Real-time Green's Functions based on the Non-Crossing Approximation

Hristiana Atanasova

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1 Impurity Model

A general impurity Hamiltonian has the form

$$\mathrm{H_{imp}} = \mathrm{H_D} + \mathrm{H_B} + \mathrm{H_{hyb}}.$$

We consider the single-orbital Anderson impurity model (AIM) with the following dot-Hamiltonian

$$\mathrm{H_D} = \sum_{\sigma\epsilon\uparrow,\downarrow} \varepsilon_\sigma \mathrm{d}_\sigma^\dagger \mathrm{d}_\sigma + \mathrm{U}\mathrm{d}_\uparrow^\dagger \mathrm{d}_\uparrow \mathrm{d}_\downarrow^\dagger \mathrm{d}_\downarrow,$$

ε_σ are the on-site energy levels and U is the interaction between electrons having opposite spins. $\mathrm{H_{imp}}$ can in general incorporate a time-dependence, but for now we will consider only time-independent impurity models. There are four possible dot eigenstates $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ corresponding to the dot being empty or occupied by either one or two electrons. The non-interacting bath Hamiltonian has the form

$$\mathrm{H_B} = \sum_{\sigma,\lambda} \varepsilon_\lambda \mathrm{b}_\lambda^\dagger \mathrm{b}_\lambda$$

and the coupling between dot and bath is given through the Hybridization

$$\mathrm{H_{hyb}} = \sum_{\sigma,\lambda} (\mathrm{t}_{\sigma\lambda} \mathrm{b}_\lambda^\dagger \mathrm{d}_\sigma + \mathrm{t}_{\sigma\lambda}^* \mathrm{d}_\sigma^\dagger \mathrm{b}_\lambda),$$

which describes processes in which electrons are hopping from the bath to the dot and vice versa.

A general procedure to evaluate expectation values $\langle \cdots \rangle$ is to split $\mathrm{H_{imp}}$ into a sum $\mathrm{H_{imp}} = \mathrm{H_0} + \mathrm{H_{int}}$. The time propagation can be calculated exactly in $\mathrm{H_0}$ while$\mathrm{H_{int}}$ is treated by pertubation expansion. For a weak electron-coupling (small U) one expands in terms of the paramter U and the rest of the Hamiltonian is treated axactly. When one is dealing with strong electron correlations (large U) $\mathrm{H_D}$and $\mathrm{H_B}$ sum up to $\mathrm{H_0}$ and the expansion is performed in terms of $\mathrm{H_{hyb}}$. The latter is called the "strong coupling approach".

2 Impurity Greens functions

2.1 Bold Propagators

We are interested in the calculation of correlation functions/Green's functions like $G^{\succ}(t,t') = -i\langle d(t)d^{\dagger}(t')\rangle$ and $G^{\prec}(t,t') = i\langle d^{\dagger}(t')d(t)\rangle$ from which we can obtain information about the system, like the spectral function $A(\omega)$, in certain regimes. The spectral functions represents the density of single particle excitations at energy ω. The times t_1, t_2 exist on the real part of the Keldysh contour. In the strong coupling approach we assume that the interaction between electrons is strong and the coupling to the bath infinitesimally weak, so we expand in terms of the hybridization H_{hyb}. The expectation value $\langle\cdots\rangle$ of an operator O at time t is given by

$$\langle O(t)\rangle = \mathrm{Tr}\left(\rho U^{\dagger}(t)\hat{O}U(t)\right),$$

with the initial density matrix ρ, that can be factorized into the dot ρ_D and the bath ρ_B density matirx, since the dot is initially decoupled from the bath. In the interaction picture the operators, here denoted by a hat $\widehat{\ }$, have the time dependency

$$\hat{O}(t) = \exp^{iH_0 t}\, O \exp^{-iH_0 t},$$

with the reduced Hamiltonian$H_0 = H_{imp} - H_{hyb}$ containing information about the coupling U. The interaction picture time evolution propagator is given by

$$U(t) = \exp^{iH_0 t}\exp^{-iHt}.$$

$U(t)$ $\left[U^{\dagger}(t)\right]$can be though of the propagation on the upper [lower] branch of the Keldysh contour obeying the differential equation

$$\begin{aligned}\frac{\partial}{\partial t}U(t) &= i\exp^{iH_0 t}(H_0 - H)\exp^{-iH_0 t}\\ &= -i\exp^{iH_0 t}H_{hyb}(\exp^{-iH_0 t}\exp^{iH_0 t})\exp^{iHt}\\ &= -i\widehat{H}_{hyb}(t)U(t).\end{aligned}$$

After integrating both sides with respect to time

$$U(t) = 1 - i\int_0^t dt_1 \widehat{H}_{hyb}(t_1)U(t_1)$$

and after repeatedly iterating we arrive at

$$U(t) = \sum_{n=0}^{\infty}(-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \widehat{H}_{hyb}(t_1)\widehat{H}_{hyb}(t_2)\cdots\widehat{H}_{hyb}(t_n)$$

with time ordering $t_1 \succ t_2 \succ \ldots \succ t_n$. The Hybridization term in the interaction picture can be written in the following form

$$\widehat{H}_{hyb}(t) = \exp^{iH_0 t} V \exp^{-iH_0 t}$$

$$= \sum_{n=0}^{\infty} \frac{i}{n!}^n (H_0 t)^n \sum_{\sigma,\lambda} (t_{\sigma\lambda} b_\sigma^\dagger d_\sigma + t_{\sigma\lambda}^\star d_\sigma^\dagger b_\lambda) \sum_{n=0}^{\infty} \frac{(-i)}{n!}^n (H_0 t)^n$$

$$= \sum_{\sigma,\lambda} \sum_{n=0}^{\infty} \frac{i}{n!}^n (\varepsilon_\sigma d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow + \varepsilon_\lambda b_\lambda^\dagger b_\lambda)^n (t)^n \sum_{\sigma,\lambda} (t_{\sigma\lambda} b_\sigma^\dagger d_\sigma + t_{\sigma\lambda}^\star d_\sigma^\dagger b_\lambda) \sum_{n=0}^{\infty} \frac{(-i)}{n!}^n (\varepsilon_\sigma d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow + \varepsilon_\lambda b_\lambda^\dagger b_\lambda)^n$$

Using $[d_\sigma, n_\uparrow n_\downarrow] = d_{\bar{\sigma}}$ and Baker-Hausdorff theorem

$$d_\sigma(t) = \exp^{iH_0 t} d_\sigma \exp^{-iH_0 t} = \exp^{-itL_{H_0}} d_\sigma,$$

where $L_{H_0} d_\sigma \equiv [d_\sigma, H_0] = \sum_{\sigma\epsilon\uparrow,\downarrow} \varepsilon_\sigma \left[d_\sigma, d_\sigma^\dagger d_\sigma\right] = \sum_{\sigma\epsilon\uparrow,\downarrow} \varepsilon_\sigma d_\sigma$, we arrive at

$$\widehat{H}_{hyb}(t) = \sum_{\sigma,\lambda} \left\{ t_{\sigma\lambda} \exp^{i(\varepsilon_\sigma + U d_\sigma^\dagger d_\sigma - \varepsilon_{\sigma\lambda})t} b_{\sigma\lambda}^\dagger d_\sigma + t_{\sigma\lambda}^\star \exp^{-i(\varepsilon_\sigma + U d_\sigma^\dagger d_\sigma - \varepsilon_{\sigma\lambda})t} d_\sigma^\dagger b_{\sigma\lambda} \right\}$$

The first step is to compute so called bold propagators $G_{\alpha\beta}(t)$ between many body states α and β containing all hybridization lines (that do not cross each other) in a given time intervall. The hybridization lines exist only on one branch and do not connects times between the two branches. Propagators on the upper and lower branch obey the relation$G_{\alpha\beta}^\dagger(t) = G_{\alpha\beta}(\bar{t})$. We start with the formal expression

$$G_{\alpha\beta}(t) = \langle\langle \alpha \mid \rho_D \exp^{-iHt} \mid \beta \rangle\rangle_B = \langle\langle \alpha \mid \rho_D \exp^{-iH_0 t} U(t) \mid \beta \rangle\rangle_B,$$

where $\langle \cdots \rangle_B = \mathrm{Tr}\{\rho_B \cdots\}$denotes that the bath degrees are traced out. We insert the expansion for U

$$G_{\alpha\alpha}(t) = \langle\langle \alpha \mid \rho_D \exp^{-iH_0 t} \mid \alpha \rangle\rangle_B + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \langle\langle \alpha \mid \rho_D \exp^{-iH_0 t} \widehat{H}_{hyb}(t_1) \widehat{H}_{hyb}(t_2) \mid \alpha \rangle\rangle_B + \cdots$$

$$= \sum_\beta \langle\langle \alpha \mid \beta \rangle\langle \beta \mid \exp^{-iH_0 t} \mid \alpha \rangle\rangle_B - \sum_\beta \sum_{\sigma,\lambda} \int dt_1 \int_0^{t_1} dt_2 \, |t_{\sigma\lambda}|^2 \times$$

$$\left(\langle\langle \alpha \mid \exp^{-iH_0 t} d_\sigma \mid \beta \rangle\langle \beta \mid d_\sigma^\dagger \hat{b}_{\sigma\lambda}^\dagger(t_1) \hat{b}_{\sigma\lambda}(t_2) \mid \alpha \rangle\rangle_B + \langle\langle \alpha \mid \exp^{-iH_0 t} d_\sigma^\dagger \mid \beta \rangle\langle \beta \mid d_\sigma \hat{b}_{\sigma\lambda}(t_2) \hat{b}_{\sigma\lambda}^\dagger(t_1) \mid \alpha \rangle\rangle_B \right) + \cdots$$

$$= \delta_{\alpha\beta}\exp^{-i\varepsilon_\alpha t} - \sum_\beta \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\alpha}(t-t_1) G^{(0)}_{\beta\beta}(t_1-t_2)\times$$

$$\left(\langle \alpha \mid d_\sigma \mid \beta\rangle\langle\beta \mid d^\dagger_\sigma \mid \alpha\rangle \sum_{\sigma,\lambda} |t_{\sigma\lambda}|^2 \langle \hat{b}^\dagger_{\sigma\lambda}(t_1)\hat{b}_{\sigma\lambda}(t_2)\rangle_B + \langle \alpha \mid d^\dagger_\sigma \mid \beta\rangle\langle\beta \mid d_\sigma \mid \alpha\rangle \sum_{\sigma,\lambda} |t_{\sigma\lambda}|^2 \langle \hat{b}_{\sigma\lambda}(t_2)\hat{b}^\dagger_{\sigma\lambda}(t_1)\rangle_B \right) G_{\alpha\alpha}$$

$$= G^{(0)}_{\alpha\alpha}(t) - \sum_\beta \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\alpha}(t-t_1) G^{(0)}_{\beta\beta}(t_1-t_2)\times$$

$$\left(\langle \alpha \mid d_\sigma \mid \beta\rangle\langle\beta \mid d^\dagger_\sigma \mid \alpha\rangle \triangle^\prec_\sigma (t_1-t_2) + \langle \alpha \mid d^\dagger_\sigma \mid \beta\rangle\langle\beta \mid d_\sigma \mid \alpha\rangle \triangle^\succ_\sigma (t_1-t_2) \right) G^{(0)}_{\alpha\alpha}(t_2) + \cdots$$

with the bare atomic state propagators $G^{(0)}_{\alpha\alpha}(t) = \exp^{-i\varepsilon_\alpha t}$ leaving the dot state invariant. Note that both the bare $G^{(0)}_{\alpha\alpha}(t)$ and bold propagator $G_{\alpha\alpha}(t)$ are diagonal for the Anderson impurity model because the trace over the bath degrees gives results only for an even number of creation and annhilation operators. Therefore only square terms of $\widehat{H}_{\rm hyb}$ appear in the expansion for G. In DMFT the hybridization function $\triangle^{\succ/\prec}_\sigma$ is obtained from the self-consistency condition. Here we will write it in terms of the coupling density $\Gamma(\omega)$ of the bath and the initial occupation probability (fermi-function)

$$\triangle^\prec(t_1,t_2) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \exp^{-i\omega(t_1-t_2)} \Gamma(\omega) f(\omega-\mu) \qquad (1)$$

and

$$\triangle^\succ(t_1,t_2) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \exp^{-i\omega(t_1-t_2)} \Gamma(\omega)(1-f(\omega-\mu)).$$

With the approximation for the self-energy, that it includes only hybridizaton lines that do not cross, the Dyson equation can be written as

$$G_{\alpha\alpha}(t) = G^{(0)}_{\alpha\alpha}(t) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\alpha}(t-t_1)\Sigma_{\alpha\alpha}(t_1-t_2) G_{\alpha\alpha}(t_2)$$

with

$$\Sigma_{\alpha\alpha}(t_1-t_2) = \sum_\sigma \sum_\beta G_{\beta\beta}(t_1-t_2)\times$$

$$\left(\langle \alpha \mid d_\sigma \mid \beta\rangle\langle\beta \mid d^\dagger_\sigma \mid \alpha\rangle \triangle^\prec_\sigma (t_1-t_2) + \langle \alpha \mid d^\dagger_\sigma \mid \beta\rangle\langle\beta \mid d_\sigma \mid \alpha\rangle \triangle^\succ_\sigma (t_1-t_2) \right).$$

For the four different initial states (denoted by the outer index α) on the dot we can derive a set of coupled Dyson equations

$$G_0(t) = G^{(0)}_0(t) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_0(t-t_1) G_\uparrow(t_1-t_2)\Delta^\prec_\uparrow(t_1-t_2) G_0(t_2) -$$
$$\int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_0(t-t_1) G_\downarrow(t_1-t_2)\Delta^\prec_\downarrow(t_1-t_2) G_0(t_2)$$

$$G_\uparrow(t) = G^{(0)}_\uparrow(t) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_\uparrow(t-t_1) G_0(t_1-t_2) \Delta^{\succ}_\uparrow(t_1-t_2) G_\uparrow(t_2) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_\uparrow(t-t_1) G_{\uparrow\downarrow}(t_1-t_2) \Delta^{\prec}_\downarrow(t_1-t_2) G_\uparrow(t_2)$$

$$G_\downarrow(t) = G^{(0)}_\downarrow(t) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_\downarrow(t-t_1) G_0(t_1-t_2) \Delta^{\succ}_\uparrow(t_1-t_2) G_\downarrow(t_2) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_\downarrow(t-t_1) G_{\uparrow\downarrow}(t_1-t_2) \Delta^{\prec}_\downarrow(t_1-t_2) G_\downarrow(t_2)$$

$$G_{\uparrow\downarrow}(t) = G^{(0)}_{\uparrow\downarrow}(t) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\uparrow\downarrow}(t-t_1) G_\downarrow(t_1-t_2) \Delta^{\succ}_\uparrow(t_1-t_2) G_{\uparrow\downarrow}(t_2) - \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\uparrow\downarrow}(t-t_1) G_\uparrow(t_1-t_2) \Delta^{\succ}_\downarrow(t_1-t_2) G_{\uparrow\downarrow}(t_2),$$

which can be solved by a self consistent iteration. All entities depend only on time differences and one can evaluate the integrals in the Fourier space, where convolutions become simple multiplications. Before starting with the first iteration, the bold propagators $G_{\alpha\alpha}(t)$ are initialized by the bare propagators $G^{(0)}_{\alpha\alpha}(t)$ from which the first self-energy is obtained. Both are inserted into the Dyson equation with the interaction times integrated over. With the updated $G_{\alpha\alpha}(t)$ one can go back to the second step and compute a new self energy for the next iteration cycle until convergence is reached.

2.2 Correlation functions

So far we have calculated propagators between many body states, which contain all non-crossing hybridization lines in a time segment on a single branch. These objects have no physical meaning, to calculate physical observables it is necessary to include hybridization lines connecting times on both branches. We introduce so called vertex functions $K_{\alpha\beta}(t,t')$ with the first[second] time index on the upper[lower] branch. A vertex funcion incorporates all non-crossing intra- and inter-branch hybrdization lines. The procedure to estimate $K_{\alpha\beta}(t,t')$ is similar to the calculation of $G_{\alpha\alpha}(t)$ with the difference that $K_{\alpha\beta}(t,t')$ is a two-times function and instead of four we have 16 equations representing the evolution of the dot from any inital state α to any final state β. For every inital state there are four coupled equations of the form

$$K_{\alpha\beta}(t,t') = K^{(0)}_{\alpha\beta}(t,t') + \sum_{\gamma\delta} \int_0^t dt_1 \int_0^{t'} dt_2 K_{\alpha\gamma}(t_1,t_2) \mathbf{\Delta}_{\gamma\delta}(t_1,t_2) G^\dagger_{\delta\beta}(t-t_1) G_{\delta\beta}(t'-t_2).$$

The vertex functions without inter-branch hybridization lines are composed by the bold propagators on the upper and lower branch

$$K^{(0)}_{\alpha\beta}(t,t') = \delta_{\alpha\beta} G^{\dagger}_{\alpha\beta}(t) G_{\alpha\beta}(t').$$

The self consistent equations for the initially unoccupied dot are

$$K_{00}(t,t') = K^{(0)}_{00}(t,t') + \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_0(t'-t_2) G_0(t-t_1) \Delta^{\prec}_{\uparrow}(t_1,t_2) K_{0\uparrow}(t_1,t_2) + \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_0(t'-t_2) G_0(t-t_1) \Delta^{\prec}_{\downarrow}(t_1,t_2) K_{0\downarrow}(t_1,t_2)$$

$$K_{0\uparrow}(t,t') = \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_{\uparrow}(t'-t_2) G_{\uparrow}(t-t_1) \Delta^{\succ}_{\uparrow}(t_1,t_2) K_{00}(t_1,t_2) + \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_{\uparrow}(t'-t_2) G_{\uparrow}(t-t_1) \Delta^{\prec}_{\downarrow}(t_1,t_2) K_{0\uparrow\downarrow}(t_1,t_2)$$

$$K_{0\downarrow}(t,t') = \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_{\downarrow}(t'-t_2) G_{\downarrow}(t-t_1) \Delta^{\succ}_{\downarrow}(t_1,t_2) K_{00}(t_1,t_2) + \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_{\downarrow}(t'-t_2) G_{\downarrow}(t-t_1) \Delta^{\prec}_{\uparrow}(t_1,t_2) K_{0\uparrow\downarrow}(t_1,t_2)$$

$$K_{0\uparrow\downarrow}(t,t') = \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_{\uparrow\downarrow}(t'-t_2) G_{\uparrow\downarrow}(t-t_1) \Delta^{\succ}_{\downarrow}(t_1,t_2) K_{0\uparrow}(t_1,t_2) + \int_0^t dt_1 \int_0^{t'} dt_2 G^{\dagger}_{\uparrow\downarrow}(t'-t_2) G_{\uparrow\downarrow}(t-t_1) \Delta^{\succ}_{\uparrow}(t_1,t_2) K_{0\downarrow}(t_1,t_2).$$

For equal times, $K_{\alpha\beta}(t,t)$ is the population probability on the dot. After initializing the vertex functions $K_{\alpha\beta}(t,t')$ with $K^{(0)}_{\alpha\beta}(t,t')$ and performing the self-consistent iteration sheme one is able to construct Greens functions in the following way

$$G^{\succ}_{\alpha\uparrow}(t,t') = -i\langle d_{\uparrow}(t) d^{\dagger}_{\uparrow}(t')\rangle = K_{\alpha 0}(t,t') * G_{\uparrow}(t-t') + K_{\alpha\downarrow}(t,t') * G_{\uparrow\downarrow}(t-t')$$

$$G^{\prec}_{\alpha\uparrow}(t,t') = i\langle d^{\dagger}_{\uparrow}(t') d_{\uparrow}(t)\rangle = K_{\alpha\uparrow}(t,t') * G_0(t-t') + K_{\alpha\uparrow\downarrow}(t,t') * G_{\downarrow}(t-t')$$

$$G^{\succ}_{\alpha\downarrow}(t,t') = -i\langle d_{\downarrow}(t) d^{\dagger}_{\downarrow}(t')\rangle = K_{\alpha 0}(t,t') * G_{\downarrow}(t-t') + K_{\alpha\uparrow}(t,t') * G_{\uparrow\downarrow}(t-t')$$

$$G^{\prec}_{\alpha\downarrow}(t,t') = i\langle d^{\dagger}_{\downarrow}(t')d_{\downarrow}(t)\rangle = K_{\alpha\downarrow}(t,t') * G_0(t-t') + K_{\alpha\uparrow\downarrow}(t,t') * G_{\uparrow}(t-t')$$

with α denoting the initial dot state. The conjugation yields to $\left(G^{\succ/\prec}(t,t')\right)^* = -G^{\succ/\prec}(t',t)$ and for particle-hole symmetric system $G^{\succ/\prec}(t,t') = -G^{\succ/\prec}(t',t)$.

The advanced and retarded Green's function are defined via the lesser and greater component as

$$G^{R}(t,t') = -i\Theta(t-t')\langle\left[d(t), d^{\dagger}(t')\right]_{+}\rangle$$

$$G^{R}(t,t') = -i\Theta(t-t')\left(\langle d(t)d^{\dagger}(t')\rangle + \langle d^{\dagger}(t')d(t)\rangle\right)$$

$$G^{R}(t,t') = \Theta(t-t')\left(G^{\succ}(t,t') - G^{\prec}(t,t')\right)$$

and

$$G^{A}(t,t') = i\Theta(t'-t)\langle\left[d(t), d^{\dagger}(t')\right]_{+}\rangle$$

$$G^{A}(t,t') = i\Theta(t'-t)\left(\langle d(t)d^{\dagger}(t')\rangle + \langle d^{\dagger}(t')d(t)\rangle\right)$$

$$G^{A}(t,t') = -\Theta(t'-t)\left(G^{\succ}(t,t') - G^{\prec}(t,t')\right).$$

They have an intuitive interpretation since the imaginary part of their Fourier transforms gives the single particle spectral function

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}G^{R} = \frac{1}{\pi}\mathrm{Im}G^{A}.$$

3 Dynamical Mean Field Theory

3.1 Systems in Equilibrium

Dynamical Mean Field Theory is a method to solve a lattice problem with many degrees of freedom by mapping it to an impurity problem consisting of a single correlated site embedded in an uncorrelated bath. The bath is formed by the residual sites of the lattice and the hybridization between the impurity and the bath (the dynamical mean field) is the two times function $\Delta(t, t')$. It resembles the exchange of particles with the rest of the lattice and must be determined self consistently as a functional of the lattice Greens function $G(t, t')$. The key approximation in DMFT is the local nature of the lattice self energy

$$\Sigma^{\mathrm{lat}}_{\mathrm{ij}}(t, t') \backsimeq \delta_{\mathrm{ij}}\Sigma^{\mathrm{imp}}(t, t')$$

that justifies the mapping.

In equilibrium all functions depend only on time-differences and can be expressed by their Fourier transforms. For time-dependent systems (e.g. an electric-field-driven lattice system) they become two-times objects and incorporate the overall temporal evolution of the system as well as quantum fluctuations. In the following the DMFT equations for systems in equilibrium (an extension to time-dependend systems follows later) will be presented. The simplest model for the description of strongly correlated systems is the single band Hubbard model representing a collection of single orbital atoms placed at the nodes of a crystal lattice

$$H_{\mathrm{Hubbard}} = -\sum_{\langle i,j\rangle,\sigma} v_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + \sum_{i} U(d^{\dagger}_{i\uparrow} d_{i\uparrow} - \frac{1}{2})(d^{\dagger}_{i\downarrow} d_{i\downarrow} - \frac{1}{2}).$$

The operators $d^{\dagger}_{i\uparrow}[d_{i\uparrow}]$ create[destroy] an electron with spin σ in an Wannier orbital at a crystal site i, v_{ij} is the hopping between neighbouring sites (it depends on the overlap of neighbouring orbitals) and U is the local Coulomb interaction between electrons. With the approximation that the lattice self energy is local in space one is able to compute the local Greens function $G^{\sigma}_{ii}(t - t') = -i\langle \mathcal{T} d_{i\sigma}(t) d^{\dagger}_{i\sigma}(t')\rangle$ from an effective impurity model described by the following action

$$S = i\int_c dt U n_{\uparrow}(t) n_{\downarrow}(t) - i\sum_{\sigma}\int_c dt dt' d^{\dagger}_{\sigma}(t) \triangle(t - t') d_{\sigma}(t').$$

From here on the spin index will be supressed for simplicity. The impurity self energy is defined via the Dyson equation

$$G^{-1}_{ii}(\omega) = \omega + \mu - \triangle(\omega) - \Sigma^{\mathrm{imp}}(\omega)$$

and will be used to obtain the lattice Greens function

$$G^{-1}_{ij}(\omega) = \delta_{ij}[\omega + \mu - \Sigma_{ii}(\omega)] - v_{ij}.$$

In real space this means that all non-local components of the lattice self energy $\Sigma_{ij}(\omega)$ are neglected and the local component is approximated by $\Sigma^{imp}(\omega)$. For a translationally invariant system ($\Sigma_{ii}(\omega) \equiv \Sigma(\omega)$) one averages over the whole Brillouin zone to get the on-site component of the lattice Green function (which is referred to as the self-consistency condition)

$$G_{ii}(\omega) = \frac{1}{L}\sum_k G_k(\omega) = \frac{1}{L}\sum_k \frac{1}{\omega + \mu + \Sigma(\omega) - \epsilon_k},$$

with $G_k(\omega)$ the momentum resolved Greens function, L the number of lattice sites and ϵ_k the dispersion relation of the non-interacting tight binding band

$$\epsilon_k = \sum_j v_{ij} exp^{ik(R_i - R_j)}.$$

Instead of performing the k-summation one can integrate over the local, non-interacting Density of states $D(\epsilon) = \frac{1}{L}\sum_k \delta(\epsilon - \epsilon_k)$

$$G_{ii}(\omega) = \int \frac{D(\epsilon)}{\omega + \mu + \Sigma(\omega) - \epsilon_k}.$$

The self-consistency condition relates for each frequency ω the dynamical mean field to the local Greens function. This functional relation G[Δ] provides a closed set of equations to determineΔ and G. This can be done by an iterative procedure that does not depend on the initial guess for Δ.

3.2 Results

We consider the Bethe lattice with nearest-neighbour hopping and an infinite coordination number, which corresponds to the limit of infinite dimensions, where DMFT becomes exact. In this case the Density of states takes a semicircular shape

$$D(\epsilon) = \frac{1}{2\pi v^2}\sqrt{4v - \epsilon^2} \tag{2}$$

and the self consistency condition collapses to the simple form

$$\Delta(t, t') = v^2 G(t, t'). \tag{3}$$

We perform the DMFT iteration scheme with the initial hybridization function calculated from 1 with $D(\epsilon)$ being the coupling density. In every iteration the hybridization is updated via 3. After the results for G are converged we are able to obtain the spectral function of the system as described in the last chapter. In the non-interacting case (U=0) we expect the spectral function to be the non-interacting Density of states $D(\epsilon)$ of the Bethe lattice with a bandwidth of $4/\Gamma$. This is furthermore a test for the performance of the impurity solver. We observe that the spectral function $A(\omega)$ [Fig. 1] deviates from the expected semicircular shape, which is down to the fact that the NCA provides reliable results only for high interactions.

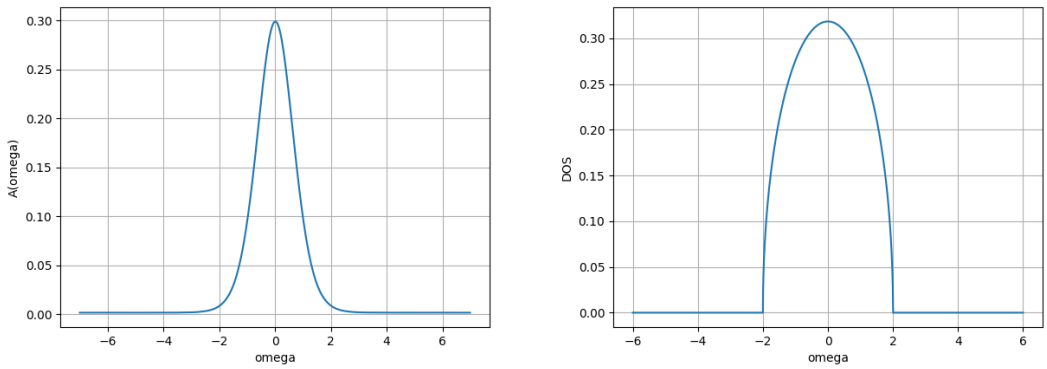

Figure 1: left side: Spectral function for U=0, $\Gamma t = 4$ and $\Gamma\beta = 1$; right side: Semicircular DOS for the Bethe lattice

With increasing interaction strenght one can observe the splitting of the spectral function into a lower and upper band indicating that the system is in an insulating phase [Fig 2]. Comparing results on different time scales [Fig. 2, Fig. 3] shows that the spectral function converges already on short timescales.

The results shown so far avarage the spectral functions over the four initial states. We can compare results on short timescales [$\sim \Gamma t = 2$] starting from different dot states and observe that for an initially unoccupied dot the lower Hubbard band forms before the upper one [Fig. 4]. The spectral function shows the reversed profile if the dot is initially in the state $|\uparrow\downarrow\rangle$. For longer timescales [$\sim \Gamma t = 4$] the spectral function equilibrates and the results become independent of the initial state.

As the temperature is lowered and the interaction reduced we observe the a Kondo-peak appearing [Fig. 5] at the chemical potential and the formation of the two side bands. The Kondo temprature is estimated from the formula $k_B T_K = U\sqrt{\frac{\Gamma}{2U}}\exp^{-\frac{\pi U}{8\Gamma}+\frac{\pi\Gamma}{2U}}$. Fig. 6 shows, that the characteristics of the Kondo physics appear on longer timescales $\sim \Gamma t = 6$.

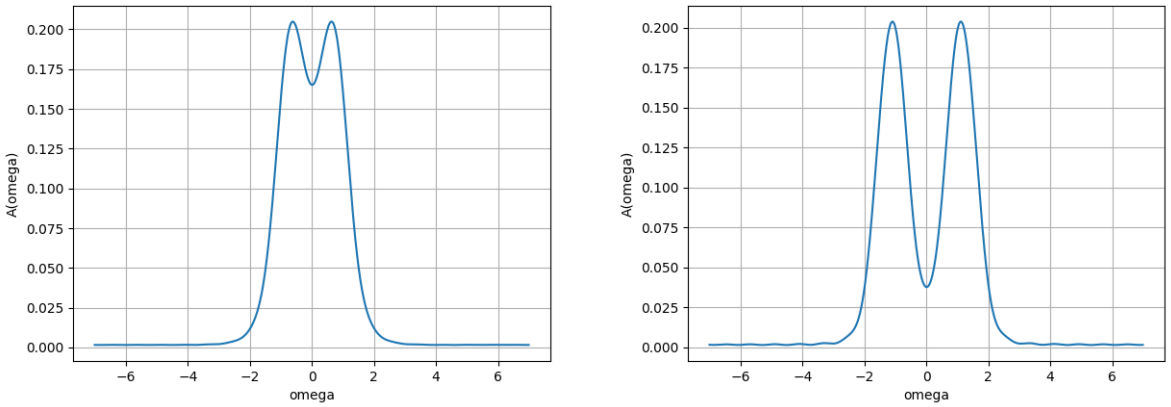

Figure 2: Splitting of the Spectral function for U=2Γ [left], U = 4Γ[left],Γt = 4 and $\Gamma\beta = 1$on a short timescale

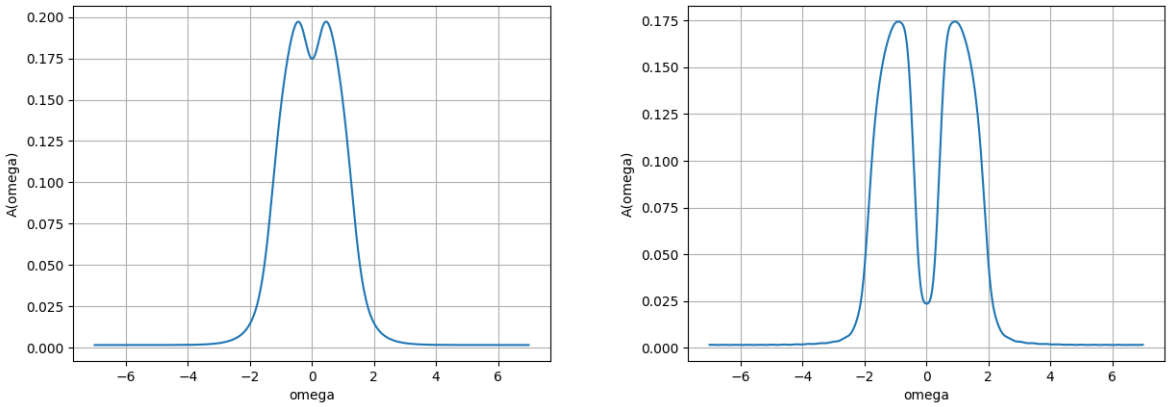

Figure 3: Splitting of the Spectral function for U=2Γ [left], U = 4Γ[left],Γt = 8 and $\Gamma\beta = 1$on a long timescale

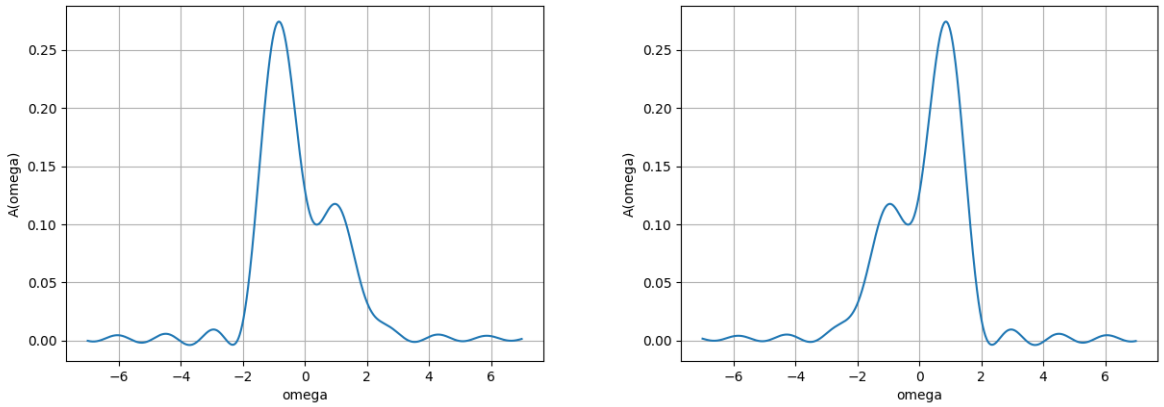

Figure 4: Spectral function for the inital dot state$|0\rangle$[left] and $|\uparrow\downarrow\rangle$[right]. The parameters areU $= 3\Gamma$, $\Gamma\beta = 1$

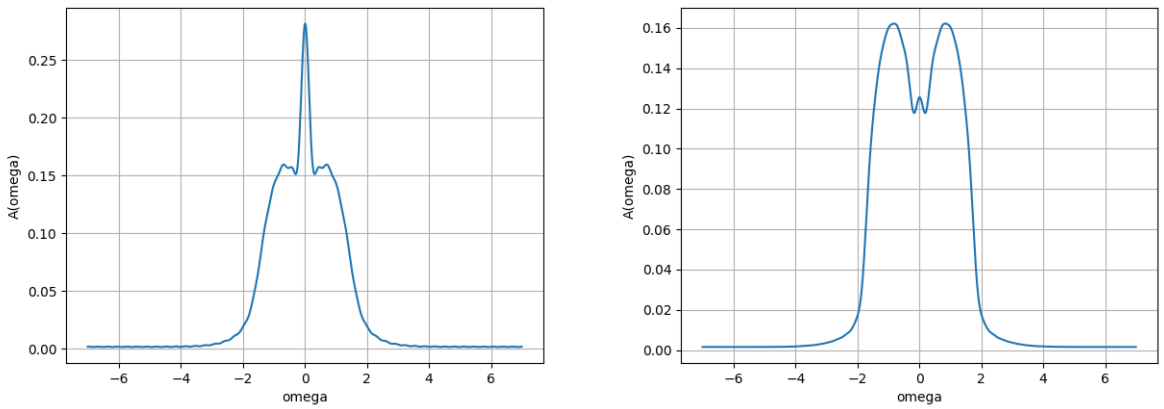

Figure 5: Kondo physics for parameters U $= 2\Gamma$ (left) and U $= 3\Gamma$ (right), $\Gamma\beta = 16$, Γt $= 10$

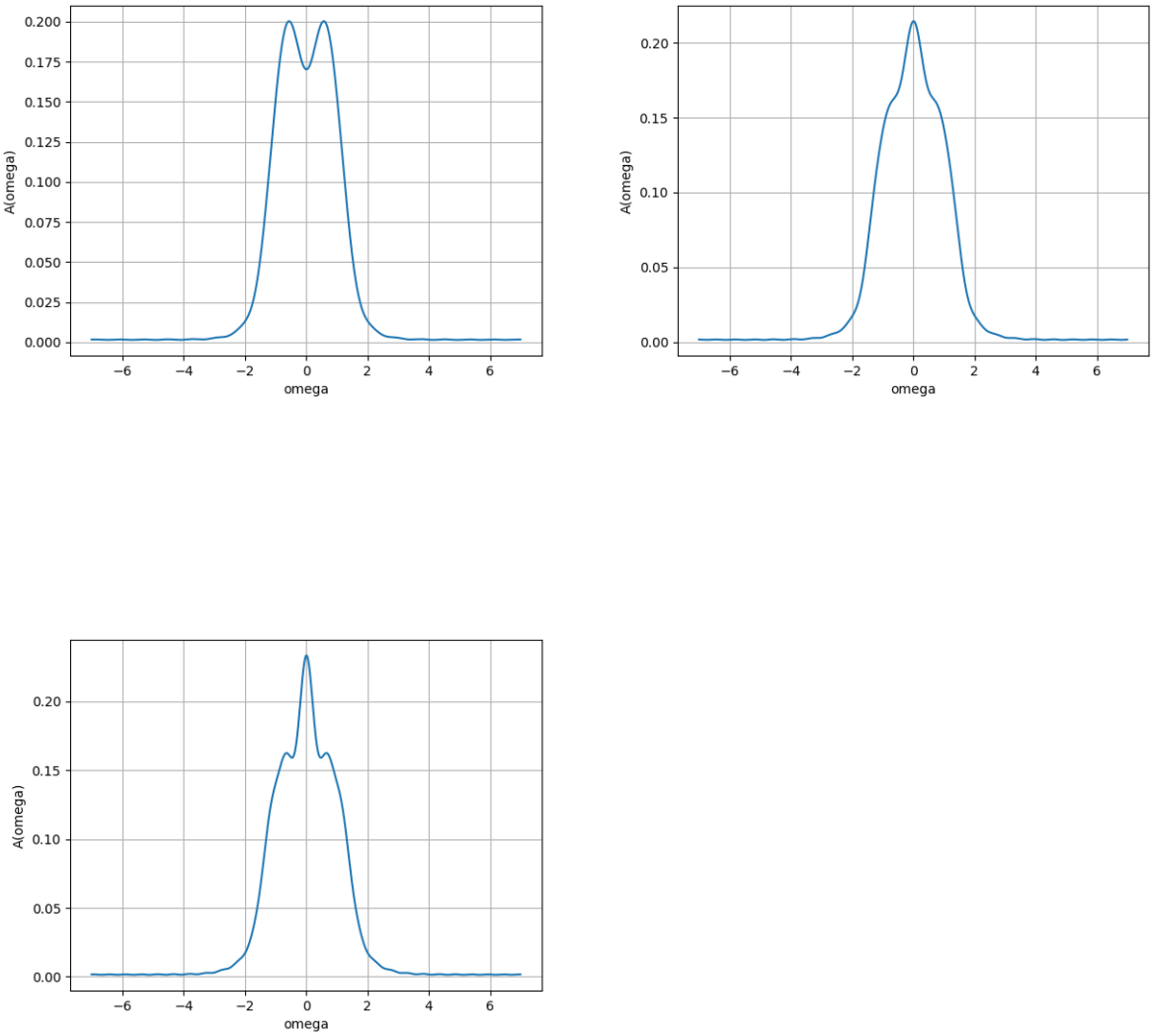

Figure 6: Emergence of the Kondo peak for different timescales $\Gamma t = 4$ [left], $\Gamma t = 5$ [middle], $\Gamma t = 6$ [right], $U = 2\Gamma$, $\Gamma\beta = 16$