DMFT with Iterated Perturbation Theory

Fabian Kugler, Hannes Herrmann and Alessandro Bottero

February 11, 2016

1   Introduction and Overview

The aim of this project is to study the metal to Mott-Insulator phase transition exhibited by the Fermi-Hubbard model.

The model consists of a lattice with a single-level *atom* at every site. The electrons can only hop from a site to a nearest neighbour one, and only interact with each other if they are at the same site. The Hamiltonian of this model is, therefore, given by:

$$\mathcal{H} = -t \sum_{<i,j>} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \mu \sum_i (n_{i,\uparrow} n_{i,\downarrow}) \tag{1}$$

where t is the hopping rate, U the strenght of the interaction, which by varying will lead to the phase transition, and μ the chemical potential.

This model is studied here by means of Dynamical Mean Field Theory (DMFT), and the quantity of interest is the local Green's function, given by:

$$G^{\sigma}_{ii}(\tau - \tau') = - \langle T c_{i\sigma}(\tau) c^{\dagger}_{i\sigma}(\tau') \rangle \tag{2}$$

by means of which it will then be possible to compute the *Spectral Function*.

The main idea behind the DMFT approach is similar in spirit to the classical mean field approximation and consists in solving the problem of a single atom coupled to a thermal bath and mapping this to our original lattice problem via a self-consistency relation. Such single atom problem is described by the Hamiltonian of a so called *Anderson Impurity Model* (AIM), given by:

$$\mathcal{H}_{AIM} = \mathcal{H}_{atom} + \mathcal{H}_{bath} + \mathcal{H}_{coupling} \tag{3}$$

where we have the following:

$$\mathcal{H}_{atom} = U n^c_{\uparrow} n^c_{\downarrow} + (\epsilon_0 - \mu)(n^c_{\uparrow} + n^c_{\downarrow})$$

$$\mathcal{H}_{bath} = \sum_{l,\sigma} \tilde{\epsilon}_l a^{\dagger}_{l\sigma} a_{l\sigma} \tag{4}$$

$$\mathcal{H}_{coupling} = \sum_{l,\sigma} V_l (a^{\dagger}_{l\sigma} c_{\sigma} + c^{\dagger}_{\sigma} a_{l\sigma})$$

here, the the a_l's describe the fermionic degrees of freedom of the bath, while the $\tilde{\epsilon}_l's$ and the V_l's are parameters which must been chosen appopriately (such that the impurity Green's funtion of (4) coincides with the local lattice one) and enter through the hybridisation function:

$$\Delta(i\omega_n) = \sum_l \frac{|V_l|^2}{i\omega_n - \tilde{\epsilon}_l} \tag{5}$$

how it can be seen from the effective action for the system, obtained integrating out the bath degrees of freedom:

$$S_{eff} = -\int_0^\beta \int_0^\beta d\tau d\tau' \sum_\sigma c_\sigma^\dagger(\tau) \mathscr{G}_0^{-1}(\tau - \tau') c_\sigma(\tau') + U \int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau) \tag{6}$$

where we have defined:

$$\mathscr{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \epsilon_0 - \Delta(i\omega_n) \tag{7}$$

At this point come into play the mean field approximation. First of all, we notice that we can define a local self-energy for the interacting Green's function of the effective AIM, $G(\tau - \tau')$, via:

$$\Sigma_{imp}(i\omega_n) \equiv \mathscr{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n) \tag{8}$$

And, of course, we can also consider the self-energy of our origina lattice problem, defined from (2), via:

$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_0 - \epsilon_\mathbf{k} - \Sigma(\mathbf{k}, i\omega_n)} \tag{9}$$

with:

$$\epsilon_\mathbf{k} \equiv t \sum_j e^{i\mathbf{k}\cdot(\mathbf{R_i} - \mathbf{R_j})} \tag{10}$$

The approximation, now, consists of saying that the lattice self-energy coincides with the impurity self-energy, resulting in vanishing off-diagonal elements of Σ_{latt}:

$$\Sigma_{ii} \simeq \Sigma_{imp} , \Sigma_{i \neq j} \simeq 0 \tag{11}$$

which is a consistent approximation only given that it uniquely determines the local Green's function, which, by assumption, is the impurity problem Green's function. We, therefore, sum (9) over $\mathbf{k}$ to obtain (2), and use (8) to arrive to the self-consistency relation:

$$\sum_\mathbf{k} \frac{1}{\Delta(i\omega_n) + G(i\omega_n)^{-1} - \epsilon_\mathbf{k}} = G(i\omega_n) \tag{12}$$

This is the idea behind the DMFT approach. In practice one use an iterative procedure, following the loop:

1. start with an initial guess for $\mathscr{G}_0$ (i.e. for Δ);

2. compute the AIM Green's function G_{imp} (by means of perturbation theory, in our case up to second order) $\rightarrow \Sigma_{imp}$ is computed;

3. compute the lattice problem local Green's function G_{loc};

4. update $\mathscr{G}_0$ via $\mathscr{G}_{0,new}^{-1} = G_{loc}^{-1} + \Sigma_{imp}$;

5. iterate till convergence.

which is what we have done in the project. Finally, once the lattice local Green's function has been obtained for the set of values $\{i\omega_n\}$, we fit it using the Padé approximation, and, eventually, we are able to compute the Spectral Function, via analytic continuation of this fit.

2 The impurity problem in 2$^{\text{nd}}$ order perturbation theory

Translating the Hamiltonian formalism into a functional integral one, we get the action

$$S = \int_0^\beta \sum_\sigma \bar{c}_\sigma(\tau) \partial_\tau c_\sigma(\tau) + \sum_{l,\sigma} \bar{a}_\sigma(\tau) \partial_\tau a_\sigma(\tau) + H_{\text{AIM}}\big(\bar{c}_\sigma(\tau), c_\sigma(\tau), \bar{a}_\sigma(\tau), a_\sigma(\tau)\big) \, \mathrm{d}\tau$$

$$= \int_0^\beta H_{\text{atom}}\big(\bar{c}_\sigma(\tau), c_\sigma(\tau)\big) \, \mathrm{d}\tau + \sum_{\sigma,\omega} \bar{c}_{\sigma,\omega}\Big(\sum_l \frac{V_l}{i\omega - \tilde{\epsilon}_l} - i\omega \Big) c_{\sigma,\omega}$$

$$+ \sum_{l,\sigma,\omega} \big(\bar{a}_{l,\sigma,\omega} + \frac{V_l}{\tilde{\epsilon}_l - i\omega} \bar{c}_{\sigma,\omega} \big)\big(\tilde{\epsilon}_l - i\omega \big)\big(a_{l,\sigma,\omega} + \frac{V_l}{\tilde{\epsilon}_l - i\omega} c_{\sigma,\omega} \big)$$

where some arrangements and usage of the usual Matsubara-Fourier transform was made. We use the convention $c_\sigma(\tau) = \sum_\omega e^{-i\omega\tau} c_{\sigma,\omega}$ where the sum runs over fermionic Matsubara frequencies and a prefactor of $1/\beta$ is understood, such that $c_{\sigma,\omega}$ has the dimension of inverse energy. Correspondingly, a Kronecker-delta of Matsubara frequencies contains a factor of β. In the above expression, the bath can easily be integrated out. The case of half filling, $\mu = U/2$, can be equivalently written with a modified interaction and zero chemical potential. Dropping a constant energy term, one has

$$S_{\text{eff}} = S_0 + S_{\text{int}} = - \sum_{\sigma,\omega} \bar{c}_{\sigma,\omega} G_{0,\omega}^{-1} c_{\sigma,\omega} + U \sum_Q \Big(\underbrace{\sum_k \bar{c}_{\uparrow,k+Q} c_{\uparrow,k} - \frac{1}{2}\delta_{Q,0}}_{C_Q} \Big)\Big(\underbrace{\sum_q \bar{c}_{\downarrow,q-Q} c_{\downarrow,q} - \frac{1}{2}\delta_{Q,0}}_{D_{-Q}} \Big).$$

A perturbative expansion of the Green's function exploits (consider w.l.o.g. $c_\omega = c_{\uparrow,\omega}$)

$$\beta G(i\omega) = -\langle c_\omega \bar{c}_\omega \rangle = -\frac{\langle c_\omega \bar{c}_\omega e^{-S_{\text{int}}} \rangle_0}{\langle e^{-S_{\text{int}}} \rangle_0} = \beta G_{0,\omega} - \frac{1}{2}\langle (c_\omega \bar{c}_\omega + \beta G_{0,\omega}) S_{\text{int}}^2 \rangle_0 + \mathcal{O}(U^3) \,.$$

Here, first order terms vanish due to Wick's theorem and the fact that without interaction, the resulting tight-binding model at zero chemical potential is half filled in the ground state,

$$\sum_\omega G_{0,\omega} = \langle n_\sigma \rangle_0 = \frac{1}{2} \quad \Rightarrow \quad \langle C_Q \rangle_0 = \big(\sum_k G_{0,\omega} - \frac{1}{2} \big) \delta_{Q,0} = 0 = \langle D_Q \rangle_0 \,.$$

For the contribution to second order, note that only mixed terms survive,

$$\langle D_{-Q_1} D_{-Q_2} \rangle_0 = \sum_{q_1,q_2} \langle c_{\downarrow,q_2} \bar{c}_{\downarrow,q_1-Q_1} \rangle_0 \langle c_{\downarrow,q_1} \bar{c}_{\downarrow,q_2-Q_2} \rangle_0 = -\delta_{Q_2,-Q_1} \sum_q G_{0,q} G_{0,q+Q_1}, \quad \text{and}$$

$$\sum_{Q_1} \langle (c_\omega \bar{c}_\omega + \beta G_{0,\omega}) C_{Q_1} C_{-Q_1} \rangle_0 = 2 \sum_{k_1,k_2,Q_1} \langle c_\omega \bar{c}_{k_1+Q_1} \rangle_0 \langle c_{k_2} \bar{c}_\omega \rangle_0 \langle c_{k_1} \bar{c}_{k_2-Q_1} \rangle_0 = -2\beta G_{0,\omega}^2 \sum_k G_{0,k} \,.$$

It follows that up to second order, the Green's function is given by

$$G(i\omega) = G_{0,\omega} - U^2 G_{0,\omega}^2 \sum_k G_{0,k} \sum_q G_{0,q} G_{0,q-k+\omega} = G_{0,\omega} + G_{0,\omega}^2 \Sigma_\omega$$

where we defined the self energy Σ in second order perturbation theory. It takes a simpler form in imaginary time space and remembering that we used an effective interaction, we summarize

$$\Sigma(\tau) = -U^2 G_0(\tau)^2 G_0(-\tau) \qquad \text{with} \quad \mu_{\text{eff}} = 0 \,. \tag{13}$$

3 On the spectral function

As a measure of single-particle excitation, we consider the spectral function, which is obtained by analytic continuation from the Matsubara Green's function with the known principles:

$$\mathcal{A}(w) = -\frac{1}{\pi}\Im G(i\omega \to \omega + i0^+), \quad \mathcal{A}(w) \geq 0, \quad \int_{-\infty}^{\infty} \mathcal{A}(w)\,\mathrm{d}\omega = 1, \quad G(-i\omega) = G(i\omega)^*. \quad (14)$$

For a basic propagator of the type $G^{-1} \propto i\omega + a, a \in \mathbb{R}$, it is easily evaluated and yields

$$G(i\omega) = \frac{c}{i\omega + a} \quad \Rightarrow \quad \mathcal{A}(w) = c\delta(w + a) \quad \Rightarrow \quad c = 1. \quad (15)$$
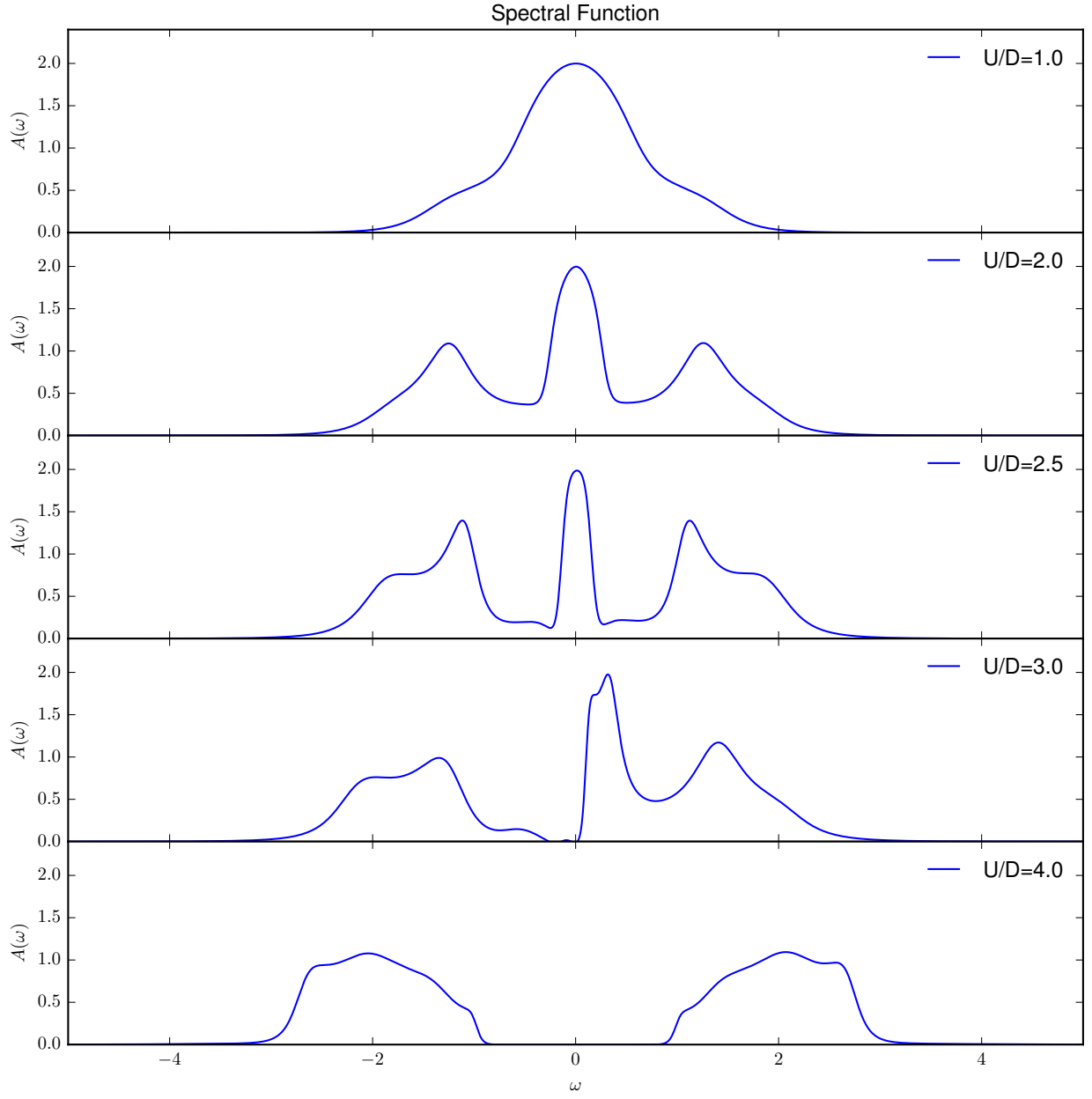
4 Results

Figure 1: Spectral function after analytic continuation. For low interaction parameter U there are single particle excitation??? at zero frequency, therefore the metalic phase. With increasing interaction parameter the spectral function develops a gap at zeros freqency, hence no excitation, ie the insulator phase.

A Matsubara Frequencies and Fast Fourier Transform

In order to solve the impurity model we have to perform several Fourier Transform. As we consider electrons, the Green's function in imaginary time is antiperiodic by shifts of β, so we have to use fermionic Matsubara frequencies $\omega_n := \frac{\pi(2n+1)}{\beta}$. The Fourier Transformations are given by:

$$G(i\omega_n) := \int_0^\beta d\tau G(\tau) e^{i\omega_n \tau} \tag{16}$$

$$G(\tau) = \frac{1}{\beta} \sum_{i\omega_n} G(i\omega_n) e^{-i\omega_n \tau} \tag{17}$$

For effient calculations we use the FFT-algorithm of the numpy package. Therefore we have to adapt our definitions to the implementation of the numpy library. The numpy library calculates its Fourier Transform by:

$$A_k = \text{FFT}(a_m) = \sum_{m=0}^{n-1} a_m \exp\left\{-2\pi i \frac{mk}{n}\right\} \qquad k = 0, \ldots, n-1. \tag{18}$$

Hence, we discretize the Matsubara Fourier transformation

$$G(i\omega_{-n}) \approx \sum_{k=0}^{N-1} \Delta\tau \, G(\Delta\tau \, k) \exp\left(i\frac{\pi(-2n+1)k}{N}\right) \tag{19}$$

$$= \frac{\beta}{N} \sum_{k=o}^{N-1} \left(G(\Delta\tau \, k) \exp\left(i\pi\frac{k}{N}\right)\right) \exp\left(i\frac{-2\pi nk}{N}\right) \tag{20}$$

$$= \frac{\beta}{N} \text{FFT}\left(G(\Delta\tau \, k) \exp\left(i\pi\frac{k}{N}\right)\right), \tag{21}$$

where $\Delta\tau = \frac{\beta}{N}$. The same can be carried out for the inverse Fourier Tranformations.

$$G(\Delta\tau k) = \frac{N}{\beta} e^{-i\pi \frac{k}{N}} \frac{1}{N} \sum_{\omega_n} G(i\omega_{-n}) e^{i2\pi nk/N} \tag{22}$$

$$= \frac{N}{\beta} e^{-i\pi \frac{k}{N}} \text{IFFT}(G(i\omega_{-n})) \tag{23}$$

Unfortunately the "naiv" implementations (21) and (23) cause numerical problems, since a typical Green's function in frequency space is of the form

$$G(i\omega_n) = \frac{1}{i\omega_n + a} = \frac{1}{i\omega_n} + \mathcal{O}\left(\frac{1}{\omega_n^2}\right). \tag{24}$$

Although a can also be frequency dependent, the first term in the expansion of G is always of the form as in (24). Carrying out the sum over frequencies of this first term does unfortunately not [more details here] converge, which is why we have to transform the $\frac{1}{i\omega_n}$ part manually. From analytical calculation the Fourier transform is given as:

$$G(\tau) = -\frac{1}{2} \quad \Leftrightarrow \quad G(i\omega_n) = \frac{1}{i\omega_n} \tag{25}$$

Consequently the improved version of our Fourier transformation is given by subtracting and adding the relevant terms before and after the transformation.

$$G(i\omega_{-n}) = \frac{1}{i\omega_{-n}} + \frac{\beta}{N} \text{FFT}\left(\left(G(\Delta\tau \, k) + \frac{1}{2}\right) \exp\left(i\pi\frac{k}{N}\right)\right) \tag{26}$$

$$G(\Delta\tau k) = -\frac{1}{2} + \frac{N}{\beta} e^{-i\pi \frac{k}{N}} \text{IFFT}\left(G(i\omega_{-n}) - \frac{1}{i\omega_{-n}}\right) \tag{27}$$
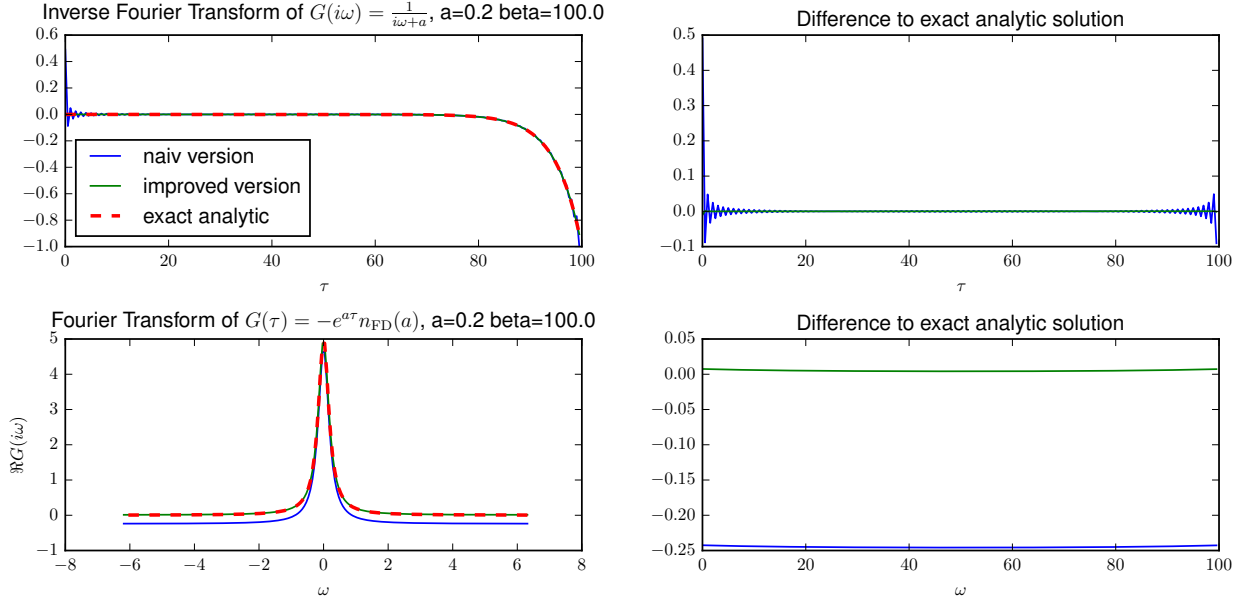
Figure 2: Comparison of the different discretized Fourier Transformations. The improved version, by manually removing the $\frac{1}{i\omega}$ factor, approximates the exact transformation significantly better.

The improvement can be seen in Figure 2, where we compare the exact Fourier transformation of $G(i\omega) = \frac{1}{i\omega + a}$ to our discretized versions. The naiv version shows significant deviations to the analytic solution, whereas our improved version approximates the exact one very well.

B Pade Approximation

Adding
Pade ap-
proxima-
tion