

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

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1 Impurity Hamiltonian

A general impurity Hamiltonian has the form

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

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

$$H_D = \sum_{\sigma \in \uparrow, \downarrow} \varepsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow},$$

ε_{σ} are the on-site energy levels and U is the interaction between electrons having opposite spins. 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

$$H_B = \sum_{\sigma, \lambda} \varepsilon_{\lambda} b_{\lambda}^{\dagger} b_{\lambda}$$

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

$$H_{\text{hyb}} = \sum_{\sigma, \lambda} (t_{\sigma\lambda} b_{\lambda}^{\dagger} d_{\sigma} + t_{\sigma\lambda}^{*} d_{\sigma}^{\dagger} b_{\lambda}),$$

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

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

2 Greens functions

2.1 Bold Propagators

We are interested in the calculation of correlation functions/Green's functions like $G^>(t_1, t_2) = -i\langle d(t_1), d^\dagger(t_2) \rangle$ and $G^<(t_1, t_2) = i\langle d^\dagger(t_2), d(t_1) \rangle$ 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 $\langle \dots \rangle$ of an operator O at time t is given by

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

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

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

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

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

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

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

After integrating both sides with respect to time

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

and after repeatedly iterating we arrive at

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

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

$$\begin{aligned}\hat{H}_{\text{hyb}}(t) &= \exp^{iH_0 t} V \exp^{-iH_0 t} \\ &= \sum_{n=0}^{\infty} \frac{i^n}{n!} (H_0 t)^n \sum_{\sigma, \lambda} (t_{\sigma\lambda} b_{\sigma}^{\dagger} d_{\sigma} + t_{\sigma\lambda}^* d_{\sigma}^{\dagger} b_{\lambda}) \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} (H_0 t)^n \\ &= \sum_{\sigma, \lambda} \sum_{n=0}^{\infty} \frac{i^n}{n!} (\varepsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow} + \varepsilon_{\lambda} b_{\lambda}^{\dagger} b_{\lambda})^n (t)^n \sum_{\sigma, \lambda} (t_{\sigma\lambda} b_{\sigma}^{\dagger} d_{\sigma} + t_{\sigma\lambda}^* d_{\sigma}^{\dagger} b_{\lambda}) \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} (\varepsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow} + \varepsilon_{\lambda} b_{\lambda}^{\dagger} b_{\lambda})^n\end{aligned}$$

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

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

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

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

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

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

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

$$\begin{aligned}G_{\alpha\alpha}(t) &= \langle \langle \alpha | \rho_D \exp^{-iH_0 t} | \alpha \rangle \rangle_B + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \langle \langle \alpha | \rho_D \exp^{-iH_0 t} \hat{H}_{\text{hyb}}(t_1) \hat{H}_{\text{hyb}}(t_2) | \alpha \rangle \rangle_B + \dots \\ &= \sum_{\beta} \langle \langle \alpha | \beta \rangle \langle \beta | \exp^{-iH_0 t} | \alpha \rangle \rangle_B - \sum_{\beta} \sum_{\sigma, \lambda} \int dt_1 \int_0^{t_1} dt_2 |t_{\sigma\lambda}|^2 \left(\langle \langle \alpha | \exp^{-iH_0 t} d_{\sigma} | \beta \rangle \langle \beta | d_{\sigma}^{\dagger} \hat{b}_{\sigma\lambda}^{\dagger}(t_1) \hat{b}_{\sigma\lambda}(t_2) | \alpha \rangle \rangle_B \right. \\ &= \delta_{\alpha\beta} \exp^{-i\varepsilon_{\alpha} t} - \sum_{\beta} \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\alpha\alpha}^{(0)}(t - t_1) G_{\beta\beta}^{(0)}(t_1 - t_2) \left(\langle \alpha | d_{\sigma} | \beta \rangle \langle \beta | d_{\sigma}^{\dagger} | \alpha \rangle \sum_{\sigma, \lambda} |t_{\sigma\lambda}|^2 \langle \hat{b}_{\sigma\lambda}^{\dagger}(t_1) \hat{b}_{\sigma\lambda}(t_2) \rangle \right. \\ &= G_{\alpha\alpha}^{(0)}(t) - \sum_{\beta} \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\alpha\alpha}^{(0)}(t - t_1) G_{\beta\beta}^{(0)}(t_1 - t_2) (\langle \alpha | d_{\sigma} | \beta \rangle \langle \beta | d_{\sigma}^{\dagger} | \alpha \rangle \triangle_{\sigma}^{\prec}(t_1 - t_2) + \langle \alpha | d_{\sigma}^{\dagger} | \beta \rangle \langle \beta | d_{\sigma} | \alpha \rangle \triangle_{\sigma}^{\succ}(t_1 - t_2))\end{aligned}$$

with the bare atomic state propagators $G_{\alpha\alpha}^{(0)}(t) = \exp^{-i\varepsilon_\alpha t}$ leaving the dot state invariant. Note that both the bare $G_{\alpha\alpha}^{(0)}(t)$ 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 annihilation operators. Therefore only square terms of \hat{H}_{hyb} appear in the expansion for G . In DMFT the hybridization function $\Delta_\sigma^{\succ/\prec}$ 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)

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

and

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

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

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

with

$$\Sigma_{\alpha\alpha}(t_1 - t_2) = \sum_{\sigma} \sum_{\beta} G_{\beta\beta}(t_1 - t_2) (\langle \alpha | d_{\sigma} | \beta \rangle \langle \beta | d_{\sigma}^{\dagger} | \alpha \rangle \Delta_{\sigma}^{\prec}(t_1 - t_2) + \langle \alpha | d_{\sigma}^{\dagger} | \beta \rangle \langle \beta | d_{\sigma} | \alpha \rangle \Delta_{\sigma}^{\succ}(t_1 - t_2))$$

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

$$\begin{aligned} G_0(t) &= G_0^{(0)}(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_0^{(0)}(t - t_1) G_{\uparrow}(t_1 - t_2) \Delta_{\uparrow}^{\prec}(t_1 - t_2) G_0(t_2) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_0^{(0)}(t - t_1) G_{\downarrow}(t_1 - t_2) \Delta_{\downarrow}^{\prec}(t_1 - t_2) G_0(t_2) \\ G_{\uparrow}(t) &= G_{\uparrow}^{(0)}(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\uparrow}^{(0)}(t - t_1) G_0(t_1 - t_2) \Delta_{\uparrow}^{\succ}(t_1 - t_2) G_{\uparrow}(t_2) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\uparrow}^{(0)}(t - t_1) G_{\downarrow}(t_1 - t_2) \Delta_{\downarrow}^{\succ}(t_1 - t_2) G_{\uparrow}(t_2) \\ G_{\downarrow}(t) &= G_{\downarrow}^{(0)}(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\downarrow}^{(0)}(t - t_1) G_0(t_1 - t_2) \Delta_{\downarrow}^{\succ}(t_1 - t_2) G_{\downarrow}(t_2) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\downarrow}^{(0)}(t - t_1) G_{\uparrow}(t_1 - t_2) \Delta_{\uparrow}^{\succ}(t_1 - t_2) G_{\downarrow}(t_2) \\ G_{\uparrow\downarrow}(t) &= G_{\uparrow\downarrow}^{(0)}(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\uparrow\downarrow}^{(0)}(t - t_1) G_{\downarrow}(t_1 - t_2) \Delta_{\uparrow}^{\prec}(t_1 - t_2) G_{\uparrow\downarrow}(t_2) + \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\uparrow\downarrow}^{(0)}(t - t_1) G_{\uparrow}(t_1 - t_2) \Delta_{\downarrow}^{\prec}(t_1 - t_2) G_{\uparrow\downarrow}(t_2) \end{aligned}$$

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 $G_{\alpha\alpha}^{(0)}(t)$ 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 function incorporates all non-crossing intra- and inter-branch hybridization 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 initial state α to any final state β . For every initial state there are four coupled equations of the form

$$K_{\alpha\beta}(t, t') = K_{\alpha\beta}^{(0)}(t, t') + \sum_{\gamma\delta} \int_{t'}^t dt_1 \int_{t'}^t dt_2 K_{\alpha\gamma}(t_1, t_2) \Delta_{\gamma\delta}(t_1, t_2) K_{\delta\beta}^{(0)}(t - t_1, t' - t_2).$$

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

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

The self consistent equations for the initially unoccupied dot are

$$K_{00}(t, t') = K_{00}^{(0)}(t, t') + \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_0^\dagger(t' - t_2) G_0(t - t_1) \Delta_\uparrow^\prec(t_1, t_2) K_{0\uparrow}(t_1, t_2) + \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_0^\dagger(t' - t_2) G_0(t - t_1) \Delta_\downarrow^\prec(t_1, t_2) K_{0\downarrow}(t_1, t_2)$$

$$K_{0\uparrow}(t, t') = \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_\uparrow^\dagger(t' - t_2) G_\uparrow(t - t_1) \Delta_\uparrow^\prec(t_1, t_2) K_{00}(t_1, t_2) + \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_\uparrow^\dagger(t' - t_2) G_\uparrow(t - t_1) \Delta_\downarrow^\prec(t_1, t_2) K_{0\downarrow}(t_1, t_2)$$

$$K_{0\downarrow}(t, t') = \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_\downarrow^\dagger(t' - t_2) G_\downarrow(t - t_1) \Delta_\downarrow^\prec(t_1, t_2) K_{00}(t_1, t_2) + \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_\downarrow^\dagger(t' - t_2) G_\downarrow(t - t_1) \Delta_\uparrow^\prec(t_1, t_2) K_{0\uparrow}(t_1, t_2)$$

$$K_{0\uparrow\downarrow}(t, t') = \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_{\uparrow\downarrow}^\dagger(t' - t_2) G_{\uparrow\downarrow}(t - t_1) \Delta_\downarrow^\prec(t_1, t_2) K_{0\uparrow}(t_1, t_2) + \int_{t'}^t dt_1 \int_{t'}^t dt_2 G_{\uparrow\downarrow}^\dagger(t' - t_2) G_{\uparrow\downarrow}(t - t_1) \Delta_\uparrow^\prec(t_1, t_2) K_{0\downarrow}(t_1, t_2)$$

After initializing the vertex functions $K_{\alpha\beta}(t, t')$ with $K_{\alpha\beta}^{(0)}(t, t')$ and performing the self-consistent iteration scheme one is able to construct Greens functions.