

1 Time-dependence for a quantum quench

See also [1, 2] for alternative derivations

Dyson equation (left and right)

$$\begin{aligned} G &= g + g \circ \tilde{\Sigma} \circ G = g + G \circ \tilde{\Sigma} \circ g \\ g^{-1} \circ G &= I + \tilde{\Sigma} \circ G \quad G \circ g^{-1} = I + G \circ \tilde{\Sigma} \end{aligned} \quad (1)$$

retarded component

$$G_r = g_r + g_r \circ \tilde{\Sigma}_r \circ G_r \quad (2)$$

or, equivalently

$$g_r^{-1} \circ G_r = I + \tilde{\Sigma}_r \circ G_r \quad (3)$$

We will consider the problem of a central region consisting of several levels described by an Hamiltonian

$$H = c^\dagger \varepsilon c . \quad (4)$$

We try to keep results valid for N levels, so that $c = (c_1, c_2, \dots, c_N)^T$, and ε is a matrix .

Some definitions

We are working in time space, so we need to specify the meaning of objects there:

- Convolution

$$A = B \circ C \leftrightarrow A(t_1, t_2) = \int dt B(t_1, t) C(t, t_2) \quad (5)$$

- Identity

$$I(t_1, t_2) = \delta(t_1 - t_2) \quad (6)$$

- It follows: inverse

$$A = B^{-1} \leftrightarrow A \circ B = I \leftrightarrow \int dt A(t_1, t) B(t, t_2) = \delta(t_1 - t_2) \quad (7)$$

Unperturbed retarded Green's function

We start with the unperturbed ($\tilde{\Sigma} = 0$) retarded Green's function.

$$g_r(t_1, t_2) = -i\theta(t_1 - t_2) \langle \{c(t_1), c^\dagger(t_2)\} \rangle$$

It satisfies the equation of motion (we consider for the moment still a time-dependent ε)

$$\begin{aligned} \partial_{t_1} g_r(t_1, t_2) &= -i\delta(t_1 - t_2) + \theta(t_1 - t_2) \langle \{[H(t_1), c(t_1)], c^\dagger(t_2)\} \rangle \\ &= -i\delta(t_1 - t_2) - \theta(t_1 - t_2)\varepsilon(t_1) \langle c(t_1), c^\dagger(t_2) \rangle \end{aligned}$$

i.e.

$$(i\partial_{t_1} - \varepsilon(t_1)) g_r(t_1, t_2) = \delta(t_1 - t_2) \quad (8)$$

in this way, one immediately recognizes the inverse of g :

$$g_r^{-1}(t_1, t_2) = (i\partial_{t_1} - \varepsilon(t_1))\delta(t_1 - t_2) \quad (9)$$

the solution of 8 with the corresponding initial conditions $g_r(t_1^+, t_1) = -i$ is given by

$$g_r(t_1, t_2) = -i\theta(t_1 - t_2) T \exp\left(-i \int_{t_2}^{t_1} \varepsilon(t) dt\right) \quad (10)$$

where T is the time-ordered product necessary because ε is a time-dependent matrix.

From here on, we consider a time-independent ε .

Retarded Green's function after a Quantum quench

We now introduce the coupling (hybridisation) to a bath which is switched on at some time, say $t = 0$ (quantum quench) $V(t) = V \theta(t)$. We have already evaluated the bath self energy ¹ (matrix). Schematically it can be

¹This is sometimes called hybridisation function in order to distinguish it from the one originating from the interaction. But we have no interactions here

written as

$$\begin{aligned}\tilde{\Sigma}(t_1, t_2) &= V(t_1)g_{bath}(t_1 - t_2)V^\dagger(t_2) = \theta(t_1)\theta(t_2)Vg_{bath}(t_1 - t_2)V^\dagger \\ &\equiv \theta(t_1)\theta(t_2)\tilde{\Sigma}(t_1 - t_2)\end{aligned}\quad (11)$$

It is thus time-translation invariant when both $t_1, t_2 > 0$.

(2) can be written explicitly

$$G_r(t_1, t_2) = g_r(t_1 - t_2) + \int dt_3 dt_4 g_r(t_1 - t_3)\theta(t_3)\theta(t_4)\tilde{\Sigma}_r(t_3 - t_4)G_r(t_4, t_2)\quad (12)$$

Consider the case $t_2 \geq 0$. Since all quantities are retarded, we have $t_1 > t_3 > t_4 > t_2 \geq 0$ so that the θ are redundant in (12). Therefore, all quantities in (12) are time translation invariant and the solution is easily obtained by Fourier (Laplace) transform, whereby the convolution becomes a product. With abuse of notation, the solution is ($z = \omega + i0^+$)

$$\bar{G}_r(z) = \left(g_r(z)^{-1} - \tilde{\Sigma}_r(z)\right)^{-1} = \left(z - \varepsilon - \tilde{\Sigma}_r(z)\right)^{-1}. \quad (13)$$

To avoid misunderstanding, we indicate by $\tilde{\Sigma}_r$ and \bar{G}_r the time-translation invariant versions of $\tilde{\Sigma}_r$ and G_r , valid when both times are positive:

$$\bar{G}_r(t_1, t_2) = \bar{G}_r(t_1 - t_2) = G_r(t_1, t_2) \quad t_1, t_2 \geq 0 \quad (14)$$

When the argument is z , then it means a Fourier (Laplace) transform.

For $0 \geq t_1 \geq t_2$, obviously $G_r = g_r$. For $t_1 > 0 \geq t_2$ the solution is obtained in the following way: We take for convenience (3) with (9), which reads for this case (here, $\delta(t_1 - t_2) = 0$):

$$(i\partial_{t_1} - \varepsilon) G_r(t_1, t_2) = \int dt_3 \tilde{\Sigma}_r(t_1 - t_3) \theta(t_3)G_r(t_3, t_2) \quad (15)$$

For fixed t_2 , this has the form ² (28) with $f(t_1) \equiv G_r(t_1, t_2)$ and $h = 0$. Following the procedure in Sec. A, we get the solution (33), which in this case translates to

$$G_r(t_1, t_2) = i G_r(t_1, 0)G_r(0, t_2) = i G_r(t_1, 0)g_r(0, t_2) \quad t_1 \geq 0, t_2 \leq 0. \quad (16)$$

²The upper limit of the integral is in fact limited to t_1 , since $\tilde{\Sigma}_r$ is a retarded function

In fact, (16) can be easily generalized (the procedure is the same as in Sec. A) for $t_1 \geq t_2 \geq t_3$

$$G_r(t_1, t_3) = iG_r(t_1, t_2)G_r(t_2, t_3) \quad (17)$$

For the advanced Green's function we have

$$G_a(t_1, t_2) = G_r^\dagger(t_2, t_1) \quad (18)$$

(Ex. 9.1) : calculate the time dependent G_r for a bath with a Lorentzian density of states.

Keldysh Green's function

The Keldysh components of the left and right Dyson equations (1) become, respectively (as usual, we can neglect g_k^{-1})

$$\begin{aligned} g_r^{-1} \circ G_k &= \tilde{\Sigma}_r \circ G_k + \tilde{\Sigma}_k \circ G_a \quad \Rightarrow \quad G_r^{-1} \circ G_k = \tilde{\Sigma}_k \circ G_a \\ G_k \circ g_a^{-1} &= G_k \circ \tilde{\Sigma}_a + G_r \circ \tilde{\Sigma}_k \quad \Rightarrow \quad G_k \circ G_a^{-1} = G_r \circ \tilde{\Sigma}_k \end{aligned} \quad (19)$$

The first one, for $t_1 > 0, t_2 = 0$ reads

$$\left((g_r^{-1} - \tilde{\Sigma}_r) \circ G_k \right) (t_1, 0) = \int dt_3 \tilde{\Sigma}_k(t_1, t_3) G_a(t_3, t_2)$$

The integral on the r.h.s. vanishes because t_3 must be < 0 due to the advanced G_a , but then $\tilde{\Sigma}_k = 0$ (cf. (11)), so we have ³

$$(i\partial_{t_1} - \varepsilon) G_k(t_1, 0) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1, t_3) G_k(t_3, 0) = 0, \quad (20)$$

which is of the form (28) with $f(t_1) = G_k(t_1, 0)$ and $h = 0$. The solution is, thus, cf. (33)

$$G_k(t, 0) = iG_r(t, 0) g_k(0, 0) = G_r(t, 0)(1 - 2n_0). \quad (21)$$

We have used that the initial value $G_k(0, 0) = g_k(0, 0)$ since $V = 0$ for negative times, and $g_k(0, 0) = -i(1 - 2n_0)$, with n_t the occupation (matrix) at time t . This is the equilibrium Keldysh Green's function at equal times.

³ t_3 is restricted to positive values because of (11)

However, we need $G_k(t_1, t_2)$ for arbitrary $t_1, t_2 > 0$. This is obtained by starting from (21) and propagating the second time via the second of (19). It is convenient to take the hermitian conjugate of that equation (which includes switching the time arguments), and using $G_a^\dagger = G_r$:

$$G_r^{-1} \circ G_k^\dagger = \tilde{\Sigma}_k^\dagger \circ G_a$$

which becomes

$$(i\partial_{t_1} - \varepsilon) G_k^\dagger(t_1, t_2) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1, t_3) G_k^\dagger(t_3, t_2) = \underbrace{\int_0^{t_2} dt_3 \tilde{\Sigma}_k^\dagger(t_1, t_3) G_a(t_3, t_2)}_{h(t_1, t_2)}. \quad (22)$$

We need this for $t_1 > t_2 > 0$, so in this case the integral on the r.h.s. does not vanish.⁴

However, since we know already $\tilde{\Sigma}_k$ and G_a , we can evaluate it. Let us call it $h(t_1, t_2)$. (22) has the form (28) with $f(t_1) = G_k^\dagger(t_1, t_2)$ and $h(t_1) = h(t_1, t_2)$. The solution (33) becomes here

$$G_k^\dagger(t_1, t_2) = iG_r(t_1, 0)G_k^\dagger(0, t_2) + \int_0^\infty dt_3 G_r(t_1 - t_3)h(t_3, t_2) \quad t_1, t_2 > 0$$

or taking the hermitian conjugate and exchanging $t_1 \leftrightarrow t_2$ yields:

$$G_k(t_1, t_2) = -iG_k(t_1, 0)G_a(0, t_2) + \int_0^\infty dt_3 h^\dagger(t_1, t_3)G_a(t_3 - t_2)$$

combining with (21), inserting the explicit expression for h from (22), and taking $G_a(t_1, t_2) = G_r(t_2, t_1)^\dagger$ yields

$$G_k(t_1, t_2) = -iG_r(t_1, 0)(1 - 2n_0)G_r(t_2, 0)^\dagger + \int_0^{t_2} dt_3 \underbrace{\int_0^{t_1} dt_4 G_r(t_1 - t_4)\tilde{\Sigma}_k(t_4 - t_3)G_r(t_2 - t_3)^\dagger}_{h^\dagger(t_1, t_3)}, \quad (23)$$

which has a more symmetric form, and we have exploited the fact that the involved times are positive.

⁴The integration limits are given by (11) and by the advanced Green's function.

Wide-band limit

We consider several baths α in the wide band limit, where their contribution to $\tilde{\Sigma}_r$ is ω -independent: $\tilde{\Sigma}_{r\alpha}(\omega) = -i\Gamma_\alpha$. The total $\tilde{\Sigma}_r$:

$$\tilde{\Sigma}_r(z) = -i\Gamma \quad \Gamma = \sum_{\alpha} \Gamma_{\alpha} \quad (24)$$

Thus, taking the Fourier transform of (13) yields (Ex.:9.2)

$$\bar{G}_r(t) = e^{-i\varepsilon t - \Gamma t} \quad (25)$$

and, for example for $t_1 > 0, t_2 < 0$ we get from (16)

$$G_r(t_1, t_2) = e^{-i\varepsilon(t_1 - t_2) - \Gamma t_1}$$

The corresponding Keldysh components $\tilde{\Sigma}_{k\alpha}(\omega) = -2i\Gamma_{\alpha}s_{\alpha}(\omega)$ is less trivial. Taking for simplicity baths with $T = 0$ and chemical potentials μ_{α} , we have $s_{\alpha}(\omega) = \text{sign}(\omega - \mu_{\alpha})$. The Fourier transform gives (CHECK: Ex. 9.3):

$$\tilde{\Sigma}_{k\alpha}(t_1 - t_2) = -\frac{2\Gamma_{\alpha}}{\pi} \frac{1}{t_1 - t_2} e^{-i\mu_{\alpha}(t_1 - t_2)}, \quad (26)$$

and again the total $\tilde{\Sigma}_k$ is just the sum of these contributions.

Interesting is the time-dependent occupation $n(t)$ of the central region given in terms of the equal-time Keldysh Green's function (here for $t > 0$)

$$-i(1 - 2n(t)) = G_k(t, t) = -ie^{-2\Gamma t}(1 - 2n_0) + e^{-2\Gamma t} \int_0^t dt_3 \int_0^t dt_4 e^{\Gamma(t_3 + t_4)} e^{-i\varepsilon(t_4 - t_3)} \sum_{\alpha} \tilde{\Sigma}_{k\alpha}(t_4 - t_3) \quad (27)$$

The first term gives the contribution from the initial occupation of the central site, which decays with a rate 2Γ , while the second part provides the tendency to reach a steady-state occupation with the baths.

A Solution of the integro-differential equation

We need the solution of (in-)homogeneous integro-differential equations (cf. (15), (20), (22)) of the form

$$(i\partial_{t_1} - \varepsilon)f(t_1) - \int_0^\infty dt_3 \tilde{\Sigma}_r(t_1 - t_3)f(t_3) = h(t_1) \quad t_1 > 0 \quad (28)$$

This is not truly a convolution since the integral starts at 0. (28) can also be written

$$\int_0^\infty dt_3 G_r^{-1}(t_1 - t_3) f(t_3) = h(t_1) \quad (29)$$

with given initial conditions at $t_1 = 0$

$$f(0) = f_0 \quad (30)$$

To solve this equation, one introduces the function

$$F(t_1) \equiv \theta(t_1)f(t_1) ,$$

coinciding with f in the region of interest.⁵ This satisfies a similar equation

$$(i\partial_{t_1} - \varepsilon)F(t_1) - \int_{-\infty}^\infty dt_3 \tilde{\Sigma}_r(t_1 - t_3)F(t_3) = i\delta(t_1)f_0 + h(t_1) . \quad (31)$$

The crucial point is that now the integral extends from $-\infty$ to ∞ , so this is a true convolution with the function $\tilde{\Sigma}_r(t_1 - t_3) = \tilde{\Sigma}_r(t_1 - t_3)$ which is translation invariant. So this can be solved by Fourier transform. Formally, we write (31), see also (14), as

$$(g_r^{-1} - \tilde{\Sigma}_r) \circ F = \bar{G}_r^{-1} \circ F = iI f_0 + h \quad \Rightarrow \quad F = i\bar{G}_r f_0 + \bar{G}_r \circ h . \quad (32)$$

So in real time (32) has the simple solution

$$F(t) = i G_r(t, 0) f_0 + \int_0^\infty dt_3 G_r(t - t_3, 0)h(t_3) \quad (33)$$

where, since all the involved times are > 0 , we replaced $\bar{G}_r(t) \rightarrow G_r(t, 0)$.

⁵This procedure is similar in spirit to the Laplace transform.

References

- [1] G. Stefanucci and C.-O. Almbladh, Phys. Rev. B **69**, 195318 (2004).
- [2] M. Cini, Phys. Rev. B **22**, 5887 (1980).