DMFT with Iterated Perturbation Theory

Fabian Kugler, Hannes Herrmann and Alessandro Bottero

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 neighbor one, and only interact with each other if they are at the same site. The Hamiltonian of this model is given by:

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

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 in the framework of Dynamical Mean Field Theory (DMFT), and the quantity of interest is the local Green's function, given by:

$$G_{\text{loc}}(\tau - \tau') = - \langle T c_{i\sigma}(\tau) c_{i\sigma}^{\dagger}(\tau') \rangle \tag{2}$$

by means of which it will then be possible to compute the *Spectral Function* as a measure of elementary excitation of the system.

The main idea behind the DMFT approach is similar in spirit to the classical mean field approximation and consists of 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 the so called *Anderson Impurity Model* (AIM), given by:

$$\mathcal{H}_{\text{AIM}} = \mathcal{H}_{\text{atom}} + \mathcal{H}_{\text{bath}} + \mathcal{H}_{\text{coupling}} \quad \text{with} \quad \mathcal{H}_{\text{atom}} = U n_{\uparrow}^c n_{\downarrow}^c - \mu(n_{\uparrow}^c + n_{\downarrow}^c),$$

$$\mathcal{H}_{\text{bath}} = \sum_{l,\sigma} \tilde{\epsilon}_l a_{l\sigma}^{\dagger} a_{l\sigma}, \quad \mathcal{H}_{\text{coupling}} = \sum_{l,\sigma} V_l(a_{l\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} a_{l\sigma}). \tag{3}$$

Here, the a_l operators describe the fermionic degrees of freedom of the bath, while the $\tilde{\epsilon}_l$ and the V_l are parameters, which must been chosen appropriately (such that the impurity Green's function of (3) coincides with the local lattice one). In section 2 we will see how, after integrating out the bath, these parameters enter into an effective action for the singled out electron. Thereby, the impurity problem is defined with a given bare propagator G_0 and a value of the interaction parameter U.

At this point, the mean field approximation comes into play. First of all, we notice that the self-energy Σ_{imp} of the effective AIM with full Green's function G is given by:

$$\Sigma_{\text{imp}}(i\omega_n) \equiv G_0^{-1}(i\omega_n) - G^{-1}(i\omega_n) \tag{4}$$

Of course we can also consider the self-energy of our original lattice problem having a dispersion relation $\varepsilon_{\mathbf{k}}$, which gives the relation:

$$G_{\text{lattice}}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu - \Sigma_{\text{lattice}}(\mathbf{k}, i\omega_n)} \quad \text{with} \quad \varepsilon_{\mathbf{k}} \equiv t \sum_j e^{i\mathbf{k} \cdot (\mathbf{R_i} - \mathbf{R_j})}. \tag{5}$$

The approximation, now, consists of assuming that at each site the lattice self-energy coincides with the impurity self-energy and has its off-diagonal elements vanish:

$$\Sigma_{ii} \simeq \Sigma_{\text{imp}} \;,\; \Sigma_{i\neq j} \simeq 0 \quad \Rightarrow \quad \Sigma_{\text{lattice}}(\mathbf{k}, i\omega_n) = \Sigma_{\text{imp}}(i\omega_n). \tag{6}$$

We average the momentum dependent Green's function (5) over $\mathbf{k}$ to obtain the local propagator (2) and use (4) to relate the impurity and lattice problem with each other:

$$G_{\text{loc}}(i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, i\omega_n) = \int \mathrm{d}\varepsilon \frac{D(\varepsilon)}{i\omega_n - \varepsilon + \mu - \Sigma_{\text{imp}}(i\omega_n)}, \tag{7}$$

where we expressed the dispersion relation with the density of states $D(\varepsilon)$.

DMFT-loop

Since the parameters of the effective model remain unknown, in order to solve the problem one uses an iterative procedure, in practice following the loop:

1. Start with an initial guess for G_0.

2. Compute the AIM self-energy Σ_{imp} by means of second order perturbation theory.

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

4. Update G_0 with imposing the self-consistency relation between the impurity Green's function and the local one, $G_{\text{loc}} \overset{!}{=} G$, therefore setting

$$G_{0,\text{new}}^{-1} = G_{\text{loc}}^{-1} + \Sigma_{\text{imp}}. \tag{8}$$

5. Iterate till convergence.

Finally, once the lattice local Green's function has been obtained for the set of values $\{i\omega_n\}$, we interpolate it using the Padé approximation, and eventually we are able to compute the Spectral Function via analytic continuation of the interpolation function.

2 The impurity problem in 2nd order perturbation theory

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

$$
\begin{aligned}
S &= \int_0^\beta \sum_\sigma \bar{c}_\sigma(\tau)\partial_\tau c_\sigma(\tau) + \sum_{l,\sigma} \bar{a}_\sigma(\tau)\partial_\tau a_\sigma(\tau) + \mathcal{H}_{\text{AIM}}\big(\bar{c}_\sigma(\tau), c_\sigma(\tau), \bar{a}_\sigma(\tau), a_\sigma(\tau)\big)\, \mathrm{d}\tau \\
&= \int_0^\beta \mathcal{H}_{\text{atom}}\big(\bar{c}_\sigma(\tau), c_\sigma(\tau)\big)\, \mathrm{d}\tau + \sum_{\sigma,\omega} \bar{c}_{\sigma,\omega}\Big(\sum_l \frac{V_l}{i\omega - \tilde{\epsilon}_l} - i\omega\Big) c_{\sigma,\omega} \\
&\quad + \sum_{l,\sigma,\omega} \big(\bar{a}_{l,\sigma,\omega} + \frac{V_l}{\tilde{\epsilon}_l - i\omega}\bar{c}_{\sigma,\omega}\big)\big(\tilde{\epsilon}_l - i\omega\big)\big(a_{l,\sigma,\omega} + \frac{V_l}{\tilde{\epsilon}_l - i\omega}c_{\sigma,\omega}\big)
\end{aligned}
$$

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 resulting in a bare propagator G_0 depending on

the parameters $\tilde{\epsilon}_l$, V_l . 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 (considering 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:

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

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

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

$$\Sigma_{\text{eff}}(\tau) = -U^2 G_0(\tau)^2 G_0(-\tau) \qquad \text{with} \quad \mu_{\text{eff}} = 0. \tag{9}$$

3 General computational aspects

For convenience, we use the Bethe lattice with infinite coordination number in our calculations. With proper rescaling, this leads to the density of states (with band-width $D = 2t$)

$$D(\varepsilon) = \frac{2}{\pi D}\sqrt{1 - \frac{\varepsilon^2}{D^2}}, \tag{10}$$

which has the handy property [1, p. 20]

$$\int_{-D}^{D} d\varepsilon \frac{D(\varepsilon)}{DB - \varepsilon} =: \tilde{D}(B) \tag{11}$$

$$\tilde{D}(B) = \frac{2}{\pi D}\Big(B\pi + \sqrt{1 - B^2}\big[\log(1 - B) - \log(B - 1)\big]\Big) \tag{12}$$

Employing (9), we note the simplified relation for (7):

$$G_{\text{loc}}(i\omega_n) = \tilde{D}\Big(\frac{i\omega_n - \Sigma_{\text{eff}}(i\omega_n)}{D}\Big). \tag{13}$$

3

For the Bethe lattice (8) further reduces to [1, p. 22]

$$G_{0,\text{new}}(i\omega) = i\omega - \frac{D^2}{4} G_{\text{loc}}(i\omega) \tag{14}$$

From the Lehmann representation, one can extract information about the Matsubara Green's function. In terms of eigenstates $\{|n\rangle\}$ of the full Hamiltonian, one has

$$G(\mathbf{k}, i\omega) = \frac{1}{\mathcal{Z}} \sum_{n,m} \frac{e^{-\beta E_n} + e^{-\beta E_m}}{i\omega + E_n - E_m} |\langle n|c_{\mathbf{k}}|m\rangle|^2 \,, \tag{15}$$

which implies $G(-i\omega) = G(i\omega)^*$. Moreover, the matrix element ensures that only energies E_n, E_m with states differing in one electron state have non-zero contribution and therefore

$$G(\mathbf{k}, i\omega) \sim \frac{1}{i\omega} \frac{1}{Z} \sum_{n,m} \left(e^{-\beta E_n} + e^{-\beta E_m} \right) |\langle n|c_{\mathbf{k}}|m\rangle|^2 = \frac{1}{i\omega} \langle \{c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger\} \rangle = \frac{1}{i\omega} \tag{16}$$

$$\text{for } |i\omega| \gg \max\left(E_n - E_m\right) \text{ s.t. } \langle n|c_{\mathbf{k}}|m\rangle| \neq 0 \,.$$

The spectral function is obtained by analytic continuation from the Matsubara Green's function and has properties proven in a similar way.

$$\mathcal{A}(w) = -\frac{1}{\pi} \Im G(i\omega \to \omega + i0^+), \quad \mathcal{A}(w) \geq 0, \quad \int_{-\infty}^{\infty} \mathcal{A}(w) \, d\omega = 1 \,. \tag{17}$$

4 Results

As a final result of our simulation, we obtained the plots of the Spectral Function for increasing values of the interaction strenght U (see Figure 1). It can cleary be seen that with increasing interaction we observe a phase transition (in our case between $3 < U < 4$) from a conductor to a Mott insulator, which is exactly what we expected to find.

This deduction from the values of the spectral function at varying U becomes clear if we recall the meaning of this function. In particular, for the Fermionic case, the single-particle Spectral Function, $\mathcal{A}(\mathbf{k}, \omega)$, can be expressed in the Lehmann representation:

$$\mathcal{A}(\omega) = \frac{1}{\mathcal{Z}} \sum_{n,m} |\langle n|c_{\sigma,i}|m\rangle|^2 (e^{-\beta E_n} + e^{-\beta E_m}) \delta(\omega + (E_n - E_m)) \tag{18}$$

where the $|n\rangle$'s are the Hamiltonian eigenstates and the E_n's are the corresponding energies. With the relations in (17) it is possible to interpret A as a probability density. In particular, usually, this is interpreted as the probability of having a fermion with energy between ω and $\omega + d\omega$.

In the light of this interpretation and of equation (18), it is clear that no gaps in the Spectral Function (as observed for low values of U) mean that we can produce excitations with any energy, leading to a conductive behavior. In contrast, if a gap is present (as for high values of U), no low-energy excitations, so that the material will behave as an insulator.
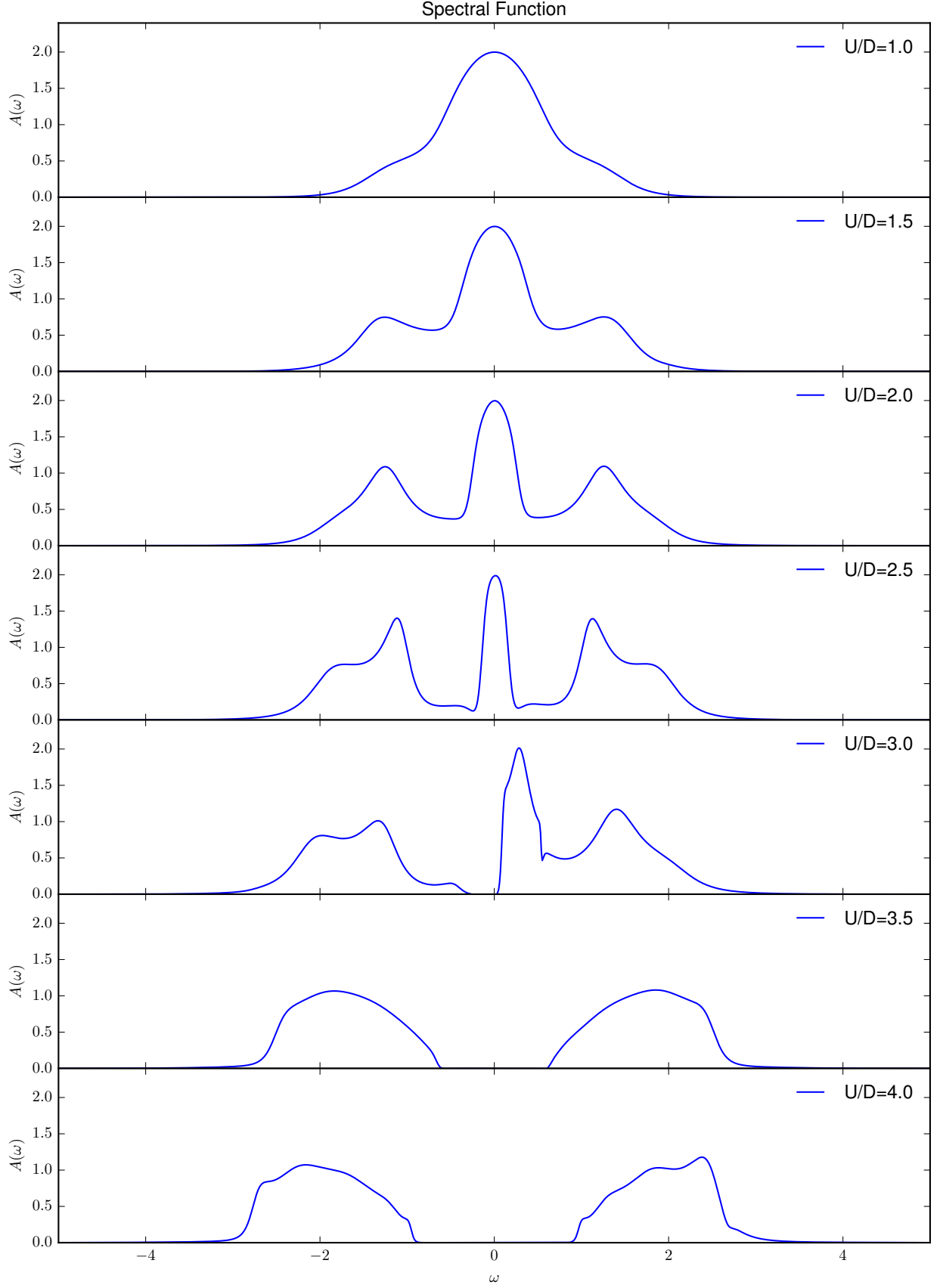
Figure 1: Spectral function for varying parameters U. For low interaction parameter U there are elementary excitation around zero frequency, which corresponds to the metallic phase. With increasing interaction parameter the spectral function develops a gap at zero freqency, hence the insulating phase.

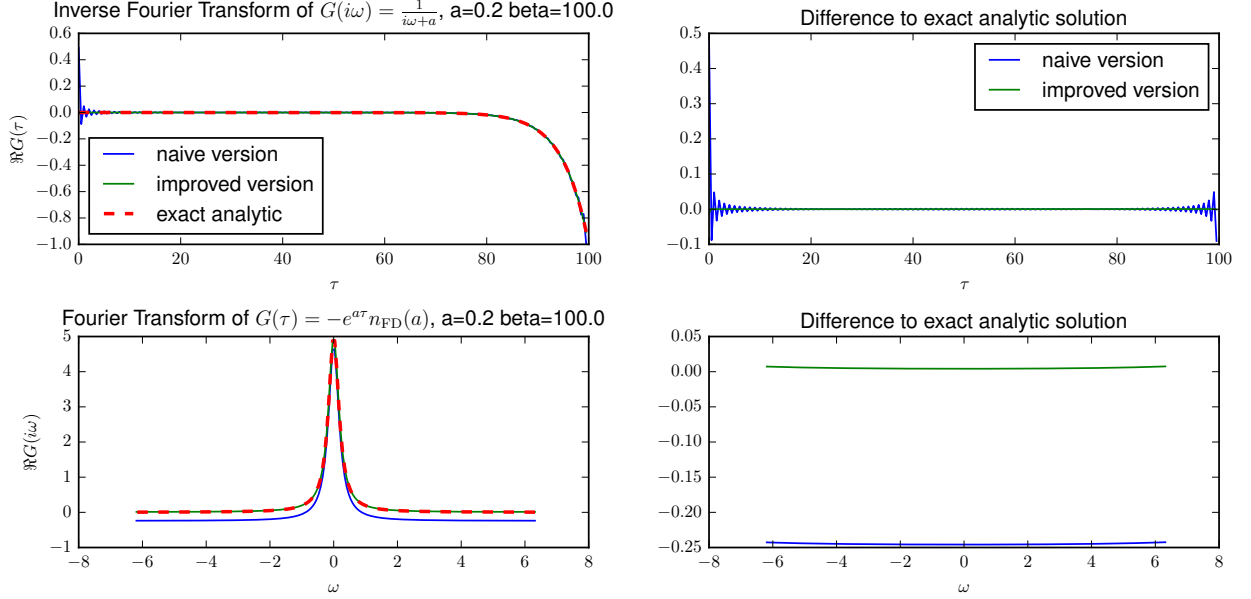# A   Matsubara Frequencies and Fast Fourier Transform

Figure 2: Comparison of the different discretized Fourier Transforms. The improved version, by manually transforming the $1/i\omega$ part, approximates the exact transformation significantly better.

In order to solve the impurity model we have to perform several Fourier Transforms. 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 $\omega_n := \pi(2n+1)/\beta$. The Fourier Transformations are given by (no more implicit β):

$$G(i\omega_n) := \int_0^\beta \mathrm{d}\tau G(\tau)e^{i\omega_n\tau}, \quad G(\tau) = \frac{1}{\beta}\sum_{i\omega_n}G(i\omega_n)e^{-i\omega_n\tau} \tag{19}$$

For efficient 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:

$$A_k = \mathrm{FFT}(a_m) = \sum_{m=0}^{n-1} a_m \exp\left\{-2\pi i\frac{mk}{n}\right\} \qquad k = 0, \ldots, n-1. \tag{20}$$

Hence, we discretize the Matsubara Fourier transformation

$$G(i\omega_{-n}) \approx \sum_{k=0}^{N-1} \Delta\tau\, G(\Delta\tau\, k) \exp\left(i\frac{\pi(-2n+1)k}{N}\right) \tag{21}$$

$$= \frac{\beta}{N}\sum_{k=o}^{N-1}\left(G(\Delta\tau\, k)\exp\left(i\pi\frac{k}{N}\right)\right)\exp\left(i\frac{-2\pi nk}{N}\right) \tag{22}$$

$$= \frac{\beta}{N}\mathrm{FFT}\left(G(\Delta\tau\, k)\exp\left(i\pi\frac{k}{N}\right)\right), \tag{23}$$

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

$$G(\Delta\tau k) = \frac{N}{\beta}e^{-i\pi\frac{k}{N}}\frac{1}{N}\sum_{\omega_n}G(i\omega_{-n})e^{i2\pi nk/N} \tag{24}$$

$$= \frac{N}{\beta}e^{-i\pi\frac{k}{N}}\text{IFFT}(G(i\omega_{-n})). \tag{25}$$

Unfortunately the "naive" implementations (23) and (25) cause numerical problems, since according to (16) Green's functions only decay as $1/i\omega_n$ in frequency space. As the frequency sum is cut off by the finite number of points used, one can strongly increase the accuracy by manually transforming the $1/i\omega_n$ part. By contour integration, it is shown that $(\tau \neq 0)$

$$G(i\omega_n) = \frac{1}{i\omega + a} \quad \Leftrightarrow \quad G(\tau) = \Theta(\tau)\frac{-e^{a\tau}}{e^{\beta a} + 1} + \Theta(-\tau)\frac{e^{a\tau}}{e^{-\beta a} + 1} \tag{26}$$

$$G(i\omega_n) = \frac{1}{i\omega_n} \quad \Leftrightarrow \quad G(\tau) = -\frac{1}{2} + \Theta(-\tau). \tag{27}$$

Consequently the improved version of our Fourier transformation for $\tau \in [0, \beta)$ is given by subtracting and adding the relevant terms before and after the transformation.

$$G(i\omega_{-n}) = \frac{1}{i\omega_{-n}} + \frac{\beta}{N}\text{FFT}\left(\left(G(\Delta\tau\, k) + \frac{1}{2}\right)\exp\left(i\pi\frac{k}{N}\right)\right) \tag{28}$$

$$G(\Delta\tau k) = -\frac{1}{2} + \frac{N}{\beta}e^{-i\pi\frac{k}{N}}\text{IFFT}\left(G(i\omega_{-n}) - \frac{1}{i\omega_{-n}}\right) \tag{29}$$

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 naive version shows significant deviations to the analytic solution, whereas our improved version approximates the exact one very well.
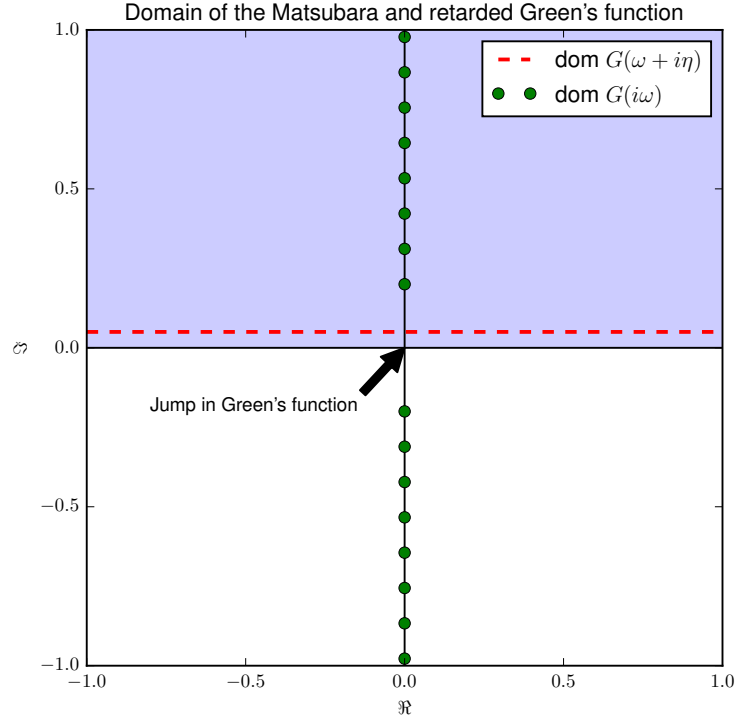
B   Analytic continuation

Figure 3: As the retarded Green's function (red) lies slightly above the real axis and the Matsubara Green's function shows discontinuous jumps at zero frequency, we only take the positive frequencies to calculate the Padé approximation. Assuming that the Green's function is analytic in the upper half plane (blue), we expect the analytic continuation with the rational function to approximate the retarded Green's function both for positive and negative frequencies.

In order to calculate the spectral function $\mathcal{A}$, we have to perform the analytic continuation of the Matsubara Green's function. This is a hard problem as we need the functional dependence of $G(i\omega_n)$ and the only information available is given by discrete points on the imaginary axis. The central idea is now to interpolate our discrete points by a rational function, called Padé approximation, and use this function to do the analytic continuation. An efficient algorithm to calculate the Padé approximation can be found in [2]. However, as the Padé approximation is continuous, whereas the Green's function exhibits non-continuous jumps, we have to think about, which values to use for the interpolation.

In the results of the DMFT-loop we observed discontinuous jumps in the Matsubara Green's function at zero frequency. As we expect the Greens function to behave non-analytically only on the real axis, we can restrict ourselves to the positive or to the negative frequencies in order to calculate the interpolation and use the symmetry of the Green's function $G(i\omega) = G(-i\omega)^*$ to get its values on the opposite half plane.

Since the retarded Green's function is given by $G(i\omega \to \omega + i0^+)$ lies slightly above the real axis, we can use the positive frequencies on the imaginary axis to calculate the interpolation and perform the analytic continuation both for positive and negative frequencies of the retarded Green's function as can be seen in Figure 3.

Furthermore, we reduced the number of values to calculate the interpolation. In some cases this proved to be more stable, which is no surprise, as interpolation polynomials of high degree often show rapid oscillations.

References

[1] Antoine Georges, Gabriel Kotliar, Werner Kraut and Marcelo J. Rozenberg *Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions*, Revwies of Modern Physics, Vol. 68, No. 1, 1996.

[2] H.J. Vidberg and J. W. Serene *Solving the Eliashberg Equations by Means of N-Point Padé Approximants*, Journal of Low Temperature Physics, Vol. 29, Nos. 3/4, 1977.