interacting Green's function can be written

$$G_\beta(\vec{k}, i\omega_n) = \frac{1}{\omega - \epsilon(\vec{k}) + \mu - \Sigma_\beta(\vec{k}, i\omega_n)} \quad (24)$$

We see that the interactions, via the self-energy Σ_β , *modifies the poles / branch cuts* and their values (in a temperature-dependant way). And because $\Sigma \in \mathbb{C}$, it can give an imaginary part to the poles and create new poles outside the real axis.

- When **interaction effects** are sufficiently weak, it only adds a real part and imaginary part to the poles, which *renormalizes their energy* and shift them out of the real axis → in the spectral function, *the diracs become lorentzians* → interactions *adds width* to the peaks → excitations have a **finite lifetime** and renormalized energies/masses.

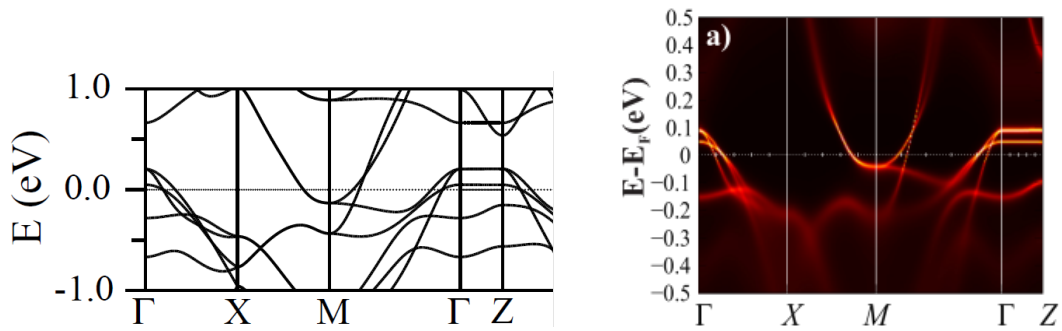


Figure 3. **Band structure** vs. spectral function of LaFeAsO by DMFT. **Washed-out peaks** ← has some width.

- When **interaction effects** are strong, poles are created and destroyed relative to $\Sigma = 0$ and the landscape of the spectral function is totally changed, and we often don't have bands anymore.

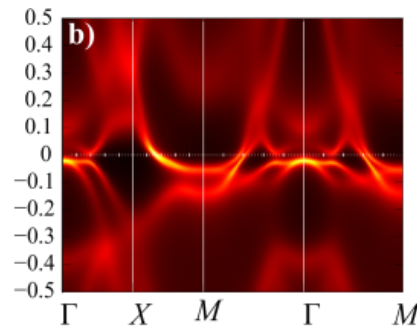


Figure 4. Heavily doped LaFeAsO_{1-x}H_x spectral function : **very washed-out, renormalized and deformed** band near ϵ_F , and fuzzy/new structures away from ϵ_F .

2.3. The LISA approximation : mapping the Hubbard model on an mean-field impurity model self-consistently

Authoritative review by Georges, Kotliar, Krauth & Rozenberg : https://www.physics.rutgers.edu/~gkguest/papers/rmp63_1996_p13_Kotliar.pdf

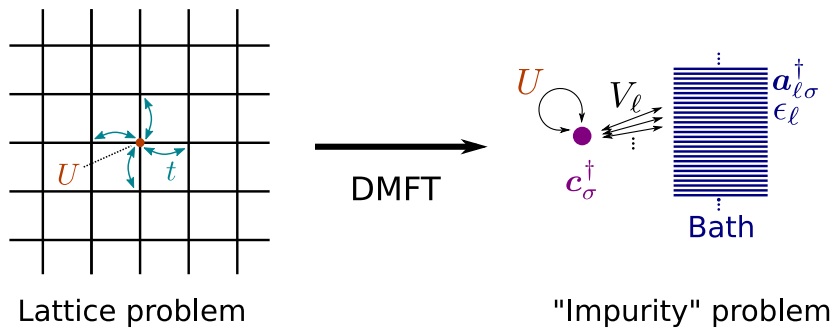
To compute the Hubbard model, we'll approximate it in a mean-field framework (which should be exact in the infinite dimensional limit), where by the law of large numbers, *fluctuations between sites vanishes*, and *quantum fluctuations become purely local*. We do not want to freeze out all fluctuations (would give Hartree-Fock), and in the LISA (Local Impurity Self-consistent Approximation) framework, we'll keep these local, temporal in nature, fluctuations, hence the name of Dynamical Mean Field Theory, or DMFT.

More precisely, in infinite dimensional limit, where the coordinance $z \rightarrow \infty$ (and with $t \mapsto t/\sqrt{z}$ to keep the kinetic energy constant), fluctuations due to neighbors vanish. Hopping fluctuations are averaged-out and are irrelevant. Remains only *local* quantum fluctuations (because it's still a quantum problem). An important consequence is that *correlations become local only* \Leftrightarrow *the self-energy becomes site-diagonal* :

$$\Sigma_{ij} = \Sigma_{ii} \delta_{ij} = \Sigma_{\text{site}} \delta_{ij}$$

where we are only left with a single number Σ_{site} because of translational invariance. It looks very much like an isolated site problem, but still we allow for on-site charge fluctuations and we still have to account for the effects of the periodic lattice, in a mean-field way : the site is *bathed* in the "field" created by its neighbors. Thus, as often in mean-field theories, the lattice problem is reduced to / mapped on a *single site model*, which is a fermionic model describing a single site with

- Coulomb **interaction** U
- **Coupled to a bath** to allow charge fluctuation, representing neighbors on the lattice in a mean-field way, just like a mean-field Ising model
- A self-consistent condition on the bath to connect back / capture the properties of the original Hubbard model : translational invariance and coherence effects of the lattice



which looks like an **Anderson impurity model** :

$$\mathbf{H}_{\text{imp}} = \mathbf{H}_{\text{site}} + \mathbf{H}_{\text{coupl}} + \mathbf{H}_{\text{bath}} \quad \text{where} \quad \begin{cases} \mathbf{H}_{\text{site}} = (\epsilon_0 - \mu) (\mathbf{n}_\uparrow + \mathbf{n}_\downarrow) + U \mathbf{n}_\uparrow \mathbf{n}_\downarrow & (\mathbf{n} = \mathbf{c}^\dagger \mathbf{c}) \\ \mathbf{H}_{\text{bath}} = \sum_{\ell\sigma} E_\ell \mathbf{a}_{\ell\sigma}^\dagger \mathbf{a}_{\ell\sigma} \\ \mathbf{H}_{\text{coupl}} = \sum_{\ell\sigma} V_\ell (\mathbf{a}_{\ell\sigma}^\dagger \mathbf{c}_\sigma + \mathbf{c}_\sigma^\dagger \mathbf{a}_{\ell\sigma}) \end{cases}$$

/!\ It is not a single-particle problem !⁶ We can't reduce to non-interacting problem if we want to describe the on-site repulsion. This is really still a N -body problem, but a much simpler one where spatial fluctuations have been eliminated.

The bath $\{\mathbf{a}_{\ell\sigma}^\dagger\}$ is described by effective energy levels E_ℓ , here discrete, but it is a band structure really, which can be *metallic* or *insulating* depending if there are states at the Fermi energy μ or not. The effective coupling constants V_ℓ and effective energy levels E_ℓ are choosen/solved so as to reproduce our initial Hubbard system self-consistently. However, it is more useful to work with an action representation of \mathbf{H}_{imp} :

$$\mathcal{S}^{\text{imp}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{c}^\dagger(\tau) \mathcal{G}_0(\tau - \tau') \mathbf{c}(\tau) + U \int_0^\beta d\tau \mathbf{n}_\uparrow(\tau) \mathbf{n}_\downarrow(\tau)$$

6. A mean-field auxiliary system, in general, is a system which is both useful (describes the original system in some sense) and such that we can solve it (at least numerically). But there is actually no specific conditions on it, in particular it does not need to be non-interacting.

where the degrees of freedom of the bath has been integrated into the bath Green's function \mathcal{G}_0

$$\mathcal{G}_0(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_0 - \Delta(i\omega_n)} \quad \text{with} \quad \Delta(i\omega_n) = \sum_{\ell} \frac{|V_{\ell}|}{i\omega_n - E_{\ell}}$$

(just like for the Ising model where neighbors have been integrated into the Weiss mean field; $\mathcal{G}_0(i\omega_n)$ is thus also called the *Weiss function*⁷)

$$\mathcal{G}_0(i\omega_n) = \frac{1}{i\omega_n + \mu + G(i\omega_n)^{-1} - R(G(i\omega_n))}$$

where R is the reciprocal function of

$$\tilde{\eta}(\zeta) = \int_{-\infty}^{+\infty} d\epsilon \frac{\eta^{\text{latt}}(\epsilon)}{\zeta - \epsilon}$$

the Hilbert transform of the density of states $\eta^{\text{latt}}(\epsilon)$ of the lattice $\{i\}$, i.e. $\zeta = R(\tilde{\eta}(\zeta))$.

Self-consistency : In the mean-field treatment of the Ising model, the self-consistent equation $m = m_{\text{MF}} = f(m)$ actually comes from *translational invariance* : a site and its neighbors actually really see the same Weiss field (up to spatial fluctuations we ignore).

2.4. The infinite dimensional limit

2.5. Solving the impurity problem. The DMFT loop.

2.6. Iterated perturbation theory approximation

⁷. Note that contrary to an Ising model where the Weiss field is only a *number*, it is here a *function* of τ , encoding local quantum fluctuations; also contrary to a Hartree-Fock approximation where we reduce everything to a single state.