

# Non-equilibrium Green functions I

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Literature:

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## 1 Basic definitions and equations

### 1.1 Equilibrium Green's functions

We define

$$G^r(x_1, t_1; x_2, t_2) = -i\Theta(t_1 - t_2)\langle\{\psi(x_1, t_1), \psi^\dagger(x_2, t_2)\}_+\rangle$$

$$G^a(x_1, t_1; x_2, t_2) = +i\Theta(t_2 - t_1)\langle\{\psi(x_1, t_1), \psi^\dagger(x_2, t_2)\}_+\rangle$$

which are called retarded and advanced Green functions (they fulfill the usual equations of motion of a Green function in the mathematical sense). Here  $\psi^\dagger(x, t)$  is a creation operator for a fermion at position  $x$ . The time dependence of the operators is determined by the time-independent Hamiltonian  $H$  of the system:

$$O(t) = O_H(t) = e^{iHt}Oe^{-iHt}$$

The bracket denotes a thermal average with the statistical operator  $\rho = e^{-\beta H}/Z$ . In order to describe a grand-canonical ensemble we have to replace  $H$  by  $H - \mu N$ . This can be accomplished by counting all single-particle energies from the chemical potential  $\mu$ . We will do that also for the Hamiltonian describing the time dependence.

In the following we also need the correlation functions

$$G^>(x_1, t_1; x_2, t_2) = -i\langle\psi(x_1, t_1)\psi^\dagger(x_2, t_2)\rangle$$

$$G^<(x_1, t_1; x_2, t_2) = +i\langle\psi^\dagger(x_2, t_2)\psi(x_1, t_1)\rangle$$

and the time-ordered Green function

$$G_c(x_1, t_1; x_2, t_2) = -i\langle\mathcal{T}_t\psi(x_1, t_1)\psi^\dagger(x_2, t_2)\rangle$$

$$= -i\Theta(t_1 - t_2)\langle\psi(x_1, t_1)\psi^\dagger(x_2, t_2)\rangle + i\Theta(t_2 - t_1)\langle\psi^\dagger(x_2, t_2)\psi(x_1, t_1)\rangle$$

$$= \Theta(t_1 - t_2)(G^>(x_1, t_1; x_2, t_2) + \Theta(t_2 - t_1)G^<(x_1, t_1; x_2, t_2))$$

Note that the retarded Green function can also be expressed by the two correlation functions

$$G^r(x_1, t_1; x_2, t_2) = \Theta(t_1 - t_2)(G^>(x_1, t_1; x_2, t_2) - G^<(x_1, t_1; x_2, t_2))$$

$$G^a(x_1, t_1; x_2, t_2) = -\Theta(t_2 - t_1)(G^>(x_1, t_1; x_2, t_2) - G^<(x_1, t_1; x_2, t_2))$$

and  $G^r - G^a = G^> - G^<$ .

In thermal equilibrium these functions depend only on the time-difference  $t = t_1 - t_2$ . Furthermore all three are linked together by the dissipation fluctuation theorem. Introducing a Fourier transform (here we suppress the dependence on variables  $x_1, x_2$  for the moment)

$$G(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} G(t) dt$$

one obtains the important relation between the two correlation functions

$$G^>(\omega) = -e^{\beta\omega} G^<(\omega)$$

Defining a spectral function

$$A(\omega) = i[G^r(\omega) - G^a(\omega)] = i[G^>(\omega) - G^<(\omega)]$$

we find

$$G^<(\omega) = if(\omega)A(\omega), \quad G^> = -i(1 - f(\omega))A(\omega)$$

where

$$f(\omega) = \frac{1}{\exp(\beta\omega) + 1}$$

is the Fermi function. Note that the Green functions and the spectral function depend also on the other variables  $x_1, x_2$ .

In the case of free conduction electrons with  $\psi(x) = \sum_k c_k e^{ikx} / \sqrt{Vol}$  we obtain after a Fourier transformation in space

$$G^{r,a}(k\omega) = \frac{1}{\omega \pm i\delta - \epsilon_k + \mu}$$

$$A(k, \omega) = 2\pi\delta(\omega - \epsilon_k + \mu)$$

Here we see that  $A(k\omega)$  contains information about the single-particle excitation spectrum, while the distribution function  $f(\omega)$  which appears in the correlation functions describes the thermal occupation of such states. In a non-equilibrium theory the distribution function will become an independent quantity. Therefore we need the correlation functions in addition to the retarded and advanced Green functions.

## 1.2 Perturbation theory for equilibrium Green functions

In order to calculate the Green function with help of a perturbation theory we split the Hamiltonian into  $H = H_0 + H^i$  where  $H_0$  describes a non-interacting electron system. Going over to the interaction representation the unitary operator for the time evolution between times  $t_0$  and  $t$  becomes

$$e^{-iH(t-t_0)} = e^{-itH_0} V(t, t_0) e^{iH_0 t_0}, \quad V(t, t_0) = \mathcal{T} \exp\left(-i \int_{t_0}^t H_0^i(t') dt'\right)$$

where the time dependence of the interaction  $H^i$  (and other operators with subscript 0) is determined by the Hamiltonian  $H_0$  of the non-interacting system:  $O_0(t) = \exp(iH_0 t) O \exp(-iH_0 t)$ .  $\mathcal{T}$  denotes a time ordering of operators on the time-axis from  $t_0$  to  $t$ . Here the time  $t_0$  is some arbitrary reference time. We can set  $t_0 = 0$ . However, for later use in the case of a time dependent interaction it has to be chosen earlier than the switch-on time of the time-dependent interaction. Later we let  $t_0 \rightarrow -\infty$ .

For fixed time  $t_1, t_2$  we then obtain

$$\langle \psi(t_1) \psi^\dagger(t_2) \rangle = \langle e^{iH_0 t_0} S(t_0, t_1) \psi_0(t_1) S(t_1, t_2) \psi_0^\dagger(t_2) S(t_2, t_0) e^{-iH_0 t_0} \rangle$$

which can also be written as

$$\langle \psi(t_1) \psi^\dagger(t_2) \rangle = \langle e^{iH_0 t_0} \mathcal{T}'_C S_C \psi_0(t_1) \psi_0^\dagger(t_2) e^{-iH_0 t_0} \rangle, \quad S_C = \exp\left(-i \int_C H_0^i(\tau) d\tau\right)$$

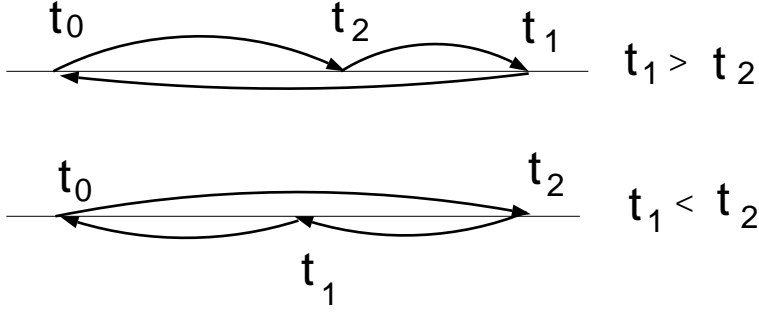


Abbildung 1: The contour  $C$  used for the perturbation theory in the time-evolution

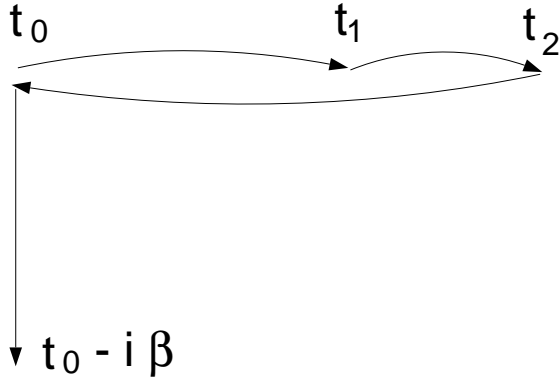


Abbildung 2: The contour  $C^i$  used for the perturbation theory including expansion of the statistical operator

where  $C$  is the contour shown in Fig. 1 and the time ordering operator  $\mathcal{T}'$  orders the interaction operators contained in  $S$  in the direction of the contour at the right places before, between, and behind the fermion operators at the fixed times  $t_1, t_2$ .

Finally we have to expand also the statistical operator, which can be expressed by

$$e^{-\beta H} = e^{-i(t_0 - i\beta)H_0} S(t_0 - i\beta, t_0) e^{it_0 H_0}$$

Then

$$\langle \mathcal{T}'_{C^i} \psi(t_1) \psi^\dagger(t_2) \rangle = \frac{\langle \mathcal{T}'_{C^i} S_{C^i} \psi_0(t_1) \psi_0^\dagger(t_2) \rangle_0}{\langle \mathcal{T}'_{C^i} S_{C^i} \rangle_0}$$

where now  $C^i$  is the contour shown in Fig. 2 and  $\langle \rangle_0$  means a thermal average performed with the statistical operator  $\rho_0 = e^{-\beta H_0} / Z_0$ .

Due to the time ordering contained in  $S$  requires that a perturbation theory

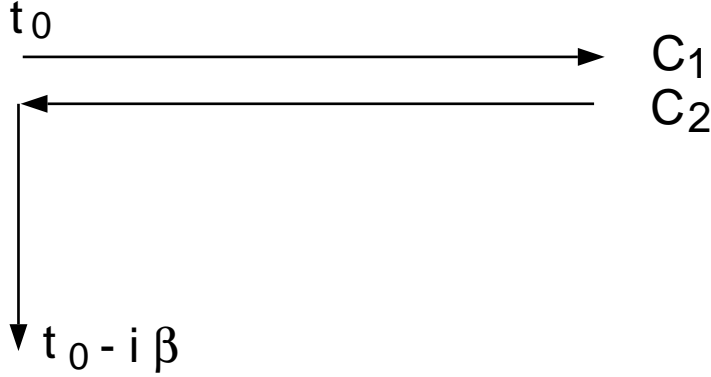


Abbildung 3: Contour  $C^i$  used for the perturbation expansion of the time-ordered Green function

for the Green function can be formulated easily only for a Green function with time-ordered operators. Therefore we define a time ordered Green function on the contour  $C^i$ :

$$G(\tau_1, \tau_2) = \begin{cases} -i \langle \psi(\tau_1) \psi^\dagger(\tau_2) \rangle & \text{for } \tau_1 >_c \tau_2 \\ +i \langle \psi^\dagger(\tau_2) \psi(\tau_1) \rangle & \text{for } \tau_1 <_c \tau_2 \end{cases}$$

where we distinguish between times  $\tau_i$  on different parts of the contour (see Fig. 3). Then for  $G$  the following perturbation expansion holds:

$$G(\tau_1, \tau_2) = -i \frac{\langle \mathcal{T}_{C^i} S_{C^i} \psi_0(\tau_1) \psi_0^\dagger(\tau_2) \rangle_0}{\langle \mathcal{T}_{C^i} S_{C^i} \rangle_0}$$

It is related to the real-time Green functions introduced above by

$$G(\tau_1, \tau_2) = \begin{cases} G_c(t_1, t_2) & \text{for } \tau_1, \tau_2 \in C_1 \\ G^>(t_1, t_2) & \text{for } \tau_1 \in C_2, \tau_2 \in C_1 \\ G^<(t_1, t_2) & \text{for } \tau_1 \in C_1, \tau_2 \in C_2 \\ G_{\bar{c}}(t_1, t_2) & \text{for } \tau_1, \tau_2 \in C_2 \end{cases}$$

The last being an antitime-ordered Green function. The retarded and advanced Green functions can be obtained from  $G^>$  and  $G^<$  in the usual way.

The purpose of this discussion was to motivate the introduction of a time-ordered Green function on the special contour  $C^i$ . This will be the basis for the following discussion of non-equilibrium Green functions. In thermal equilibrium it is possible to simplify this contour considerably: As in thermal equilibrium all Green functions depend only on the time difference we can replace  $C^i$  by a

contour  $C^{th}$  which runs from  $t_0$  to  $t_0 - i\beta$ , where we can put  $t_0 \rightarrow 0$  without loss of generality. One then defines a time-ordered Green function on the imaginary axis. The physical retarded and advanced Green functions are then obtained by an analytical continuation in frequency space. This is the Matsubara technique.

### 1.3 Green functions with time dependent perturbation

A non-equilibrium situation is obtained if we add to the Hamiltonian  $H$  of the system a time-dependent perturbation  $H'_t$  describing for instance the interaction with an external time-dependent field:

$$\mathcal{H}_t = H + H'_t$$

with  $H = H_0 + H^i$ . We assume that the time dependent interaction  $H'_t$  vanishes for times  $t < t_0$ . The time dependent interaction can be treated by a perturbation expansion in a similar way as the internal interaction. The final result for the Green function can be written as a double expansion:

$$G(\tau_1, \tau_2) = -i \frac{\langle \mathcal{T}_{C^i} S_{C^i} S_C \psi_0(\tau_1) \psi_0^\dagger(\tau_2) \rangle_0}{\langle \mathcal{T}_{C^i} S_{C^i} S_C \rangle_0}$$

where

$$S_{C^i} = \exp\left(-i \int_{C^i} d\tau H_0^i(\tau)\right)$$

$$S_C = \exp\left(-i \int_C d\tau H'_{\tau,0}(\tau)\right)$$

and both interaction operators are Heisenberg operators constructed with  $H_0$ . Note that  $H'_{\tau,0}$  contains an implicit time dependence through the external field. Here the contour  $C$  starts and ends at  $t_0$ , while the contour  $C^i$  starts at  $t_0$  and ends at  $t_0 - i\beta$ .

The principal significance of this result is that for the time-ordered Green function on the contour  $C^i$  the usual perturbation expansion in form of Feynman graphs as in the case of equilibrium Green function can be applied. In particular if the Hamiltonian  $H_0$  is bilinear in fermionic operators Wick' theorem can be applied. It states that in each order of the perturbation theory the result for the Green function can be expressed by products of single particle Green functions of the non-interacting system. The same holds for the statistical operator. Therefore the denominator cancels against non-connected graphs in the numerator, leaving

us with an expansion containing only connected graphs. For these, finally, a Dyson equation can be formulated, which will be the basis of the following discussion.

## 1.4 Dyson equation

In order to be specific let us assume a time-dependent interaction of the form

$$H'_t = \int dx \psi^\dagger(x) U(x, t) \psi(x)$$

then the time-ordered Green function on the contour fulfills the following Dyson equation

$$G(1, 2) = G_0(1, 2) + \int d3 G_0(1, 2) U(3) G(3, 2) \\ \int d3 \int d4 G_0(1, 3) \Sigma(3, 4) G(4, 2)$$

where  $(i)$  is a short-hand notation for  $(x_i, \tau_i)$  and  $\int di = \int dx \int_{C^i} d\tau_i$ . We did not specify the internal interaction further. It is contained in the (irreducible) self-energy  $\Sigma$ . The self-energy can be calculated and expressed by single-particle Green functions in any specific case. In principle the time-integrations have to be performed on the contour  $C^i$ . A simplification occurs if we put  $t_0 \rightarrow -\infty$ . Then the contribution from the path  $t_0$  to  $t_0 - i\beta$  can be neglected, if the internal interactions wash out the memory of initial conditions. Then for the internal integrations we may use the contour  $C$  (Fig. 4) extending from  $-\infty$  to  $+\infty$  (part  $C_1$ ) and back (part  $C_2$ ). This will be called the Keldysh contour in the following.

There still remains the problem of expressing the integrations of products of different functions by integrations over the usual time axis  $-\infty < t < +\infty$ . This will be the task of the following section.

## 1.5 Langreth rules, Keldysh formalism

In the Dyson equations appear integrations over the contour of products of two and three functions. Let us start with the investigation of a folding of two functions of the form (here we suppress the dependence on the spatial variables)

$$C(\tau_1, \tau_2) = \int_C d\tau_3 A(\tau_1, \tau_3) B(\tau_3, \tau_2)$$

Our aim is to express this integral on  $C$  by integrals over the simple time-axis  $-\infty < t < +\infty$ . The result depends on the choice of variables on the contour. If

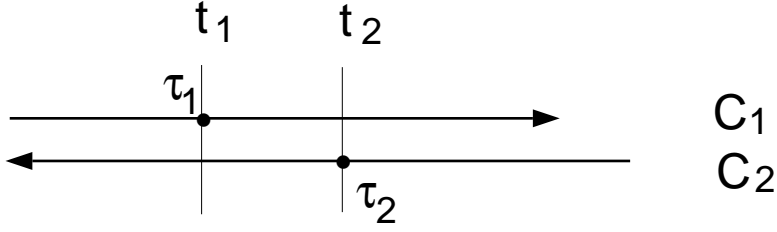


Abbildung 4: Relation between real times and times on the different branches of the Keldish contour

we are interested, for instance, in  $C^<(t_1, t_2)$  we place as in Fig. 4  $\tau_1$  on  $C_1$  and  $\tau_2$  on  $C_2$  and evaluate the integrals on the contour. Then we obtain:

$$C^<(t_1, t_2) = \int_{-\infty}^{+\infty} dt [A^r(t_1, t)B^<(t, t_2) + A^<(t_1, t)B^a(t, t_2)]$$

For a derivation of this result we split the integrals:

$$C^<(t_1, t_2) = \int_{C_1} d\tau A(\tau_1, \tau)B(\tau, \tau_2) + \int_{C_2} d\tau A(\tau_1, \tau)B(\tau, \tau_2)$$

On  $C_1$  the function  $B$  is a function  $B^<$  while  $A = A_c$ . On  $C_2$  the function  $A$  is a function  $A^>$  while  $B = B_{\bar{c}}$ . Then for the first integral we obtain

$$\begin{aligned} \int_{C_1} d\tau A(\tau_1, \tau)B(\tau, \tau_2) &= \int_{-\infty}^{+\infty} dt A_c(t_1, t)B^<(t, t_2) \\ &= \int_{-\infty}^{t_1} dt A^>(t_1, t)B^<(t, t_2) + \int_{t_1}^{+\infty} dt A^<(t_1, t)B^>(t, t_2) \end{aligned}$$

For the second integral we find

$$\begin{aligned} \int_{C_2} d\tau A(\tau_1, \tau)B(\tau, \tau_2) &= \int_{+\infty}^{-\infty} dt A^>(t_1, t)B_{\bar{c}}(t, t_2) \\ &= - \int_{-\infty}^{t_2} dt A^>(t_1, t)B^>(t, t_2) - \int_{t_2}^{+\infty} dt A^>(t_1, t)B^<(t, t_2) \end{aligned}$$

Using the relations  $A^r(t_1, t_2) = \Theta(t_1 - t_2)(G^>(t_1, t_2) - G^<(t_1, t_2))$  and  $A^a(t_1, t_2) = -\Theta(t_2 - t_1)(G^>(t_1, t_2) - G^<(t_1, t_2))$  we can show the equivalence of the two results.

In a similar way we can show

$$C^>(t_1, t_2) = \int_{-\infty}^{+\infty} dt [A^r(t_1, t)B^>(t, t_2) + A^>(t_1, t)B^a(t, t_2)]$$



and

$$C^r(t_1, t_2) = \int_{-\infty}^{+\infty} dt A^r(t_1, t) B^r(t, t_2), \quad C^a(t_1, t_2) = \int_{-\infty}^{+\infty} dt A^a(t_1, t) B^a(t, t_2)$$

In the Dyson equation we also encounter a folding of the form

$$C(\tau_1, \tau_2) = \int_C d\tau A(\tau_1, \tau) U(\tau) B(\tau, \tau_2)$$

this is transformed into

$$C^<(t_1, t_2) = \int_{-\infty}^{+\infty} dt [A^r(t_1, t) U(t) B^<(t, t_2) + A^<(t_1, t) U(t) B^r(t, t_2)]$$

For a product of three functions we obtain similar rules, for instance, let

$$D(\tau_1, \tau_2) = \int_C d\tau_3 d\tau_4 A(\tau_1, \tau_3) B(\tau_3, \tau_4) C(\tau_4, \tau_2)$$

then

$$D^< = \int dt [A^r B^r C^< + A^r B^< C^a + A^< B^a C^a]$$

The rules for foldings of products can also be cast into matrix multiplication form (Keldish matrices) by writing:

$$\hat{A} = \begin{pmatrix} A^r & A^{<,>} \\ 0 & A^a \end{pmatrix}$$

then in the above example

$$\hat{D} = \hat{A} \hat{B} \hat{C}$$

A table of rules for all the other combinations necessary to calculate the self-energy can be found in Haug/Jauho.

As an example let us study the linear response of the density of free conduction electrons on a scalar potential. Here the self-energy is absent and we have the equation:

$$\delta G(x_1, \tau_1; x_2, \tau_2) = \int_C d\tau_3 \int dx_3 G_0(x_1, \tau_1; x_3, \tau_3) U(x_3, \tau_3) G_0(x_3, \tau_3; x_2, \tau_2)$$

The density is directly described by the function  $n(x, t) = -iG^<(x, t; x, t)$ . For this quantity we obtain

$$\delta n(x, t) = \int dx_3 \int_{-\infty}^{+\infty} dt_3 [G_0^r(x - x_3, t - t_3) U(x_3, t_3) G_0^<(x_3 - x, t_3 - t) \\ G_0^<(x - x_3, t - t_3) U(x_3, t_3) G_0^a(x_3 - x, t_3 - t)]$$

where we already have used that the equilibrium Green functions depend only on the difference of arguments.

For a time-dependence of the scalar potential of the form

$$U(x, t) = \delta U \exp(iqx - i\Omega t)$$

and going over to a Fourier representation

$$G_0(x, t) = \frac{1}{Vol} \sum_k \int \frac{d\omega}{2\pi} G_0(k, \omega) \exp(ikx - i\omega t)$$

we find

$$\delta n(x, t) = -i\delta U \exp(iqx - i\Omega t) \frac{1}{Vol} \int \frac{d\omega}{2\pi} [G_0^r(k+q, \omega+\Omega)G_0^<(k, \omega) \\ G_0^<(k+q, \omega+\Omega)G_0^a(k, \omega)]$$

Now we use the equilibrium relation:

$$G^<(k, \omega) = if(\omega)A(k, \omega) = 2\pi if(\omega)\delta(\omega - \epsilon_k + \mu), \quad G^{r,a}(k\omega) = \frac{1}{\omega - \epsilon_k + \mu \pm i\delta}$$

and obtain

$$\delta n(x, t) = \frac{1}{Vol} \sum_k \frac{f(\epsilon_k - \mu) - f(\epsilon_{k+q} - \mu)}{\Omega + \epsilon_k - \epsilon_{k+q} + i\delta} U(x, t)$$

Here we recover the well-known Lindhard function.