DMFT with Iterated Perturbation Theory

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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, therefore, 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 by means 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 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:

$$\begin{gathered} \mathcal{H}_{\text{AIM}} = \mathcal{H}_{\text{atom}} + \mathcal{H}_{\text{bath}} + \mathcal{H}_{\text{coupling}} \qquad \text{with} \quad \mathcal{H}_{\text{atom}} = U n_{\uparrow}^{c} n_{\downarrow}^{c} - \mu (n_{\uparrow}^{c} + n_{\downarrow}^{c}), \\ \mathcal{H}_{\text{bath}} = \textstyle\sum_{l,\sigma} \tilde{\epsilon}_l a_{l\sigma}^{\dagger} a_{l\sigma}, \quad \mathcal{H}_{\text{coupling}} = \textstyle\sum_{l,\sigma} V_l (a_{l\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} a_{l\sigma}) \,. \end{gathered} \tag{3}$$

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 (3) coincides with the local lattice one). In chapter 2 we will see how, upon 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 we can define a local self-energy for the interacting Green's function of the effective AIM with full Green's function G via:

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

And, of course, we can also consider the self-energy of our original lattice problem, defined from (2), having a dispersion relation $\varepsilon_{\mathbf{k}}$, via:

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

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

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

This 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 (5) over $\mathbf{k}$ to obtain (2), and use (4) to arrive to relate impurity and lattice problem:

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

where we cast the dispersion relation into a density of states $D(\varepsilon)$.

In practice one uses an iterative procedure, following the loop:

1. start with an initial guess for G_0
2. compute the AIM Green's function G (by means of perturbation theory, in our case up to second order) $\rightarrow \Sigma_{\text{imp}}$ is computed
3. compute the lattice problem local Green's function G_{loc} and require the self-consistency relation to the impurity Greens's function, $G_{\text{loc}} = G$
4. update G_0 with the above requirement, $G^{-1}_{0,\text{new}} = G^{-1}_{\text{loc}} + \Sigma_{\text{imp}}$,
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 interpolate it using the Padé approximation, and, eventually, we are able to compute the Spectral Function, via analytic continuation of function.

2 The impurity problem in 2nd order perturbation theory

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

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

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

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

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

$$\Sigma(\tau) = -U^2 G_0(\tau)^2 G_0(-\tau) \qquad \text{with} \quad \mu_{\text{eff}} = 0\,. \tag{8}$$

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 $D = 2t$)

$$D(\varepsilon) = \frac{2}{\pi D}\sqrt{1 - \frac{\varepsilon^2}{D^2}} \tag{9}$$

which has the handy property

$$\int_{-D}^{D} \mathrm{d}\varepsilon \frac{D(\varepsilon)}{DB - \varepsilon} = \tilde{D}(B) \quad \text{which reads for} \quad \Im B \neq 0, -1 \leq \Re B \leq 1: \tag{10}$$

$$\tilde{D}(B) = \frac{2}{\pi D}\Big(B\pi + \sqrt{1-B^2}\,\big[\log(1-B) - \log(B-1)\big]\Big) \tag{11}$$

Employing (8), we note the simplified relation for (7):

$$G_{\text{loc}}(i\omega_n) = \tilde{D}\Big(\frac{i\omega_n - \Sigma(i\omega_n)}{D}\Big)\,. \tag{12}$$

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

$$G(\mathbf{k}, i\omega) = \frac{1}{Z}\sum_{n,m} \frac{e^{-\beta E_n} + e^{-\beta E_m}}{i\omega + E_n - E_m} |\langle n | c_{\mathbf{k}} | m \rangle|^2\,, \tag{13}$$

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. Thus, $E_n - E_m$ is strongly bounded and for high frequencies, one has

$$G(\mathbf{k}, i\omega) \sim \frac{1}{i\omega}\frac{1}{Z}\sum_{n,m}\left(e^{-\beta E_n} + e^{-\beta E_m}\right)|\langle n|c_{\mathbf{k}}|m\rangle|^2 = \frac{1}{i\omega} \quad \text{for } |i\omega| \gg E_n - E_m, \langle n|c_{\mathbf{k}}|m\rangle| \neq 0\,. \tag{14}$$

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

$$\mathcal{A}(w) = -\frac{1}{\pi}\Im G(i\omega \to \omega + i0^+), \quad \mathcal{A}(w) \geq 0, \quad \int_{-\infty}^{\infty} \mathcal{A}(w)\,\mathrm{d}\omega = 1\,. \tag{15}$$

4 Results

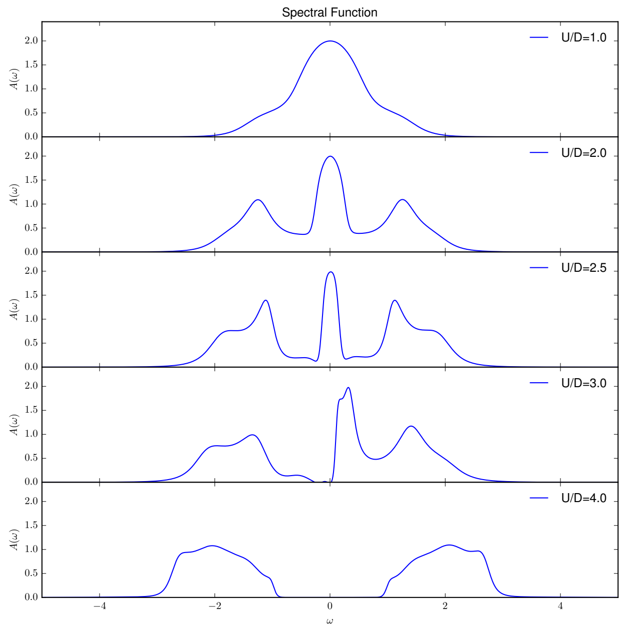

Figure 1: Spectral function after analytic continuation. For low interaction parameter U there are single particle excitation??? at zero frequency, therefore the metalic phase. With increasing interaction parameter the spectral function develops a gap at zeros freqency, hence no excitation, ie the insulator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

As 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 be cleary 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 exspected 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, $\mathscr{A}(\mathbf{k}, \omega)$, can be expressed in the Lehmann representation:

$$\mathscr{A}_\sigma(\mathbf{k}, \omega) = \frac{1}{\mathcal{Z}}\sum_{n,m} |\,\langle m|c^\dagger_{\sigma,\mathbf{k}}|n\rangle\,|^2(e^{-\beta E_n} + e^{-\beta E_m})\delta(\omega + (E_n - E_m))) \tag{16}$$

where the $|n\rangle$'s are the Hamiltonian eigenstates and the E_n's are the corresponding energies. Starting from this expression it is also possible to show that the following sum rule holds:

$$\int_{-\infty}^{\infty} \mathscr{A}_\sigma(\mathbf{k},\omega)d\omega = 1 \tag{17}$$

If one notice, moreover, that $\mathscr{A}_\sigma \geq 0$, it is, then, possible to interpret it as a probability density. In particular, usually, this is interpreted as the probability of having a fermion with energy between ω and $\omega + d\omega$.

One could also consider the single-particle density of states, $D(\omega)$, which is given by:

$$D(\omega) = \frac{1}{V}\sum_{\mathbf{k},\sigma} \mathscr{A}_\sigma(\mathbf{k},\omega) \tag{18}$$

at the light of this expression and of equation (16), it is clear, then, that no gaps in the Spectral Function (as in our plots for low values of U) means that we can produce exitations with any energy, leading to a conductor behaviour. Whereas, if a gap is present (as in the last plot of Refenrence ??) it means that no exitations can be produced with thise energy, so that the material will behave as an insulator.

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 (no implicit β):

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

For 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:

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

Hence, we discretize the Matsubara Fourier transformation

$$\begin{aligned} G(i\omega_{-n}) &\approx \sum_{k=0}^{N-1} \Delta\tau\, G(\Delta\tau\, k) \exp\left(i\frac{\pi(-2n+1)k}{N}\right) && (21) \\ &= \frac{\beta}{N} \sum_{k=o}^{N-1} \left(G(\Delta\tau\, k) \exp\left(i\pi\frac{k}{N}\right)\right) \exp\left(i\frac{-2\pi nk}{N}\right) && (22) \\ &= \frac{\beta}{N} \mathrm{FFT}\left(G(\Delta\tau\, k) \exp\left(i\pi\frac{k}{N}\right)\right), && (23) \end{aligned}$$

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

$$\begin{aligned} G(\Delta\tau k) &= \frac{N}{\beta} e^{-i\pi\frac{k}{N}} \frac{1}{N} \sum_{\omega_n} G(i\omega_{-n}) e^{i2\pi nk/N} && (24) \\ &= \frac{N}{\beta} e^{-i\pi\frac{k}{N}} \mathrm{IFFT}(G(i\omega_{-n})) && (25) \end{aligned}$$

Unfortunately the "naive" implementations (23) and (25) cause numerical problems, since according to (14) Green's function 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 strongly increase the accuracy by manually transforming the $1/i\omega_n$ part. With contour integration, it is commonly 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 is given by subtracting and adding the relevant terms before and after the transformation.

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

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

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 naiv version shows significant deviations to the analytic solution, whereas our improved version approximates the exact one very well.

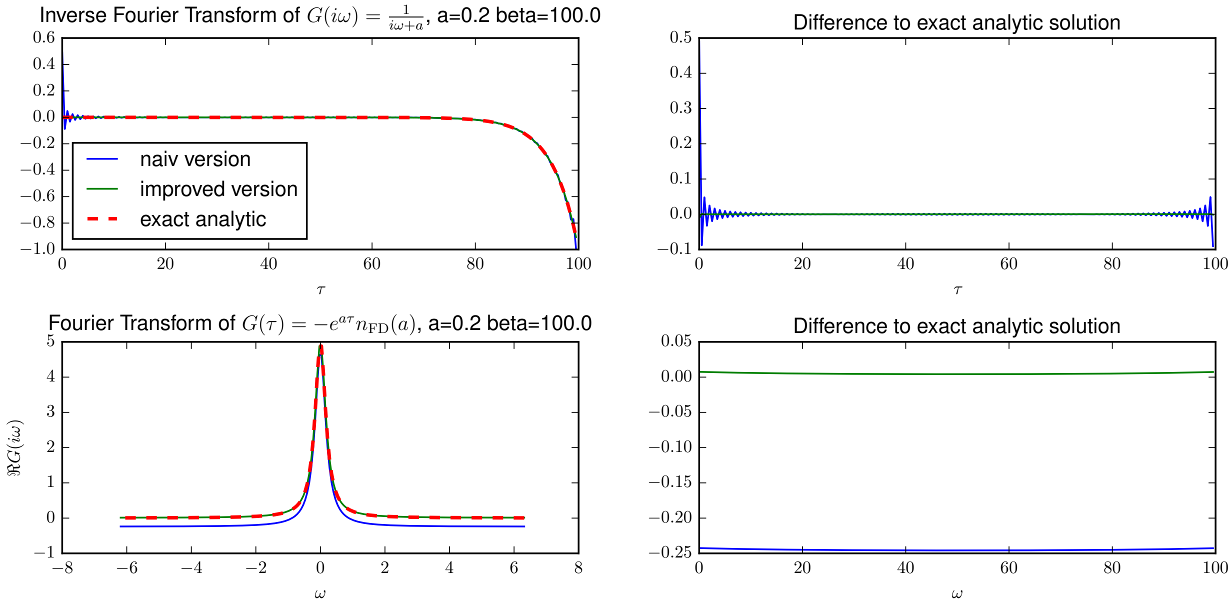

Figure 2: Comparison of the different discretized Fourier Transformations. The improved version, by manually removing the $\frac{1}{i\omega}$ factor, approximates the exact transformation significantly better.

B Analytic continuation

In order to calculate the spectral function A, we have to perform the anlytic 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 Pade approximation, and use this function to do the analytic continuation. An efficient algortihm to calculalte the Padé approximation can be found in [1]. However, as the Padé approximation is continous, whereas the Green's function exhibits non-continous jumps, we have to think about, which values to use for the fit.

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

Since the retared Green's function given by $G(i\omega \to w + io^+)$ lies slightly above the real axis, we can use the positive freqencies on the imaginary axis to calculate the fit 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 homogeneously reduced the number of values to calculate the fit. In some cases this proved to be more stable, which is no surprise, as interpolation polynomials of high degree often shows rapid oscillations.

References

[1] 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.

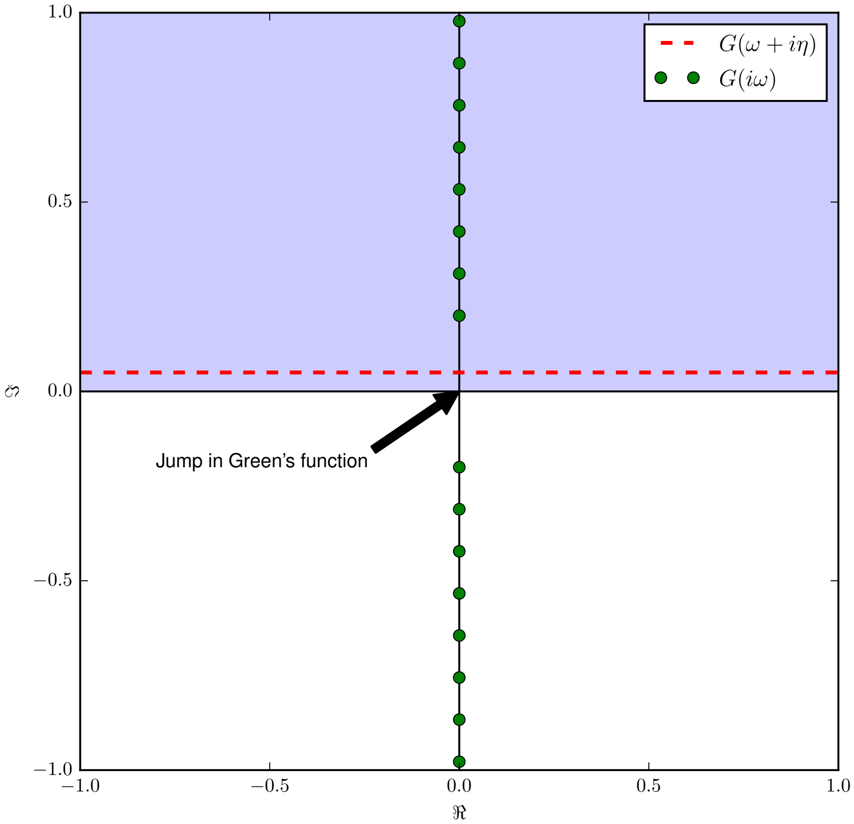

Figure 3: As the retarded Green's function (red) lies slightly above the real axis and the Matsubara Green's function shows discontinous jumps at zero frequency, we only take the postive frequencies to calculate the Padé approximation. Assuming that the Green's function is analytic in the upper half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