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

Hristiana Atanasova

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1 Impurity Hamiltonian

A general impurity Hamiltonian has the form

$$\mathrm{H} = \mathrm{H_D} + \mathrm{H_B} + \mathrm{V}.$$

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. There are four possible states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ corresponding to the dot being empty or occupied by either one or two electrons. The bath Hamiltonian is non interacting and has the form

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

The coupling between dot and bath is given through the Hybridization

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

which either adds or removes an electron from the dot to the bath.

2 Greens functions

2.1 Bold Propagators

We are interested in the calculation of correlation functions/Green's functions like $\mathrm{G}^{\succ}(\mathrm{t}_1, \mathrm{t}_2) = -\mathrm{i}\langle \mathrm{d}(\mathrm{t}_1), \mathrm{d}^\dagger(\mathrm{t}_2)\rangle$ and $\mathrm{G}^{\prec}(\mathrm{t}_1, \mathrm{t}_2) = \mathrm{i}\langle \mathrm{d}^\dagger(\mathrm{t}_2), \mathrm{d}(\mathrm{t}_1)\rangle$ from which we can obtain e.g. the spectral function A(w) of a system in a certain regime. The times $\mathrm{t}_1, \mathrm{t}_2$ exist on the real part of the Keldysh contour. In general the

expectation value $\langle \cdots \rangle$ is computed by splitting the Hamiltonian into a part in which the time evolution can be computed exactlty and another one which is treated by pertubative expansion. 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 strength V. In the interaction picture the expectation value $\langle \cdots \rangle$ of any operator O at time t is given by

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

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 coulped to the bath at t=0. Operators in the interaction picture are denoted by a hat $\hat{}$ and have the time dependency

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

where $\mathrm{H_0} = \mathrm{H} - \mathrm{V}$. The time evolution propagator is

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

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

$$\begin{aligned}\frac{\partial}{\partial \mathrm{t}}\mathrm{U(t)} &= \mathrm{i}\exp^{\mathrm{iH_0 t}}(\mathrm{H_0} - \mathrm{H})\exp^{-\mathrm{iH_0 t}} \\ &= -\mathrm{i}\exp^{\mathrm{iH_0 t}}\mathrm{V}(\exp^{-\mathrm{iH_0 t}}\exp^{\mathrm{iH_0 t}})\exp^{\mathrm{iHt}} \\ &= -\mathrm{i}\hat{\mathrm{V}}(\mathrm{t})\mathrm{U(t)}.\end{aligned}$$

After integrating both sides with respect to time

$$\mathrm{U(t)} = 1 - \mathrm{i}\int_0^{\mathrm{t}} \mathrm{dt_1}\hat{\mathrm{V}}(\mathrm{t_1})\mathrm{U}(\mathrm{t_1})$$

and after repeatedly iterating we arrive at

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

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

$$\begin{aligned}\hat{\mathrm{V}}(\mathrm{t}) &= \exp^{\mathrm{iH_0 t}}\mathrm{V}\exp^{-\mathrm{iH_0 t}} \\ &= \sum_{\mathrm{n}=0}^{\infty}\frac{\mathrm{i}}{\mathrm{n!}}^{\mathrm{n}}(\mathrm{H_0 t})^{\mathrm{n}}\sum_{\sigma,\lambda}(\mathrm{t_{\sigma\lambda}}\mathrm{b}_{\sigma}^{\dagger}\mathrm{d}_{\sigma} + \mathrm{t}_{\sigma\lambda}^{\star}\mathrm{d}_{\sigma}^{\dagger}\mathrm{b}_{\lambda})\sum_{\mathrm{n}=0}^{\infty}\frac{(-\mathrm{i})^{\mathrm{n}}}{\mathrm{n!}}(\mathrm{H_0 t})^{\mathrm{n}}\end{aligned}$$

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

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

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

The first step is to compute the bold atomic state propagators $G_{\alpha\beta}(t)$ between many body states α and β that contain all non crossing hybridization lines in a time segment of one branch. The propagators on the upper and lower branch have the simple relation$G_{\alpha\beta}^\dagger(t) = G_{\alpha\beta}(\bar{t})$.

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

where $\langle \cdots \rangle_B = \mathrm{Tr}\{\rho_B \cdots\}$. We insert the expansion for U

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

$$= \sum_\beta \langle\langle \alpha \mid \beta \rangle\langle \beta \mid \exp^{-iH_0 t} \mid \alpha \rangle\rangle_B - \sum_\beta \sum_{\sigma,\lambda} \int dt_1 \int_0^{t_1} dt_2 \, |t_{\sigma\lambda}|^2 \Big(\langle\langle \alpha \mid \exp^{-iH_0 t} d_\sigma \mid \beta \rangle\langle \beta \mid d_\sigma^\dagger \hat{b}_{\sigma\lambda}^\dagger(t_1) \hat{b}_{\sigma\lambda}(t_2$$

$$= \delta_{\alpha\beta} \exp^{-i\varepsilon_\alpha t} - \sum_\beta \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\alpha\alpha}^{(0)}(t - t_1) G_{\beta\beta}^{(0)}(t_1 - t_2) \left(\langle \alpha \mid d_\sigma \mid \beta \rangle\langle \beta \mid d_\sigma^\dagger \mid \alpha \rangle \sum_{\sigma,\lambda} |t_{\sigma\lambda}|^2 \langle \hat{b}_{\sigma\lambda}^\dagger(t_1) \hat{b}_{\sigma\lambda}($$

$$= G_{\alpha\alpha}^{(0)}(t) - \sum_\beta \int_0^t dt_1 \int_0^{t_1} dt_2 G_{\alpha\alpha}^{(0)}(t - t_1) G_{\beta\beta}^{(0)}(t_1 - t_2) \left(\langle \alpha \mid d_\sigma \mid \beta \rangle\langle \beta \mid d_\sigma^\dagger \mid \alpha \rangle \triangle_\sigma^\prec (t_1 - t_2) + \langle \alpha \mid d_\sigma^\dagger \mid \beta \rangle\langle \right.$$

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 annhilation operators. Therefore only square terms of $\hat{V}$ appear in the expansipon of G. In DMFT the hybridization function $\triangle_\sigma^{\succ/\prec}$ is obtained from the self-consistency condition.

For the pure impurity model it can be expressed through the coupling density $\Gamma(\omega)$ of the bath and the initial occupation probability (fermi-function)

$$\triangle^{\prec}(\mathrm{t}_1,\mathrm{t}_2) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\pi} \exp^{-\mathrm{i}\omega(\mathrm{t}_1-\mathrm{t}_2)} \mathit{\Gamma}(\omega)\mathrm{f}(\omega-\mu)$$

and

$$\triangle^{\succ}(\mathrm{t}_1,\mathrm{t}_2) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\pi} \exp^{-\mathrm{i}\omega(\mathrm{t}_1-\mathrm{t}_2)} \mathit{\Gamma}(\omega)(1-\mathrm{f}(\omega-\mu)).$$

We can write the Dyson equation

$$\mathrm{G}_{\alpha\alpha}(\mathrm{t}) = \mathrm{G}^{(0)}_{\alpha\alpha}(\mathrm{t}) + \int_0^{\mathrm{t}} \mathrm{dt}_1 \int_0^{\mathrm{t}_1} \mathrm{dt}_2 \mathrm{G}^{(0)}_{\alpha\alpha}(\mathrm{t}-\mathrm{t}_1)\mathit{\Sigma}_{\alpha\alpha}(\mathrm{t}_1-\mathrm{t}_2)\mathrm{G}_{\alpha\alpha}(\mathrm{t}_2),$$

with the self energy

$$\mathit{\Sigma}_{\alpha\alpha}(\mathrm{t}_1-\mathrm{t}_2) = \sum_{\beta} \mathrm{G}^{(0)}_{\beta\beta}(\mathrm{t}_1-\mathrm{t}_2)\left(\langle\alpha \mid \mathrm{d}_\sigma \mid \beta\rangle\langle\beta \mid \mathrm{d}^\dagger_\sigma \mid \alpha\rangle \triangle^{\prec}_\sigma(\mathrm{t}_1-\mathrm{t}_2) + \langle\alpha \mid \mathrm{d}^\dagger_\sigma \mid \beta\rangle\langle\beta \mid \mathrm{d}_\sigma \mid \alpha\rangle \triangle^{\succ}_\sigma(\mathrm{t}_1-\mathrm{t}_2)\right.$$

containing all non crossing hybidization lines. Renormalizing the self energy leads to replacing the bare propagators with bold ones. For the four different initial states (denoted by the outer index α) on the dot we can derive a set of coupled Dyson equations

$$\mathrm{G}_0(\mathrm{t}) = \mathrm{G}^{(0)}_0(\mathrm{t}) + \int_0^{\mathrm{t}} \mathrm{dt}_1 \int_0^{\mathrm{t}_1} \mathrm{dt}_2 \mathrm{G}^{(0)}_0(\mathrm{t}-\mathrm{t}_1)\mathrm{G}_\uparrow(\mathrm{t}_1-\mathrm{t}_2)\Delta^{\prec}_\uparrow\mathrm{G}_0(\mathrm{t}_2) + \int_0^{t} dt_1 \int_0^{t_1} dt_2 G^{(0)}_0(t-t_1)G_\downarrow(t_1-t_2)\Delta^{\prec}_\downarrow$$

$$\mathrm{G}_\uparrow(\mathrm{t}) = \mathrm{G}^{(0)}_\uparrow(\mathrm{t}) + \int_0^{\mathrm{t}} \mathrm{dt}_1 \int_0^{\mathrm{t}_1} \mathrm{dt}_2 \mathrm{G}^{(0)}_\uparrow(\mathrm{t}-\mathrm{t}_1)\mathrm{G}_0(\mathrm{t}_1-\mathrm{t}_2)\Delta^{\succ}_\uparrow\mathrm{G}_\uparrow(\mathrm{t}_2) + \int_0^{t} dt_1 \int_0^{t_1} dt_2 G^{(0)}_\uparrow(t-t_1)G_0(t_1-t_2)\Delta^{\prec}_\downarrow$$

$$\mathrm{G}_\downarrow(\mathrm{t}) = \mathrm{G}^{(0)}_\downarrow(\mathrm{t}) + \int_0^{\mathrm{t}} \mathrm{dt}_1 \int_0^{\mathrm{t}_1} \mathrm{dt}_2 \mathrm{G}^{(0)}_\downarrow(\mathrm{t}-\mathrm{t}_1)\mathrm{G}_0(\mathrm{t}_1-\mathrm{t}_2)\Delta^{\prec}_\uparrow\mathrm{G}_\downarrow(\mathrm{t}_2) + \int_0^{t} dt_1 \int_0^{t_1} dt_2 G^{(0)}_\downarrow(t-t_1)G_0(t_1-t_2)\Delta^{\succ}_\downarrow$$

$$\mathrm{G}_{\uparrow\downarrow}(\mathrm{t}) = \mathrm{G}^{(0)}_{\uparrow\downarrow}(\mathrm{t}) + \int_0^{\mathrm{t}} \mathrm{dt}_1 \int_0^{\mathrm{t}_1} \mathrm{dt}_2 \mathrm{G}_{\uparrow\downarrow}(\mathrm{t}-\mathrm{t}_1)\mathrm{G}^{(0)}_\downarrow(\mathrm{t}_1-\mathrm{t}_2)\Delta^{\succ}_\uparrow\mathrm{G}_\uparrow(\mathrm{t}_2) + \int_0^{t} dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\uparrow\downarrow}(t-t_1)G_\uparrow(t_1-t_2)\Delta$$

The initial propagators are simply the bare propagators $\mathrm{G}^{(0)}_{\alpha\alpha}(\mathrm{t})$ and with every iteration one ads a new hybridization line to the self energy and integrates over all times.

2.2 Correlation functions