Nonequilibrium DMFT

1 Green's function

The Kadanoff contour-ordered Green's function is defined as

$$G(t,t') = -i\langle T_C c(t) c^\dagger(t')\rangle. \tag{1.1}$$

The Green's function has 9 components that

$$G(t,t') = \begin{pmatrix} G^{11} & G^{12} & G^{13} \\ G^{21} & G^{22} & G^{23} \\ G^{31} & G^{32} & G^{33} \end{pmatrix}, \tag{1.2}$$

where the 1st branch is the '+' branch, 2nd is the '-' branch, and 3rd is the imaginary branch.

2 Lattice Green's function

Consider the lattice Green's function

$$G_{ij}(t,t') = -i\langle T_C c_i(t) c_j^\dagger(t')\rangle, \tag{2.1}$$

its Dyson equation is

$$G_{ij}(t,t') = G_{ij}^{(0)}(t,t') + \sum_{kl}\int \mathrm{d}t_1 \mathrm{d}t_2 G_{ik}^{(0)}(t,t_1)\Sigma_{kl}(t_1,t_2)G_{lj}(t_2,t'). \tag{2.2}$$

In momentum space, we have

$$G_k(t,t') = G_k^{(0)}(t,t') + \int \mathrm{d}t_1 \mathrm{d}t_2 G_k^{(0)}(t,t_1)\Sigma_k(t_1,t_2)G_k(t_2,t'). \tag{2.3}$$

Employing the approximation that $\Sigma_k(t_1,t_2) \approx \Sigma(t_1,t_2)$, we have

$$G_k(t,t') = G_k^{(0)}(t,t') + \int \mathrm{d}t_1 \mathrm{d}t_2 G_k^{(0)}(t,t_1)\Sigma(t_1,t_2)G_k(t_2,t'). \tag{2.4}$$

Once $\Sigma(t,t')$ is known, in principle $G_k(t,t')$ can be obtained via this equation.

3 Impurity Green's function

3.1 Free impurity

For free impurity, we denote the Green's function as $g(t,t') = -i\langle T_C c(t) c^\dagger(t')\rangle$. Differentiation it on t gives

$$\partial_t g(t,t') = -\varepsilon(t)\langle T_C c(t) c(t')\rangle - i\delta(t,t'), \tag{3.1}$$

here we have used the relation $\partial_t c(t) = i[H, c(t)] = -ic(t)$, or we can write it as

$$i\partial_t g(t,t') - \varepsilon(t) g(t,t') = \delta(t,t'). \tag{3.2}$$

It can been seen that the inverse operator g^{-1} is (it can be seen that g^{-1} is a linear operator)

$$g^{-1} = i\partial_t - \varepsilon(t). \tag{3.3}$$

3.2 With hybridization

When the bath is present, we denote the Green's function as $G_0(t,t')$, and we have the dyson equation

$$G_0(t,t') = g(t,t') + \int \mathrm{d}t_1 \mathrm{d}t_2\, g(t,t_1)\Delta(t_1,t_2)G_0(t_2,t'), \tag{3.4}$$

Applying g^{-1} to the equation, we have

$$i\partial_t G_0(t,t') - \varepsilon(t)G_0(t,t') = \delta(t,t') + \int \Delta(t,t_1)G_0(t_1,t')\mathrm{d}t_1, \tag{3.5}$$

or

$$i\partial_t G_0(t,t') - \varepsilon(t)G_0(t,t') - \int \Delta(t,t_1)G_0(t_1,t')\mathrm{d}t_1 = \delta(t,t'). \tag{3.6}$$

Then we have

$$G_0^{-1} = i\partial_t - \varepsilon(t) - \Delta(t,t_1). \tag{3.7}$$

3.3 With interaction

With the interaction, we have the final Green's function as

$$G(t,t') = G_0(t,t') + \int \mathrm{d}t_1 \mathrm{d}t_2 G_0(t,t_1)\Sigma(t_1,t_2)G(t_2,t'). \tag{3.8}$$

Applying G_0^{-1} to the equation, we have

$$i\partial_t G(t,t') - \varepsilon(t)G(t,t') - \int \Delta(t,t_1)G(t_1,t')\mathrm{d}t_1 - \int \Sigma(t,t_1)G(t_1,t')\mathrm{d}t_1 = \delta(t,t'), \tag{3.9}$$

or

$$i\partial_t G(t,t') - \varepsilon(t)G(t,t') - \int [\Sigma(t,t_1) + \Delta(t,t_1)]G(t_1,t')\mathrm{d}t_1 = \delta(t,t'). \tag{3.10}$$

Solving this Volterra integral equation gives us $\Sigma(t,t')$ in principle.