

# LISA DMFT for the Hubbard model

## 1. Green's functions framework

Nice review in the PES framework : <https://arxiv.org/pdf/1303.1438.pdf>. Very interesting resource : [http://perso.neel.cnrs.fr/xavier.blase/OLDER/GF1\\_Blase.pdf](http://perso.neel.cnrs.fr/xavier.blase/OLDER/GF1_Blase.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

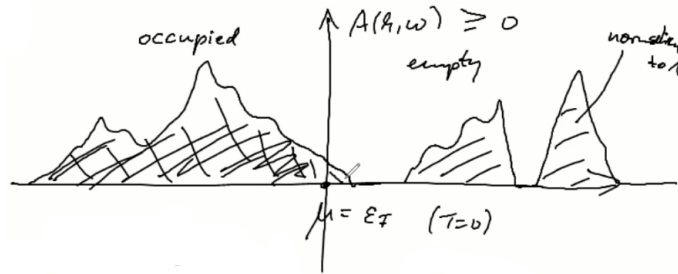
$$\begin{aligned} -\epsilon_{\alpha} &= \mathcal{E}_{0, \text{GC}}^{(N)} - \mathcal{E}_{\alpha, \text{GC}}^{(N+1)} = \mathcal{E}_0^{(N)} + \mu - \mathcal{E}_{\alpha}^{(N+1)} \simeq \mathcal{E}_0^{(N+1)} - \mathcal{E}_{\alpha}^{(N+1)} \\ -\epsilon_{\beta} &= \mathcal{E}_{0, \text{GC}}^{(N)} - \mathcal{E}_{\beta, \text{GC}}^{(N-1)} = \mathcal{E}_0^{(N)} - \mu - \mathcal{E}_{\beta}^{(N-1)} \simeq \mathcal{E}_0^{(N-1)} - \mathcal{E}_{\beta}^{(N-1)} \end{aligned}$$

are excitation energies under a chemical potential  $\mu$ , 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  $\omega$ .

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  $A_0(\omega) = \int \frac{d\vec{k}}{V_{\text{BZ}}} A_0(\vec{k}, \omega) = \int \frac{d\vec{k}}{V_{\text{BZ}}} \delta(\omega - (\epsilon(\vec{k}) - \mu)) = \eta(\mu + \omega)$  is the *density of states* relative to the Fermi energy  $\mu$ .

## 1.2. Green's function

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

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

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.)<sup>2</sup>. For arbitrary  $t$ , we define the *time-ordered Green function* ( $\neq$  advanced and retarded ones)<sup>3</sup>

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

which actually defines an operator  $\mathbf{G}(t) = \sum_{\ell,m} |\ell\rangle G_{\ell,m}(t) \langle m|$  in the single-particle Hilbert space.

The 1-body Green's function can be considered as a time-dependent generalization of the 1-body density matrix. In the position basis,  $G(\vec{x}, t, \vec{x}', t') = -i \langle \text{GS} | \mathbf{T} \Psi(\vec{x}, t) \Psi^{\dagger}(\vec{x}', t') | \text{GS} \rangle$ , and for an homogeneous time-independant system ( $\vec{r} = \vec{x} - \vec{x}'$ ,  $t' = 0$ ), its spatial Fourier transform is

$$G(\vec{k}, t) = \int_{\mathbb{R}^d} d\vec{r} G(\vec{r}, t) e^{i\vec{k} \cdot \vec{r}} = -i \langle \text{GS} | \mathbf{T} \mathbf{c}_{\vec{k}}(t) \mathbf{c}_{\vec{k}}^{\dagger}(0) | \text{GS} \rangle = \langle \vec{k} | \mathbf{G}(t) | \vec{k} \rangle \quad (7)$$

i.e.  $\mathbf{G}(t)$  is diagonal in the  $|\vec{k}\rangle$  basis. Let's define its time Fourier transform :

$$\mathbf{G}(\omega) = \int_{-\infty}^{+\infty} dt \mathbf{G}(t) e^{i\omega t} \iff \mathbf{G}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \mathbf{G}(\omega) e^{-i\omega t} \quad (8)$$

By inserting closure relations for  $\alpha$  (for  $t > 0$ ) and  $\beta$  basis (for  $t < 0$ ), we get the spectral representation

$$i G(\vec{k}, t) = \begin{cases} +\sum_{\alpha} e^{+i(\mathcal{E}_0^{(N)} - \mathcal{E}_{\alpha}^{(N+1)} + \mu)t} \left| \langle \Psi_{\text{GS}}^{(N)} | \mathbf{c}_{\vec{k}} | \Psi_{\alpha}^{(N+1)} \rangle \right|^2 & \text{for } t > 0 \\ -\sum_{\beta} e^{-i(\mathcal{E}_0^{(N)} - \mathcal{E}_{\beta}^{(N-1)} - \mu)t} \left| \langle \Psi_{\text{GS}}^{(N)} | \mathbf{c}_{\vec{k}}^{\dagger} | \Psi_{\beta}^{(N-1)} \rangle \right|^2 & \text{for } t < 0 \end{cases} \quad (9)$$

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

$$\boxed{G(\vec{k}, \omega) = \int_{-\infty}^{+\infty} d\omega' \frac{A(\vec{k}, \omega')}{\omega - \omega' + i0^+ \text{sgn } \omega'}} \quad (10)$$

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

$$\boxed{A(\vec{k}, \omega) = -\frac{1}{\pi} \Im(G(\vec{k}, \omega))} \quad (11)$$

Note that we can *prove* (rather than define) that the spectral function is (1) (*Lehmann representation*) in the framework of **linear response theory** of an observable  $\mathbf{O}$  to a perturbation  $\mathbf{W}(t) : \langle \mathbf{O} \rangle(t) = \langle \mathbf{O} \rangle_0 + \int_{-\infty}^t dt' G_{\mathbf{O}\mathbf{W}}(t, t')$  where  $G_{\mathbf{O}\mathbf{W}}(t, t') = -i \langle \text{GS} | [\mathbf{O}_{\text{I}}(t), \mathbf{W}_{\text{I}}(t')] | \text{GS} \rangle$  (for  $t > t'$ ). Then, the spectral function is defined as  $\langle \mathbf{W}(0) \mathbf{O}(t) \rangle = \text{FT}^{-1}[A]$ , the Fourier transform of the correlation function, and we have the same relation with the Green function.

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.

3. In general, for bosons/fermions  $\eta = \mp$ , we define  $\mathbf{T}_{\eta} \mathbf{A}(t) \mathbf{B}(t') = \mathbf{A}(t) \mathbf{B}(t')$  for  $t > t'$  and  $-\eta \mathbf{B}(t') \mathbf{A}(t')$  for  $t' > t$ .

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

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

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

$$G_0(\vec{k}, \omega) = \frac{1}{\omega - \epsilon(\vec{k}) + \mu + i0^+ \text{sgn}(\epsilon(\vec{k}) - \mu)} \in \mathbb{R} \quad (12)$$

### 1.3. 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 :

$$\langle m | \mathbf{G}_\beta(t) | \ell \rangle = \frac{1}{Z} \text{tr} (e^{-\beta \mathbf{H}_{\text{gc}}} \mathbf{T} \mathbf{c}_\ell(t) \mathbf{c}_m^\dagger(0)) \quad \text{with} \quad Z(\beta, \mu) = \text{tr}(e^{-\beta \mathbf{H}_{\text{gc}}}) \quad (13)$$

But from time evolution  $\mathbf{c}(t) = e^{-i\mathbf{H}_{\text{gc}}t} \mathbf{c} e^{i\mathbf{H}_{\text{gc}}t}$ , 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  $\mathbf{O}$ , define<sup>4</sup>

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

where  $\tau \in \mathbb{R}$  is called the *Matsubara time*, and then define the Green's function in Matsubara space :

for  $0 < \tau, \tau' < \beta$ ,  $\langle m | \mathbf{G}_\beta(\tau, \tau') | \ell \rangle := \frac{1}{Z} \text{tr}(e^{-\beta \mathbf{H}_{\text{gc}}} \mathbf{T} \mathbf{c}_\ell(\tau) \mathbf{c}_m^\dagger(\tau'))$

(15)

The second reason for using Matsubara time is that we'll use Quantum Monte Carlo to solve the problem. The hamiltonian being time-independent,  $G_\beta(\tau, \tau')$  depends only on  $\tau - \tau'$ , and thus is a function of  $\tau \in ]-\beta, +\beta[$ . Notice that, **at least for the diagonal case**  $\ell = m$ , the Matsubara Green's function is *real*. In the following, we'll implicitly use the  $\vec{k}$  basis, where  $\mathbf{G}$  is diagonal for homogeneous systems ( $\ell = m = \vec{k}$ ). Why do we restrict to  $0 < \tau, \tau' < \beta$  ? Because all information is contained in this interval as we'll see. We thus decompose it as a Fourier series :

$$\mathbb{R} \ni G_\beta(\tau) = \frac{1}{\beta} \sum_{p \in \mathbb{Z}} e^{-2\pi i p \tau / 2\beta} \tilde{G}_\beta(p) \iff \tilde{G}_\beta(p) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau G(\tau) e^{2\pi i p \tau / 2\beta} \quad (= \tilde{G}_\beta(-p)^*)$$

Using  $\mathbf{T}$  and cyclicity of the trace, we show that  $\forall \tau \in ]-\beta, 0[$ ,  $G(\tau) = -\eta G(\tau + \beta)$ , where  $\eta = +1$  for fermions (i.e. the minus sign stems from the fermionic  $\mathbf{c}\mathbf{c}^\dagger = -\mathbf{c}^\dagger\mathbf{c}$ ). Thus, in the interval  $[-\beta, +\beta]$ , it is **anti-periodic** with period  $\beta$  (and  $\beta$ -periodic for bosons). Then,  $\tilde{G}_\beta(p) = \frac{1-\eta(-1)^p}{2} \int_0^\beta d\tau G(\tau) e^{i\frac{\pi p}{\beta}\tau}$  : even frequencies  $\tilde{G}_\beta(2n)$  vanish, and for odd frequencies  $p = 2n + 1$ ,  $G_\beta(i\omega_n) := \int_0^\beta d\tau G(\tau) e^{i\omega_n\tau}$ . Then,

$G_\beta(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\omega_n\tau} G_\beta(i\omega_n) \quad \text{where } \omega_n = \frac{2n+1}{\beta} \pi \text{ are Matsubara frequencies}$

(16)

For  $G(\tau)$  to be real, we must have  $G(i\omega_n)^* = G_\beta(-i\omega_n)$ , i.e.  $\begin{cases} \Im G_\beta(i\omega_{-n-1}) = -\Im G(i\omega_n) \\ \Re G_\beta(i\omega_{-n-1}) = +\Re G(i\omega_n) \end{cases}$ . Thus, we only have to know  $G(i\omega_n)$  for frequencies  $n \in \llbracket 0, +\infty \rrbracket$ , and

$$G_\beta(\tau) = \frac{1}{\beta} \sum_{n=0}^{+\infty} 2 \Re(e^{-i\omega_n\tau} G_\beta(i\omega_n))$$

<sup>4. Warning !</sup> The imaginary time Heisenberg rep. does not preserve the conjugation operation :  $(\mathbf{O}(\tau))^\dagger = \mathbf{O}(-\tau) \neq \mathbf{O}^\dagger(\tau)$ . Moreover, we should write  $\mathbf{O}(-i\tau)$  to keep coherent notations. But whatever.

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

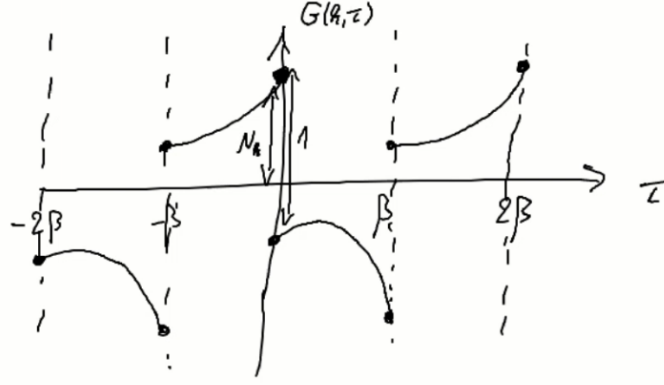


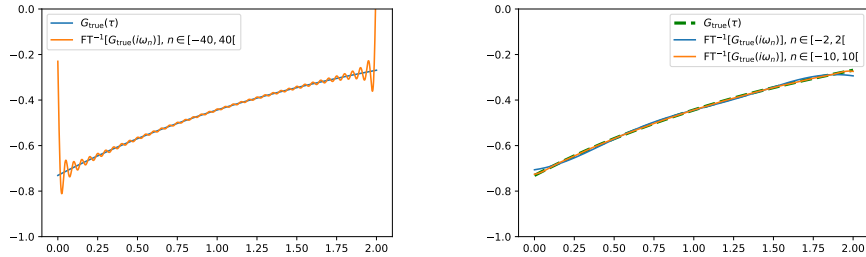
Figure 2. Rough picture of Green's function in Matsubara space.

### Numerical considerations

This discontinuity is very annoying because it is the cause of the slow decay in frequency space, e.g.

$$G(i\omega_n) = \frac{1}{i\omega_n - \epsilon + \mu - \Sigma(i\omega_n)} \underset{n \gg 1}{\approx} \frac{1}{i\omega_n}$$

which would need to evaluate Matsubara sums (16) with high  $n$  cutoffs to obtain a reasonable result. And even with large  $n$ 's, this is far from ideal because of Gibbs ringing (left figure) :



The nice thing is that this jump is always 1, so we can simply singularize it :

$$G(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\omega_n \tau} G(i\omega_n) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\omega_n \tau} \underbrace{\left( G(i\omega_n) - \frac{1}{i\omega_n} \right)}_{=: G^b(i\omega_n)} + \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} \frac{e^{-i\omega_n \tau}}{i\omega_n} = -\frac{1}{2} \text{sgn}(\tau)$$

where we defined a jump-free auxiliary function  $G^b(i\omega_n)$ . Now the leading order in  $G^b(i\omega_n)$  should be  $1/(i\omega_n)^2$ , so the sum is absolutely convergent, and we should be able to take a finite cutoff for any arbitrary precision. It indeed works very well (figure above at the right), even for small cutoffs.

To compute a *one-body* observable  $O = \sum_{\ell m} O_{\ell m} c_{\ell}^{\dagger} c_m$  from Green's function in Matsubara space :

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

( $0^-$  to commute  $c_{\ell}^{\dagger} \leftrightarrow c_m$ ). In particular, the momentum distribution is given by  $\langle n_{\vec{k}} \rangle = G(\vec{k}, \tau = 0^-)$ . We are in this situation, for any equilibrium property, which only looks at *equal times* ( $c^{\dagger} c \leftrightarrow \tau = 0$ ).

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<sup>5</sup> (indexed by  $\alpha$ ) against what was the ground state  $|\Psi_{\text{GS}}^{(N)}\rangle$ , and

5. 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  $\langle \Psi_{\gamma}^{(N)} | c_{\vec{k}}^{\dagger}$ , only remains  $|\Psi_{\alpha}^{(N+1)}\rangle$  states. Moreover, we restrict ourselves to  $\tau > 0$  because it is enough to know  $\tau < 0$  thanks to anti-periodicity.

now is the thermal mixture of  $N$  particules states (indexed by  $\gamma$ ) :

$$\begin{aligned}
G_\beta(\vec{k}, \tau) &= -\frac{1}{Z} \sum_{\gamma} e^{-\beta \mathcal{E}_{\gamma, \text{GC}}^{(N)}} \langle \Psi_{\gamma}^{(N)} | e^{\mathbf{H}_{\text{GC}} \tau} \mathbf{c}_{\vec{k}} e^{-\mathbf{H}_{\text{GC}} \tau} \mathbf{c}_{\vec{k}}^\dagger | \Psi_{\gamma}^{(N)} \rangle \\
&= -\frac{1}{Z} \sum_{\gamma} \sum_{\alpha} e^{-\beta \mathcal{E}_{\gamma, \text{GC}}^{(N)}} \langle \Psi_{\gamma}^{(N)} | e^{\mathbf{H}_{\text{GC}} \tau} \mathbf{c}_{\vec{k}} e^{-\mathbf{H}_{\text{GC}} \tau} | \Psi_{\alpha}^{(N+1)} \rangle \langle \Psi_{\alpha}^{(N+1)} | \mathbf{c}_{\vec{k}}^\dagger | \Psi_{\gamma}^{(N)} \rangle \\
&= -\frac{1}{Z} \sum_{\gamma, \alpha} e^{-\beta \mathcal{E}_{\gamma, \text{GC}}^{(N)}} e^{(\mathcal{E}_{\gamma, \text{GC}}^{(N)} - \mathcal{E}_{\alpha, \text{GC}}^{(N+1)}) \tau} |\langle \Psi_{\alpha}^{(N+1)} | \mathbf{c}_{\vec{k}}^\dagger | \Psi_{\gamma}^{(N)} \rangle|^2
\end{aligned}$$

And then, going to frequency space and using  $\int_0^\beta d\tau e^{(\mathcal{E}_{\gamma} - \mathcal{E}_{\alpha}) \tau} e^{i\omega_n \tau} = \frac{e^{(i\omega_n + \mathcal{E}_{\gamma} - \mathcal{E}_{\alpha}) \beta} - 1}{i\omega_n + \mathcal{E}_{\gamma} - \mathcal{E}_{\alpha}}$  and  $e^{i\omega_n \beta} = -1$ ,

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

The finite-temperature spectral function being, for  $\omega > 0$ ,

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

(which has the same interpretation as the  $T=0$  spectral function,  $\int d\omega A_\beta(\vec{k}, \omega) = 1$ , ...), it verifies the same relation with the Green's function (except the  $i0^+$  is not needed anymore because  $i\omega_n \notin \mathbb{R}$ ) :

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

The Matsubara Green's function  $G_\beta(i\omega_n)$  is simply the analytic continuation of the (retarded, not time-ordered) usual Green's function (13), evaluated on the imaginary axis  $t = -i\tau \Leftrightarrow i\omega_n = \omega + i0^+$ . By the way, we see that restricting ourselves to  $-\beta < \tau < \beta$  is mandatory if we want  $e^{i\omega_n \beta} = -1$ , which is a necessary step to allow us to extract usefull information from the Matsubara Green's function. The more general justification is that the perturbative expansion (as we do in Quantum Monte Carlo) only uses  $G_\beta(\tau = \beta/m \leq \beta)$ , so  $G_\beta(\tau > \beta)$  is of no use. Anyhow, we show<sup>6</sup> that (and again,  $G_\beta(\tau) \in \mathbb{R}$ )

$$G_\beta(\vec{k}, \tau) = - \int_{-\infty}^{+\infty} d\omega A_\beta(\vec{k}, \omega) \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} \quad (20)$$

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.

It looks simpler to invert (19) because there is no exponential tail, but (19) and (20) are directly (linearly) related so if the problem is ill-defined/hard for (20), it is also for (19). Choosing to invert from  $G(i\omega_n)$  or  $G(\tau)$  is then just a matter of taste or practical considerations.

For the **non-interacting** electron gas, the Green's function is, using (4) and (19),

$$G_{0, \beta}(\vec{k}, i\omega_n) = \frac{1}{i\omega_n - \epsilon(\vec{k}) + \mu} \quad (21)$$

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

c.f. the table at [https://en.wikipedia.org/wiki/Matsubara\\_frequency#Green's\\_function\\_related](https://en.wikipedia.org/wiki/Matsubara_frequency#Green's_function_related).

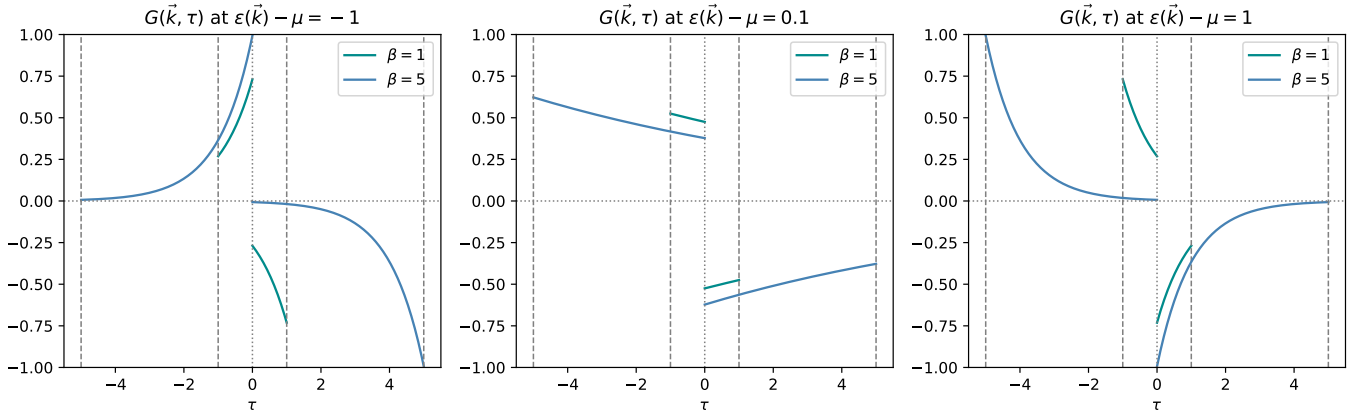
[ Direct computation from the hamiltonian  $\mathbf{H} = \sum_{\vec{k}} \epsilon(\vec{k}) c_{\vec{k}}^\dagger c_{\vec{k}}$  : <http://folk.ntnu.no/johnof/green-2013.pdf> p. 18. ] which is *independent of the temperature*. Computing the Matsubara sum, we get (again from the tables)

$$G_{0,\beta}(\vec{k}, \tau) = -e^{(\epsilon(\vec{k}) - \mu)(\beta - \tau)} f_{\beta}^{\text{FD}}(\epsilon(\vec{k}) - \mu) \quad \text{for } \tau \in ]0, \beta[ \quad \text{with} \quad f_{\beta}^{\text{FD}}(\epsilon) = \frac{1}{e^{\beta\epsilon} + 1}$$

But it turns out that in this case, we can compute it directly from the definition (15) : solving the Heisenberg equations of motion gives  $c_{\vec{k}}(\tau) = e^{-(\epsilon(\vec{k}) - \mu)\tau} c_{\vec{k}}$ , and then, using  $\langle c_{\vec{k}}^\dagger c_{\vec{k}} \rangle_{\beta} = f_{\beta}^{\text{FD}}(\epsilon(\vec{k}) - \mu)$ , we have

$$G_{0,\beta}(\vec{k}, \tau) = -e^{(\epsilon(\vec{k}) - \mu)\tau} \left( (1 - f_{\beta}^{\text{FD}}) \mathbb{1}_{\tau > 0} - f_{\beta}^{\text{FD}} \mathbb{1}_{\tau < 0} \right) \quad \forall \tau \in \mathbb{R}$$

which is clearly non- $\beta$ -anti-periodic. Is is only if we restrict to  $-\beta < \tau < \beta$  (which we can, and should). Then we compute  $G_{0,\beta}(\vec{k}, i\omega_n) = \int_0^\beta d\tau G_{0,\beta}(\vec{k}, \tau) e^{i\omega_n \tau}$  and obtain  $\frac{1}{i\omega_n - \epsilon(\vec{k}) + \mu}$  indeed.



**Figure 3.** Matsubara Green function for **non-interacting** fermions system, for two temperatures. Left : below Fermi surface ( $n_k \simeq 1$  @  $\beta = 5$ ). Center : slightly above Fermi surface. Right : above Fermi surface ( $n_k \simeq 0$  @  $\beta = 5$ ).

At  $T = 0$ ,  $\beta \rightarrow \infty$  and  $G_{\beta=\infty}(\tau)$  is no more periodic, and the Matsubara frequencies  $i\omega_n \propto \beta^{-1}$  become a continuum. Then, (16) becomes an integral :

$$G_{\beta}(\tau) = \frac{1}{\beta} \int \frac{d\omega}{2\pi} e^{-i\omega\tau} G_{\beta}(i\omega) = \text{FT}_{\omega}^{-1}[G_{\beta}(i\omega)](\tau) \iff G_{\beta}(i\omega) = \text{FT}_{\tau}[G_{\beta}(\tau)](\omega)$$

We should really look at the effect of non-zero temperatures ( $\Leftrightarrow$  finite  $\beta$ ) just like the effect of a finite length  $L$  in a system which induces spatial inhomogeneity, i.e. spatial gradients. A finite temperature then induces  $\partial_{\tau}$  gradients.

If we have particle-hole symmetry, then  $A(-\omega) = A(+\omega)$ . As a consequence, it is easy to check that

$$G(i\omega_n)^* = G(-i\omega_n) \stackrel{(19)}{=} -G(i\omega_n) \Rightarrow \Re G_{\beta}(i\omega_n) = 0 \Rightarrow G_{\beta}(\beta - \tau) = G_{\beta}(\tau) \quad (22)$$

## 1.4. 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

$$\mathbf{H}_0^{(1)} |\varphi_{\nu\vec{k}}\rangle = \epsilon_{\nu}(\vec{k}) |\varphi_{\nu\vec{k}}\rangle$$

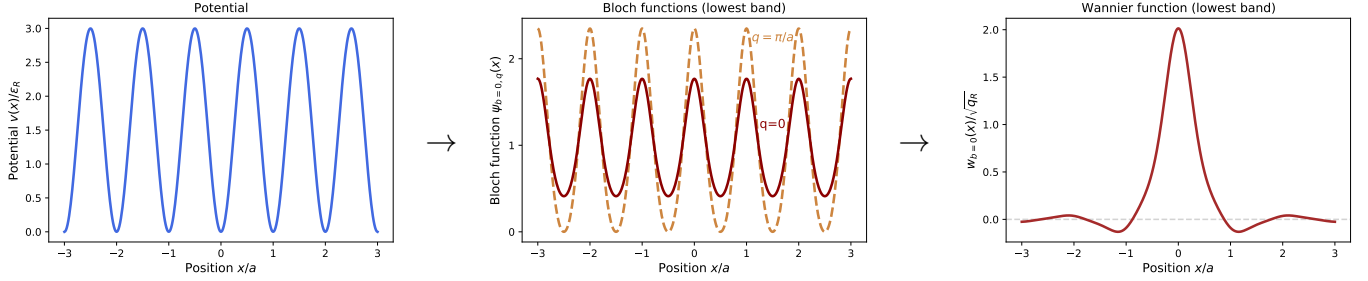
then the Wannier function for band  $\nu$  and atomic site  $\vec{X}$  is defined by

$$\mathcal{W}_{\vec{X},\nu}(\vec{x}) = \int_{\text{BZ}} \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \varphi_{\nu\vec{k}}(\vec{x}) e^{-i\vec{k}\cdot\vec{X}} \quad (23)$$

which verifies  $\mathcal{W}_{\vec{0},\nu}(\vec{x} - \vec{X}) = \mathcal{W}_{\vec{X},\nu}(\vec{x})$ , i.e. the Wannier function at site  $\vec{X}$  is simply the translation of the Wannier function at site  $\vec{0}$ . Note that this definition is not unique because  $\varphi_{\nu\vec{k}}$  is defined up to a global phase  $e^{i\alpha(\nu,\vec{k})}$ . This phase can be chosen such that  $\mathcal{W}(\vec{x})$ 's are well localized around site  $\vec{X}$ , as in the figure bellow. Wannier functions form a discrete basis ( $\int d\vec{x} \mathcal{W}_{\vec{X}}(\vec{x}) \mathcal{W}_{\vec{X}'}(\vec{x})^* = \delta_{\vec{X}\vec{X}'}$ ), and we write

$$\Psi_{\sigma}^{\dagger}(\vec{x}) = \sum_{\vec{X},\nu} \mathcal{W}_{\vec{X}\nu\sigma}(\vec{x})^* c_{\vec{X}\nu\sigma}^{\dagger} \quad (24)$$

↑ creates a Wannier state at site  $\vec{X}$



**Figure 4.** Wannier function (site  $x=0$ ) of the lowest band from a  $V(x) = V_0 \sin^2(\pi x/a)$  potential of period  $a$ .  $q_R = \pi/a$ ,  $\epsilon_R = \hbar^2 q_R^2 / 2m$ . Here  $V_0 = 3 \epsilon_R$ .

Now

$$G(\vec{x}, \vec{x}', t) = \sum_{\vec{X},\nu} \sum_{\vec{X}',\nu'} \mathcal{W}_{\vec{X}\nu}(\vec{x}) \mathcal{W}_{\vec{X}'\nu'}(\vec{x}')^* G_{\nu\nu'}^{\mathcal{W}}(\vec{X}, \vec{X}', t)$$

with  $G_{\nu\nu'}^{\mathcal{W}}(\vec{X}, \vec{X}', t) = -i \langle \text{GS} | \mathbf{T} c_{\vec{X}\nu}(t) c_{\vec{X}'\nu'}^{\dagger}(0) | \text{GS} \rangle$  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. It is often denoted simply  $G_{ij}(\cdot) := G^{\mathcal{W}}(\vec{X}_i, \vec{X}_j, \cdot)$ , where  $\{i\}$  indexes the lattice sites.

The spatial Fourier transform (7) of the Green's function  $G(\vec{r}, t)$  has now a much more convenient form (here for an homogeneous system and forgetting  $\nu$ 's) :

$$G(\vec{k}, t) = \sum_{\vec{R}} G^{\mathcal{W}}(\vec{R}, t) e^{i\vec{k} \cdot \vec{R}} \longleftrightarrow G^{\mathcal{W}}(\vec{R}, t) = \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} G(\vec{k}, t) e^{-i\vec{k} \cdot \vec{R}} \quad (25)$$

Note that for a finite system with  $N$  sites, we use  $\frac{1}{N} \sum_{\vec{k}} =: \sum'_{\vec{k}}$  rather than  $\int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}}$ .

An important quantity in DMFT is the **local Green's function**  $G_{\text{loc}} := G_{ii}$  (i.e.  $\vec{R} = \vec{0}$ ), which describes the process “an electron stays on the site”. The **non-interacting** local Green's function in frequency space (here Matsubara frequencies) takes a nice form in the Wannier basis if we express it with the **density of states**

$$\eta^{\text{latt}}(\epsilon) = \int_{\text{BZ}} \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \delta(\epsilon - \epsilon(\vec{k})) \quad (26)$$

Indeed, from (21),

$$G_{0,\text{loc}}(i\omega_n) = G_0^{\mathcal{W}}(\vec{0}, i\omega_n) = \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \frac{e^{-i\vec{k} \cdot \vec{0}}}{i\omega_n - \epsilon(\vec{k}) + \mu} = \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \int d\epsilon \frac{\delta(\epsilon - \epsilon(\vec{k}))}{i\omega_n - \epsilon + \mu} = \int d\epsilon \frac{\eta^{\text{latt}}(\epsilon)}{i\omega_n - \epsilon + \mu}$$

which is nothing else than the *Hilbert transform*  $\tilde{\eta}$  of the density of states of our lattice :

$$\tilde{\eta}(\zeta) = \int_{-\infty}^{+\infty} d\epsilon \frac{\eta^{\text{latt}}(\epsilon)}{\zeta - \epsilon} \quad (27)$$

evaluated at  $\zeta = i\omega_n + \mu$  :

$$G_{0,\text{loc}}(i\omega_n) = \tilde{\eta}(\zeta = i\omega_n + \mu) \quad (28)$$

It is also a direct consequence of (19) together with the fact that  $\sum_{\vec{k}} A_0(\vec{k}, \omega) = \eta(\mu + \omega)$ .

## 2. The Hubbard model and the DMFT LISA approximation

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

$$\mathbf{H} = - \underbrace{\sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})}_{\text{hopping / tight-binding / Bloch hybridization}} + \underbrace{U \sum_i n_{i\uparrow} n_{i\downarrow}}_{\text{Coulomb repulsion / double occ. cost}} \quad (29)$$

### 2.1. Limits

#### 2.1.1. Non-interacting limit

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 (provided  $t_{ij}$ 's are translationally invariant)

$$\mathbf{H} = - \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) = \sum_{\vec{k}, \sigma} \epsilon(\vec{k}) c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} \quad \text{with} \quad \epsilon(\vec{k}) \stackrel{\text{def}}{=} \sum_j -t_{ij} e^{i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)} \quad (30)$$

$\rightarrow A_0(\vec{k}, \omega) = \delta(\omega - \epsilon(\vec{k}))$ . We immediately recover the non-interacting Green's function (21).

#### 2.1.2. Atomic limit

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

	state	$n$	$\epsilon$	$\epsilon_{\text{GC}}$
para	$ \emptyset\rangle$	0	0	0
	$\frac{1}{\sqrt{2}}(c_\uparrow^\dagger + c_\downarrow^\dagger) \emptyset\rangle$	1	0	$-\mu$
	$\frac{1}{\sqrt{2}}(c_\uparrow^\dagger - c_\downarrow^\dagger) \emptyset\rangle$	1	0	$-\mu$
	$ \uparrow\downarrow\rangle = c_\uparrow^\dagger c_\downarrow^\dagger  \emptyset\rangle$	2	$U$	$U - 2\mu$

By imposing the condition  $\langle \mathbf{n}_{i\uparrow} + \mathbf{n}_{i\downarrow} \rangle_{\text{GC}} = 1$ , we get  $\mu = U/2$  (indep. of  $\beta$ ). The spectral function is then

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

This is the *atomic limit*. The Green's function is then computed with (10) :

$$G(\omega) = \frac{1}{2} \frac{1}{\omega - \frac{U}{2} + i0^+} + \frac{1}{2} \frac{1}{\omega + \frac{U}{2} - i0^+} \quad (31)$$

For finite temperature, we can compute  $A_\beta(\sigma, \omega)$  using (18), with  $\alpha = \uparrow\downarrow$  and  $\gamma = \text{para}$  states. The matrix elements and  $\delta\left(\omega - \frac{U}{2}\right)$  are unchanged, and it turns out that  $\frac{1}{Z} (e^{-\beta\epsilon_{\gamma, \text{GC}}^{(N)}} + e^{-\beta\epsilon_{\alpha, \text{GC}}^{(N+1)}}) = \frac{e^{\beta U/2} + 1}{1 + 2e^{\beta U/2} + 1} = \frac{1}{2}$  so that  $\beta \neq \infty$  changes nothing  $\rightarrow A_\beta(\sigma, \omega) = A(\sigma, \omega)$ . The Matsubara Green's function is then

$$G_\beta(i\omega_n) = \frac{1}{2} \frac{1}{i\omega_n - \frac{U}{2}} + \frac{1}{2} \frac{1}{i\omega_n + \frac{U}{2}} = \frac{-i\omega_n}{\omega_n^2 + \left(\frac{U}{2}\right)^2} \Leftrightarrow G_\beta(\tau) = -\frac{1}{2} \frac{e^{-\tau U/2}}{1 + e^{-\beta U/2}} - \frac{1}{2} \frac{e^{+\tau U/2}}{1 + e^{+\beta U/2}}$$

### 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  $G_0 = G|_{U=0, \text{ fixed } \mu}$  Green's functions (as operators) :

$$\Sigma(i\omega_n) := G_0(i\omega_n)^{-1} - G(i\omega_n)^{-1} \quad (32)$$



This is the **Dyson equation**<sup>7</sup>, and is actually a *result* with a suitable definition of the self-energy which allows to interpret it diagrammatically. The self-energy *encodes all 1-body interactions properties* : Hartree energy, exchange and correlations.  $\Delta$  It is non-linear (matrix) equation, and thus *does not transform* under Fourier transform  $t \leftrightarrow \omega$  or  $\tau \leftrightarrow i\omega_n$ <sup>8</sup>. However, it turns out it is the same with Matsubara or real time, i.e.  $\Sigma(i\omega_n)$  is indeed the analytic continuation of  $\Sigma(\omega)$  as for the Green's functions. Note that we stopped writing  $G_\beta$  or  $\Sigma_\beta$  for Matsubara time functions and this will always be implicit in the following. Because  $G$  is diagonal in the  $|\vec{k}\rangle$  basis, the matrix inversions are straightforward and

$$\Sigma(\vec{k}, i\omega_n) = G_0(\vec{k}, i\omega_n)^{-1} - G(\vec{k}, i\omega_n)^{-1} \quad (33)$$

but it not true anymore with  $G_{ij}(i\omega_n)$  and  $\Sigma_{ij}(i\omega_n) := \sum_{\vec{k}} \Sigma(\vec{k}, i\omega_n) e^{-i\vec{k} \cdot \vec{R}_{ij}}$  which are true matrices. In the atomic limit, and whatever the temperature, (31)

$$\Sigma(\omega) \underset{U \gg t}{=} \frac{U}{2} + \left(\frac{U}{2}\right)^2 \frac{1}{\omega + i0^+}, \quad \Sigma(i\omega_n) \underset{U \gg t}{=} \frac{U}{2} + \left(\frac{U}{2}\right)^2 \frac{1}{i\omega_n} \quad (34)$$

The  $U/2$  term is the Hartree term. It is sometimes absorbed into the chemical potential, such that  $\mu = 0$ . 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).

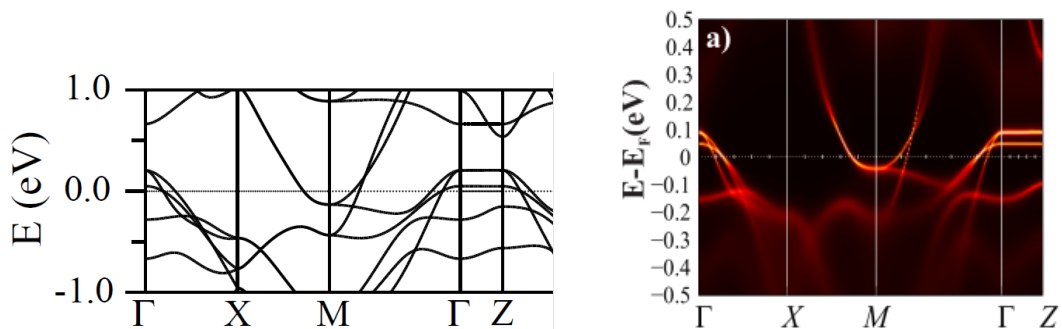
Moreover, in the site / Wannier basis,  $\Sigma_{ij}$  has no reason to be diagonal, *even if the coulombic interactions are purely local* ( $U \sum_i \mathbf{n}_{i\uparrow} \mathbf{n}_{i\downarrow}$ , i.e. does not involve  $\mathbf{n}_i \mathbf{n}_j$  terms<sup>9</sup>). This means that the effects of the interaction (encoded in  $\Sigma_{ij}$ ) are non-local even if the interaction is local  $\Rightarrow$  *non-local correlations*.

Because the **non-interacting** problem has a known solution in term of a band  $\epsilon(\vec{k})$ ,  $G_0$  is known (21) :  $G_0(\vec{k}, i\omega_n)^{-1} = i\omega_n - \epsilon(\vec{k}) + \mu$ . Then, the **interacting** Green's function can be written

$$G(\vec{k}, i\omega_n) = \frac{1}{i\omega_n - \epsilon(\vec{k}) + \mu - \Sigma(\vec{k}, i\omega_n)} \quad (35)$$

We see that the interactions, via the self-energy  $\Sigma$ , *modifies the poles / branch cuts* and their values (in a temperature-dependant way). And because  $\Sigma \in \mathbb{C}$  in general, 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.



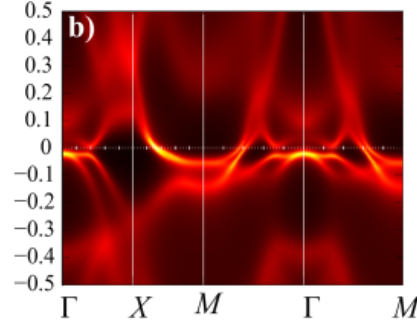
**Figure 5.** Band structure vs. spectral function of LaFeAsO by DMFT. Washed-out peaks ← has some width.

7. It looks very much like the Dyson equation in perturbation theory (if  $H = H_0 + V$  and  $G$  is the resolvent operator, then  $G = G_0 + G_0 V G \Leftrightarrow G^{-1} = G_0^{-1} + V$ ), where the self-energy plays the role of the perturbation. This is not a coincidence : type "dyson equation green function" in your favorite search engine for more info.

8. However, in the litterature, we often find the Dyson equation as  $\Sigma(t) = G_0(t)^{-1} - G(t)^{-1}$ . This means that in these cases, we are *not talking about the same self-energy*, i.e.  $\Sigma(\omega) \neq \text{FT}[\Sigma(t)]$ . But in this document, the self-energies will really be Fourier transforms of each other and the Dyson equation is valid only in the  $(\vec{k}, i\omega_n)$  basis.

9. 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.

→ 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 6.** Heavily doped  $\text{LaFeAsO}_{1-x}\text{H}_x$  spectral function : **very washed-out, renormalized and deformed** band near  $\epsilon_F$ , and fuzzy/new structures away from  $\epsilon_F$ .

[ Much more details and quantitative physical interpretation (energy shift, effective mass, Fermi liquid and relation to ARPES) on the self-energy in <https://www.physique.usherbrooke.ca/tremblay/cours/phy-892/jouvence.pdf>, sec. 3.5 p. 80. ]

From (35), the **local Green's function**  $G_{\text{loc}}(i\omega_n) = G_{ii}(i\omega_n) = \sum_{\vec{k}}' G(\vec{k}, i\omega_n)$ , useful in DMFT, can be expressed as a function of the density of states of the non-interacting problem : exactly as for (28), we have

$$G_{\text{loc}}(i\omega_n) = \tilde{\eta}(\zeta) \quad \text{with} \quad \zeta(i\omega_n) = i\omega_n + \mu - \Sigma_{\text{loc}}(i\omega_n) \quad (36)$$

where  $\tilde{\eta}$  is the Hilbert transform of the density of states (27).  $\triangle$  And we see that  $\Sigma_{\text{loc}} \neq G_{0,\text{loc}}^{-1} - G_{\text{loc}}^{-1}$  because  $G_{0,\text{loc}}(i\omega_n) = \tilde{\eta}(i\omega_n + \mu)$ , which backs up our warning above.

### 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](https://www.physics.rutgers.edu/~gkguest/papers/rmp63_1996_p13_Kotliar.pdf) (GKKR)

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 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* :

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

where we are only left with a single number  $\Sigma_{\text{loc}}$  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 :

$$\Sigma_{ij} \stackrel{\text{DMFT}}{\approx} \Sigma_{\text{loc}} \delta_{ij} \quad \Leftrightarrow \quad \Sigma(\vec{k}) \approx \Sigma_{\text{loc}} \quad (37)$$

(recall that  $\Sigma(\vec{k}) = \sum_j \Sigma_{ij} e^{i\vec{k} \cdot \vec{R}_{ij}}$  whatever  $i$ ) and the Green's function (35) becomes

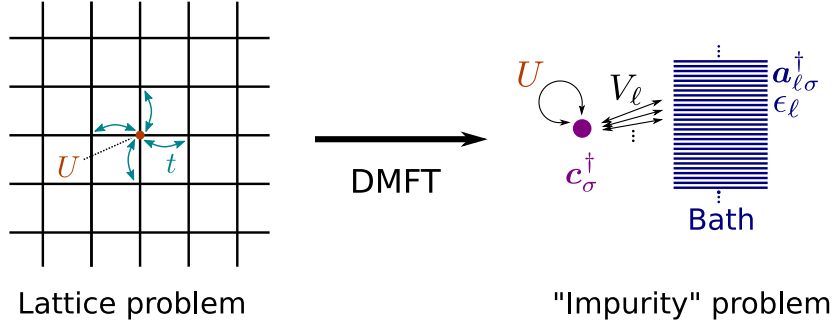
$$G(\vec{k}, i\omega_n) \stackrel{\text{DMFT}}{\approx} \frac{1}{i\omega_n - \epsilon(\vec{k}) + \mu - \Sigma_{\text{loc}}(i\omega_n)} \quad (38)$$

## 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<sup>10</sup>

- 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



which looks like an *Anderson impurity model* :

$$H_{\text{imp}}^{\text{GC}} = H_{\text{site}} + H_{\text{coupl}} + H_{\text{bath}} \quad \text{where} \quad \begin{cases} H_{\text{site}} = (\epsilon_0 - \mu)(n_{\uparrow} + n_{\downarrow}) + U n_{\uparrow} n_{\downarrow} & (n = c^\dagger c) \\ H_{\text{bath}} = \sum_{\ell\sigma} \epsilon_\ell a_{\ell\sigma}^\dagger a_{\ell\sigma} \\ H_{\text{coupl}} = \sum_{\ell\sigma} V_\ell (a_{\ell\sigma}^\dagger c_\sigma + c_\sigma^\dagger a_{\ell\sigma}) \end{cases} \quad (39)$$

⚠ It is not a single-particle problem !<sup>11</sup> We can't reduce to non-interacting problem if we want to describe the on-site repulsion. This is really still a many-body problem, the site being described by creation operators  $c_\sigma^\dagger$ , 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 problem, the Green's function describes processes on-site  $\vec{R} \rightarrow \vec{R}$  ( $G_{ii} \equiv G_{\text{loc}}$ , the *local part of the Green's function*) but also *between sites*  $\vec{R}_i \rightarrow \vec{R}_j$  ( $G_{ij} = G^{\mathcal{W}}(\vec{R}_i, \vec{R}_j)$ ). However, in the impurity model, there is only the impurity Green's function

$$G_\sigma^{\text{imp}}(t) := -i \langle T c_\sigma(t) c_\sigma^\dagger(0) \rangle \quad (\text{and } G^{\text{imp}}(i\omega_n)) \quad (40)$$

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

The spirit of DMFT is to simply forget about non-local self-energy, cf. (37), and we can only impose

$$\text{local Hubbard} \rightarrow \boxed{G_{\text{loc}}^{\text{latt}} \stackrel{!}{=} G^{\text{imp}}} \leftarrow \text{impurity} \quad (41)$$

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.

10. Color code : ■ non-interacting properties ■ interacting properties ( $U \neq 0$ ) ■ impurity ■ bath (should be ■ also)

11. 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.

The bath  $\{\mathbf{a}_{\ell\sigma}^\dagger\}$  is described by effective energy levels  $E_\ell$ , here discrete, but it is a band structure really, which can be *metallic* or *insulating* depending if there are states at the Fermi energy  $\mu$  or not. The effective coupling constants  $V_\ell$  and effective energy levels  $E_\ell$  are *chosen/solved so as to reproduce our initial Hubbard system self-consistently* at a given  $U$ . However, there is an unnecessary freedom of choice and complexity in this description and we'd better of using an action representation<sup>12</sup> of  $\mathbf{H}_{\text{imp}}^{\text{GC}}$  :

$$\mathcal{S}^{\text{imp}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \mathbf{c}^\dagger(\tau) \frac{1}{\mathcal{G}_0(\tau - \tau')} \mathbf{c}(\tau) + U \int_0^\beta d\tau \mathbf{n}_\uparrow(\tau) \mathbf{n}_\downarrow(\tau) \quad (42)$$

(and  $\sum_\sigma \mathbf{c}_\sigma^\dagger(\tau) \mathcal{G}_{0,\sigma}(\tau - \tau')^{-1} \mathbf{c}_\sigma(\tau)$  is there is magnetic order) where the degrees of freedom of the bath has been formally integrated<sup>13</sup> into the *bath Green's function*  $\mathcal{G}_0$  :

$$\mathcal{G}_0(i\omega_n) = \frac{1}{i\omega_n - \epsilon_0 + \mu - \Delta(i\omega_n)} \quad \text{with} \quad \Delta(i\omega_n) = \sum_\ell \frac{|V_\ell|^2}{i\omega_n - E_\ell} \quad (43)$$

(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 field*, or the *dynamical mean field*<sup>14</sup>). The  $\mathbf{c}^\dagger(\tau) \mathcal{G}_0(\tau - \tau')^{-1} \mathbf{c}(\tau)$  process is : "an electron comes on the site, waits a bit  $(\tau - \tau')$  depending on the coupling with the bath (described by  $\mathcal{G}_0(i\omega_n) \Leftrightarrow \Delta(i\omega_n)$ ) and goes back somewhere in the bath"<sup>15</sup>. The second term  $U \mathbf{n}_\uparrow(\tau) \mathbf{n}_\downarrow(\tau)$  describes coulombic interaction.

At fixed bath  $\mathcal{G}_0$ , in the non-interacting limit  $U = 0$  of the impurity model, (42) 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 the impurity model. [todo; see mesm-silke-4.mp4 @ 1:35:30]

⚠ It is however *not*, in general, the non-interacting Green's function of the original problem  $G_{0,\text{loc}}^{\text{latt}}$  because the bath  $\mathcal{G}_0$  is an *effective quantity* coming from the original Hubbard problem, which depends on  $U^{\text{latt}}$  ! Of course, if  $U^{\text{latt}} = 0$ , it is the case :  $\mathcal{G}_0|_{U=0} = G_{0,\text{loc}}^{\text{latt}} = \tilde{\eta}(i\omega_n + \mu)$ . But whatever, we already knew that. [ 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

The previous remark is very useful : from the general definition of the self-energy  $\Sigma = G_0^{-1} - G^{-1}$  (32) on the impurity side (we assume that the spins are non-polarized so that the impurity problem basis is a single state) :

$$\Sigma^{\text{imp}}(i\omega_n) = \frac{1}{\mathcal{G}_0(i\omega_n)} - \frac{1}{G^{\text{imp}}(i\omega_n)} \quad (44)$$

Using (41)  $G_{\text{loc}}^{\text{latt}} = G^{\text{imp}}$  and the additional hypothesis  $\Sigma_{\text{loc}}^{\text{latt}} = \Sigma^{\text{imp}}$  (proven by the cavity method, §2.8),

$$\boxed{\Sigma_{\text{loc}} = \frac{1}{\mathcal{G}_0} - \frac{1}{G_{\text{loc}}}} \quad (45)$$

And so what ?

Just as for the Ising model, we have to compute the mean field acting on the impurity,  $\mathcal{G}_0$ . Without knowing it, we have already all the ingredients on the table. Indeed, in (45),  $\Sigma_{\text{loc}}$  and  $G_{\text{loc}}$  are not independant : on the lattice site, recall that (32) also implies the relation (36) which stems from the evaluation of  $G_{\text{loc}}(i\omega_n) = \sum_k' \frac{1}{i\omega_n - \epsilon_k + \mu - \Sigma_{\text{loc}}(i\omega_n)}$ , connecting  $\Sigma_{\text{loc}}$  and  $G_{\text{loc}}$  through the density of states of the lattice :

$$G_{\text{loc}} = \tilde{\eta}(\zeta) \quad \text{with} \quad \zeta(i\omega_n) = i\omega_n + \mu - \Sigma_{\text{loc}}(i\omega_n), \quad \Leftrightarrow \quad \zeta = R(G_{\text{loc}})$$

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

13. The hamiltonian  $\mathbf{H}_{\text{imp}}$  is *quadratic* in  $\mathbf{a}_{\ell\sigma}^\dagger, \mathbf{a}_{\ell\sigma}$ 's, allowing integration of bath degrees of freedom.

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

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

where  $R$  is the reciprocal function of  $\tilde{\eta}(\zeta)$ , i.e.  $\zeta = R(\tilde{\eta}(\zeta))$ . Then, equation (45) can be expressed as a self-consistent equation :  $\mathcal{G}_0^{-1} = \Sigma_{\text{loc}} + G_{\text{loc}}^{-1} = i\omega_n + \mu - \zeta + G_{\text{loc}}^{-1}$  so that

$$\begin{aligned} \mathcal{G}_0(i\omega_n)^{-1} &= i\omega_n + \mu + G_{\text{loc}}(i\omega_n)^{-1} - R(G_{\text{loc}}(i\omega_n)) \\ &=: \text{DMF}[G_{\text{loc}}](i\omega_n)^{-1} \end{aligned} \quad (46)$$

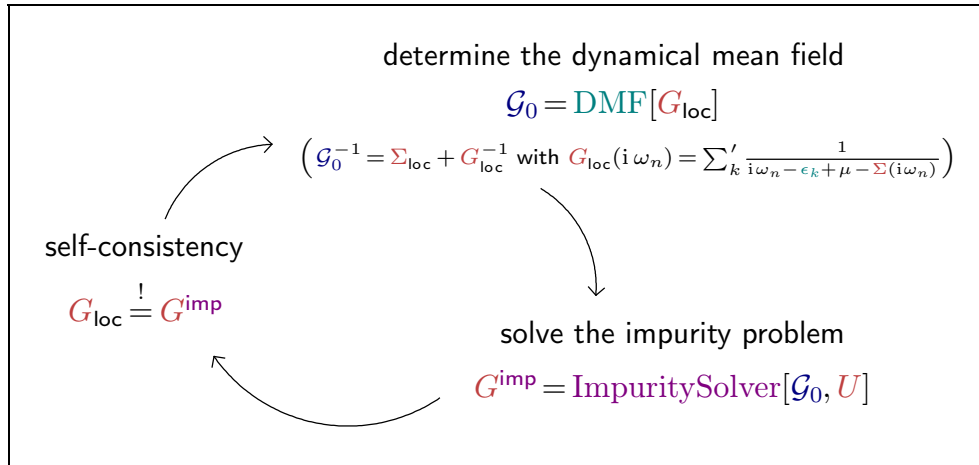
What have we done here ? We encoded the properties of the Hubbard lattice (lattice **hybridization** and **translational invariance**<sup>16</sup>) in an expression for the bath / *dynamical mean field*  $\mathcal{G}_0 = \text{DMF}[G_{\text{loc}}]$ , just like in the Weiss treatment of the Ising model where we encode properties of the lattice in a Weiss field :

	Ising model	Hubbard model
Hamiltonian	$H = -\sum_{ij} J_{ij} s_i s_j$	$H = -\sum_{ij} t_{ij} c_i^\dagger c_j + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (29)$
Local observable	$m = \langle s_i \rangle$	$G_{\text{loc}}(\tau) = -\langle c_i^\dagger(\tau) c_i(0) \rangle$
Spatial correlations	$\langle s_i s_j \rangle$	$G_{ij}(\tau) = -\langle c_i^\dagger(\tau) c_j(0) \rangle$
Single-site model	$H_{\text{MF}}^{(1)} = -B_{\text{Weiss}} \cdot s$	$H_{\text{imp}} \mid \mathcal{G}^{\text{imp}} = -\int \int \frac{c^\dagger(\tau) c(\tau)}{\mathcal{G}_0(\tau - \tau')} + U \int n_\uparrow n_\downarrow \quad (42)$
Mean field / Bath	$B_{\text{Weiss}} = Jz m$	$\mathcal{G}_0(\tau) = \text{DMF}[G_{\text{loc}}] \quad (45, 46, 52) \quad (\Leftrightarrow \{V_\ell, E_\ell\})$
Self-consistency	$m \stackrel{!}{=} m_{\text{MF}}(B_{\text{Weiss}})$	$G_{\text{loc}} \stackrel{!}{=} G^{\text{imp}}(\mathcal{G}_0) \quad (41)$
Solving	$m_{\text{MF}} = \tanh(\beta B_{\text{Weiss}})$	Let the computer work ! $(\S 2.7)$

Note that LISA and these self-consistent equations can be derived from the Hubbard model itself, allowing to understand better and to control the approximations which lead to (42). See §2.8 for the **cavity method**.

## 2.5. The DMFT self-consistent loop

If we have a solver for the impurity model, **ImpuritySolver**, giving us  $G^{\text{imp}}$  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 an implicit system. As usual, the only way is to **solve in an iterative manner self-consistently** :



**Figure 7.** The LISA DMFT self-consistent loop.

<sup>16</sup>. 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).

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

$$\begin{aligned} G^{(m)} &= \text{ImpuritySolver}[\mathcal{G}_0^{(m)}, U] && \leftarrow \text{needs } i\omega_n \text{ or } \tau \\ &&& \text{dep'ing on the solver} \\ \mathcal{G}_0^{(m+1)} &= \text{DMF}[G^{(m)}] && \leftarrow \text{needs } i\omega_n \end{aligned} \quad (46)$$

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

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

Note that a priori,  $\Sigma^{\text{imp}} \neq \Sigma^{\text{latt}}$ , but the self-energies are actually equal, as we see by comparing (44) and (53). It is then equivalent (at least on paper, numerically it depends) to work the self-energy  $\Sigma$  rather than  $G$  with using  $\Sigma = \mathcal{G}_0^{-1} - G^{-1}$  if self-consistent convergence is achieved. Note that we write bare  $\Sigma$ 's and  $G$ 's here, without precising “imp” or “latt” because until convergence, these do not have physical meaning, and at convergence “imp” and “latt” are identical (41).

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  $\beta$ .

At the end of the day, we want  $A_\beta(\vec{k}, \omega)$ , which we have to invert from  $G_\beta(\vec{k}, \tau)$  or  $G_\beta(\vec{k}, i\omega_n)$ . To obtain the latter, we just compute it from  $\Sigma_{\text{loc}}$  and  $\epsilon_{\vec{k}}$  using (38).

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  $\mathcal{G}_0^{(0)}$*  (metallic or insulating density of states) *can lead to different lattice states* (metallic or Mott insulator).

## 2.6. Lattices

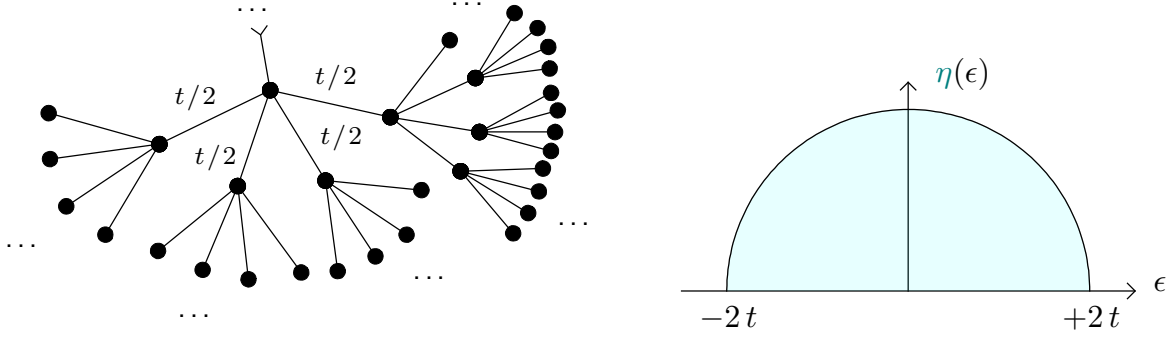
The density of states  $\eta^{\text{latt}}(\epsilon)$ , or DMF (46), contains all the properties we need for the LISA DMFT. For DMFT to be valid, we should look at infinite dimensional lattices, i.e. each site has an infinite number of neighbors, a number which we call  $z$ , the coordinance ( $z = 2d$  for a cubic lattice).

But for the kinetic/hopping energy  $\epsilon(\vec{k})$  to stay finite in the limit  $d \rightarrow \infty$ , the hopping amplitudes must scale<sup>17</sup> as  $t_{ij} \propto 1/\sqrt{z}$ .

<sup>17</sup>. Indeed,  $\epsilon(\vec{k})$  is a Fourier transform of the  $t_{ij}$ 's, so is basically a sum  $\sum_{n=1}^d t \cos(k)$  of randomly alternating sum, for which  $t$  must be of the order of  $d^{-1/2}$  in order to stay constant with  $d$ . [GKKR p. 20]

### 2.6.1. The Bethe lattice

Also called the Cayley tree. Represents a lattice in hyperbolic geometry. Mostly used because the mean field equation takes a simple analytical form in the limit of infinite coordinance  $z$ .



**Figure 8.** The Bethe lattice  $z = 4$ . Density of states of the  $z = \infty$  Bethe lattice.

Two ways to obtain the bath for the impurity model :

- Let's start from (50) :  $\Delta = \sum_{i,j} t_{oi} t_{oj} G_{ij}^{(o)}$ . For a Bethe lattice  $z \rightarrow \infty$  with  $t_{ij} = t/\sqrt{z}$ , removing a site does not make any difference and  $G_{ij}^{(o)} = G_{ij}$ , and  $G_{ij}^{(o)} = \delta_{ij} G_{ii}^{(o)}$  (since neighbors of  $o$  are completely disconnected on this lattice once the cavity has been introduced), which yields

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

and injecting in  $\mathcal{G}_0^{-1} = i\omega_n + \mu - \Delta$  (43), we get the simple mean field

$$\boxed{\mathcal{G}_0(i\omega_n)^{-1} = i\omega_n + \mu - t^2 G_{\text{loc}}(i\omega_n)} \quad (47)$$

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

$$\eta_{\text{Bethe}}(\epsilon) = \frac{1}{2\pi t^2} \sqrt{4t^2 - \epsilon^2} \quad \text{for } |\epsilon| < 2t \quad (48)$$

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

$$\widetilde{\eta_{\text{Bethe}}}(\zeta) = \frac{1}{2t^2} \left( \zeta - \text{sgn}(\Re \zeta) \sqrt{\zeta^2 - 4t^2} \right) \Leftrightarrow \begin{matrix} R_{\text{Bethe}}(x) = t^2 x + x^{-1} \\ (x \in [-1, 1] \times i[-1, 1]) \end{matrix}$$

Now, injecting this result in (46)  $\mathcal{G}_0^{-1} = i\omega_n + \mu + G_{\text{loc}}^{-1} - R(G_{\text{loc}})$ ,  $G_{\text{loc}}^{-1}$  simplifies and we get

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

### 2.6.2. The cubic lattice in infinite dimensions

Nearest neighbors hopping  $t_{ij} = \delta_{\langle i,j \rangle} t/\sqrt{z}$  with coordinance  $z = 2d \rightarrow \infty$ . Density of states :

$$\eta_{\text{cubic}}(\epsilon) = \frac{1}{t\sqrt{2\pi}} e^{-\epsilon^2/2t^2} = \frac{1}{\sqrt{\pi}} e^{-\epsilon^2} \text{ with } t = 1/\sqrt{2}$$

of Hilbert transform (which can't be inverted explicitly)

$$\tilde{\eta}_{\text{cubic}}(\zeta) = -is\sqrt{\pi} \exp(-\zeta^2) \text{erfc}(-is\zeta) \quad \text{with } s = \text{sgn}(\Im \zeta)$$



## 2.7. Solving the impurity problem $G^{\text{imp}} = \text{ImpuritySolver}[\mathcal{G}_0, U]$

There are many techniques to solve the impurity problem (42). This is still a quantum many-body problem (with a single site, but with an arbitrary bath), so it is not trivial, and is actually the most difficult part.

Whether we work with Matsubara time  $\tau$  or frequencies  $i\omega_n$ , we have to discretize  $\tau$  or set an upper frequency  $n_{\text{max}}$  for  $\mathcal{G}_0$  to be numerically represented. Then the problem reduces to a finite number of coupled equations, which we hope is enough to obtain an accurate result. This is usually not an issue.

### 2.7.1. Quantum Monte Carlo techniques

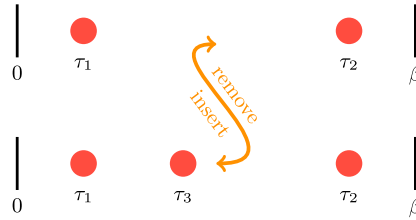
The goal is to compute  $G^{\text{imp}}(t) = -i \langle T c(t) c^\dagger(0) \rangle$  (40), or rather  $G_\beta^{\text{imp}}(\tau)$ . Being an average, Monte Carlo methods are well suited to compute it, with the condition of using Matsubara time rather than real time. As always, computing such an average reduces to computing the partition function  $Z = \text{tr}(e^{-\beta H_{\text{GC}}^{\text{imp}}})$ .

Ref : [https://www.theorie.physik.uni-muenchen.de/activities/schools/archiv/asc\\_school\\_17/extramaterial/parcollet\\_slides\\_3.pdf](https://www.theorie.physik.uni-muenchen.de/activities/schools/archiv/asc_school_17/extramaterial/parcollet_slides_3.pdf)

*Continuous-time Quantum Monte Carlo* (CT-QMC) amounts to writing  $Z$  in a perturbative way :

$$\begin{aligned} H = H_a + H_b &\Rightarrow Z = \text{tr} \left( T_\tau e^{-\beta H_a} \exp \left( - \int_0^\beta d\tau H_b(\tau) \right) \right) \\ &= \sum_{n \geq 0} (-1)^n \int_0^\beta d\tau_1 \dots \int_{\tau_{n-1}}^\beta d\tau_n \text{tr} (e^{-\beta H_a} H_b(\tau_n) \dots H_b(\tau_1)) \\ &= \sum_{c \in \mathcal{C}} p(c) \quad \text{where configurations are } c = (n, \tau_1, \dots, \tau_n, \gamma) \end{aligned}$$

To evaluate this sum, we use a Monte Carlo method, where moves are adding/removing “interaction terms”, i.e.  $c = (n, \tau_1, \dots, \tau_n) \rightarrow c' = (n, \tau_1, \dots, \tau_n, \tau_{n+1})$  with  $\tau_{n+1} \in [0, \beta]$  :



For solving the impurity problem (42), there are two ways to write the problem perturbatively :

→ either in the *interaction*  $U$  (this is CT-INT-QMC) :

$$\frac{Z}{Z_0} = 1 - U \int_0^\beta d\tau_1 \langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) \rangle_0 + \frac{U^2}{2} \iint_0^\beta d\tau_1 d\tau_2 \langle T_\tau n_\uparrow(\tau_1) n_\downarrow(\tau_1) n_\uparrow(\tau_2) n_\downarrow(\tau_2) \rangle_0 + \dots$$

→ either in the *bath/hybridization*  $\Delta(i\omega_n)$  (this is CT-HYB-QMC).

Writing an efficient CT-QMC is not an easy task. QMC methods are versatile and work at any temperature, but there are slow/noisy and may suffer from the sign problem.

### 2.7.2. Iterated Perturbation Theory approximation

Applicable *only at half-filling*. It is a second order perturbation theory in  $U$ , where the self-energy reads

$$\boxed{\Sigma^{\text{imp}}(i\omega_n) \simeq \frac{U}{2} + U^2 \int_0^\beta d\tau e^{i\omega_n \tau} \mathcal{G}'_0(\tau)^3} \quad \text{where} \quad \frac{1}{\mathcal{G}'_0(i\omega_n)} = \frac{1}{\mathcal{G}_0(i\omega_n)} - \frac{U}{2} \quad (49)$$

Together with the usual DMFT loop, this is called the *Iterated Perturbation Theory* (IPT) approximation.



It turns out that this approximation is not only exact in the non-interacting limit ( $\Sigma^{\text{imp}} = 0$ ) and very good up to  $U / (V_{\ell_0} \eta_{\text{bath}}(0)) \approx 6$  where, but it is *also exact in the strong-coupling limit* (which is a fortunate coincidence, which does not survive if we are not at half-filling anymore) ! Indeed, in the atomic limit (34), the lattice effectively disappear and we can forget about the dispersion  $\epsilon(\vec{k})$  in (38) so that  $G_{\text{loc}} = \sum_{\vec{k}} G(\vec{k}, i\omega_n) = G(\vec{k}, i\omega_n)$  :

$$G_{\text{loc}} = \frac{1}{i\omega_n + \mu - \Sigma_{\text{loc}}} \Rightarrow \frac{1}{\mathcal{G}_0} = \Sigma_{\text{loc}} + G_{\text{loc}}^{-1} = i\omega_n + \mu = i\omega_n + \frac{U}{2} \Rightarrow \frac{1}{\mathcal{G}'_0(i\omega_n)} = i\omega_n$$

Thus,  $\mathcal{G}'_0(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathcal{G}'_0(i\omega_n) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \frac{1}{i\omega_n} = -\frac{1}{2}$ , and then the IPT self-energy reads

$$\Sigma^{\text{imp}}(i\omega_n) = \frac{U}{2} + U^2 \int_0^\beta d\tau e^{i\omega_n \tau} \left(-\frac{1}{2}\right)^3 = \frac{U}{2} - \frac{U^2}{8} \frac{\overbrace{e^{i\omega_n \beta} - 1}^{-1}}{i\omega_n} = \frac{U}{2} + \frac{U^2}{4} \frac{1}{i\omega_n} = \Sigma_{\text{at}}(i\omega_n) \quad (34)$$

Thus, if it captures the insulating (atomic limit) and the metallic (non-interacting limit) phases, the IPT must show a phase transition somewhere. And actually, *at half-filling*, it reproduces quite well more refined results, so it interpolates quite well between the two limits.

The shift  $\mathcal{G}'_0^{-1} = \mathcal{G}_0^{-1} - U/2$  effectively removes the Hartree part of the self-energy, and makes  $\mathcal{G}'_0$  particle-hole symmetric (i.e.  $\Re \mathcal{G}'_0(i\omega_n) = 0$ ). A good way to improve numerical stability would be to enforce this in the code, as well as enforcing the particle-hole symmetry of  $G_{\text{loc}}(i\omega_n)$ .

### 2.7.3. Real time methods

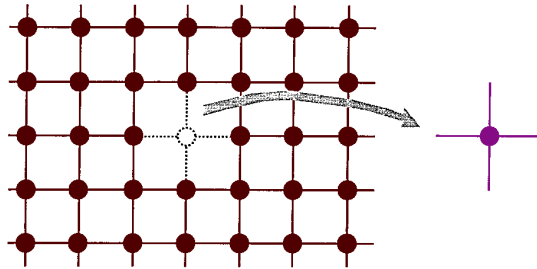
The issue with previous techniques is that we must work with Matsubara time  $\tau/i\omega_n$ , and then perform continuation to real time  $t/\omega$  to compute observables. This is a hard task in itself, and one may want to work only in real time. To solve the impurity problem in real time, we must use the hamiltonian formulation (39)

$$\mathbf{H} = \mathbf{H}_{\text{site}} + \mathbf{H}_{\text{coupl}} + \mathbf{H}_{\text{bath}}$$

where the bath has been discretized from  $\mathcal{G}'_0(\tau)$  (note that there are infinitely many  $\{V_\ell, E_\ell\}$  for a given bath, an choosing is a problem in itself). Then, this hamiltonian can be diagonalized (this is *exact diagonalization*), or solved by techniques such as NRG or DMRG.

## 2.8. Deriving LISA using the cavity method

Let's derive the action  $\mathcal{S}^{\text{imp}}$  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  $\mathcal{S}_{\text{eff}}$ , and then performing a mean-field approximation by removing many terms which disappear in  $d \rightarrow \infty$ , we eventually get the action (42) with  $\mathcal{G}_0^{-1} = i\omega_n + \mu - \Delta$  with

$$\begin{aligned} \Delta(i\omega_n) &\underset{d \rightarrow \infty}{\simeq} \sum_{i,j} t_{oi} t_{oj} G_{ij}^{(o)}(i\omega_n) \\ &= \sum_{i,j} t_{oi} t_{oj} G_{ij} - \frac{1}{G_{oo}} \left( \sum_i t_{oi} G_{io} \right)^2 \end{aligned} \quad (50)$$

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  $\epsilon(\vec{k}) = \text{FT}[-t_{ij}](\vec{k})$  (30) and its density of states  $\eta^{\text{latt}}(\epsilon) = \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \delta(\epsilon - \epsilon(\vec{k}))$ . For example, the term

$$\begin{aligned} \sum_i t_{oi} G_{io} &= - \sum_i \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} e^{i\vec{k} \cdot (-\vec{R}_i)} \epsilon(\vec{k}) \int \frac{d\vec{k}'}{\mathcal{V}_{\text{BZ}}} e^{i\vec{k}' \cdot \vec{R}_i} G(\vec{k}') \\ &= - \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \epsilon(\vec{k}) G(\vec{k}) \quad \text{because} \quad \sum_i e^{i(\vec{k}' - \vec{k}) \cdot \vec{R}_i} = \delta(\vec{k}' - \vec{k}) \\ \text{and similarly, } \sum_{i,j} t_{oi} t_{oj} G_{ij} &= \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \epsilon(\vec{k})^2 G(\vec{k}) \\ \text{and } G_{oo} &= \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} G(\vec{k}) \end{aligned}$$

Now, using the DMFT expression of the Hubbard lattice Green's function (38)  $G(\vec{k}, i\omega_n)^{-1} = \zeta - \epsilon(\vec{k})$  with  $\zeta = i\omega_n + \mu - \Sigma_{\text{loc}}(i\omega_n)$ , these three terms reads (for  $l = 1, 2, 0$  resp.)

$$\int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \frac{(-\epsilon(\vec{k}))^l}{\zeta - \epsilon(\vec{k})} = \int d\epsilon \frac{(-\epsilon)^l}{\zeta - \epsilon} \int \frac{d\vec{k}}{\mathcal{V}_{\text{BZ}}} \delta(\epsilon - \epsilon(\vec{k})) \stackrel{\text{def}}{=} (-1)^l \underbrace{\int d\epsilon \eta(\epsilon) \frac{\epsilon^l}{\zeta - \epsilon}}_{=: h_l(\zeta)}$$

Then,

$$\Delta = h_2(\zeta) - h_1(\zeta)^2 / h_0(\zeta) \quad (51)$$

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  $\int d\epsilon \eta(\epsilon) \epsilon = t_{oo} = 0$ ), 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 (27).

Now, we have to inject back in  $\mathcal{G}_0^{-1} = i\omega_n + \mu - \Delta$  (43, with  $\epsilon_0 = 0$ ) to obtain the bath Green's function from the Hubbard model :  $\mathcal{G}_0^{-1} = \zeta + \Sigma_{\text{loc}} - (\zeta - 1 / \tilde{\eta}(\zeta))$ , or

$$\boxed{\mathcal{G}_0(i\omega_n)^{-1} = \Sigma_{\text{loc}}(i\omega_n) + \frac{1}{\tilde{\eta}(\zeta(i\omega_n))} \quad \text{with} \quad \zeta(i\omega_n) \stackrel{(38)}{=} i\omega_n + \mu - \Sigma_{\text{loc}}(i\omega_n)} \quad (52)$$

We can express this Weiss field as a function of  $G_{\text{loc}}$ , hiding  $\tilde{\eta}$ , by using  $G_{\text{loc}} = G_{oo} = h_0(\zeta) = \tilde{\eta}(\zeta)$  (36) :

$$\boxed{\Sigma_{\text{loc}} = \frac{1}{\mathcal{G}_0} - \frac{1}{G_{\text{loc}}}} \quad (53)$$

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

$$\boxed{\mathcal{G}_0(i\omega_n)^{-1} = i\omega_n + \mu + G_{\text{loc}}(i\omega_n)^{-1} - R(G_{\text{loc}}(i\omega_n))} \quad (54)$$

These self-consistent equations are the one we already derived using general considerations in §2.4.2.

## 2.9. Practical considerations. Random things to do.

- Ferromagnetic order : gkkp p31
- Read GKKR section VII p59
- En pratique, on fixe  $t = 1$ , et on travaille avec  $U/t, \beta t$ .

- For the itinerant ferromagnetism : mean field [13/11 @38:40]
- Calcul de la conductivity : en linear-response theory, nécessite la 2-body Green function (+ sa continuation analytique...)  $\langle \mathbf{T} \mathbf{j}_\alpha^P(\vec{r}_1, \tau_1) \mathbf{j}_\beta^P(\vec{r}_2, \tau_2) \rangle$ , or on a accès qu'aux propriétés 1-body ? Alternativement, on pourrait induire un champ  $\vec{E}$  à la main dans le modèle de Hubbard (peut être juste avoir un hopping  $t_{ij} \neq t_{ji}$  ?), et simplement regarder  $\langle \mathbf{T} \mathbf{j}_\alpha^P(\vec{r}, \tau) \rangle$  qui est 1-body, calculable directement depuis  $G(i\omega_n)$  (mais nécessite la continuation analytique ?)

For a rectangular lattice of dimension  $d$  of hoppings  $t_m$  and lattice constants  $a_m$  in directions  $\vec{e}_m$ , if we add to the hopping  $t_1$  an asymmetry  $+\varepsilon$  in the direction  $+\vec{e}_1$  and  $-\varepsilon$  in the direction  $-\vec{e}_1$ , then

$$\begin{aligned}
 \epsilon'(\vec{k}) &= \sum_j -t_{ij} e^{i\vec{k} \cdot \vec{R}_{ij}} = - \sum_{m=1}^d (t_{m,\rightarrow} e^{ik_m a_m} + t_{m,\leftarrow} e^{-ik_m a_m}) \\
 &= -(t_1 + \varepsilon) e^{ik_1 a_1} - (t_1 - \varepsilon) e^{-ik_1 a_1} - \sum_{m=2}^d t_m (e^{ik_m a_m} + e^{-ik_m a_m}) \\
 &= -2\varepsilon i \sin(k_1 a_1) - \sum_{m=1}^d 2 t_m \cos(k_m a_m)
 \end{aligned}$$