Non-Equilibrium Green's functions and Transport

Quantum Matter Summer School - Materials & Concepts

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Contents

1 Time-dependent perturbation theory

We have a system with dynamics governed by a time-dependent Hamiltonian. We write it as

$$H(t) = H_0 + V(t) + H_{\text{int}}, \tag{1}$$

where H_0 is an "easy" independent particle Hamiltonian, $V(t)$ is a, possibly, time-dependent single-particle term and H_{int} takes into account interactions between the particles. The initial state of the system, at a reference time t_0, is described by the density matrix $\rho(t_0)$. Always this assumption can be relaxed, we will assume that initial state if the grand-canonical density matrix for the "easy" Hamiltonian H_0. Therefore, we have

$$\rho(t_0) = \rho_0 = \frac{1}{Z_0} e^{-\beta(H_0 - \mu N)}, \tag{2}$$

where μ is the chemical potential and $Z_0 = \text{Tr}\left[e^{-\beta(H_0-\mu N)}\right]$ is the partition function. We will assume that after the time t_0 a time dependent perturbation is turned on, which is included in $V(t)$. We will treat $V(t) + H_{\text{int}}$ as a perturbation. Our goal is to develop a perturbation scheme to evaluate the expectation value of a certain observable O at times $t > t_0$. That is we want to evaluate

$$\langle O \rangle (t) = \text{Tr}\left[\rho(t) O\right], \tag{3}$$

where $\rho(t)$ is the density matrix in the Schrödinger picture, obbeys

$$i\hbar \frac{d}{dt}\rho(t) = \left[H(t), \rho(t)\right], \tag{4}$$

which is the Schrödinger equation for the density matrix.

1.1 The interaction picture

We can write $\rho(t)$ as

$$\rho(t) = U(t, t_0)\, \rho(t_0)\, U(t_0, t), \tag{5}$$

where $U(t, t_0)$ is the time-evolution operator, which is obeys the equations

$$i\hbar \frac{\partial}{\partial t} U(t, t') = H(t) U(t, t'), \tag{6}$$

$$-i\hbar \frac{\partial}{\partial t'} U(t, t') = U(t, t')\, H(t'), \tag{7}$$

with initial condition $U(t, t) = 1$. The evolution operator also satisfies $U(t, t_1)\, U(t_1, t') = U(t, t')$ and $U^{-1}(t, t') = U^{\dagger}(t, t') = U(t', t)$.

In order to do perturbation theory on $V(t) + H_{\text{int}}$, we will switch to the interaction picture. This is achieved by writing the time-evolution operator as

$$U(t, t') = U_0(t, t_0)\, S(t, t')\, U(t_0, t'), \tag{8}$$

where $U_0(t, t') = e^{-\frac{i}{\hbar} H_0 (t - t')}$ is the time-evolution operator due to the "easy" Hamiltonian. It is easy to see that $S(t, t')$ obeys the equations

$$i\hbar \frac{\partial}{\partial t} S(t, t') = W(t) U(t, t'), \tag{9}$$

$$-i\hbar \frac{\partial}{\partial t'} S(t, t') = U(t, t')\, W(t'), \tag{10}$$

where

$$W(t) = U_0(t_0, t)\left[V(t) + H_{\text{int}}\right] U(t, t_0), \tag{11}$$

is the perturbation in the interaction picture. Eqs. (9) and (10) are supplemented by the initial condition $S(t,t) = 1$. The solution for $S(t,t')$ can be formally written as

$$S(t,t') = \begin{cases} Te^{-\frac{i}{\hbar}\int_{t'}^{t} dt_1 W(t_1)}, & t > t' \\ \bar{T}e^{\frac{i}{\hbar}\int_{t}^{t'} dt_1 W(t_1)}, & t < t' \end{cases}, \tag{12}$$

where T is the time-ordering operator and $\bar{T}$ is the anti-time-ordering operator. These act as

$$T\left[A(t_1)B(t_2)\right] = \begin{cases} A(t_1)B(t_2), & t_1 > t_2 \\ \zeta B(t_2)A(t_1), & t_1 < t_2 \end{cases}, \tag{13}$$

$$\bar{T}\left[A(t_1)B(t_2)\right] = \begin{cases} \zeta B(t_2)A(t_1), & t_1 > t_2 \\ A(t_1)B(t_2), & t_1 < t_2 \end{cases}, \tag{14}$$

with the factor $\zeta = -1$ for fermionic operators or $\zeta = +1$ for bosonic operators (or even number of fermionic operators).

Therefore, we can write in terms of the S operator

$$\langle O\rangle(t) = \text{Tr}\left[\rho(t_0)S(t_0,t)O(t)S(t,t_0)\right], \tag{15}$$

where $O(t) = U_0(t,t_0)O(t)U_0(t,t_0)$ is the operator in the interaction picture. Assuming that $\rho(t_0) = \rho_0 = e^{-\beta(H_0-\mu N)}/Z_0$ we obtain

$$\langle O\rangle(t) = \langle S(t_0,t)O(t)S(t,t_0)\rangle_0, \tag{16}$$

where $\langle ...\rangle_0 = \text{Tr}\left[\rho_0 ...\right]$ is the expectation value with respect to ρ_0.

More explicitly, expanding the S-operator in Taylor series we obtain

$$\begin{aligned}\langle O\rangle(t) = \sum_{n,m}\frac{1}{n!m!}\left(\frac{i}{\hbar}\right)^n\left(-\frac{i}{\hbar}\right)^m\int_{t_0}^{t}dt_1...\int_{t_0}^{t}dt_n\int_{t_0}^{t}dt'_1...\int_{t_0}^{t}dt'_m\times \\ \times\left\langle\bar{T}\left[W(t_1)...W(t_n)\right]O(t)T\left[W(t'_1)...W(t'_n)\right]\right\rangle_0.\end{aligned} \tag{17}$$

We have reduced the problem to the evaluation of a series of products of operators with respect to the the "easy" density matrix.

1.2 Wick's theorem

Now we notice that after time-ordering, the expectation values in Eq. (17), reduce to the expectation value of strings of creation/annihilation operators, such that

$$\left\langle a^{\nu_1}_{n_1}(t_1)a^{\nu_2}_{n_2}(t_2)...a^{\nu_N}_{n_N}(t_N)\right\rangle_0, \tag{18}$$

where $a^{\dagger}_{n_i}(t_i) = a^{+}_{n_i}(t_i)$ is a creation operator and $a_{n_i}(t_i) = a^{-}_{n_i}(t_i)$ is an annihilation. Since the expectation value is taken with respect to a density matrix of independent particles, it can be evaluated using Wick's theory. Wick's theorem states that for an even number of operators we have

$$\left\langle a^{\nu_1}_{n_1}a^{\nu_2}_{n_2}...a^{\nu_N}_{n_N}\right\rangle_0 = \sum_{\text{pairings}}\zeta^P\left\langle a^{\nu_{P(1)}}_{n_{P(1)}}a^{\nu_{P(2)}}_{n_{P(2)}}\right\rangle_0...\left\langle a^{\nu_{P(N-1)}}_{n_{P(N-1)}}a^{\nu_{P(N)}}_{n_{P(N)}}\right\rangle_0, \tag{19}$$

where we sum over all possible combinations of the N operators and P is the parity of the permutation that brings the operators in the order appearing in the LHS into the order of the operators in each

term of the RHS, with $\zeta = +1$ for bosons and ζ =-1 for fermions. Furthermore, in the absence of superconductivity, the only non-zero expecation values are of the form $\langle a^\dagger_{n_i} a_{n_j} \rangle_0$ and $\left\langle a_{n_i} a^\dagger_{n_j} \right\rangle_0$. Wick's theorem can be understood in the following way: (i) For independent particles, the expectation value of a string of operators should only depend on single-particles properties. (ii) Single particle properties are encoded into expectation values of the form $\langle a^{\nu_i}_{n_i} a^{\nu_j}_{n_j} \rangle_0$. (iii) Therefore, the expectation value of a string or operators should factorize into products of pairs of operators, $\langle a^{\nu_i}_{n_i} a^{\nu_j}_{n_j} \rangle_0$. (iv) Since the particles are identical, we should consider all possible ways of pairings of the operators. (v) Finally, we should take into account the fermionic/bosonic nature of the operators for each possible factorization, we can a $\pm$ sign for each possible factorization. Since bosons commute, we always get a $+$ sign. For fermions, we get $\pm$ sign for each term, depending on the number of operator commutations that had to be performed to bring the operators in the order of each term. Now let us see an example:

Let us compute

$$\left\langle c_1 c_2^\dagger c_3^\dagger c_4 \right\rangle_0 \tag{20}$$

where all the operators are fermionic. According to Eq. (19), we have

$$\begin{aligned} \left\langle c_1 c_2^\dagger c_3^\dagger c_4 \right\rangle_0 = & \left\langle c_1 c_2^\dagger \right\rangle_0 \langle c_3 c_4 \rangle_0 \\ & - \left\langle c_1 c_3^\dagger \right\rangle \left\langle c_2^\dagger c_4 \right\rangle_0 \\ & + \langle c_1 c_4 \rangle_0 \left\langle c_2^\dagger c_3^\dagger \right\rangle_0 . \end{aligned} \tag{21}$$

In the first term, we get $+$ sign, because we did not alter the order of the operators. In the second term, we get a minus sign, because we made the anti-commutation $c_2^\dagger c_3^\dagger \to -c_3^\dagger c_2^\dagger$. Finally, in the last term, we get a plus sign due to the commutations: $c_1 c_2^\dagger c_3^\dagger c_4 \to -c_1 c_2^\dagger c_4 c_3^\dagger \to (-1)^2 c_1 c_4 c_2^\dagger c_3^\dagger$. Furthermore, using the fact that $\langle c_1 c_4 \rangle_0 = \left\langle c_2^\dagger c_3^\dagger \right\rangle_0 = 0$, we get two terms

$$\begin{aligned} \left\langle c_1 c_2^\dagger c_3^\dagger c_4 \right\rangle_0 = & \left\langle c_1 c_2^\dagger \right\rangle_0 \langle c_3 c_4 \rangle_0 \\ & - \left\langle c_1 c_3^\dagger \right\rangle \left\langle c_2^\dagger c_4 \right\rangle_0 . \end{aligned} \tag{22}$$

Representing expectation values of the two operators, a contraction of two operators, with the notation

$$\left\langle a^{\nu_i}_{n_i} a^{\nu_j}_{n_j} \right\rangle_0 = \overbrace{a^{\nu_i}_{n_i} a^{\nu_j}_{n_j}} \tag{23}$$

We can write Eq. (22) as

$$\left\langle c_1 c_2^\dagger c_3^\dagger c_4 \right\rangle_0 = \overbrace{c_1 c_2^\dagger} \overbrace{c_3^\dagger c_4} + \overbrace{c_1 \overbrace{c_2^\dagger c_3^\dagger} c_4} \tag{24}$$

with the understanding that when reshuffling the operators to bring contracted operators next to each other, we obtain a -1 whenever we commute two fermionic operators. A simple way to determine the sign, in the case of fermions, corresponding to each contraction is to count the number of intersecting lines, corresponding to contractions of fermionic operators. If the number of intersections is even, we get a $+$ sign; if the number is odd, we get a $-$ sign.

A complete proof of Wick's theorem can be found in Appendix A.

1.3 Contour ordering

Now, armed with Wick's theorem, we know how to evaluate each term in the perturbative expansion of Eq. (17). However, it still have a double Taylor expansion, instead of a single one, which would be more desirable. To achieve such a single expansion, we start by noticing that in the products

$$\left\langle \bar{T} \left[W(t_1) ... W(t_n) \right] O(t) T \left[W(t'_1) ... W(t'_n) \right] \right\rangle_0$$

from left to right, the operotors first appear all time-ordered and then all anti-time-ordered. We can consider a directed double-time contour, C, that goes first, forwards, from t_0 to $t_{\max}$ (where $t_{\max}$ is greater than any t we are interested) and then, backwards, from $t_{\max}$ to t_0. Such double-time contour can be paremetrized by its arclength, s, that goes from 0 to $2\left(t_{\max}-t_0\right)$, and

$$t_C(s)=\begin{cases} t_0+s, & s\in[0,t_{\max}-t_0] \\ t_{\max}-\left(s-t_{\max}+t_0\right), & s\in[t_{\max}-t_0,2\left(t_{\max}-t_0\right)] \end{cases}. \tag{25}$$

Therefore we write

$$C=C^{+}\cup C^{-},$$

where $C^{+/-}$ is the forward/backwards contour. Introducing the C-contour-ordering operator as

$$T_C\left[A(s_1)B(s_2)\right]=\begin{cases} A(s_1)B(s_2), & s_1>s_2 \\ \zeta B(s_2)A(s_1), & s_1<s_2 \end{cases}. \tag{26}$$

Noticing that in C^{+} C-ordering corresponds to time-ordering, while in C^{-} C-ordering corresponds to anti-time-ordering, we can write

$$\begin{aligned} \langle O\rangle(t) &= \langle S(t_0,t)O(t)S(t,t_0)\rangle_0 \\ &= \langle S(t_0,t)S(t,t_{\max})S(t_{\max},t)O(t)S(t,t_0)\rangle_0 \\ &= \langle T_C S(t_0,t)S(t,t_{\max})S(t_{\max},t)O(t)S(t,t_0)\rangle_0 \\ &= \langle T_C S(t_0,t)S(t,t_{\max})S(t_{\max},t)S(t,t_0)O(t)\rangle_0 \\ &= \langle T_C S_C(t_0,t_0)O(t)\rangle_0 , \end{aligned}$$

where we introduced

$$S_C(t_0,t_0)=T_C\exp\left[-\frac{i}{\hbar}\int_C dsW(s)\right], \tag{27}$$

and $W(s)\equiv W(t_C(s))$. One is free to take $t_{\max}\to\infty$. We point out that all that the operator T_C is doing is keeping the booking of which operators appear time-ordered or anti-time-ordered. If one is not interested in transient dynamics, we can take the limit $t_0\to-\infty$, in which case, C is usually refereed to as the Schwinger-Keldysh contour.

With this trick, we obtain a single perturbative series expansion for $\langle O\rangle(t)$:

$$\begin{aligned} \langle O\rangle(t) &= \langle T_C S_C(t_0,t_0)O(t)\rangle_0 \\ &= \sum_n \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_C ds_1 ... \int_C ds_n \left\langle T_C W(s_1)...W(s_n)O(t)\right\rangle_0 . \end{aligned} \tag{28}$$

The price we have to pay is that the integrals $\int_C ds_i$ are taken over the double-time contour C.

2 Real-time Green's functions

2.1 Time-ordered, anti-time-ordered, greater and lesser Green's functions

When applying Wick's theorem to terms like

$$\left\langle \bar{T}\left[W(t_1)...W(t_n)\right]O(t)T\left[W(t_1')...W(t_n')\right]\right\rangle_0$$

we obtain different kinds of contractions: (i) contractions between two operators that are time-ordered, (ii) two operators that are anti-time ordered, (ii) contractions between two operators that have a fixed

order. For this reason, we introduce the following kinds of Green's functions

$$\text{Time-ordered Green's function: } G^T_{ab}(t,t') = -\frac{i}{\hbar}\left\langle T\hat{c}_a(t)\hat{c}^\dagger_b(t)\right\rangle, \tag{29}$$

$$\text{Anti-time-ordered Green's function: } G^{\bar{T}}_{ab}(t,t') = -\frac{i}{\hbar}\left\langle \bar{T}\hat{c}_a(t)\hat{c}^\dagger_b(t)\right\rangle, \tag{30}$$

$$\text{Greater Green's function: } G^{>}_{ab}(t,t') = -\frac{i}{\hbar}\left\langle \hat{c}_a(t)\hat{c}^\dagger_b(t)\right\rangle, \tag{31}$$

$$\text{Lesser Green's function: } G^{<}_{ab}(t,t') = -\zeta\frac{i}{\hbar}\left\langle \hat{c}^\dagger_b(t)\hat{c}_a(t)\right\rangle, \tag{32}$$

where the operators $\hat{O}(t)$ evolve in the Heisenberg picture with $H(t)$. One can also define corresponding unperturbed Green's functions, where the operators evolve with H_0, the "easy" Hamiltonian, and the expectation value is taken with respect to ρ_0. These unperturbed Green's function are usually denoted by a lower case g or with a index $_0$.

Notice that the 4 Green's functions are not linearly independent, but instead

$$G^{>}_{ab}(t,t') + G^{<}_{ab}(t,t') = G^{T}_{ab}(t,t') + G^{\bar{T}}_{ab}(t,t'). \tag{33}$$

2.2 Retarded and Advanced Green's functions

It is also normal to introduce the Retarded and Advanced Green's functions as

$$\text{Retarded Green's function: } G^R_{ab}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\left\langle\left[\hat{c}_a(t),\hat{c}^\dagger_b(t)\right]_\zeta\right\rangle, \tag{34}$$

$$\text{Advanced Green's function: } G^A_{ab}(t,t') = \frac{i}{\hbar}\Theta(t'-t)\left\langle\left[\hat{c}_a(t),\hat{c}^\dagger_b(t)\right]_\zeta\right\rangle, \tag{35}$$

where $[A,B]_\zeta = AB - \zeta BA$ is the commutator for the bosonic case, with $\zeta = +1$, of anti-commutator for the fermionic case, with $\zeta = -1$.

The Retarded and Advanced Green's functions are related to the previous ones as

$$G^R_{ab}(t,t') = G^T_{ab}(t,t') - G^<_{ab}(t,t') = G^>_{ab}(t,t') - G^{\bar{T}}_{ab}(t,t'), \tag{36}$$

$$G^A_{ab}(t,t') = G^T_{ab}(t,t') - G^>_{ab}(t,t') = G^<_{ab}(t,t') - G^{\bar{T}}_{ab}(t,t'). \tag{37}$$

We also have the two additional relations

$$G^R_{ab}(t,t') - G^A_{ab}(t,t') = G^>_{ab}(t,t') - G^<_{ab}(t,t'), \tag{38}$$

$$G^R_{ab}(t,t') + G^A_{ab}(t,t') = G^T_{ab}(t,t') - G^{\bar{T}}_{ab}(t,t'). \tag{39}$$

It is also useful to introduce the spectral function

$$\begin{aligned} A_{ab}(t,t') &= i\left[G^R_{ab}(t,t') - G^A_{ab}(t,t')\right] \\ &= \frac{1}{\hbar}\left\langle\left[\hat{c}_a(t),\hat{c}^\dagger_b(t)\right]_\zeta\right\rangle, \end{aligned} \tag{40}$$

which, as we will later see, for equilibrium system encodes the information about the spectrum of the system.

2.3 Green's functions for equilibrium independent particles

Let us assume we have a single particle Hamiltonian

$$H_0 = \sum_n \epsilon_n c^\dagger_n c_n. \tag{41}$$

Then the operators involve in time as $c_n(t) = e^{-i\epsilon_n t/\hbar} c_n$, $c_n(t) = e^{-i\epsilon_n t/\hbar} c_n$ and we have the expectation values $\left\langle c_n^\dagger c_n \right\rangle = n_\zeta(\epsilon_n)$ and $\left\langle c_n c_n^\dagger \right\rangle = 1 + \zeta n_\zeta(\epsilon_n)$, where $n_\zeta(\epsilon) = \left[e^{\beta(\epsilon-\mu)} - \zeta\right]^{-1}$. Therefore, we obtain

$$g_n^>(t,t') = -\frac{i}{\hbar}\left[1 + \zeta n(\epsilon_n)\right] e^{-i\epsilon_n\left(t-t'\right)/\hbar}, \tag{42}$$

$$g_n^<(t,t') = -\frac{i}{\hbar}\zeta n(\epsilon_n) e^{-i\epsilon_n\left(t-t'\right)/\hbar}, \tag{43}$$

$$g_n^R(t,t') = -\frac{i}{\hbar}\Theta(t-t') e^{-i\epsilon_n\left(t-t'\right)/\hbar}, \tag{44}$$

$$g_n^A(t,t') = \frac{i}{\hbar}\Theta(t'-t) e^{-i\epsilon_n\left(t-t'\right)/\hbar}. \tag{45}$$

We see that the Green's functions are only a function of the time difference $t - t'$. This is a general feature of translationally invariant systems (either in thermal equilibrium or in a stationary system). Making a Fourier transform in time

$$g(t-t') = \int \frac{d\omega}{2\pi} e^{-i\omega t} g(\omega), \tag{46}$$

$$g(\omega) = \int dt e^{i\omega t} g(t), \tag{47}$$

we obtain

$$g_n^>(\omega) = -i\left[1 + \zeta n(\epsilon_n)\right] 2\pi\delta\left(\hbar\omega - \epsilon_n\right), \tag{48}$$

$$g_n^<(\omega) = -i\zeta n(\epsilon_n) 2\pi\delta\left(\hbar\omega - \epsilon_n\right) \tag{49}$$

$$g_n^R(\omega) = \frac{1}{\hbar\omega + i0^+ - \epsilon_n}, \tag{50}$$

$$g_n^A(\omega) = \frac{1}{\hbar\omega - i0^+ - \epsilon_n}. \tag{51}$$

Notice that in order to evaluate $g_n^{R/A}(\omega)$ one needs to regularize the integration over time. For $g^R(\omega)$ this is done by multiplying the integrand by $e^{-\eta t}$ in the limit of $\eta \to 0^+$, while for $g^A(\omega)$ the integrand is multiplied by $e^{+\eta t}$. The spectral function is given by

$$\begin{aligned} a_n(\omega) &= i\left[g_n^R(\omega) - g_n^A(\omega)\right] \\ &= 2\pi\delta\left(\hbar\omega - \epsilon_n\right) \end{aligned} \tag{52}$$

2.4 Thermodynamic equilibrium: the fluctuation-dissipation theorem

Notice that for independent particles in thermal equilibrium, the lesser and greater green's functions can be expressed in terms of the spectral function:

$$g_n^>(\omega) = -i\left[1 + \zeta n_\zeta(\omega)\right] a_n(\omega),$$
$$g_n^<(\omega) = -i\zeta n_\zeta(\omega) a_n(\omega).$$

This is actually a general property of equilibrium systems. Ultimately, this is due to the fact that in equilibrium systems, both the state of the system, described by the canonical density matrix ρ, and the time-evolution of the system are both determined by the Hamiltonian H. The spectral function encodes information about the spectrum of the system and therefore all other Green's functions can be written in terms of it.

This relation property of system in thermodynamic equilibrium is the Fluctuation-Dissipation theorem, which states that

$$G_{ab}^>(\omega) = -i\left[1 + \zeta n_\zeta(\omega)\right] A_{ab}(\omega), \tag{53}$$

$$G_{ab}^<(\omega) = -i\zeta n_\zeta(\omega) A_{ab}(\omega), \tag{54}$$

where $n_\zeta(\epsilon) = \left[e^{\beta(\epsilon-\mu)} - \zeta\right]^{-1}$ is the Bose-Einstein (for $\zeta = +1$) of Fermi-Dirac (for $\zeta = -1$) distribution function.

3 Contour ordered Green's function

3.1 Definition

Motivated by the fact that in $\langle O\rangle(t) = \langle T_C S_C(t_0,t_0)O(t)\rangle_0$ all operators appear ordered along the contour C we introduce the contour ordered Green's function

$$G(s,s') = -\frac{i}{\hbar}\left\langle T_C \hat{c}_a(s)\hat{c}_b^\dagger(s')\right\rangle, \tag{55}$$

where the operators $\hat{O}(s)$ evolve along the contour following the Heisenberg equation in the C contour

$$\frac{d}{ds}\hat{O}(s) = \frac{i}{\hbar}\left[\hat{H}(s),\hat{O}(s)\right] \tag{56}$$

with the C contour evolution operator

$$\hat{O}(s) = U_C(s_0,s)OU_C(s,s_0), \tag{57}$$

where $U_C(s,s')$ obeys the Schrödinger equation in the contour

$$i\hbar\frac{d}{ds}U_C(s,s') = H(s)U(s,s') \tag{58}$$

$$-i\hbar\frac{d}{ds'}U_C(s,s') = U(s,s')H(s') \tag{59}$$

where $H(s) = H(t_C(s))$. We will often write $t^\pm$ to refer to a time variable in the $C^\pm$ contour. We notice that $\hat{O}(t^-) = \hat{O}(t^+)$. To see this, we start by noticing that

$$\hat{O}(t^-) = U_C(t_0,t^-)OU_C(t^-,t_0). \tag{60}$$

Now we write the contour evolution operator as

$$\begin{aligned} U_C(t^-,t_0) &= U_C(t^-,t_{\max})U_C(t_{\max},t^+)U_C(t^+,t_0)\\ &= U(t,t_{\max})U(t_{\max},t)U(t,t_0)\\ &= U_C(t^+,t_0). \end{aligned} \tag{61}$$

Once again, we see that T_C is just a bookkeeping tool to take into account the ordering of the operators. Therefore the contour ordered Green's function is just a convenient tool to encode different kinds of Green's functions.

3.1.1 Relation to real-time Green's functions

Depending on whether the arguments of $G^C_{ab}(s,s')$ lie in the C^+ or C^- contour, the contour ordered Green's functions deduces to different real-time Green's functions. Namelly

$$G(t_+,t'_+) = -\frac{i}{\hbar}\left\langle T_C \hat{c}_a(t_+)\hat{c}_b^\dagger(t'_+)\right\rangle = -\frac{i}{\hbar}\left\langle T \hat{c}_a(t)\hat{c}_b^\dagger(t')\right\rangle = G^T_{ab}(t,t'), \tag{62}$$

$$G(t_+,t'_-) = -\frac{i}{\hbar}\left\langle T_C \hat{c}_a(t_+)\hat{c}_b^\dagger(t'_-)\right\rangle = -\zeta\frac{i}{\hbar}\left\langle \hat{c}_b^\dagger(t'_-)\hat{c}_a(t_+)\right\rangle = G^<_{ab}(t,t'), \tag{63}$$

$$G(t_-,t'_+) = -\frac{i}{\hbar}\left\langle T_C \hat{c}_a(t_-)\hat{c}_b^\dagger(t'_+)\right\rangle = -\frac{i}{\hbar}\left\langle \hat{c}_a(t_-)\hat{c}_b^\dagger(t'_+)\right\rangle = G^>_{ab}(t,t'), \tag{64}$$

$$G(t_-,t'_-) = -\frac{i}{\hbar}\left\langle T_C \hat{c}_a(t_-)\hat{c}_b^\dagger(t'_-)\right\rangle = -\frac{i}{\hbar}\left\langle \bar{T} \hat{c}_a(t)\hat{c}_b^\dagger(t')\right\rangle = G^{\bar{T}}_{ab}(t,t'), \tag{65}$$

where we used the facts that then both variables lie in C^+ contour-ordering reduces to time-ordering, when both variables lie in C^- contour-ordering reduces to anti-time-ordering and when one variable lies in C^+ and the other in C^-, contour-ordering always puts the operator in C^- on the left.

3.2 Perturbation by a single-particle potential

We will now focus on the problem of a system that is governed by an independent particle Hamiltonian

$$H(t) = H_0 + V(t), \tag{66}$$

$$H_0 = \sum_{ab} h_{ab} c_a^\dagger c_b, \tag{67}$$

$$V(t) = \sum_{ab} V_{ab}(t) c_a^\dagger c_b. \tag{68}$$

We will treat $V(t)$ as a perturbation. We want to determine the equation of motion obeyed by $G^C_{ab}(s_1, s_2)$. Recalling that

$$G(s_1, s_2) = \Theta(s_1 - s_2) \left(-\frac{i}{\hbar}\right) \left\langle \hat{c}_a(s_1) \hat{c}_b^\dagger(s_2) \right\rangle + \Theta(s_2 - s_1) \left(-\zeta \frac{i}{\hbar}\right) \left\langle \hat{c}_b^\dagger(s_2) \hat{c}_a(s_1) \right\rangle, \tag{69}$$

we can calculate

$$\begin{aligned} i\hbar \frac{\partial}{\partial s} G(s_1, s_2) = {} & \delta(s_1 - s_2) \left\langle \hat{c}_a(s_1) \hat{c}_b^\dagger(s_2) \right\rangle - \delta(s_2 - s_1) \zeta \left\langle \hat{c}_b^\dagger(s_2) \hat{c}_a(s_1) \right\rangle \\ & + \left(-\frac{i}{\hbar}\right) \left\langle \frac{\partial}{\partial s} \hat{c}_a(s_1) \hat{c}_b^\dagger(s_2) \right\rangle. \end{aligned} \tag{70}$$

In the first line, we can set $s' = s$ in the operators and thus obtain a (anti-)commutator. For the second term, we obtain

$$\begin{aligned} \frac{\partial}{\partial s} \hat{c}_a(s) &= \left[\hat{H}(s), \hat{c}_a(s)\right] \\ &= \sum_{bc} \left(h_{bc} + V_{bc}(s)\right) \left[\hat{c}_b^\dagger(s) \hat{c}_c(s), \hat{c}_a(s)\right] \\ &= -\sum_{bc} \left(h_{bc} + V_{bc}(s)\right) \delta_{ba} \hat{c}_c(s) \\ &= -\sum_{b} \left(h_{ab} + V_{ab}(s)\right) \hat{c}_b(s). \end{aligned} \tag{71}$$

Therefore, we obtain

$$\sum_c \left[i\hbar \frac{\partial}{\partial s} \delta_{ac} - h_{ac} \right] G_{cb}(s_1, s_2) = \delta(s_1 - s_2) \delta_{ab} + \sum_c V_{ac}(s_1) G(s_1, s_2). \tag{72}$$

The integral form of this differential equation is

$$G_{ab}(s_1, s_2) = g_{ab}(s_1, s_2) + \sum_{a_3 b_3} \int_C ds_3 g_{aa_3}(s_1, s_3) V_{a_3 b_3}(s_3) G_{b_3 b}(s_3, s_2), \tag{73}$$

where $g_{ab}(s_1, s_2)$ is the contour ordered Green's function for the unperturbed Hamiltonian H_0. This is nothing more than a Lipmann-Schwinger equation for the contour ordered Green's function.

Now we notice that the the integration over the contour C can be written as

$$\int_C ds_3 (...) = \int dt_3 \left[(...)_{s_3 = t_3^+} - (...)_{s_3 = t_3^-} \right]. \tag{74}$$

Now we go back to real-time Green's functions by replacing $(s_1, s_2) \to (t_1^{\varsigma_1}, t_2^{\varsigma_2})$, such that $G(s_1, s_2) \to G_{ab}(t_1^{\varsigma_1}, t_2^{\varsigma_2})$, where where the indices ς_1, ς_2 take values $\pm$, indicating if the variables lies in the $C^\pm$ contour. We will refer to this indices as Keldysh indices. Therefore we can write

$$G_{ab}(t_1^{\varsigma_1}, t_2^{\varsigma_2}) = g_{ab}(t_1^{\varsigma_1}, t_2^{\varsigma_2}) + \sum_{a_3 b_3} \sum_{\varsigma_3} \int dt_3 g_{aa_3}(t_1^{\varsigma_1}, t_3^{\varsigma_3}) \varsigma_3 V_{a_3 b_3}(t_3^{\varsigma_3}) G_{b_3 b}(t_3^{\varsigma_3}, t_2^{\varsigma_2}). \tag{75}$$

This can be recast into a matrix form as

$$\begin{bmatrix} G^T_{ab}(t_1,t_2) & G^<_{ab}(t_1,t_2) \\ G^>_{ab}(t_1,t_2) & G^{\bar{T}}_{ab}(t_1,t_2) \end{bmatrix} = \begin{bmatrix} g^T_{ab}(t_1,t_2) & g^<_{ab}(t_1,t_2) \\ g^>_{ab}(t_1,t_2) & g^{\bar{T}}_{ab}(t_1,t_2) \end{bmatrix} + \\ + \sum_{a_3 b_3} \int dt_3 \begin{bmatrix} g^T_{aa_3}(t_1,t_3) & g^<_{aa_3}(t_1,t_3) \\ g^>_{aa_3}(t_1,t_3) & g^{\bar{T}}_{aa_3}(t_1,t_3) \end{bmatrix} \begin{bmatrix} V_{a_3 b_3}(t_3) & 0 \\ 0 & -V_{a_3 b_3}(t_3) \end{bmatrix} \begin{bmatrix} G^T_{b_3 b}(t_3,t_2) & G^<_{b_3 b}(t_3,t_2) \\ G^>_{b_3 b}(t_3,t_2) & G^{\bar{T}}_{b_3 b}(t_3,t_2) \end{bmatrix}, \tag{76}$$

where we recalled the relation between the contour ordered Green's functions and the different real-time Green's functions Eq. (62)-(65).

3.3 Linear transformations in Keldysh indices

As we have stated before, the 4 Green's functions G^T, $G^<$, $G^>$ and $G^{\bar{T}}$ are not all linearly independent, but are instead related via $G^T + G^{\bar{T}} = G^> + G^<$. This means that it should be possible to eliminate one of the Green's functions from Eq. (76). This can be achieve by applying a linear transformation to the matrix in Keldysh space

$$\begin{bmatrix} G^T_{ab}(t_1,t_2) & G^<_{ab}(t_1,t_2) \\ G^>_{ab}(t_1,t_2) & G^{\bar{T}}_{ab}(t_1,t_2) \end{bmatrix} \to L^{-1} \cdot \begin{bmatrix} G^T_{ab}(t_1,t_2) & G^<_{ab}(t_1,t_2) \\ G^>_{ab}(t_1,t_2) & G^{\bar{T}}_{ab}(t_1,t_2) \end{bmatrix} \cdot Q^{-1}.$$

We will write Eq. (76) in a compact notation, representing the Green's function via

$$G^{a_1}{}_{b_2} = G_{a_1 b_2}(t_1^{\varsigma_1}, t_2^{\varsigma_2}), \tag{77}$$

where all the indices a_1, t_1, ς_1 are encoded in the superindex a_1 (abusing the notation a bit). With this notation, we can write the Lippmann-Schwinger equation as

$$G^{a_1}{}_{b_2} = g^{a_1}{}_{b_2} + g^{a_1}{}_{a_3} V^{a_3}{}_{b_3} G^{b_3}{}_{b_2}, \tag{78}$$

where repeated indices are summed over (i.e., summed over orbital index a, integrated over time and summed over Keldysh indices). In this notation, we have

$$V^a{}_b \to \sigma^z_{\varsigma_a \varsigma_b} V_{ab}(t_a) \delta(t_a - t_b)$$

where we have attributed a structure in Keldysh space to the potential. Using Matrix notation we can write

$$G = g + g \cdot V \cdot G.$$

Performing the linear transformation in Keldysh indices, we obtain

$$\begin{aligned} \hat{G} &= L^{-1} \cdot G \cdot Q^{-1} \\ &= L^{-1} \cdot [g + g \cdot V \cdot G] \cdot Q^{-1} \\ &= L^{-1} \cdot g \cdot Q^{-1} + L^{-1} \cdot g \cdot V \cdot G \cdot Q^{-1} \\ &= \left(L^{-1} \cdot g \cdot Q^{-1}\right) + \left(L^{-1} \cdot g \cdot Q^{-1}\right) \cdot (Q \cdot V \cdot L) \cdot \left(L^{-1} \cdot G \cdot Q^{-1}\right) \\ &= \hat{g} + \hat{g} \cdot \hat{V} \cdot \hat{G}. \end{aligned}$$

Therefore, if we make a linear transformation in the Keldysh indices of a Green's function as

$$G^a{}_b \to \hat{G}^a{}_b = \left(L^{-1}\right)^a{}_{a'} \cdot G^{a'}{}_{b'} \cdot \left(Q^{-1}\right)^{b'}{}_b, \tag{79}$$

the potential changes as

$$V^a{}_b \to \hat{V}^a{}_b = Q^a{}_{a'} V^{a'}{}_{b'} L^{b'}{}_b. \tag{80}$$

Now we have a great freedom great freedom in the choice of the matrices L and Q. Some common choices are:

3.3.1 *RAL* representation

In this representation, one chooses

$$L^{-1} = \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix}, \qquad Q^{-1} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}, \tag{81}$$

and

$$L = \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix}, \qquad Q = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}. \tag{82}$$

With this transformation, we obtain

$$\begin{aligned} L^{-1} \cdot \begin{bmatrix} G^T & G^< \\ G^> & G^{\bar{T}} \end{bmatrix} \cdot Q^{-1} &= \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \cdot \begin{bmatrix} G^T & G^< \\ G^> & G^{\bar{T}} \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \\ &= \begin{bmatrix} G^T - G^< & G^< \\ G^T + G^{\bar{T}} - G^> - G^< & G^< - G^{\bar{T}} \end{bmatrix} \\ &= \begin{bmatrix} G^R & G^< \\ 0 & G^A \end{bmatrix}. \end{aligned}$$

We also notice that a single-particle potential changes as

$$Q \cdot \sigma^z \cdot L = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

In this representation, we only work with retarded, advanced and lesser Green's functions.

3.3.2 *RAG* representation

In this representation, one chooses

$$L^{-1} = \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix}, \qquad Q^{-1} = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}, \tag{83}$$

with

$$L = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \qquad Q = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}. \tag{84}$$

The Green's function therefore changes as

$$\begin{aligned} L^{-1} \cdot \begin{bmatrix} G^T & G^< \\ G^> & G^{\bar{T}} \end{bmatrix} \cdot Q^{-1} &= \begin{bmatrix} 1 & -1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} G^T & G^< \\ G^> & G^{\bar{T}} \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} \\ &= \begin{bmatrix} G^T - G^> & G^T - G^> - G^< + G^{\bar{T}} \\ G^> & G^> - G^{\bar{T}} \end{bmatrix} \\ &= \begin{bmatrix} G^A & 0 \\ G^< & G^R \end{bmatrix}. \end{aligned} \tag{85}$$

We also notice that a single-particle potential changes as

$$Q \cdot \sigma^z \cdot L = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{86}$$

In this representation, we only work with retarded, advanced and greater Green's functions.

3.3.3 *RAK* representation

The another common representation, we choose

$$L^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad Q^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}, \tag{87}$$

with

$$L = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \qquad Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}, \tag{88}$$

such that

$$\begin{aligned} L^{-1} \cdot \begin{bmatrix} G^T & G^< \\ G^> & G^{\bar{T}} \end{bmatrix} \cdot Q^{-1} &= \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} G^T & G^< \\ G^> & G^{\bar{T}} \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} \\ &= \frac{1}{2} \begin{bmatrix} \left(G^T - G^<\right) + \left(G^> - G^{\bar{T}}\right) & G^T + G^> + G^< + G^{\bar{T}} \\ 0 & \left(G^T - G^>\right) + \left(G^< - G^{\bar{T}}\right) \end{bmatrix} \\ &= \begin{bmatrix} G^R & G^K \\ 0 & G^A \end{bmatrix}, \end{aligned} \tag{89}$$

where we introduced the so called Keldysh Green's function

$$G^K_{ab}(t,t') = G^>_{ab}(t,t') + G^<_{ab}(t,t') = G^T_{ab}(t,t') + G^{\bar{T}}_{ab}(t,t'). \tag{90}$$

We also have that

$$Q \cdot \sigma^z \cdot L = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{91}$$

3.4 Dyson and Keldysh equations

Now let us assume we have an interacting system. It is possible to prove that in the perturbative expansion, terms that correspond to diagrams with disconnect parts do not contribute. As such, it is possible to reorganize the perturbative expansion as a Dyson equation in the C contour:

$$\begin{aligned} G_{ab}(s_1,s_2) = g_{ab}(s_1,s_2) &+ \sum_{a_3 b_3} \int_C ds_3 g_{aa_3}(s_1,s_3) V_{a_3 b_3}(s_3) G_{b_3 b}(s_3,s_2) \\ &+ \sum_{a_3 b_4} \int_C ds_3 \int_C ds_4 g_{aa_3}(s_1,s_3) \Sigma_{a_3 b_4}(s_3,s_4) G_{b_4 b}(s_4,s_2). \end{aligned} \tag{92}$$

where $\Sigma_{ab}(s,s')$ is the self-energy in the contour. Writing the integral in the contour as double integral over time

$$\int_C ds_i(...) = \sum_{\varsigma_i} \int dt_i \varsigma_i (...)_{s_i = t_i^{\varsigma_i}} \tag{93}$$

we obtain

$$\begin{aligned} G_{ab}(t_1^{\varsigma_1}, t_2^{\varsigma_2}) = g_{ab}(t_1^{\varsigma_1}, t_2^{\varsigma_2}) &+ \sum_{a_3 b_3} \sum_{\varsigma_3} \int dt_3 g_{aa_3}(t_1^{\varsigma_1}, t_3^{\varsigma_3}) \varsigma_3 V_{a_3 b_3}(t_3^{\varsigma_3}) G_{b_3 b}(t_3^{\varsigma_3}, t_2^{\varsigma_2}) \\ &+ \sum_{a_3 b_4} \sum_{\varsigma_3, \varsigma_4} g_{aa_3}(t_1^{\varsigma_1}, t_3^{\varsigma_3}) \varsigma_3 \Sigma_{a_3 b_4}(t_3^{\varsigma_3}, t_4^{\varsigma_4}) \varsigma_4 G_{b_3 b}(t_3^{\varsigma_3}, t_2^{\varsigma_2}). \end{aligned} \tag{94}$$

In matrix form this becomes

$$\begin{aligned}\begin{bmatrix} G^T_{ab}(t_1,t_2) & G^<_{ab}(t_1,t_2) \\ G^>_{ab}(t_1,t_2) & G^{\bar{T}}_{ab}(t_1,t_2) \end{bmatrix} &= \begin{bmatrix} g^T_{ab}(t_1,t_2) & g^<_{ab}(t_1,t_2) \\ g^>_{ab}(t_1,t_2) & g^{\bar{T}}_{ab}(t_1,t_2) \end{bmatrix} + \\ &+ \sum_{a_3b_3} \int dt_3 \begin{bmatrix} g^T_{aa_3}(t_1,t_3) & g^<_{aa_3}(t_1,t_3) \\ g^>_{aa_3}(t_1,t_3) & g^{\bar{T}}_{aa_3}(t_1,t_3) \end{bmatrix} V_{a_3b_3}(t_3)\sigma^z \begin{bmatrix} G^T_{b_3b}(t_3,t_2) & G^<_{b_3b}(t_3,t_2) \\ G^>_{b_3b}(t_3,t_2) & G^{\bar{T}}_{b_3b}(t_3,t_2) \end{bmatrix} \\ +\sum_{a_3b_4} \int dt_3 \int dt_4 \begin{bmatrix} g^T_{aa_3}(t,t_1) & g^<_{aa_3}(t,t_1) \\ g^>_{aa_3}(t,t_1) & g^{\bar{T}}_{aa_3}(t,t_1) \end{bmatrix} \sigma_z \begin{bmatrix} \Sigma^T_{a_3a_4}(t_3,t_4) & \Sigma^<_{a_3a_4}(t_3,t_4) \\ \Sigma^>_{a_3a_4}(t_3,t_4) & \Sigma^{\bar{T}}_{a_3a_4}(t_3,t_4) \end{bmatrix} \sigma_z \begin{bmatrix} G^T_{b_4b}(t_2,t') & G^<_{b_4b}(t_2,t') \\ G^>_{b_4b}(t_4,t') & G^{\bar{T}}_{b_4b}(t_2,t') \end{bmatrix}.\end{aligned} \tag{95}$$

Now we can perform a linear transformation in the Keldysh indices. Assuming that the self-energy satisfies

$$\Sigma^T_{ab}(t,t') + \Sigma^{\bar{T}}_{ab}(t,t') = \Sigma^>_{ab}(t,t') + \Sigma^<_{ab}(t,t'),$$

which is inherited from the properties of the Green's functions, we can also simplify the equation by eliminating one of the entries of the matrices. For example, by performing a linear transformation to the RAL representation, we obtain

$$\begin{aligned}\begin{bmatrix} G^R_{ab}(t_1,t_2) & G^<_{ab}(t_1,t_2) \\ 0 & G^A_{ab}(t_1,t_2) \end{bmatrix} &= \begin{bmatrix} g^R_{ab}(t_1,t_2) & g^<_{ab}(t_1,t_2) \\ 0 & g^A_{ab}(t_1,t_2) \end{bmatrix} + \\ &+ \sum_{a_3b_3} \int dt_3 \begin{bmatrix} g^R_{aa_3}(t_1,t_3) & g^<_{aa_3}(t_1,t_3) \\ 0 & g^A_{aa_3}(t_1,t_3) \end{bmatrix} V_{a_3b_3}(t_3) \begin{bmatrix} G^R_{b_3b}(t_3,t_2) & G^<_{b_3b}(t_3,t_2) \\ 0 & G^A_{b_3b}(t_3,t_2) \end{bmatrix} \\ +\sum_{a_3b_4} \int dt_3 \int dt_4 \begin{bmatrix} g^R_{aa_3}(t,t_1) & g^<_{aa_3}(t,t_1) \\ 0 & g^A_{aa_3}(t,t_1) \end{bmatrix} \sigma_z \begin{bmatrix} \Sigma^R_{a_3a_4}(t_3,t_4) & \Sigma^<_{a_3a_4}(t_3,t_4) \\ 0 & \Sigma^A_{a_3a_4}(t_3,t_4) \end{bmatrix} \sigma_z \begin{bmatrix} G^R_{b_4b}(t_2,t') & G^<_{b_4b}(t_2,t') \\ 0 & G^A_{b_4b}(t_2,t') \end{bmatrix}.\end{aligned} \tag{96}$$

From this we obtain the Dyson equation for the retarded and the advanced equations:

$$\boldsymbol{G}^R = \boldsymbol{g}^R + \boldsymbol{g}^R \cdot \boldsymbol{V} \cdot \boldsymbol{G}^R + \boldsymbol{g}^R \cdot \boldsymbol{\Sigma}^R \cdot \boldsymbol{G}^R \tag{97}$$

$$\boldsymbol{G}^A = \boldsymbol{g}^A + \boldsymbol{g}^A \cdot \boldsymbol{V} \cdot \boldsymbol{G}^A + \boldsymbol{g}^A \cdot \boldsymbol{\Sigma}^A \cdot \boldsymbol{G}^A \tag{98}$$

(using a compact notation where $\cdot$ represents integration over time and summation over orbital indices).

As for the lesser Green's function we obtain

$$\begin{aligned}\boldsymbol{G}^< = \boldsymbol{g}^< &+ \boldsymbol{g}^R \cdot \boldsymbol{V} \cdot \boldsymbol{G}^< + \boldsymbol{g}^< \cdot \boldsymbol{V} \cdot \boldsymbol{G}^A \\ &+ \boldsymbol{g}^R \cdot \boldsymbol{\Sigma}^R \cdot \boldsymbol{G}^< + \boldsymbol{g}^R \cdot \boldsymbol{\Sigma}^< \cdot \boldsymbol{G}^A + \boldsymbol{g}^< \cdot \boldsymbol{\Sigma}^A \cdot \boldsymbol{G}^A.\end{aligned} \tag{99}$$

We can act on this equation with the operator $i\hbar\partial_t - \boldsymbol{h}$. Using the fact that

$$(i\hbar\partial_t - \boldsymbol{h}) \cdot \boldsymbol{g}^R(t,t') = \delta(t-t') \tag{100}$$

$$(i\hbar\partial_t - \boldsymbol{h}) \cdot \boldsymbol{g}^<(t,t') = 0 \tag{101}$$

we obtain

$$(i\hbar\partial_t - \boldsymbol{h}) \cdot \boldsymbol{G}^< = \boldsymbol{V} \cdot \boldsymbol{G}^< + \boldsymbol{\Sigma}^R \cdot \boldsymbol{G}^< + \boldsymbol{\Sigma}^< \cdot \boldsymbol{G}^A. \tag{102}$$

Which we can write this as

$$\left(i\hbar\partial_t - \boldsymbol{h} - \boldsymbol{V} - \boldsymbol{\Sigma}^R\right) \cdot \boldsymbol{G}^< = \boldsymbol{\Sigma}^< \cdot \boldsymbol{G}^A. \tag{103}$$

Notice that if we act with $i\hbar\partial_t - \boldsymbol{h}$ on the Dyson equation for the retarded Green's function, we obtain

$$\left(i\hbar\partial_t - \boldsymbol{h} - \boldsymbol{V} - \boldsymbol{\Sigma}^R\right) \cdot \boldsymbol{G}^R = \mathbf{1}.$$

Therefore, we obtain

$$\boldsymbol{G}^{<} = \boldsymbol{C} + \boldsymbol{G}^{R} \cdot \boldsymbol{\Sigma}^{<} \cdot \boldsymbol{G}^{A}.$$

where

$$\left(i\hbar\partial_t - \boldsymbol{h} - \boldsymbol{V} - \boldsymbol{\Sigma}^{R}\right) \cdot \boldsymbol{C} = 0.$$

Since at $t, t' = t_0, t_0$ we must recover $\boldsymbol{G}^{<}(t_0, t_0)$ we have that

$$\begin{aligned}\boldsymbol{G}^{<}(t,t') = \boldsymbol{G}^{R}(t,t_0) \cdot \boldsymbol{G}^{<}(t_0,t_0) \cdot \boldsymbol{G}^{A}(t_0,t') \\ + \int dt_1 \int dt_2 \boldsymbol{G}^{R}(t,t_1) \cdot \boldsymbol{\Sigma}^{<}(t_1,t_2) \cdot \boldsymbol{G}^{A}(t_2,t').\end{aligned} \tag{104}$$

In interacting or open system, one expects that the system will lose memory of its initial state, $\lim_{t\to\infty} \boldsymbol{G}^{R}(t,t_0) = \lim_{t\to\infty} \boldsymbol{G}^{A}(t_0,t) = 0$. In that case, we have

$$\boldsymbol{G}^{<}(t,t') = \int dt_1 \int dt_2 \boldsymbol{G}^{R}(t,t_1) \cdot \boldsymbol{\Sigma}^{<}(t_1,t_2) \cdot \boldsymbol{G}^{A}(t_2,t').$$

which is the so called Keldysh equation.

3.5 Langreth Rules

Langreth's rules allow us to write results for contour ordered Green's functions, in terms of real-time Green's functions. Although it is always possible to work with time-ordered, anti-time-ordered, lesser and greater Green's functions, it is more common to represent results in terms of retarded, advanced and lesser/greater/Keldysh Green's functions. In the following, we will list some common Langreth's rules.

3.5.1 Convolution

In perturbative expansions, one commonly encounters convolutions of the form

$$C(s,s') = \int_C ds_1 A(s,s_1) B(s_1,s'), \tag{105}$$

where C, A and B and Green's functions/self-energies. We have already encountered this kind of convolution in the Dyson equation. We saw the result in the RAL representation. It is also possible to do a transformation to the RAG representation, the result is similar. One obtains

$$C^{\lessgtr}(t,t') = \int dt_1 \left[A^{R}(t,t_1)B^{\lessgtr}(t_1,t') + A^{\lessgtr}(t,t_1)B^{A}(t_1,t')\right]. \tag{106}$$

The retarded and advanced components are given by

$$C^{R/A}(t,t') = \int dt_1 A^{R/A}(t,t_1) B^{R/A}(t_1,t'). \tag{107}$$

3.5.2 Parallel product

It is also common to appear terms of the form

$$C(s,s') = A(s,s')B(s,s'). \tag{108}$$

In this case it is easy to obtain the greater and lesser components:

$$C^{>}(t,t') = C(t_-,t'_+) = A(t_-,t'_+)B(t_-,t'_+) = A^{>}(t,t')B^{>}(t,t'), \tag{109}$$

$$C^{<}(t,t') = C(t_+,t'_-) = A(t_+,t'_-)B(t_+,t'_-) = A^{<}(t,t')B^{<}(t,t'). \tag{110}$$

The time-ordered and anti-time-ordered components are obtained from

$$C^T(t,t') = C(t_+,t'_+) = A(t_+,t'_+)B(t_+,t'_+) = A^T(t,t')B^T(t,t') \tag{111}$$
$$C^{\bar{T}}(t,t') = C(t_-,t'_-) = A(t_-,t'_-)B(t_-,t'_-) = A^{\bar{T}}(t,t')B^{\bar{T}}(t,t') \tag{112}$$

Recalling that $G^R = G^T - G^<$, the retarded component can be obtained as

$$\begin{aligned} C^R(t,t') &= C^T(t,t') - C^<(t,t') \\ &= A^T(t,t')B^T(t,t') - A^<(t,t')B^<(t,t') \\ &= \left[A^R(t,t') + A^<(t,t')\right]\left[B^R(t,t') + B^<(t,t')\right] - A^<(t,t')B^<(t,t') \\ &= A^R(t,t')B^R(t,t') + A^<(t,t')B^R(t,t') + A^R(t,t')B^<(t,t'). \end{aligned} \tag{113}$$

Noticing that $A^R(t,t')B^A(t,t') = A^A(t,t')B^R(t,t') = 0$, it is also possible to write

$$\begin{aligned} C^R(t,t') &= A^R(t,t')B^R(t,t') + A^<(t,t')B^R(t,t') + A^R(t,t')B^<(t,t') \\ &= \left[A^R(t,t') - A^A(t,t') + A^<(t,t')\right]B^R(t,t') + A^R(t,t')B^<(t,t') \\ &= A^>(t,t')B^R(t,t') + A^R(t,t')B^<(t,t') \end{aligned} \tag{114}$$

or

$$\begin{aligned} C^R(t,t') &= A^R(t,t')B^R(t,t') + A^<(t,t')B^R(t,t') + A^R(t,t')B^<(t,t') \\ &= A^R(t,t')\left[B^R(t,t') - B^A(t,t') + B^<(t,t')\right] + A^<(t,t')B^R(t,t') \\ &= A^R(t,t')B^>(t,t') + A^<(t,t')B^R(t,t'). \end{aligned} \tag{115}$$

Summarizing, we have

$$C^R(t,t') = A^R(t,t')B^R(t,t') + A^<(t,t')B^R(t,t') + A^R(t,t')B^<(t,t') \tag{116}$$
$$= A^>(t,t')B^R(t,t') + A^R(t,t')B^<(t,t') \tag{117}$$
$$= A^<(t,t')B^R(t,t') + A^R(t,t')B^>(t,t'). \tag{118}$$

Likewise for the advanced component, recalling that $G^A = G^< - G^{\bar{T}}$, we obtain

$$\begin{aligned} C^A(t,t') &= C^<(t,t') - C^{\bar{T}}(t,t') \\ &= A^<(t,t')B^<(t,t') - A^{\bar{T}}(t,t')B^{\bar{T}}(t,t') \\ &= A^<(t,t')B^<(t,t') - \left[A^<(t,t') - A^A(t,t')\right]\left[B^<(t,t') - B^A(t,t')\right] \\ &= A^<(t,t')B^A(t,t') + A^A(t,t')B^<(t,t') - A^A(t,t')B^A(t,t') \end{aligned} \tag{119}$$

which can be rewritten as

$$C^A(t,t') = A^<(t,t')B^A(t,t') + A^A(t,t')B^<(t,t') - A^A(t,t')B^A(t,t'), \tag{120}$$
$$= A^>(t,t')B^A(t,t') + A^A(t,t')B^<(t,t'), \tag{121}$$
$$= A^<(t,t')B^A(t,t') + A^A(t,t')B^>(t,t'). \tag{122}$$

3.5.3 Anti-parallel product

Another kind of term that appears frequently is

$$D(s,s') = A(s,s')B(s',s). \tag{123}$$

In this case, we obtain

$$D^{>}(t,t') = A^{>}(t,t')B^{<}(t',t) \tag{124}$$
$$D^{<}(t,t') = A^{<}(t,t')B^{>}(t',t) \tag{125}$$

and

$$D^{T}(t,t') = A^{T}(t,t')B^{T}(t',t), \tag{126}$$
$$D^{\bar{T}}(t,t') = A^{\bar{T}}(t,t')B^{\bar{T}}(t',t). \tag{127}$$

The retarded component can be obtained as

$$\begin{aligned} D^{R}(t,t') &= D^{T}(t,t') - D^{<}(t,t') \\ &= A^{T}(t,t')B^{T}(t',t) - A^{<}(t,t')B^{<}(t',t) \\ &= \left[A^{R}(t,t') + A^{<}(t,t')\right]\left[B^{R}(t',t) + B^{<}(t',t)\right] - A^{<}(t,t')B^{<}(t',t) \\ &= A^{R}(t,t')B^{R}(t',t) + A^{<}(t,t')B^{R}(t,t') + A^{R}(t,t')B^{<}(t,t'). \end{aligned} \tag{128}$$

Since $A^{R}(t,t')B^{R}(t',t) = 0$, we obtain

$$D^{R}(t,t') = A^{<}(t,t')B^{R}(t,t') + A^{R}(t,t')B^{<}(t,t'). \tag{129}$$

As for the advanced component

$$\begin{aligned} D^{A}(t,t') &= D^{<}(t,t') - D^{\bar{T}}(t,t') \\ &= A^{<}(t,t')B^{>}(t',t) - A^{\bar{T}}(t,t')B^{\bar{T}}(t',t) \\ &= A^{<}(t,t')B^{<}(t',t) - \left[A^{<}(t,t') - A^{A}(t,t')\right]\left[B^{<}(t',t) - B^{A}(t',t)\right] \\ &= A^{<}(t,t')B^{A}(t,t') + A^{A}(t,t')B^{<}(t,t') - A^{A}(t,t')B^{A}(t',t). \end{aligned} \tag{130}$$

Since $A^{A}(t,t')B^{A}(t',t) = 0$, we obtain

$$D^{A}(t,t') = A^{<}(t,t')B^{A}(t,t') + A^{A}(t,t')B^{<}(t,t'). \tag{131}$$

3.6 Transformation in Keldysh indices for general interaction terms

We have seen that under a linear transformation in Keldysh space for the Green's functions

$$G^{a}{}_{b} \to \hat{G}^{a}{}_{b} = \left(L^{-1}\right)^{a}{}_{a'} \cdot G^{a'}{}_{b'} \cdot \left(Q^{-1}\right)^{b'}{}_{b}, \tag{132}$$

a single particle potential changes as as

$$V^{a}_{\ b} \to \hat{V}^{a}_{\ b} = Q^{a}{}_{a'} V^{a'}{}_{b'} L^{b'}{}_{b}. \tag{133}$$

The same holds more generally for more general interaction terms. Let us assume we have an interaction term, with M incomming particles and N outgoing particles

$$H_{\text{int}} = \sum U^{a_1 \ldots a_N}_{b_1 \ldots b_M} c^{\dagger}_{a_1} \ldots c_{a_N} c_{b_1} \ldots c_{b_M}, \tag{134}$$

then under a linear transformation in Keldysh space, the interaction vertex changes as

$$\hat{U}^{a_1 \ldots a_N}_{b_1 \ldots b_M} \to \hat{U}^{a_1 \ldots a_N}_{b_1 \ldots b_M} = \left(Q^{a_1}{}_{a'_1} \ldots Q^{a_N}{}_{a'_N}\right) U^{a'_1 \ldots a'_N}_{b'_1 \ldots b'_M} \left(L^{b'_1}{}_{b_1} \ldots L^{b'_M}{}_{b_M}\right), \tag{135}$$

with the Kelsysh structure of the interaction vertex before the transformation being being

$$V^{a_1 \ldots a_N}_{b_1 \ldots b_M} = \begin{cases} +1, & a_1 = \ldots = a_N = b_1 = \ldots = b_M = + \\ -1, & a_1 = \ldots = a_N = b_1 = \ldots = b_M = - \\ 0, & \text{otherwise} \end{cases}. \tag{136}$$

4 Mesoscopic transport

We will now see how the non-equilibrium Green's function formalism can be used to describe transport in the stationary regime through a mesoscopic device that is subject to a potential bias.

4.1 Setup

We will consider the problem of mesoscopic transport in a two-terminal setup. This means we will consider that we have a device or central region (C), that is connect to two leads, left (L) and right (R), which will act as source and drain electrodes. We will consider a "partitioned setup"[1] for initial state of the system. In this description, for times smaller than t_0 the leads are disconned from the central region and kept at different chemical potentials μ_L and μ_R. At instant t_0, it is established contact between the leads and the central region and current starts flowing, driven by the potential imbalence of the leads $\mu_L - \mu_R$. We will assume that the leads are non-interacting, but wil allow (for now) for itneractions to occur in the central region.

Since in the "partitioned setup", at times $t > t_0$, the leads are disconnected from the central device, we can write the density matrix as

$$\rho(t_0) = \rho_L \otimes \rho_C \otimes \rho_R,$$

where we assume that each region is in local thermodynamic equilibrium. For times $t > t_0$ the Hamiltonian of the system reads

$$H = H_C + \sum_{\ell=R,L} H_\ell + \sum_\ell \left(H_{C,\ell} + H_{\ell,C}\right), \tag{137}$$

where H_C is the Hamiltonian of the central region, H_ℓ with $\ell = R, C$ is the Hamiltonian of the isolated leads and $H_{C,\ell}$ descibes the hopping of electrons from lead ℓ to the central region (with $H_{\ell,C} = H_{C,\ell}^\dagger$) which is switched on at t_0. We write

$$H_{C,\ell} = \sum_{ab} V_{C,\ell}^{ab} c_{C,a}^\dagger c_{\ell,b}$$

4.2 Current in the stationary regime

We define the current flowing from the left lead to the central region as

$$I_{L\to C} = -\left(-e\right)\frac{dN_L}{dt}, \tag{138}$$

is the electron number operator in lead L. We can evaluate

$$\begin{aligned}
\frac{dN_L}{dt} &= \frac{i}{\hbar}\left[H, N_L\right] \\
&= \frac{i}{\hbar}\left[H_{C,L} + H_{L,C}, N_L\right] \\
&= \frac{i}{\hbar}\left[\sum_{ab}\left(V_{C,L}^{ab} c_{C,a}^\dagger c_{L,b} + V_{L,C}^{ba} c_{L,b}^\dagger c_{C,a}\right), \sum_c c_{L,c}^\dagger c_{L,c}\right] \\
&= \frac{i}{\hbar}\sum_{ab}\left(V_{C,L}^{ab} c_{C,a}^\dagger c_{L,b} - V_{L,C}^{ba} c_{L,b}^\dagger c_{C,a}\right).
\end{aligned}$$

[1] This is to be contrasted with the "partion-free setup", in which leads and central region are connected from the begining an in equilibrium for times before t_0. At the instant t_0 a potential bias is applied to the leads and current starts flowing. Since this are two different physical situations, the current in the transiend regime will be different in the two setups. However, due to a loss of memory of the initial conditions, the two approaches agree on the current in the stationary regime.

Therefore the expectation value of the current is given by

$$\begin{aligned}\langle I_{L\to C}\rangle(t) &= e\left\langle \frac{dN_L}{dt}\right\rangle(t)\\ &= e\frac{i}{\hbar}\sum_{ab}\left(V^{ab}_{C,L}\left\langle \hat{c}^\dagger_{C,a}(t)\hat{c}_{L,b}(t)\right\rangle - V^{ba}_{L,C}\left\langle \hat{c}^\dagger_{L,b}(t)\hat{c}_{C,a}(t)\right\rangle\right)\\ &= e\sum_{ab}\left(V^{ab}_{C,L}G^<_{L,b;C,a}(t,t) - V^{ba}_{L,C}G^<_{C,a;L,b}(t,t)\right).\end{aligned}$$

Using a matrix notation for the orbital indices, we can write

$$\langle I_{L\to C}\rangle(t) = e\mathrm{Tr}\left[\boldsymbol{V}_{C,L}\cdot\boldsymbol{G}^<_{L,C}(t,t)\right] - e\mathrm{Tr}\left[\boldsymbol{V}_{L,C}\cdot\boldsymbol{G}^<_{C,L}(t,t)\right]. \tag{139}$$

4.2.1 Integrating out the leads

Now we procede by treating the central region-lead couplings as perturbations and using the Lippmann-Schwinger equations on the C contour, we write

$$\boldsymbol{G}_{\ell,C}(s,s') = \int_C ds_1 \boldsymbol{g}_{\ell,\ell}(s,s_1)\cdot\boldsymbol{V}_{\ell,C}\cdot\boldsymbol{G}_{C,C}(s_1,s'), \tag{140}$$

$$\boldsymbol{G}_{C,\ell}(s,s') = \int_C ds_1 \boldsymbol{G}_{\ell,\ell}(s,s_1)\cdot\boldsymbol{V}_{C,\ell}\cdot\boldsymbol{g}_{\ell,\ell}(s_1,s'), \tag{141}$$

where we write $\boldsymbol{g}$ to represent the Green's functions for disconnected system. The Lippmann-Schwinger equation for the central region Green's functions reads

$$\boldsymbol{G}_{C,C}(s,s') = \boldsymbol{G}_{C,C}(s,s') + \sum_{\ell=L,R}\int_C ds_1 \boldsymbol{g}_{C,C}(s,s_1)\cdot\boldsymbol{V}_{C,\ell}\cdot\boldsymbol{G}_{\ell,C}(s_1,s'). \tag{142}$$

Combining this with Eq. (140), we obtain

$$\boldsymbol{G}_{C,C}(s,s') = \boldsymbol{G}_{C,C}(s,s') + \sum_{\ell=L,R}\int_C ds_1\int_C ds_2 \boldsymbol{g}_{C,C}(s,s_1)\cdot\boldsymbol{\Sigma}_\ell(s_1,s_2)\cdot\boldsymbol{G}_{C,C}(s_2,s'), \tag{143}$$

where we have inroduced the self-energy induced by the leads

$$\boldsymbol{\Sigma}_\ell(s,s') = \boldsymbol{V}_{C,\ell}\cdot\boldsymbol{g}_{\ell,\ell}(s,s')\cdot\boldsymbol{V}_{\ell,C}. \tag{144}$$

Appying Langreth's rules to Eqs. (140) and (141), we obtain for the lesser components

$$\boldsymbol{G}^<_{L,C}(t,t') = \int dt_1\left[\boldsymbol{g}^<_{L,L}(t,t_1)\cdot\boldsymbol{V}_{L,C}\cdot\boldsymbol{G}^A_{C,C}(t_1,t') + \boldsymbol{g}^R_{L,L}(t,t_1)\cdot\boldsymbol{V}_{L,C}\cdot\boldsymbol{G}^<_{C,C}(t_1,t')\right], \tag{145}$$

$$\boldsymbol{G}^<_{C,L}(s,s') = \int dt_1\left[\boldsymbol{G}^<_{C,C}(t,t_1)\cdot\boldsymbol{V}_{C,L}\cdot\boldsymbol{g}^A_{L,L}(t_1,t') + \boldsymbol{G}^R_{C,C}(t,t_1)\cdot\boldsymbol{V}_{C,L}\cdot\boldsymbol{g}^<_{L,L}(t_1,t')\right]. \tag{146}$$

Using these equations, we can write the current as

$$\begin{aligned}\langle I_{L\to C}\rangle(t) = e\int dt_1 &\left(\mathrm{Tr}\left[\boldsymbol{\Sigma}^<_L(t,t_1)\cdot\boldsymbol{G}^A_{C,C}(t_1,t)\right] + \mathrm{Tr}\left[\boldsymbol{\Sigma}^R_L(t,t_1)\cdot\boldsymbol{G}^<_{C,C}(t_1,t)\right]\right)\\ - e\int dt_1 &\left(\mathrm{Tr}\left[\boldsymbol{G}^<_{C,C}(t,t_1)\cdot\boldsymbol{\Sigma}^A_L(t_1,t)\right] + \mathrm{Tr}\left[\boldsymbol{G}^R_{C,C}(t,t_1)\cdot\boldsymbol{\Sigma}^<_L(t_1,t)\right]\right).\end{aligned} \tag{147}$$

where we identified the retarded, advanced, lesser and greater components of the lead induced self-energy

$$\boldsymbol{\Sigma}^{R/A/</>}_\ell(t,t') = \boldsymbol{V}_{C,\ell}\cdot\boldsymbol{g}^{R/A/</>}_{\ell,\ell}(t,t')\cdot\boldsymbol{V}_{\ell,C}. \tag{148}$$

Using the fact that $G^R(t,t') = \Theta(t-t')\left[G^>(t,t') - G^<(t,t')\right]$, and $G^A(t,t') = -\Theta(t'-t)\left[G^>(t,t') - G^<(t,t')\right]$ we can rewrite Eq. (147) as

$$\begin{aligned}\langle I_{L\to C}\rangle(t) = e\int_{t_0}^{t} dt_1 \left(\mathrm{Tr}\left[\boldsymbol{\Sigma}_L^>(t,t_1)\cdot\boldsymbol{G}_{C,C}^<(t_1,t)\right] - \mathrm{Tr}\left[\boldsymbol{\Sigma}_L^<(t,t_1)\cdot\boldsymbol{G}_{C,C}^>(t_1,t)\right]\right)\\ + e\int_{t_0}^{t} dt_1 \left(\mathrm{Tr}\left[\boldsymbol{G}_{C,C}^<(t,t_1)\cdot\boldsymbol{\Sigma}_L^>(t_1,t)\right] - \mathrm{Tr}\left[\boldsymbol{G}_{C,C}^>(t,t_1)\cdot\boldsymbol{\Sigma}_L^<(t_1,t)\right]\right).\end{aligned} \tag{149}$$

4.2.2 The stationary limit

We will now be interested in the limit $t - t_0 \to \infty$, were we will assume a stationary limit is reached. In a stationary state, we recover translational invariance and therefore all two-time quantities become only a function of the time differences. Therefore, we can write

$$\boldsymbol{G}(t,t_1) \simeq \boldsymbol{G}(t-t_1) = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')}\boldsymbol{G}(\omega). \tag{150}$$

This allows us to write

$$\begin{aligned}\langle I_{L\to C}\rangle(t) = e\int_{t_0}^{t} dt_1 \int\frac{d\omega}{2\pi}\int\frac{d\omega'}{2\pi} e^{-i(\omega-\omega')(t-t_1)}\left(\mathrm{Tr}\left[\boldsymbol{\Sigma}_L^>(\omega)\cdot\boldsymbol{G}_{C,C}^<(\omega')\right] - \mathrm{Tr}\left[\boldsymbol{\Sigma}_L^<(\omega)\cdot\boldsymbol{G}_{C,C}^>(\omega')\right]\right)\\ + e\int_{t_0}^{t} dt_1 \int\frac{d\omega}{2\pi}\int\frac{d\omega'}{2\pi} e^{i(\omega-\omega')(t-t_1)}\left(\mathrm{Tr}\left[\boldsymbol{G}_{C,C}^<(\omega')\cdot\boldsymbol{\Sigma}_L^>(\omega)\right] - \mathrm{Tr}\left[\boldsymbol{G}_{C,C}^>(\omega')\cdot\boldsymbol{\Sigma}_L^<(\omega)\right]\right).\end{aligned} \tag{151}$$

Evaluating the integrals we obtain

$$\int_{t_0}^{t} dt_1 e^{-i(\omega-\omega')(t-t')} = \frac{1-e^{-i(\omega-\omega')(t-t_0)}}{i(\omega-\omega')}, \tag{152}$$

$$\int_{t_0}^{t} dt_1 e^{i(\omega-\omega')(t-t_1)} = -\frac{1-e^{i(\omega-\omega')(t-t_0)}}{i(\omega-\omega')}, \tag{153}$$

such that

$$\langle I_{L\to C}\rangle(t) = e\int\frac{d\omega}{2\pi}\int\frac{d\omega'}{2\pi}\frac{2\sin\left[(\omega-\omega')(t-t_0)\right]}{(\omega-\omega')}\left(\mathrm{Tr}\left[\boldsymbol{\Sigma}_L^>(\omega)\cdot\boldsymbol{G}_{C,C}^<(\omega')\right] - \mathrm{Tr}\left[\boldsymbol{\Sigma}_{L,L}^<(\omega)\cdot\boldsymbol{G}_{C,C}^>(\omega')\right]\right). \tag{154}$$

In the long time limit, we obtain

$$\lim_{t-t_0\to\infty}\frac{2\sin\left[(\omega-\omega')(t-t_0)\right]}{(\omega-\omega')} = 2\pi\delta(\omega-\omega'), \tag{155}$$

and we obtain the following result for the current in the stationary regime

$$J_{L\to R} = \lim_{t-t_0\to\infty}\langle I_{L\to C}\rangle(t) = e\int\frac{d\omega}{2\pi}\left(\mathrm{Tr}\left[\boldsymbol{\Sigma}_L^>(\omega)\cdot\boldsymbol{G}_{C,C}^<(\omega)\right] - \mathrm{Tr}\left[\boldsymbol{\Sigma}_L^<(\omega)\cdot\boldsymbol{G}_{C,C}^>(\omega)\right]\right). \tag{156}$$

This expression if the starting point for a series of approximations.

4.3 Ballistic transport: the Landauer formula

Now, we will assume that the system is non-interacting. Our starting point is Eq. (156). We will use the Keldysh equation to write

$$\boldsymbol{G}_{C,C}^{\lessgtr}(\omega) = \boldsymbol{G}_{C,C}^R(\omega)\cdot\boldsymbol{\Sigma}_{C,C}^{\lessgtr}(\omega)\cdot\boldsymbol{G}_{C,C}^A(\omega). \tag{157}$$

Where the self-energy is given by the contribution from the two leads:

$$\boldsymbol{\Sigma}^{\lessgtr}_{C,C}(\omega) = \boldsymbol{\Sigma}^{\lessgtr}_{L}(\omega) + \boldsymbol{\Sigma}^{\lessgtr}_{R}(\omega). \tag{158}$$

Combining Eqs. (156), (157) and (158), we obtain the following expression for the current

$$\begin{aligned} J_L = & e \int \frac{d\omega}{2\pi} \mathrm{Tr}\left[\boldsymbol{\Sigma}^{>}_{L}(\omega) \cdot \boldsymbol{G}^{R}_{C,C}(\omega) \cdot \boldsymbol{\Sigma}^{<}_{R}(\omega) \cdot \boldsymbol{G}^{A}_{C,C}(\omega)\right] \\ & - e \int \frac{d\omega}{2\pi} \mathrm{Tr}\left[\boldsymbol{\Sigma}^{<}_{L}(\omega) \cdot \boldsymbol{G}^{R}_{C,C}(\omega) \cdot \boldsymbol{\Sigma}^{>}_{R}(\omega) \cdot \boldsymbol{G}^{A}_{C,C}(\omega)\right]. \end{aligned} \tag{159}$$

Now we will use the fact that $\boldsymbol{g}^{\lessgtr}_{\ell,\ell}(\omega)$ are Green's functions for the disconnect system, which is in thermodynamic equilibrium. Therefore, we can use the fluctuation-dissipation theorem to write

$$\boldsymbol{g}^{>}_{\ell,\ell}(\omega) = -i\left(1 - f_\ell(\omega)\right) i\left[\boldsymbol{g}^{R}_{\ell,\ell}(\omega) - \boldsymbol{g}^{A}_{\ell,\ell}(\omega)\right] \tag{160}$$

$$\boldsymbol{g}^{<}_{\ell,\ell}(\omega) = i f_\ell(\omega) i\left[\boldsymbol{g}^{R}_{\ell,\ell}(\omega) - \boldsymbol{g}^{A}_{\ell,\ell}(\omega)\right], \tag{161}$$

such that

$$\boldsymbol{\Sigma}^{>}_{\ell}(\omega) = -i\left(1 - f_\ell(\omega)\right) \boldsymbol{\Gamma}_\ell(\omega) \tag{162}$$

$$\boldsymbol{\Sigma}^{<}_{\ell,\ell}(\omega) = i f_\ell(\omega) \boldsymbol{\Gamma}_\ell(\omega). \tag{163}$$

where we introduced the $\boldsymbol{\Gamma}_\ell(\omega)$ matrices as

$$\boldsymbol{\Gamma}_\ell(\omega) = i\left[\boldsymbol{\Sigma}^{R}_{\ell}(\omega) - \boldsymbol{\Sigma}^{A}_{\ell}(\omega)\right] = i\boldsymbol{V}_{C,\ell}\left[\boldsymbol{g}^{R}_{\ell,\ell}(\omega) - \boldsymbol{g}^{A}_{\ell,\ell}(\omega)\right]\boldsymbol{V}_{\ell,C}. \tag{164}$$

The current is thus given by

$$J_L = e \int \frac{d\omega}{2\pi} \left[f_R(\omega) - f_L(\omega)\right] \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega) \cdot \boldsymbol{G}^{R}_{C,C}(\omega) \cdot \boldsymbol{\Gamma}_R(\omega) \cdot \boldsymbol{G}^{A}_{C,C}(\omega)\right], \tag{165}$$

this equation is the so called Caroli formula. This is one of the possible representations of the celebrated Landauer formula, with the quantity

$$\mathcal{T}(\omega) = \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega) \cdot \boldsymbol{G}^{R}_{C,C}(\omega) \cdot \boldsymbol{\Gamma}_R(\omega) \cdot \boldsymbol{G}^{A}_{C,C}(\omega)\right], \tag{166}$$

being the transmission function.

4.4 Transport in the proportionate coupling case

Let us go back to the general expression for the stationary current, Eq. (156),

$$J_{L\to C} = e \int \frac{d\omega}{2\pi} \left(\mathrm{Tr}\left[\boldsymbol{\Sigma}^{>}_{L}(\omega) \cdot \boldsymbol{G}^{<}_{C,C}(\omega)\right] - \mathrm{Tr}\left[\boldsymbol{\Sigma}^{<}_{L}(\omega) \cdot \boldsymbol{G}^{>}_{C,C}(\omega)\right]\right).$$

We will now use the fluctuation-dissipation theorem to write

$$\boldsymbol{\Sigma}^{<}_{L}(\omega) = i f_L(\omega) \boldsymbol{\Gamma}_L(\omega), \tag{167}$$

$$\boldsymbol{\Sigma}^{>}_{L}(\omega) = -i\left(1 - f_L(\omega)\right) \boldsymbol{\Gamma}_L(\omega), \tag{168}$$

obtaining

$$\begin{aligned} J_{L\to C} &= e \int \frac{d\omega}{2\pi} \left(-i\left(1 - f_L(\omega)\right) \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega) \cdot \boldsymbol{G}^{<}_{C,C}(\omega)\right] - i f_L(\omega) \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega) \cdot \boldsymbol{G}^{>}_{C,C}(\omega)\right]\right) \\ &= e \int \frac{d\omega}{2\pi} \left(-i \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega) \cdot \boldsymbol{G}^{<}_{C,C}(\omega)\right] - f_L(\omega) \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega) \cdot i\left(\boldsymbol{G}^{>}_{C,C}(\omega) - \boldsymbol{G}^{<}_{C,C}(\omega)\right)\right]\right). \end{aligned} \tag{169}$$

We recognize the spectral function of the central region

$$\begin{aligned}\boldsymbol{A}_{C,C}(\omega) &= i\left[\boldsymbol{G}^{>}_{C,C}(\omega) - \boldsymbol{G}^{<}_{C,C}(\omega)\right] \\ &= i\left[\boldsymbol{G}^{R}_{C,C}(\omega) - \boldsymbol{G}^{A}_{C,C}(\omega)\right],\end{aligned} \tag{170}$$

such that we obtain the Meir-Wingreen formula for current

$$J_{L\to C} = e\int\frac{d\omega}{2\pi}\left(\mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega)\cdot(-i)\,\boldsymbol{G}^{<}_{C,C}(\omega)\right] - f_L(\omega)\mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega)\cdot\boldsymbol{A}_{C,C}(\omega)\right]\right). \tag{171}$$

Now the current, measured as flowing from the right electrode to the central device is given by

$$J_{R\to C} = e\int\frac{d\omega}{2\pi}\left(\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(\omega)\cdot(-i)\,\boldsymbol{G}^{<}_{C,C}(\omega)\right] - f_R(\omega)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(\omega)\cdot\boldsymbol{A}_{C,C}(\omega)\right]\right). \tag{172}$$

In the stationary limit, there is no charge accumulation in the central region and therefore

$$J_{R\to C} = -J_{L\to C}. \tag{173}$$

Therefore, we are free to write the current (measured as flowing from the left to the right electrode) as

$$J_{L\to R} = xJ_{R\to C} - (1-x)J_{L\to C}, \tag{174}$$

for any value of x. We therefore, obtain

$$\begin{aligned}J_{L\to R} = {}& xe\int\frac{d\omega}{2\pi}\left(\mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega)\cdot(-i)\,\boldsymbol{G}^{<}_{C,C}(\omega)\right] - f_L(\omega)\mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega)\cdot\boldsymbol{A}_{C,C}(\omega)\right]\right) \\ & - (1-x)e\int\frac{d\omega}{2\pi}\left(\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(\omega)\cdot(-i)\,\boldsymbol{G}^{<}_{C,C}(\omega)\right] - f_R(\omega)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(\omega)\cdot\boldsymbol{A}_{C,C}(\omega)\right]\right).\end{aligned} \tag{175}$$

We will assume that the $\boldsymbol{\Gamma}_{L/R}(\omega)$ functions are proportional $\boldsymbol{\Gamma}_R(\omega) = \lambda\boldsymbol{\Gamma}_L(\omega)$, such that we obtain

$$\begin{aligned}J_{L\to R} = {}& e\int\frac{d\omega}{2\pi}\left[x-(1-x)\lambda\right]\mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega)\cdot(-i)\,\boldsymbol{G}^{<}_{C,C}(\omega)\right] \\ & - e\int\frac{d\omega}{2\pi}\left[xf_L(\omega)-(1-x)\lambda f_R(\omega)\right]\mathrm{Tr}\left[\boldsymbol{\Gamma}_L(\omega)\cdot\boldsymbol{A}_{C,C}(\omega)\right].\end{aligned} \tag{176}$$

We choose x such that the first term vanishes $x-(1-x)\lambda = 0$, such that $x = \lambda/(1+\lambda)$. We thus obtain

$$J_{L\to R} = e\int\frac{d\omega}{2\pi}\left[f_R(\omega)-f_L(\omega)\right]\mathrm{Tr}\left[\frac{\lambda}{1+\lambda}\boldsymbol{\Gamma}_L(\omega)\cdot\boldsymbol{A}_{C,C}(\omega)\right]. \tag{177}$$

Which we can write as

$$J_{L\to R} = e\int\frac{d\omega}{2\pi}\left[f_R(\omega)-f_L(\omega)\right]\mathrm{Tr}\left[\frac{\boldsymbol{\Gamma}_L(\omega)\boldsymbol{\Gamma}_R(\omega)}{\boldsymbol{\Gamma}_L(\omega)+\boldsymbol{\Gamma}_R(\omega)}\cdot\boldsymbol{A}_{C,C}(\omega)\right]. \tag{178}$$

This expression still has the form of a Landauer formula, even though it remains true for the interacting case (provided the proportionality condition is satisfied).

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A Wick/Gaudin's theorem

We wish to evaluate

$$\left\langle a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right\rangle_0$$

where $a_n^+ = a_n^\dagger$ is a creation operator and $a_n^- = a_n$ is an annihilation operator for a particle on state n. We will assume the operators are written in the basis that diagonalise the single particle operator H_0

$$H_0 = \sum_n \epsilon_n a_n^\dagger a_n$$

and that the expectation value is taken with respect the grand-canonical density matrix associated with H_0. We will write $\bar{H}_0 = H_0 - \mu N$. We will start to prove that

$$\left\langle a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right\rangle_0 = \sum_{m=2}^{N} \zeta^m \left\langle a_{n_1}^{\nu_1} a_{n_m}^{\nu_m} \right\rangle_0 \left\langle a_{n_2}^{\nu_2} ... a_{n_{m-1}}^{\nu_{m-1}} a_{n_{m+1}}^{\nu_{m+1}} ... a_{n_N}^{\nu_N} \right\rangle_0$$

where $\zeta = +1$ for bosons and $\zeta = -1$ for fermions.

The prove consists of two steps:

1. Show that $\mathrm{Tr}\left[e^{-\beta \bar{H}_0} a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N}\right] \propto \mathrm{Tr}\left[e^{-\beta \bar{H}_0} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} a_{n_1}^{\nu_1}\right]$.

2. Use (anti-)commutation properties to bring the operator $a_{n_1}^{\nu_1}$ to its original position, obtaining

$$\mathrm{Tr}\left[e^{-\beta \bar{H}_0} a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N}\right] \propto \mathrm{Tr}\left[e^{-\beta \bar{H}_0} a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N}\right] + \\ + \text{terms generated by the (anti-)commutations.}$$

Step 1. We will start to define

$$a_n^\nu(\tau) = e^{\tau \bar{H}_0} a_n^\nu a^{-\tau \bar{H}_0},$$

which obeys the Heisenberg equation in imaginary time:

$$\frac{d a_n^\nu(\tau)}{d\tau} = \left[\bar{H}_0, a_n^\nu(\tau)\right]. \tag{179}$$

We have that

$$\frac{d a_n^\dagger(\tau)}{d\tau} = \bar{\epsilon}_n \left[a_n^\dagger(\tau) a_n(\tau), a_n^\dagger(\tau)\right] = \bar{\epsilon}_n a_n^\dagger(\tau), \tag{180}$$

$$\frac{d a_n(\tau)}{d\tau} = \bar{\epsilon}_n \left[a_n^\dagger(\tau) a_n(\tau), a_n(\tau)\right] = -\bar{\epsilon}_n a_n(\tau), \tag{181}$$

which we can write in a unified way as

$$a_n^\nu(\tau) = \nu \bar{\epsilon}_n a_n^\nu(\tau). \tag{182}$$

The solution of this equation is

$$a_n^\nu(\tau) = e^{\nu \bar{\epsilon}_n \tau} a_n^\nu. \tag{183}$$

Therefore, we conclude that

$$a_n^\nu(\tau) = e^{\tau \bar{H}_0} a_n^\nu e^{-\tau \bar{H}_0} = e^{\nu \bar{\epsilon}_n \tau} a_n^\nu. \tag{184}$$

Setting $\tau = -\beta$, we obtain $e^{-\beta \bar{H}_0} a_n^\nu e^{\beta \bar{H}_0} = e^{-\nu \bar{\epsilon}_n \beta} a_n^\nu$, which allows us to write

$$e^{-\beta \bar{H}_0} a_n^\nu = e^{-\nu \beta \bar{\epsilon}_n} a_n^\nu e^{-\beta \bar{H}_0}. \tag{185}$$

Therefore we can write $\left\langle a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right\rangle_0$ as

$$\begin{aligned}\left\langle a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right\rangle_0 &= \frac{1}{\mathcal{Z}_0} \mathrm{Tr}\left[e^{-\beta \bar{H}_0} a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right] \\ &= \frac{1}{\mathcal{Z}_0} e^{-\nu_1 \beta \bar{\epsilon}_{n_1}} \mathrm{Tr}\left[a_{n_1}^{\nu_1} e^{-\beta \bar{H}_0} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right]. \end{aligned} \tag{186}$$

Using the cyclic property of the trace, we get

$$\left\langle a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \right\rangle_0 = \frac{1}{\mathcal{Z}_0} e^{-\nu \beta \bar{\epsilon}_{n_1}} \mathrm{Tr}\left[e^{-\beta \bar{H}_0} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} a_{n_1}^{\nu_1} \right]. \tag{187}$$

Step 2: Our goal is now to bring $a_{n_1}^{\nu_1}$ to its original position. To do this, we have to (anti-)commute the operator $a_{n_1}^{\nu_1}$ with the remaing operators $a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N}$. Let us start with a particular case: $a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} a_{n_1}^{\nu_1}$. First, we (anti-)commute the operators $a_{n_4}^{\nu_4}$ and $a_{n_1}^{\nu_1}$.

$$a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} a_{n_1}^{\nu_1} = a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} \left(\zeta a_{n_1}^{\nu_1} a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta \right). \tag{188}$$

Which we can rewrite as

$$a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} a_{n_1}^{\nu_1} = \zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_1}^{\nu_1} a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3}. \tag{189}$$

We continue the proccedure, first for $a_{n_3}^{\nu_3} a_{n_1}^{\nu_1}$ and next for $a_{n_2}^{\nu_2} a_{n_1}^{\nu_1}$. We obtain:

$$\begin{aligned} a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} a_{n_1}^{\nu_1} &= \zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_1}^{\nu_1} a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3}. \\ &= \zeta a_{n_2}^{\nu_2} \left(\zeta a_{n_1}^{\nu_1} a_{n_3}^{\nu_3} + \left[a_{n_3}^{\nu_3}, a_{n_1}^{\nu_1} \right]_\zeta \right) a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} \\ &= \zeta^2 a_{n_2}^{\nu_2} a_{n_1}^{\nu_1} a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} + \zeta \left[a_{n_3}^{\nu_3}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} \\ &= \zeta^2 \left(\zeta a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} + \left[a_{n_2}^{\nu_2}, a_{n_1}^{\nu_1} \right]_\zeta \right) a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} + \zeta \left[a_{n_3}^{\nu_3}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} \\ &= \zeta^3 a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} + \zeta^2 \left[a_{n_2}^{\nu_2}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_3}^{\nu_3} a_{n_4}^{\nu_4} + \zeta \left[a_{n_3}^{\nu_3}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_4}^{\nu_4} + \left[a_{n_4}^{\nu_4}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} a_{n_3}^{\nu_3}. \end{aligned} \tag{190}$$

Extrapolating this result, we propose that

$$a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} a_{n_1}^{\nu_1} = \zeta^{N-1} a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} + \sum_{m=2}^{N} \zeta^{N-m} \left[a_{n_m}^{\nu_2}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} ... a_{n_{m-1}}^{\nu_{m-1}} a_{n_{m+1}}^{\nu_{m+1}} ... a_{n_N}^{\nu_N}. \tag{191}$$

This can be proved by induction. It is true to the $N = 2$ case, by the very definition of (anti-)commutator $\left[a_{n_2}^{\nu_2}, a_{n_1}^{\nu_1} \right]_\zeta$:

$$a_{n_2}^{\nu_2} a_{n_1}^{\nu_1} = \zeta a_{n_1}^{\nu_1} a_{n_2}^{\nu_2} + \left[a_{n_2}^{\nu_2}, a_{n_1}^{\nu_1} \right]_\zeta$$

Now, assuming it is true for N, let us prove for $N + 1$. We start by writing

$$\begin{aligned} a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} a_{n_{N+1}}^{\nu_{N+1}} a_{n_1}^{\nu_1} &= a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} \left((\zeta) a_{n_1}^{\nu_1} a_{n_{N+1}}^{\nu_{N+1}} + \left[a_{n_{N+1}}^{\nu_{N+1}}, a_{n_1}^{\nu_1} \right]_\zeta \right) \\ &= \zeta a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N} a_{n_1}^{\nu_1} a_{n_{N+1}}^{\nu_{N+1}} + \left[a_{n_{N+1}}^{\nu_{N+1}}, a_{n_1}^{\nu_1} \right]_\zeta a_{n_2}^{\nu_2} ... a_{n_N}^{\nu_N}. \end{aligned} \tag{192}$$

Now using the result for N, Eq. (191), we obtain

$$
\begin{aligned}
a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}a_{n_{N+1}}^{\nu_{N+1}}a_{n_1}^{\nu_1} = \\
&= \zeta^N a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}a_{n_{N+1}}^{\nu_{N+1}} + \sum_{m=2}^{N}\zeta^{N+1-m}\left[a_{n_m}^{\nu_2},a_{n_1}^{\nu_1}\right]_\zeta a_{n_2}^{\nu_2}...a_{n_{m-1}}^{\nu_{m-1}}a_{n_{m+1}}^{\nu_{m+1}}...a_{n_N}^{\nu_N}a_{n_{N+1}}^{\nu_{N+1}} \\
&\qquad + \left[a_{n_{N+1}}^{\nu_{N+1}},a_{n_1}^{\nu_1}\right]_\zeta a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N} \\
&= \zeta^N a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}a_{n_{N+1}}^{\nu_{N+1}} + \sum_{m=2}^{N+1}\zeta^{N+1-m}\left[a_{n_m}^{\nu_2},a_{n_1}^{\nu_1}\right]_\zeta a_{n_2}^{\nu_2}...a_{n_{m-1}}^{\nu_{m-1}}a_{n_{m+1}}^{\nu_{m+1}}...a_{n_N}^{\nu_N}a_{n_{N+1}}^{\nu_{N+1}}. \qquad (193)
\end{aligned}
$$

Now, let us put together steps 1 and 2: using Eq. (191) in Eq. (187), yields

$$
\begin{aligned}
\left\langle a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}\right\rangle_0 &= \frac{1}{\mathcal{Z}_0}e^{-\nu\beta\bar{\epsilon}_{n_1}}\mathrm{Tr}\left[e^{-\beta\bar{H}_0}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}a_{n_1}^{\nu_1}\right] \\
&= e^{-\nu\beta\bar{\epsilon}_{n_1}}\zeta^{N-1}\frac{1}{\mathcal{Z}_0}\mathrm{Tr}\left[e^{-\beta\bar{H}_0}a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}\right] \\
&+ e^{-\nu\beta\bar{\epsilon}_{n_1}}\sum_{m=2}^{N}\zeta^{N-m}\left[a_{n_m}^{\nu_m},a_{n_1}^{\nu_1}\right]_\zeta\frac{1}{\mathcal{Z}_0}\mathrm{Tr}\left[e^{-\beta\bar{H}_0}a_{n_2}^{\nu_2}...a_{n_{m-1}}^{\nu_{m-1}}a_{n_{m+1}}^{\nu_{m+1}}...a_{n_N}^{\nu_N}\right]. \qquad (194)
\end{aligned}
$$

We can write the above result as

$$
\left(e^{\nu_1\beta\bar{\epsilon}_{n_1}}-\zeta^{N-1}\right)\left\langle a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}\right\rangle_0 = \sum_{m=2}^{N}\zeta^{N-m}\left[a_{n_m}^{\nu_2},a_{n_1}^{\nu_1}\right]_\zeta\left\langle a_{n_2}^{\nu_2}...a_{n_{m-1}}^{\nu_{m-1}}a_{n_{m+1}}^{\nu_{m+1}}...a_{n_N}^{\nu_N}\right\rangle_0. \qquad (195)
$$

If N is odd, applying this result recursively, we eventually obtain terms involving $\langle a_n^\nu\rangle_0 = 0$. Therefore, we onlu obtain a non-zero result if N is even, in which case $\zeta^N = 1$. For N even we can therefore write

$$
\left\langle a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}\right\rangle_0 = \sum_{m=2}^{N}\zeta^m\frac{\left[a_{n_m}^{\nu_2},a_{n_1}^{\nu_1}\right]_\zeta}{e^{\nu_1\beta\bar{\epsilon}_{n_1}}-\zeta}\left\langle a_{n_2}^{\nu_2}...a_{n_{m-1}}^{\nu_{m-1}}a_{n_{m+1}}^{\nu_{m+1}}...a_{n_N}^{\nu_N}\right\rangle_0. \qquad (196)
$$

It is easy to check that

$$
\frac{\left[a_{n_m}^{\nu_m},a_{n_1}^{\nu_1}\right]_\zeta}{e^{\nu_1\beta\bar{\epsilon}_{n_1}}-\zeta} = \left\langle a_{n_1}^{\nu_1}a_{n_m}^{\nu_m}\right\rangle_0. \qquad (197)
$$

Explicitly, we have

$$
\left\langle a_{n_1}^{+}a_{n_m}^{-}\right\rangle_0 = \delta_{n_1,n_m}n_\pm\left(\epsilon_{n_1}\right) = \frac{\delta_{n_1,n_m}}{e^{\beta\bar{\epsilon}_{n_1}}-\zeta}, \qquad (198)
$$

$$
\left\langle a_{n_1}^{-}a_{n_m}^{+}\right\rangle_0 = \delta_{n_1,n_m}\left(1+\zeta n_\zeta\left(\epsilon_{n_1}\right)\right) = \frac{-\zeta\delta_{n_1,n_m}}{e^{-\beta\bar{\epsilon}_{n_1}}-\zeta}, \qquad (199)
$$

$$
\left\langle a_{n_1}^{+}a_{n_m}^{+}\right\rangle_0 = 0, \qquad (200)
$$

$$
\left\langle a_{n_1}^{-}a_{n_m}^{-}\right\rangle_0 = 0. \qquad (201)
$$

Therefore, we obtain

$$
\left\langle a_{n_1}^{\nu_1}a_{n_2}^{\nu_2}...a_{n_N}^{\nu_N}\right\rangle_0 = \sum_{m=2}^{N}\zeta^m\left\langle a_{n_1}^{\nu_1}a_{n_m}^{\nu_2}\right\rangle_0\left\langle a_{n_2}^{\nu_2}...a_{n_{m-1}}^{\nu_{m-1}}a_{n_{m+1}}^{\nu_{m+1}}...a_{n_N}^{\nu_N}\right\rangle_0. \qquad (202)
$$

This form of Wick's theorem (without time ordering) is generally called Gaudin's theorem.

For the time ordering case, we first order the operators and then apply Gaudin's theorem. Since the operators are ordered, we can restore the time-ordering operators.

B Fluctuation-dissipation theorem

In order to prove the fluctuation-dissipation theorem, we will use the Lehmann for Green's functions in thermodynamic equilibrium. We will consider an eigenbasis of the Hamiltonian of the system, $\{|n\rangle\}$, where $|n\rangle$ is teh state with E_n and particle number N_n:

$$H|n\rangle = E_n|n\rangle\,, \tag{203}$$
$$N|n\rangle = N_n|n\rangle\,. \tag{204}$$

In this basis, we can write for the greater Green's functions

$$\begin{aligned} G^{>}_{AB}(t,t') &= -\frac{i}{\hbar}\left\langle A(t)B^\dagger(t')\right\rangle \\ &= -\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\mathrm{Tr}\left(e^{-\beta(H-\mu N)}e^{iHt/\hbar}Ae^{-iHt/\hbar}e^{iHt'/\hbar}B^\dagger e^{-iHt'/\hbar}\right) \\ &= -\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_n \langle n|\, e^{-\beta(H-\mu N)}e^{iHt/\hbar}Ae^{-iHt/\hbar}e^{iHt'/\hbar}B^\dagger e^{-iHt'/\hbar}\,|n\rangle \\ &= -\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_n e^{-\beta(E_n-\mu N_n)}e^{iE_n\left(t-t'\right)/\hbar}\langle n|\, Ae^{-iHt/\hbar}e^{iHt'/\hbar}B^\dagger\,|n\rangle\,. \end{aligned} \tag{205}$$

Inserting the resolution of identity, $\mathbf{1} = \sum_m |m\rangle\langle m|$, we get

$$\begin{aligned} G^{>}_{AB}(t,t') &= -\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_n e^{-\beta(E_n-\mu N_n)}e^{iE_n\left(t-t'\right)/\hbar}\langle n|\, A\mathbf{1}e^{-iHt/\hbar}e^{iHt'/\hbar}B^\dagger\,|n\rangle \\ &= -\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_{n,m} e^{-\beta(E_n-\mu N_n)}e^{iE_n\left(t-t'\right)/\hbar}\langle n|\, A\,|m\rangle\langle m|\, e^{-iHt/\hbar}e^{iHt'/\hbar}B^\dagger\,|n\rangle \\ &= -\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_{n,m} e^{-\beta(E_n-\mu N_n)}e^{i(E_n-E_m)\left(t-t'\right)/\hbar}\langle n|\, A\,|m\rangle\langle m|\, B^\dagger\,|n\rangle\,. \end{aligned} \tag{206}$$

This is the Lehmann representation for the greater Green's function. Making a Fourier transform, we obtain

$$G^{>}_{AB}(\omega) = -\frac{i}{\mathcal{Z}}\sum_{n,m} e^{-\beta(E_n-\mu N_n)}2\pi\delta\left(\hbar\omega + E_n - E_m\right)\langle n|\, A\,|m\rangle\langle m|\, B^\dagger\,|n\rangle\,. \tag{207}$$

Likewise, for the lesser function, we obtain

$$\begin{aligned} G^{<}_{AB}(t,t') &= \mp\frac{i}{\hbar}\left\langle B^\dagger(t')A(t)\right\rangle \\ &= \mp\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\mathrm{Tr}\left(e^{-\beta(H-\mu N)}e^{iHt'/\hbar}B^\dagger e^{-iHt'/\hbar}e^{iHt/\hbar}Ae^{-iHt/\hbar}\right) \\ &= \mp\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_{n,m} \langle n|\, e^{-\beta(H-\mu N)}e^{iHt'/\hbar}B^\dagger\,|m\rangle\langle m|\, e^{-iHt'/\hbar}e^{iHt/\hbar}Ae^{-iHt/\hbar}\,|n\rangle \\ &= \mp\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_{n,m} e^{-\beta(E_n-\mu N_n)}e^{iE_nt'/\hbar}\langle n|\, B^\dagger\,|m\rangle\, e^{-iE_mt'/\hbar}e^{iE_mt/\hbar}\langle m|\, A\,|n\rangle\, e^{-iE_nt/\hbar} \\ &= \mp\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_{n,m} e^{-\beta(E_n-\mu N_n)}e^{i(E_m-E_n)\left(t-t'\right)/\hbar}\langle m|\, A\,|n\rangle\langle n|\, B^\dagger\,|m\rangle\,. \end{aligned} \tag{208}$$

Exchanging $m \leftrightarrow n$, we get

$$G^{<}_{AB}(t,t') = -\zeta\frac{i}{\hbar}\frac{1}{\mathcal{Z}}\sum_{n,m} e^{-\beta(E_m-\mu N_m)}e^{i(E_n-E_m)\left(t-t'\right)/\hbar}\langle n|\, A\,|m\rangle\langle m|\, B^\dagger\,|n\rangle\,. \tag{209}$$

Making a Fourier transform give us

$$G^{<}_{AB}(\omega) = -\zeta \frac{i}{\mathcal{Z}} \sum_{n,m} e^{-\beta(E_m - \mu N_m)} 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle$$

Recalling the expression of the spectral function in terms of greater and lesser Green's functions, we have

$$\begin{aligned} A_{AB}(t,t') &= i\left(G^{>}_{AB}(t,t') - G^{<}_{AB}(t,t')\right) \\ &= \frac{1}{\hbar}\frac{1}{\mathcal{Z}} \sum_{n,m} \left(e^{-\beta(E_n - \mu N_n)} - \zeta e^{-\beta(E_m - \mu N_m)}\right) e^{i(E_n - E_m)\left(t-t'\right)/\hbar} \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle . \end{aligned} \quad (210)$$

Making a Fourier transform, we obtain the Lehmann representation of the spectral function

$$A_{AB}(\omega) = \frac{1}{\mathcal{Z}} \sum_{n,m} \left(e^{-\beta(E_n - \mu N_n)} - \zeta e^{-\beta(E_m - \mu N_m)}\right) 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle . \quad (211)$$

Using the δ-Dirac function, we can write the previous result as

$$A_{AB}(\omega) = \frac{1}{\mathcal{Z}} \sum_{n,m} \left(1 - \zeta e^{-\beta(E_m - E_n - \mu(N_m - N_n))}\right) e^{-\beta(E_n - \mu N_n)} 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle . \quad (212)$$

For $B^{\dagger} = a^{\dagger}$, a creation operator, e $A = a$, an annihilation operator, we have that $N_m = N_n + 1$, which allows us to write

$$\begin{aligned} A_{AB}(\omega) &= \frac{1}{\mathcal{Z}} \sum_{n,m} \left(1 - \zeta e^{-\beta(\hbar\omega - \mu)}\right) e^{-\beta(E_n - \mu N_n)} 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle \\ &= \left(1 - \zeta e^{-\beta(\hbar\omega - \mu)}\right) \frac{1}{\mathcal{Z}} \sum_{n,m} e^{-\beta(E_n - \mu N_n)} 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle \\ &= iG^{>}_{AB}(\omega)\left(1 - \zeta e^{-\beta(\hbar\omega - \mu)}\right) . \end{aligned} \quad (213)$$

Likewise, we can write

$$\begin{aligned} A_{AB}(\omega) &= \frac{1}{\mathcal{Z}} \sum_{n,m} \left(e^{-\beta(E_n - E_m - \mu(N_n - N_m))} - \zeta\right) e^{-\beta(E_m - \mu N_m)} 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{n,m} \left(e^{\beta(\hbar\omega - \mu)} - \zeta\right) e^{-\beta(E_m - \mu N_m)} 2\pi\delta\left(\hbar\omega + E_n - E_m\right) \langle n| A |m\rangle \langle m| B^{\dagger} |n\rangle \\ &= \pm iG^{<}_{AB}(\omega)\left(e^{\beta(\hbar\omega - \mu)} - \zeta\right) . \end{aligned} \quad (214)$$

Rewriting the previous two results, we obtain the fluctuation-dissipation theorem

$$iG^{>}_{AB}(\omega) = \frac{1}{1 - \zeta e^{-\beta(\hbar\omega - \mu)}} A_{AB}(\omega) = \left[1 + \zeta n_{\zeta}\left(\hbar\omega\right)\right] A_{AB}(\omega), \quad (215)$$

$$\zeta iG^{<}_{AB}(\omega) = \frac{1}{e^{\beta(\hbar\omega - \mu)} - \zeta} A_{AB}(\omega) = n_{\zeta}\left(\hbar\omega\right) A_{AB}(\omega). \quad (216)$$

where

$$n_{\zeta}\left(\hbar\omega\right) = \frac{1}{e^{\beta(\hbar\omega - \mu)} - \zeta} \quad (217)$$

is the Bose-Einstein / Fermi-Dirac distribution function.

C Cancellation of disconnected diagrams

Each term in the perturbation expansion can be pictorially represented in terms of Feynman diagrams. We will know show that a certain class of diagrams, the so called disconnected diagrams, do not contribute the expansion. Let us consider the evaluation of

$$\left\langle T_C W(s_1)...W(s_n)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_0 . \tag{218}$$

We say that term with a vertex arising from $W(s_i)$ is connect, if the corresponding diagram has lines that connect it to either $c_\alpha(s)$ or $c^\dagger_\beta(s')$. In the evaluation of Eq. (218), we can organize the different terms by the number of vertices that are connected. For the n-th order term, let usa say that m vertices are connected and $n-m$ as disconnected. How many such terms are there. Since all the $W(s_1)...W(s_n)$ are equivalent, and we want to pick m vertices out of n, there are

$$\binom{n}{m} = \frac{n!}{m!\,(m-n)!}.$$

Therefore, we can write

$$\begin{aligned}\left\langle T_C W(s_1)...W(s_n)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_0 = \\ = \sum_{m=0}^{n} \frac{n!}{m!\,(n-m)!}\left\langle T_C W(s_1)...W(s_m)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_{0,\text{connected}} \langle T_C W(s_{m+1})...W(s_n)\rangle_0 .\end{aligned} \tag{219}$$

Therefore, we can write

$$\begin{aligned}G^C_{\alpha\beta}(s,s') &= \sum_n \left(-\frac{i}{\hbar}\right)^{n+1}\frac{1}{n!}\int_C ds_1...\int_C ds_n \left\langle T_C W(s_1)...W(s_n)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_0 \\ &= \sum_n \left(-\frac{i}{\hbar}\right)^{n+1}\frac{1}{n!}\sum_{m=0}^{n}\frac{n!}{m!\,(n-m)!}\int ds_{m+1}...\int_C ds_n \langle T_C W(s_{m+1})...W(s_n)\rangle_0 \times \\ &\qquad \times \int_C ds_1...\int_C ds_m \left\langle T_C W(s_1)...W(s_m)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_{0,\text{connected}} .\end{aligned} \tag{220}$$

Now we write $k = n-m$, such that

$$\begin{aligned}G^C_{\alpha\beta}(s,s') = \left(-\frac{i}{\hbar}\right)\sum_n \sum_{m,k=0}^{+\infty}\delta_{n,k+m}\left(-\frac{i}{\hbar}\right)^k \frac{1}{k!}\int_C ds'_1...\int_C ds'_k \langle T_C W(s'_1)...W(s'_k)\rangle_0 \times \\ \times \left(-\frac{i}{\hbar}\right)^m \frac{1}{m!}\int_C ds_1...\int_C ds_m \left\langle T_C W(s_1)...W(s_m)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_{0,\text{connected}} .\end{aligned} \tag{221}$$

Now the sum over n can be trivially performed, and we obtain

$$\begin{aligned}G^C_{\alpha\beta}(s,s') = \left(-\frac{i}{\hbar}\right)\sum_{k=0}^{+\infty}\left(-\frac{i}{\hbar}\right)^k \frac{1}{k!}\int_C ds'_1...\int_C ds'_k \langle T_C W(s'_1)...W(s'_k)\rangle_0 \times \\ \times \sum_{m=0}^{+\infty}\left(-\frac{i}{\hbar}\right)^m \frac{1}{m!}\int_C ds_1...\int_C ds_m \left\langle T_C W(s_1)...W(s_m)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_{0,\text{connected}} .\end{aligned} \tag{222}$$

Now we notice that

$$\sum_{k=0}^{+\infty}\left(-\frac{i}{\hbar}\right)^k \frac{1}{k!}\int_C ds'_1...\int_C ds'_k \langle T_C W(s'_1)...W(s'_k)\rangle_0 = \langle T_C S_C(t_0,t_0)\rangle_0 , \tag{223}$$

and

$$\langle T_C S_C(t_0,t_0)\rangle_0 = \langle S(t_0,t_{\max})S(t_{\max},t_0)\rangle_0 = \langle 1\rangle_0 = 1. \tag{224}$$

Therefore we conclude that

$$\begin{aligned} G^C_{\alpha\beta}(s,s') &= -\frac{i}{\hbar}\left\langle T_C S_C(s_0,s_0)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_0 \\ &= \left(-\frac{i}{\hbar}\right)\sum_{m=0}^{+\infty}\left(-\frac{i}{\hbar}\right)^m \frac{1}{m!}\int_C ds_1 ... \int_C ds_m \left\langle T_C W(s_1)...W(s_m)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_{0,\text{connected}} \\ &= -\frac{i}{\hbar}\left\langle T_C S_C(s_0,s_0)c_\alpha(s)c^\dagger_\beta(s')\right\rangle_{0,\text{connected}}, \end{aligned} \tag{225}$$

only connected diagrams contribute to the Green's function.