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-particule 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, $I(\vec{k}_{\|},\epsilon=\hbar\omega)\propto|\text{matrix elem}|^2\, f^{\text{FD}}(\epsilon)\, A(\vec{k},\omega)$), and what we're interested at the end of the day. Defined as

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

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

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

and where $\left\{|\Psi_\beta^{(N-1)}\rangle\right\}_\beta$ 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

$$\boldsymbol{H}_{\text{GC}}=\boldsymbol{H}-\mu\,\boldsymbol{N} \tag{2}$$

The spectral function verifies

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

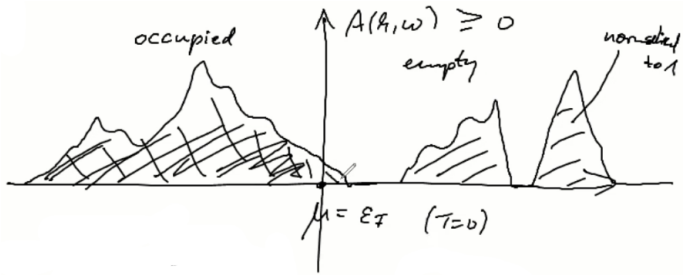


Figure 1. Illustation of a spectral function $A(\vec{k},\omega)$ at a given $\vec{k}$, as function of ω.

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 $\left\{\vec{k}_1,\dots,\vec{k}_N,(\vec{k}_{N+1}=\vec{k})\right\}$, $\Psi_{\text{GS}}^{(N)}$ is a Fermi sea so $\vec{k}_1,\dots,\vec{k}_N$ are fixed in the sum ($|\Psi_\alpha^{(N+1)}\rangle$ must be $\boldsymbol{c}_{\vec{k}}^\dagger\,|\Psi_{\text{GS}}^{(N)}\rangle$), $\epsilon_\alpha=\epsilon(\vec{k})-\mu$, and are simply left with

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

The k-summed spectral function $A_0(\omega)=\int\mathrm{d}\vec{k}\,A_0(\vec{k},\omega)=\int\mathrm{d}\vec{k}\,\delta\big(\omega-(\epsilon(\vec{k})-\mu)\big)$ 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

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

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

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

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

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

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

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

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

$$\boxed{G(\vec{k},\omega)=\int_{-\infty}^{+\infty}\mathrm{d}\omega'\,\frac{A(\vec{k},\omega')}{\omega-\omega'+\mathrm{i}\,0^+\,\mathrm{sgn}\,\omega'}} \tag{8}$$

Using that $\lim\limits_{\eta\to0^+}\frac{1}{x+\mathrm{i}\,\eta}=\mathrm{pp}\big(\frac{1}{x}\big)+\mathrm{i}\pi\,\delta(x)$, we can get the reciprocical relation

$$\boxed{A(\vec{k},\omega)=-\tfrac{1}{\pi}\,\mathfrak{Im}\big(G(\vec{k},\omega)\big)} \tag{9}$$

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

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

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

$$G_0(\vec{k},\omega)=\frac{1}{\omega-\epsilon(\vec{k})+\mu+\mathrm{i}\,0^+\,\mathrm{sgn}\,(\epsilon(\vec{k})-\mu)} \tag{10}$$

1.3. Green's function in Wannier basis

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

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

1. Because we're looking at $|\Psi_{\mathrm{GS}}\rangle$.
2. Note that if $\boldsymbol{c}(t)=\boldsymbol{U}^{-1}(t)\,\boldsymbol{c}\,\boldsymbol{U}(t)$, then $\boldsymbol{c}(t)^\dagger=\boldsymbol{U}(t)^\dagger\,\boldsymbol{c}^\dagger\,\boldsymbol{U}^{-1}(t)^\dagger=\boldsymbol{U}^{-1}(t)\,\boldsymbol{c}^\dagger\,\boldsymbol{U}(t)=\boldsymbol{c}^\dagger(t)$ as expected.

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

$$\mathcal{W}_{\vec{R},\nu}(\vec{r}) \;=\; \int \frac{\mathrm{d}\vec{k}}{\mathcal{V}_0}\, \varphi_{\nu\vec{k}}(\vec{r})\, \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{R}} \tag{11}$$

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

$$\boldsymbol{\Psi}^\dagger_\sigma(\vec{r},t) \;=\; \sum_{\vec{R},\nu} \mathcal{W}_{\vec{R}\nu\sigma}(\vec{r})^*\, \boldsymbol{c}^\dagger_{\vec{R}\nu\sigma} \tag{12}$$

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

Now

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

with $G^{\mathcal{W}}_{\nu\nu'}(\vec{R},\vec{R}',t) = -\mathrm{i}\,\langle \mathrm{GS}|\, \boldsymbol{T}\boldsymbol{c}_{\vec{R}\nu}(t)\, \boldsymbol{c}^\dagger_{\vec{R}'\nu'}(0)\,|\mathrm{GS}\rangle$ 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 :

$$G(\vec{k},t) = \sum_{\vec{R}} G^{\mathcal{W}}(\vec{R},t)\, \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}} \quad\longleftrightarrow\quad G^{\mathcal{W}}(\vec{R},t) = \int \frac{\mathrm{d}\vec{k}}{\mathcal{V}_0} G(\vec{k},t)\, \mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{R}} \tag{13}$$

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 :

$$G_\beta(\vec{k},t) \;=\; \frac{1}{Z}\,\mathrm{tr}\big(\mathrm{e}^{-\beta \boldsymbol{H}_{\mathrm{GC}}}\, \boldsymbol{T}\boldsymbol{c}_{\vec{k}}(t)\, \boldsymbol{c}^\dagger_{\vec{k}}(0)\big) \quad \text{with} \quad Z(\beta) = \mathrm{tr}(\mathrm{e}^{-\beta \boldsymbol{H}_{\mathrm{GC}}})$$

But from time evolution $\boldsymbol{c}(t) = \mathrm{e}^{-\mathrm{i}\boldsymbol{H}_{\mathrm{GC}}\,t}\, \boldsymbol{c}\, \mathrm{e}^{\mathrm{i}\boldsymbol{H}_{\mathrm{GC}}\,t}$, we would then get a nasty $\mathrm{e}^{-(\beta+\mathrm{i}t)\boldsymbol{H}_{\mathrm{GC}}}$ which destoys 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 $\boldsymbol{O}$, define[3]

$$\boldsymbol{O}(\tau) \;:=\; \mathrm{e}^{\boldsymbol{H}_{\mathrm{GC}}\,\tau}\, \boldsymbol{O}\, \mathrm{e}^{-\boldsymbol{H}_{\mathrm{GC}}\,\tau} \tag{14}$$

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

$$\boxed{G_\beta(\vec{k},\tau) \;:=\; \frac{1}{Z}\,\mathrm{tr}\big(\mathrm{e}^{-\beta \boldsymbol{H}_{\mathrm{GC}}}\, \boldsymbol{T}\boldsymbol{c}_{\vec{k}}(\tau)\, \boldsymbol{c}^\dagger_{\vec{k}}(0)\big)} \tag{15}$$

(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 $\boldsymbol{c}\boldsymbol{c}^\dagger = \boldsymbol{c}^\dagger\boldsymbol{c}$. For bosons, it would be β-periodic. Anyway, we can restrict to the $[0,\beta]$ interval and expand as a Fourier series

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

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

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

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

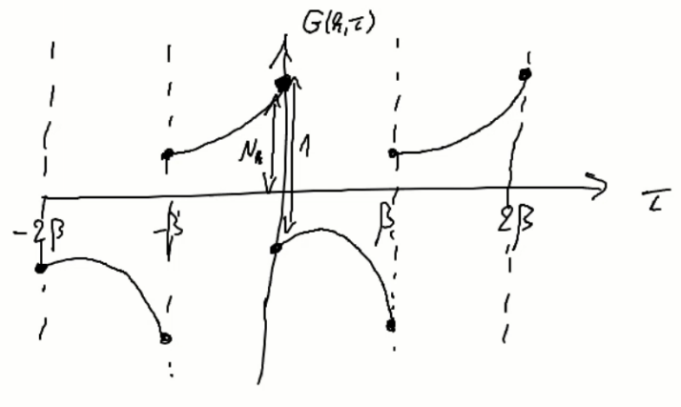


Figure 2. Rough picture of Green's function in Matsubara space.

To compute an observable $\boldsymbol{O}$ from Green's function in Matsubara space :

$$\langle \boldsymbol{O} \rangle_\beta = \frac{1}{Z(\beta)} \mathrm{tr}\big(\mathrm{e}^{-\beta \boldsymbol{H}_{\mathrm{GC}}} \boldsymbol{O}\big) = \sum_{\vec{k}} O_{\vec{k}} G_\beta(\vec{k}, \tau = 0^-)$$

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 $N+1$ particules eigenstates[4] (indexed by α) against what was the ground state $|\Psi_{\mathrm{GS}}^{(N)}\rangle$, and now is the thermal mixture of N particules states (indexed by γ) :

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

[todo : pourquoi $\mathrm{e}^{\cdots} + \mathrm{e}^{\cdots}$ et pas $\times$?]

and define a finite-temperature spectal function

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

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

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

[pas de $\mathrm{i}\,0^+$ comme avant ?] Then, for the non-interacting electron gas, the Green's function is, using (4),

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

Also, from (19), we show[5] that

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

4. As for the $T = 0$ case, we take the closure relation on the full Fock space (all $N \in \mathbb{N}$ a priori) obviously, but because of the $\langle \Psi_\gamma^{(N)}| \boldsymbol{c}_{\vec{k}}$, only remains $|\Psi_\alpha^{(N+1)}\rangle$ states. And for negative times / frequencies ? We forget it, or it has no meaning with Matsubara time ?

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

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

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 $\mathrm{e}^{-\tau\omega}$ 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 invertion methods.

It looks simpler to invert (19) because there is no exponential tail, but (19) and (21) are directly (linearly) related so if the problem is ill-defined/hard for (21), it is also for (19). Choosing to invert from $G(\mathrm{i}\,\omega_n)$ or $G(\tau)$ is then just a matter of taste.

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 $\{i\}$:

$$\boxed{\boldsymbol{H} = \underbrace{-\sum_{\langle i,j\rangle,\sigma} t_{ij}\,(\boldsymbol{c}^\dagger_{i\sigma}\,\boldsymbol{c}_{j\sigma} + \boldsymbol{c}^\dagger_{j\sigma}\,\boldsymbol{c}_{i\sigma})}_{\substack{\text{hopping / tight-binding}\\ \text{/ Bloch hybridization}}} + \underbrace{U\sum_i \boldsymbol{n}_{i\uparrow}\,\boldsymbol{n}_{i\downarrow}}_{\substack{\text{Coulomb repulsion}\\ \text{/ double occ. cost}}}} \tag{22}$$

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 method

$$\boldsymbol{H} = -\sum_{\langle i,j\rangle,\sigma} t_{ij}\,(\boldsymbol{c}^\dagger_{i\sigma}\,\boldsymbol{c}_{j\sigma} + \boldsymbol{c}^\dagger_{j\sigma}\,\boldsymbol{c}_{i\sigma}) = \sum_{\vec{k},\sigma} \epsilon(\vec{k})\,\boldsymbol{c}^\dagger_{\vec{k}\sigma}\,\boldsymbol{c}_{\vec{k}\sigma} \quad \text{with} \quad \epsilon(\vec{k}) = \sum_{i,j} t_{ij}\,\mathrm{e}^{\mathrm{i}\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} \tag{23}$$

$\to A_0(\vec{k},\omega) = \delta(\omega - \epsilon(\vec{k}))$. We immediately recover the non-interacting Green's function (20).

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

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

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

$$A_\sigma(\omega) = \tfrac{1}{2}\,\delta\Big(\omega - \tfrac{U}{2}\Big) + \tfrac{1}{2}\,\delta\Big(\omega + \tfrac{U}{2}\Big)$$

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

$$G(\omega) = \tfrac{1}{2}\,\frac{1}{\omega - \frac{U}{2} + \mathrm{i}\,0^+} + \tfrac{1}{2}\,\frac{1}{\omega + \frac{U}{2} - \mathrm{i}\,0^+} \tag{24}$$

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 :

$$\Sigma := G_0^{-1} - G^{-1} \tag{25}$$

(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 (24),

$$\Sigma \underset{U \gg t}{=} \left(\frac{U}{2}\right)^2 \frac{1}{\omega + \mathrm{i}\,0^+}$$

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* ($U \sum_i \boldsymbol{n}_{i\uparrow} \boldsymbol{n}_{i\downarrow}$, i.e. does not involve $\boldsymbol{n}_i \boldsymbol{n}_j$ terms[6]). 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*.

In Matsubara time, $\Sigma_{ij}(\mathrm{i}\omega_n) := G_{0,ij}(\mathrm{i}\omega_n)^{-1} - G_{ij}(\mathrm{i}\omega_n)^{-1}$ in the site basis, or in the wavevector basis $\Sigma(\vec{k}, \mathrm{i}\omega_n) := G_0(\vec{k}, \mathrm{i}\omega_n)^{-1} - G(\vec{k}, \mathrm{i}\omega_n)^{-1}$. Using that $G_0(\vec{k}, \mathrm{i}\omega_n)^{-1} = \mathrm{i}\,\omega_n - \epsilon(\vec{k}) + \mu$ (20), the interacting Green's function can be written

$$\boxed{G_\beta(\vec{k}, \mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\,\omega_n - \epsilon(\vec{k}) + \mu - \Sigma_\beta(\vec{k}, \mathrm{i}\omega_n)}} \tag{26}$$

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.

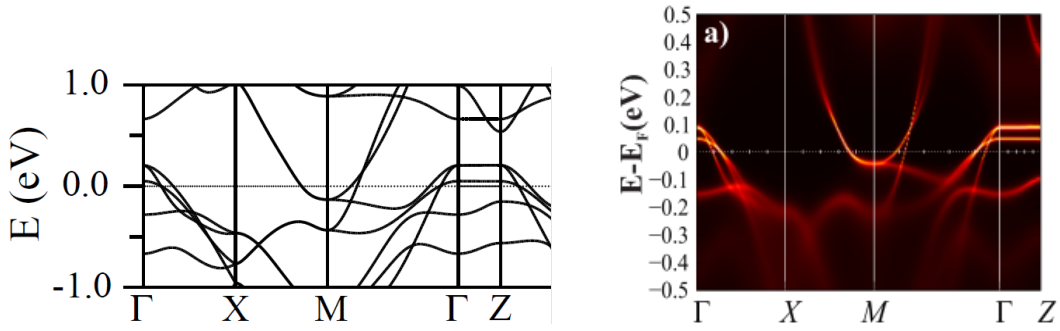


Figure 3. Band structure vs. spectral function of $\mathrm{LaFeAsO}$ by DMFT. Washed-out peaks ← has some width.

→ 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.

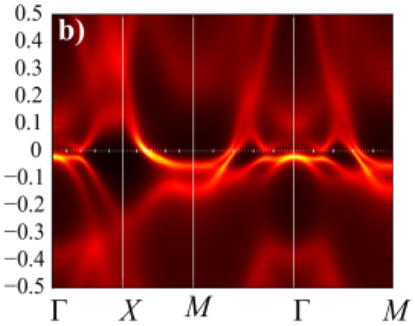


Figure 4. Heavily dopped $\mathrm{LaFeAsO}_{1-x}\mathrm{H}_x$ spectral function : very washed-out, renormalized and deformed band near ϵ_F, and fuzzy/new structures away from ϵ_F.

6. 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.

2.3. The Hubbard model in infinite dimensions : towards a DMFT

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 present framework, we'll keep these local, temporal in nature, fluctuations, hence the name of Dynamical Mean Field Therory, or DMFT.

More precisely, in infinite dimensional limit, where the coordinance $z \to \infty$ (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* :

$$\Sigma_{ij} \overset{d=\infty}{=} \Sigma_{ii}\,\delta_{ij} = \Sigma_{\text{loc}}\,\delta_{ij}$$

where we are only left with a single number Σ_{loc} 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.

And we'll use this approximation in finite dimensions :

$$\boxed{\Sigma_{ij} \overset{\text{DMFT}}{\approx} \Sigma_{\text{loc}}\,\delta_{ij}} \quad \Leftrightarrow \quad \Sigma(\vec{k}) \approx \Sigma_{\text{loc}} \tag{27}$$

and the Green's function (26) becomes

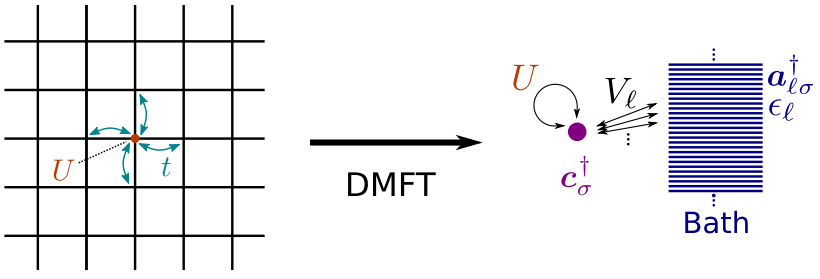
$$\boxed{G_\beta(\vec{k}, \mathrm{i}\omega_n) \overset{\text{DMFT}}{\approx} \frac{1}{\mathrm{i}\,\omega_n - \epsilon(\vec{k}) + \mu - \Sigma^{\text{loc}}_\beta(\mathrm{i}\omega_n)}} \tag{28}$$

2.4. The LISA framework

2.4.1. An impurity model on which the Hubbard model is reduced

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[7]

- → Coulomb interaction U (the same U as before in standard DMFT)
- → 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



Lattice problem "Impurity" problem

7. Color code : non-interacting properties interacting properties ($U \neq 0$) impurity bath

which looks like an *Anderson impurity model* :

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

/!\ It is not a single-particule problem ![8] We can't reduce to non-interacting problem if we want to describe the on-site repeulsion. This is really still a N-body problem, the site being described by creation operators $\boldsymbol{c}^\dagger_\sigma$, but a much simpler one where spatial fluctuations have been eliminated.

The natural framework for relating the initial Hubbard model and the impurity model is the one of Green's functions. In the initial probem, the Green's function describes processes on-site $\vec{R} \to \vec{R}$ ($G_{ii} \equiv G_{\mathsf{loc}}$, the *local part of the Green's function*) but also *between* sites $\vec{R}_i \to \vec{R}_j$ ($G_{ij} = G^{\mathcal{W}}(\vec{R}_i, \vec{R}_j)$). However, in the impurity model, there is only the impurity Green's function

$$G^{\mathsf{imp}}_\sigma(t) := -\mathrm{i}\,\langle \boldsymbol{T}\boldsymbol{c}_\sigma(t)\,\boldsymbol{c}^\dagger_\sigma(0)\rangle \quad (\text{and } G^{\mathsf{imp}}_\beta(\mathrm{i}\omega_n))$$

As always, if there is no magnetic order, $G_\uparrow = G_\downarrow$ and we can drop σ.

The spirit of DMFT is to simply forget about non-local self-energy, cf. (27), and we can only impose

$$\text{local Hubbard} \to \boxed{G^{\mathsf{latt}}_{\mathsf{loc}} \overset{!}{=} G^{\mathsf{imp}}} \leftarrow \text{impurity} \tag{29}$$

This is the **LISA framework** (Local Impurity Self-consistent Approximation). Only the *local part* of the Green's functions are required to be the same. If we'd want to have non-local Green's functions, it would be much more complicated (would need more than a single site). If we took a "movie" of a single site in the Hubbard model, it will be the same [is is true ?] than in the impurity model, only spatial fluctuations would be not reproduced.

The bath $\{\boldsymbol{a}^\dagger_{\ell\sigma}\}$ is described by effective energy levels E_ℓ, here discrete, but it is a band structure really, which can be *metalic* 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, there is an unnecessary freedom of choice and complexity in this description and we'd better of using an action representation[9] of $\boldsymbol{H}^{\mathrm{GC}}_{\mathrm{imp}}$:

$$\boldsymbol{S}^{\mathsf{imp}} = -\int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau'\,\boldsymbol{c}^\dagger(\tau)\,\frac{1}{\mathcal{G}_0(\tau-\tau')}\,\boldsymbol{c}(\tau) + U\int_0^\beta \mathrm{d}\tau\,\boldsymbol{n}_\uparrow(\tau)\,\boldsymbol{n}_\downarrow(\tau) \tag{30}$$

(and $\sum_\sigma \boldsymbol{c}^\dagger_\sigma(\tau)\,\mathcal{G}_{0,\sigma}(\tau-\tau')^{-1}\,\boldsymbol{c}_\sigma(\tau)$ is there is magnetic order) where the degrees of freedom of the bath has been formally integrated[10] into the *bath Green's function* $\mathcal{G}_0$:

$$\mathcal{G}_0(\mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n - \epsilon_0 + \mu - \Delta(\mathrm{i}\omega_n)} \quad \text{with} \quad \Delta(\mathrm{i}\omega_n) = \sum_\ell \frac{|V_\ell|^2}{\mathrm{i}\omega_n - E_\ell} \tag{31}$$

(just like for the Ising model where neighbors have been integrated into the Weiss mean field; $\mathcal{G}_0(\mathrm{i}\omega_n)$ is thus also called the *Weiss field*, or the *dynamical mean field*[11]). The $\boldsymbol{c}^\dagger(\tau)\,\mathcal{G}_0(\tau-\tau')^{-1}\,\boldsymbol{c}(\tau)$ process is : "an electron comes on the site, waits a bit $(\tau-\tau')$ depending on the coupling with the bath (described by $\mathcal{G}_0(\mathrm{i}\omega_n) \Leftrightarrow \Delta(\mathrm{i}\omega_n)$) and goes back somewhere in the bath"[12]. The second term $U\,\boldsymbol{n}_\uparrow(\tau)\,\boldsymbol{n}_\downarrow(\tau)$ describes coulombic interaction.

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8. 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.

9. See it as an action appearing in a path integral $Z = \int \mathrm{D}\boldsymbol{c}^\dagger\,\mathrm{D}\boldsymbol{c}\,\mathrm{e}^{-\boldsymbol{S}[\boldsymbol{c}^\dagger,\boldsymbol{c}]}$.

10. The hamiltonian $\boldsymbol{H}_{\mathsf{imp}}$ is *quadratic* in $\boldsymbol{a}^\dagger_{\ell\sigma}$, $\boldsymbol{a}_{\ell\sigma}$'s, allowing integration of bath degrees of freedom.

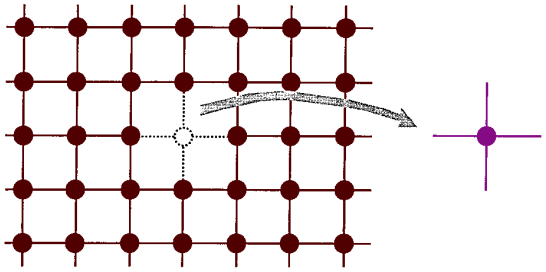
11. Note that contrary to an Ising model where the Weiss field is only a *number*, it is here a *function* of τ, encoding local quantum fluctuations; also contrary to a Hartree-Fock approximation where we reduce everything to a single state.

12. More comments : `mesm-silke-4.mp4` @ 1:26:20

In the non-interacting limit $U=0$, (30) can be solved and yields $G_0^{\text{imp}} = \mathcal{G}_0$, so $\mathcal{G}_0$ is already the non-interacting Green's function (of both the impurity model, and the original problem locally) [todo; see `mesm-silke-4.mp4` @ 1:35:30; it would be interesting to see exactly how can we go from the non-interacting tight-binding model to the impurity action]

2.4.2. Computing the mean field $\mathcal{G}_0$ describing the bath : Self-consistency

Just as for the Ising model, we have to compute the mean field acting on the impurity. For that, we must derive the action S^{imp} directly from the Hubbard model. The simplest way is using the **cavity method** [GKKR section III.A, p. 21].



The big picture is the following : by tracing out neighbors degrees of freedom of a given site, yielding an effective action for an isolated site S_{eff}, and then performing a mean-field approximation by removing many terms which disapear in $d\to\infty$, we eventually get the action (30) with $\mathcal{G}_0^{-1} = \mathrm{i}\omega_n + \mu - \Delta$ with

$$\begin{aligned}\Delta(\mathrm{i}\omega_n) &\underset{d\to\infty}{\simeq} \sum_{i,j} t_{oi}\, t_{oj}\, G_{ij}^{(o)}(\mathrm{i}\omega_n) \\ &= \sum_{i,j} t_{oi}\, t_{oj}\, G_{ij} - \frac{1}{G_{oo}}\Big(\sum_i t_{oi}\, G_{io}\Big)^2\end{aligned} \tag{32}$$

where $G_{ij}^{(o)} = G_{ij} - \frac{G_{io}\,G_{oj}}{G_{oo}}$ is the Green's function for the Hubbard lattice without site o, and G_{ij} the one for the full Hubbard lattice.

We want to replace the nasty hopping amplitudes t_{ij} by the band structure, that is $\epsilon(\vec{k}) = \mathrm{FT}[t_{ij}](\vec{k})$ (23) and its density of states $\eta^{\text{latt}}(\epsilon) = \sum_{\vec{k}} \delta(\epsilon - \epsilon(\vec{k}))$. For example, the term

$$\begin{aligned}\sum_i t_{oi}\, G_{io} &= \sum_i \sum_{\vec{k}} \mathrm{e}^{\mathrm{i}\vec{k}\cdot(-\vec{R}_i)}\,\epsilon(\vec{k}) \sum_{\vec{k}'} \mathrm{e}^{\mathrm{i}\vec{k}'\cdot\vec{R}_i}\, G(\vec{k}') \\ &= \sum_{\vec{k}} \epsilon(\vec{k})\, G(\vec{k}) \quad \text{because} \quad \sum_i \mathrm{e}^{\mathrm{i}(\vec{k}'-\vec{k})\cdot\vec{R}_i} = \delta(\vec{k}'-\vec{k})\end{aligned}$$

$$\text{and similarly,} \quad \sum_{i,j} t_{oi}\, t_{oj}\, G_{ij} = \sum_{\vec{k}} \epsilon(\vec{k})^2\, G(\vec{k})$$

$$\text{and} \quad G_{oo} = \sum_{\vec{k}} G(\vec{k})$$

Now, using the DMFT expression of the Hubbard lattice Green's function (28) $G(\vec{k},\mathrm{i}\omega_n)^{-1} = \zeta - \epsilon(\vec{k})$ with $\zeta = \mathrm{i}\omega_n + \mu - \Sigma_{\text{loc}}(\mathrm{i}\omega_n)$, these three terms reads (for $l=1,2,0$ resp.)

$$\sum_{\vec{k}} \frac{\epsilon(\vec{k})^l}{\zeta - \epsilon(\vec{k})} = \int \mathrm{d}\epsilon\, \frac{\epsilon^l}{\zeta-\epsilon} \sum_{\vec{k}} \delta(\epsilon - \epsilon(\vec{k})) \overset{\text{def}}{=} \int \mathrm{d}\epsilon\, \eta(\epsilon)\, \frac{\epsilon^l}{\zeta-\epsilon} =: h_l(\zeta)$$

Then,

$$\Delta = h_2(\zeta) - h_1(\zeta)^2 / h_0(\zeta)$$

Using the properties $h_1(\zeta) = \zeta \cdot h_0(\zeta) - 1$ and $h_2(\zeta) = \zeta \cdot h_1(\zeta)$ (which are valid if $\int \mathrm{d}\epsilon\, \eta(\epsilon)\, \epsilon = t_{oo} = 0$), we finally have $\Delta = \zeta - \frac{1}{h_0(\zeta)}$. In fact, $h_0(\zeta)$ is the Hilbert transform $\tilde{\eta}$ of the density of states $\eta(\epsilon) = \eta^{\text{latt}}(\epsilon)$ of the lattice $\{i\}$:

$$\tilde{\eta}(\zeta) = \int_{-\infty}^{+\infty} \mathrm{d}\epsilon \, \frac{\eta^{\text{latt}}(\epsilon)}{\zeta - \epsilon} \tag{33}$$

Now, we have to inject back in $\mathcal{G}_0^{-1} = \mathrm{i}\,\omega_n + \mu - \Delta$ (31, with $\epsilon_0 = 0$) to obtain the bath Green's function from the Hubbard model : $\mathcal{G}_0^{-1} = \cancel{\zeta} + \Sigma_{\text{loc}} - (\cancel{\zeta} - 1/\tilde{\eta}(\zeta))$, or

$$\boxed{\mathcal{G}_0(\mathrm{i}\,\omega_n)^{-1} = \Sigma_{\text{loc}}(\mathrm{i}\,\omega_n) + \frac{1}{\tilde{\eta}\big(\zeta(\mathrm{i}\,\omega_n)\big)} \quad \text{with} \quad \zeta(\mathrm{i}\,\omega_n) \overset{(28)}{=} \mathrm{i}\,\omega_n + \mu - \Sigma_{\text{loc}}(\mathrm{i}\omega_n)} \tag{34}$$

We can express this Weiss field as a function of G_{loc}, hiding $\tilde{\eta}$, by remarking that

$$G_{\text{loc}} \overset{(28)}{=} \textstyle\sum_{\vec{k}} G(\vec{k}) = h_0(\zeta) = \tilde{\eta}(\zeta)$$

so we obtain the **Dyson equation**

$$\boxed{\Sigma_{\text{loc}} = \frac{1}{\mathcal{G}_0} - \frac{1}{G_{\text{loc}}}} \tag{35}$$

A third expression can be obtained from the above ones : $\mathcal{G}_0^{-1} = \Sigma_{\text{loc}} + G_{\text{loc}}^{-1} = \mathrm{i}\,\omega_n + \mu - \zeta + G_{\text{loc}}^{-1}$ and

$$G_{\text{loc}} = \tilde{\eta}(\zeta) \quad \Leftrightarrow \quad \zeta = R(G_{\text{loc}})$$

where R is the reciprocal function of $\tilde{\eta}(\zeta)$, i.e. $\zeta = R(\tilde{\eta}(\zeta))$, so that

$$\boxed{\mathcal{G}_0(\mathrm{i}\,\omega_n)^{-1} = \mathrm{i}\,\omega_n + \mu + G_{\text{loc}}(\mathrm{i}\,\omega_n)^{-1} - R(G_{\text{loc}}(\mathrm{i}\,\omega_n))} \tag{36}$$

Pfffew. Let's recap : we encoded the properties of the Hubbard lattice (lattice **hybridization** and **translational invariance**[13]) in an expression for the dynamical mean field $\mathcal{G}_0 = \mathrm{DMF}[G_{\text{loc}}]$, as a function of the wanted result itself, the Green's function of the site.

	Ising model	Hubbard model
Hamiltonian	$H = -\sum_{ij} J_{ij}\, s_i\, s_j$	$\boldsymbol{H} = -\sum_{ij} t_{ij}\, \boldsymbol{c}_i^\dagger\, \boldsymbol{c}_j + U \sum_i \boldsymbol{n}_{i\uparrow}\, \boldsymbol{n}_{i\downarrow}$ (22)
Local observable	$m = \langle s_i \rangle$	$G_{\text{loc}}(\tau) = -\langle \boldsymbol{c}_i^\dagger(\tau)\, \boldsymbol{c}_i(0) \rangle$
Spatial correlations	$\langle s_i\, s_j \rangle$	$G_{ij}(\tau) = -\langle \boldsymbol{c}_i^\dagger(\tau)\, \boldsymbol{c}_j(0) \rangle$
Single-site model	$H_{\text{MF}}^{(1)} = -B_{\text{Weiss}} \cdot s$	$\boldsymbol{H}_{\text{imp}} \mid \boldsymbol{S}^{\text{imp}} = -\int\int \frac{\boldsymbol{c}^\dagger(\tau)\, \boldsymbol{c}(\tau)}{\mathcal{G}_0(\tau - \tau')} + U \int \boldsymbol{n}_\uparrow\, \boldsymbol{n}_\downarrow$ (30)
Mean field / Bath	$B_{\text{Weiss}} = J\, z\, m$	$\mathcal{G}_0(\tau) = \mathrm{DMF}[G_{\text{loc}}]$ (34,35,36) ($\Leftrightarrow \{V_\ell, E_\ell\}$)
Self-consistency	$m \overset{!}{=} m_{\text{MF}}(B_{\text{Weiss}})$	$G_{\text{loc}} \overset{!}{=} G^{\text{imp}}(\mathcal{G}_0)$ (29)
Solving	$m_{\text{MF}} = \tanh(\beta\, B_{\text{Weiss}})$	Let the computer work ! (§2.7)

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

2.5. The DMFT self-consistent loop

If we have a solver for the impurity model, $\mathrm{ImpuritySolver}$, giving us G^{imp} (or Σ^{imp}) as a function of the bath $\mathcal{G}_0$ and the interaction U, we now have a closed system together with the mean field equation, but it is still an implicit system. As usual, the only way is to **solve self-consistently** with a loop :

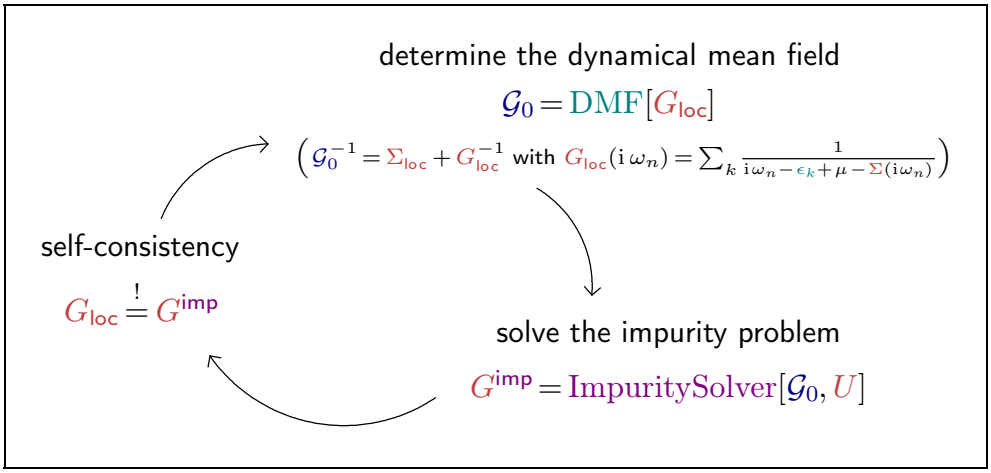


Figure 5. The LISA DMFT self-consistent loop.

We start with an educated guess for the bath $\mathcal{G}_0^{(0)}$, and then we repeat

$$\begin{aligned} G^{(m)} &= \mathrm{ImpuritySolver}\big[\mathcal{G}_0^{(m)}, U\big] && \leftarrow \text{needs } \mathrm{i}\,\omega_n \text{ or } \tau \text{ dep}^{\mathrm{ing}} \text{ on the solver} \\ \mathcal{G}_0^{(m+1)} &= \mathrm{DMF}\big[G^{(m)}\big] \quad (36) && \leftarrow \text{needs } \mathrm{i}\,\omega_n \end{aligned}$$

and hope that the scheme will converge to a self-consistent solution after a reasonable number of steps, i.e. such that $\|G^{(m_{\mathrm{sc}}+1)} - G^{(m_{\mathrm{sc}})}\| < \varepsilon_{\mathrm{thresh}}$. Then this $G^{(m_{\mathrm{sc}})}$ is a self-consistent solution of the system $\{G_{\mathrm{loc}} = G^{\mathrm{imp}}, \mathrm{ImpuritySolver}\,@\,U, \mathrm{DMF}\}$, so up to approximations in the impurity solver and up to the approximative nature of DMFT, we can finally affirm that

$$G_{ii}^{\mathrm{latt}} \approx G^{(m_{\mathrm{sc}})}\,, \quad \Sigma_{ij}^{\mathrm{latt}} \approx \Sigma^{(m_{\mathrm{sc}})}\,\delta_{ij}\,, \quad \Sigma^{\mathrm{latt}}(\vec{k}) \approx \Sigma^{(m_{\mathrm{sc}})}$$

Is is obviously equivalent (at least on paper, numerically it depends) to work the self-energy Σ rather than G with using $\Sigma = \mathcal{G}_0^{-1} - G^{-1}$ (35) if self-consistent convergence is achieved. Note that we write bare Σ's and G's here, without precising "imp" or "latt" because until convergence, these do not have physical meaning, and at convergence they "imp" and "latt" are identical

Physically, we could say that we are relaxing from a non-equilibrium $\mathcal{G}_0^{(0)}$ towards the equilibrium grand-canonical system at inverse temperature β.

Note that in general, there is not a unique solution to the problem. Indeed, as often with phase transitions, there are hysteresis cycles. Then, close to a critical point, *different initial* $\mathcal{G}_0^{(0)}$ (metalic or insulating density of states) *can lead to different lattice states* (metalic or Mott insulator).

2.6. Lattices

Todo :

- Scaling of t with z : $t_{ij} = t/\sqrt{z}$, GKKR eq (18)

2.6.1. The Bethe lattice with infinite coordinance

Figure 6. The Bethe lattice for $z = 4$ and its density of states.

Two ways to obtain the bath for the impurity model :

- Let's start from (32) : $\Delta = \sum_{i,j} t_{oi}\, t_{oj}\, G^{(o)}_{ij}$. For a Bethe lattice $z \to \infty$ with $t_{ij} = t/\sqrt{z}$, removing a site does not make any difference and $G^{(o)}_{ij} = G_{ij}$, and $G^{(o)}_{ij} = \delta_{ij}\, G^{(o)}_{ii}$ (since neighbors of o are completely disconnected on this lattice once the cavity has been introduced), which yields

$$\Delta = \sum_{i,j} \underbrace{t_{oi}\, t_{oj}}_{t^2/z} \underbrace{G_{ii}}_{G_{\text{loc}}} \delta_{ij} = t^2\, G_{\text{loc}}$$

  and injecting in $\mathcal{G}_0^{-1} = \mathrm{i}\,\omega_n + \mu - \Delta$ (31), we get the simple Dyson equation

$$\boxed{\mathcal{G}_0(\mathrm{i}\,\omega_n)^{-1} = \mathrm{i}\,\omega_n + \mu - t^2\, G_{\text{loc}}(\mathrm{i}\,\omega_n)} \tag{37}$$

- Alternatively, we can start from the density of states, which is semi-circular :

$$\eta_{\text{Bethe}}(\epsilon) = \frac{1}{2\,\pi\,t^2}\,\sqrt{4\,t^2 - \epsilon^2} \quad \text{for} \quad |\epsilon| < 2\,t \tag{38}$$

  and compute its Hilbert transform, which is quite simple and admits a very simple reciprocal :

$$R_{\text{Bethe}}(x) = t^2\, x + x^{-1}$$

  Now, injecting this result in (36) $\mathcal{G}_0^{-1} = \mathrm{i}\,\omega_n + \mu + G_{\text{loc}}^{-1} - R(G_{\text{loc}})$, G_{loc}^{-1} simplifies and we get

$$\mathcal{G}_0(\mathrm{i}\,\omega_n)^{-1} = \mathrm{i}\,\omega_n + \mu - t^2\, G_{\text{loc}}(\mathrm{i}\,\omega_n)$$

2.7. Solving the impurity problem

2.7.1. Quantum Monte Carlo techniques

2.7.2. Iterated perturabtion theory approximation

2.8. Practical considerations. Random things

- Half-filling symmetry considerations for the IPT to be numerically stable [27/11 @27:00]
- Practical representation considerations for $G(\mathrm{i}\,\omega_n)$ and n-cutoff [27/11 @31:00]