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9 Keldysh Green function

This is a lecture note of the theory of condensed matter IV, on Jun. 17. We are interested in a steady-state transport through a system of a quantum dot (QD). When the applied bias is very small, we rely on the linear-response theory and can obtain the linear conductance. What happens when we apply a finite bias? For that purpose, we introduce Keldysh non-equilibrium Green function method. While here we only discuss static problem and a steady state current, it is straightforward to extend to the time-dependent perturbation or transient dynamics in the Keldysh non-equilibrium formalism. Several basic properties of Keldysh Green function are explained. Explicit application to the evaluation of the current through single level quantum dot coupled with two reservoirs is shown in the next (final) lecture.

9.1 Closed time path

The explanation in this section is based on the book[1]. The nonequilibrium problem is stated as follows: We consider a system evolving under the Hamiltonian

$$\hat{\mathcal{H}}(t) \equiv \hat{\mathcal{H}}_0 + \hat{H}'(t), \tag{1}$$

where the time-independent part $\hat{\mathcal{H}}_0$ may include complicated interactions. However, in this note, we neglect the effect of electron interaction and $\hat{\mathcal{H}}_0$ is a sum of "free" Hamiltonians. The perturbation part, $\hat{H}'(t)$, which is absent for times $t < t_0$, could be, *e.g.,* an electric field, a light excitation pulse, or a coupling to contacts at different electro-chemical potentials. Before the perturbation is turned on, the system is described by the thermal equilibrium density operator, (canonical distribution)

$$\hat{\chi}(\hat{\mathcal{H}}_0) = \frac{e^{-\beta\hat{\mathcal{H}}_0}}{\mathrm{Tr}\left[e^{-\beta\hat{\mathcal{H}}_0}\right]}. \tag{2}$$

In the electrical or thermal transport discussed in this lecture, the free hamiltonian $\hat{\mathcal{H}}_0$ is made of several components which represents independent physical systems, namely, source and drain electrodes, and quantum dot or quantum wire, *etc.* Therefore, $\hat{\mathcal{H}}_0 = \sum_{i=1}^{N_s} \hat{\mathcal{H}}_{0i}$, where N_s is the total number of the relevant systems. These independent systems are in *locally* thermal-equilibria, which are characterized by the local inverse temperatures β_i and by the local chemical potentials μ_i, hence, (grand canonical distribution)

$$\hat{\chi}(\hat{\mathcal{H}}_0) = \hat{\rho}_1(\hat{\mathcal{H}}_{01}) \otimes \hat{\rho}_2(\hat{\mathcal{H}}_{02}) \otimes \cdots \hat{\rho}_{N_s}(\hat{\mathcal{H}}_{0N_s}) = \prod_{i=1}^{N_s\otimes} \frac{e^{-\beta(\hat{\mathcal{H}}_{0i}-\mu_i\hat{n}_i)}}{\mathrm{Tr}\left[e^{-\beta_i(\hat{\mathcal{H}}_{0i}-\mu_i\hat{n}_i)}\right]}, \tag{3}$$

where $\hat{n}_i$ are the (electron) number operator in i-th component system. Our task is to calculate the expectation value of a quantum mechanical operator $\hat{O}$, for $t \geq t_0$,

$$\left\langle \hat{O} \right\rangle (t) \equiv \mathrm{Tr}\left[\hat{\chi}(t)\hat{O}\right], \tag{4}$$

where $\hat{\chi}(t)$ is the density operator at time t, defined as $\hat{\chi}(t) = \hat{W}(t,t_0)\hat{\chi}(\hat{\mathcal{H}}_0)\hat{W}^\dagger(t,t_0)$, where the time-evolution operator $\hat{W}(t,t_0)$ obeys the differential equation

$$i\hbar\frac{d}{dt}\hat{W}(t,t_0) = \hat{\mathcal{H}}(t)\hat{W}(t,t_0), \tag{5}$$

and the initial condition $\hat{W}(t_0,t_0)=\hat{I}$ (identity). Using the property of the cyclic invariance of the trace operator

$$\left\langle \hat{O} \right\rangle(t) = \mathrm{Tr}\left[\hat{\chi}(\hat{\mathcal{H}}_0)\hat{W}^\dagger(t,t_0)\hat{O}\hat{W}(t,t_0)\right] \equiv \mathrm{Tr}\left[\hat{\chi}(\hat{\mathcal{H}}_0)\hat{O}_{\mathcal{H}}(t)\right] \equiv \left\langle \hat{O}_{\mathcal{H}}(t) \right\rangle_0, \tag{6}$$

where the average is $\langle\hat{O}\rangle_0 \equiv \mathrm{Tr}\left[\hat{\chi}(\hat{\mathcal{H}}_0)\hat{O}\right]$. The subscript $\mathcal{H}$ put to an operator means the time-evolution by the full Hamltonian, $\hat{\mathcal{H}}(t)$, (Heisenberg representation) and explicitly $\hat{O}_{\mathcal{H}}(t) = \hat{W}^\dagger(t,t_0)\hat{O}\hat{W}(t,t_0)$. Hence, $\hat{O}_{\mathcal{H}}(t)$ satisfies Heisenberg equation of motion,

$$\frac{d}{dt}\hat{O}_{\mathcal{H}}(t) = \frac{i}{\hbar}\left[\hat{\mathcal{H}}_{\mathcal{H}}(t), \hat{O}_{\mathcal{H}}(t)\right]. \tag{7}$$

We then introduce the time-evolution operator in the interaction picture,

$$\hat{V}(t,t_0) = e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{W}(t,t_0), \tag{8}$$

with the initial condition $\hat{V}(t_0,t_0)=\hat{I}$. Therefore

$$\hat{O}_{\mathcal{H}}(t) = \hat{V}^\dagger(t,t_0)e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{O}e^{-\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{V}(t,t_0) = \hat{V}^\dagger(t,t_0)\tilde{O}(t)\hat{V}(t,t_0). \tag{9}$$

The time-derivative of Eq. (8) is

$$\begin{aligned}
\frac{d}{dt}\hat{V}(t,t_0) &= \frac{i}{\hbar}e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{\mathcal{H}}_0\hat{W}(t,t_0) + e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\left\{-\frac{i}{\hbar}\hat{\mathcal{H}}(t)\hat{W}(t,t_0)\right\} \\
&= \frac{i}{\hbar}e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\left[\hat{\mathcal{H}}_0 - \hat{\mathcal{H}}_0 - \hat{H}'(t)\right]\hat{W}(t,t_0) \\
&= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{H}'(t)e^{-\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{W}(t,t_0) \\
&= -\frac{i}{\hbar}\tilde{H}'(t)\hat{V}(t,t_0).
\end{aligned} \tag{10}$$

Here, $\tilde{O}(t)$ and $\tilde{H}'(t)$ are in the interaction representation,

$$\tilde{O}(t) = e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{O}e^{-\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}, \tag{11}$$

$$\tilde{H}'(t) = e^{\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}\hat{H}'(t)e^{-\frac{i}{\hbar}\hat{\mathcal{H}}_0(t-t_0)}. \tag{12}$$

The solution of Eq. (10) is[1]

$$\hat{V}(t,t_0) = \hat{\mathcal{T}}\left\{\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}dt'\tilde{H}'(t')\right]\right\}, \tag{13}$$

where $\hat{\mathcal{T}}$ is the time-ordering operator. It should be noted that if the order of operators containing odd numbers of fermions is reversed, minus (-) sign should be added. However, $\tilde{\mathcal{H}}(t')$ is assumed made of even number of fermion operators. One my note the following identity

$$\hat{V}^\dagger(t,t_0) = \hat{V}(t_0,t) = \tilde{\mathcal{T}}\left\{\exp\left[-\frac{i}{\hbar}\int_{t}^{t_0}dt'\tilde{H}'(t')\right]\right\}, \tag{14}$$

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[1] By integrating Eq. (10) with time, we have

$$\hat{V}(t,t_0) = \hat{I} - \frac{i}{\hbar}\int_{t_0}^{t}dt_1\tilde{H}'(t_1)\hat{V}(t_1,t_0),$$

and putting this into Eq. (10),

$$\frac{d}{dt}\hat{V}(t,t_0) = -\frac{i}{\hbar}\tilde{H}'(t) + \left(-\frac{i}{\hbar}\right)^2\tilde{H}'(t)\int_{t_0}^{t}dt_1\hat{H}'(t_1)\hat{V}(t_1,t_0).$$

Integrating this equation again,

$$\hat{V}(t,t_0) = \hat{I} - \frac{i}{\hbar}\int_{t_0}^{t}dt_1\tilde{H}'(t_1) + \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t}dt_1\tilde{H}'(t_1)\int_{t_0}^{t_1}dt_2\hat{H}'(t_2)\hat{V}(t_2,t_0).$$

where we introduced anti-time-ordering operator $\tilde{\mathcal{T}}$. We then introduce the contour-ordered quantity:

$$\hat{O}_{\mathcal{H}}(t) = \hat{\mathcal{T}}_C \left\{ \exp\left[-\frac{i}{\hbar} \int_C d\tau \tilde{H}'(\tau) \right] \tilde{O}(t) \right\}, \tag{15}$$

where $\hat{\mathcal{T}}_C$ is the time-ordering operator along the contour C. It can be shown that Eq.(9) is equivalent to Eq.(15). The contour C starts from t_0 and propagates along the path C_1 until the time t and then return backward to t_0 via C_2 as shown in Fig. 1(a).

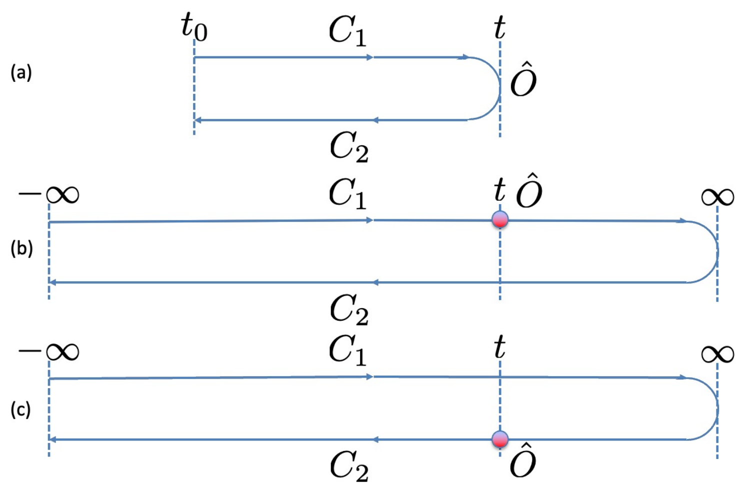

Figure 1: Schematics of the closed-time contours. (a) (top): The contour C made of C_1 starting from t_0 to t and of C_2 starting from t back to t_0. (b) (middle): The contour C starting from $-\infty$ via t with $\hat{O}$ to ∞ (C_1) and then back to $-\infty$ (C_2). (c) (bottom): The contour C starting from $-\infty$ to ∞ (C_1) and then back via t with $\hat{O}$ to $-\infty$ (C_2).

By setting $t_0 \to -\infty$ and modifying the contour C as starting from $-\infty$ to $+\infty$ (C_1) and back to $-\infty$ again (C_2),

$$\begin{aligned}\left\langle \hat{O} \right\rangle (t) &= \mathrm{Tr}\left[\hat{\chi}(\hat{\mathcal{H}}_0) \hat{\mathcal{T}}_C \left\{ \exp\left[-\frac{i}{\hbar} \int_C d\tau \tilde{H}'(\tau) \right] \tilde{O}(t) \right\} \right] \\ &\equiv \left\langle \hat{\mathcal{T}}_C \left\{ \exp\left[-\frac{i}{\hbar} \int_C d\tau \tilde{H}'(\tau) \right] \tilde{O}(t) \right\} \right\rangle_0, \end{aligned} \tag{16}$$

where the measurement time t of the observable $\hat{O}$ could be located either on C_1 (Fig. 1(b)) or C_2 (Fig. 1(c)). In the Appendix A, the first order expansion of the exponential operator is shown to be the linear response theory.

Repeating these procedures iteratively, we have an infinite perturbative series expansion

$$\begin{aligned}\hat{V}(t, t_0) &= \hat{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt_1 \tilde{H}'(t_1) + \left(-\frac{i}{\hbar} \right)^2 \int_{t_0}^{t} dt_1 \tilde{H}'(t_1) \int_{t_0}^{t_1} dt_2 \hat{H}'(t_2) \\ &+ \left(-\frac{i}{\hbar} \right)^3 \int_{t_0}^{t} dt_1 \tilde{H}'(t_1) \int_{t_0}^{t_1} dt_2 \tilde{H}'(t_2) \int_{t_0}^{t_2} dt_3 \tilde{H}'(t_3) + O(\tilde{H}')^4 \\ &= \hat{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt_1 \tilde{H}'(t_1) + \left(-\frac{i}{\hbar} \right)^2 \frac{1}{2} \hat{\mathcal{T}} \left[\int_{t_0}^{t} dt_1 \tilde{H}'(t_1) \int_{t_0}^{t} dt_2 \hat{H}'(t_2) \right] \\ &+ \left(-\frac{i}{\hbar} \right)^3 \frac{1}{3!} \hat{\mathcal{T}} \left[\int_{t_0}^{t} dt_1 \tilde{H}'(t_1) \int_{t_0}^{t} dt_2 \tilde{H}'(t_2) \int_{t_0}^{t} dt_3 \tilde{H}'(t_3) \right] + O(\tilde{H}')^4 \\ &= \hat{\mathcal{T}} \left\{ \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} dt' \tilde{H}'(t') \right] \right\},\end{aligned}$$

with the time-ordering operator $\hat{\mathcal{T}}$.

9.2 Contour-ordered Green function

The idea of the contour-ordered path (closed-time path) goes back to Scgwinger (1961)[2] and the associated contour-ordered Green function was introduced by Keldysh (1965)[3]. We define the contour-ordered (Keldysh) Green function:

$$G(1,1') \equiv -\frac{i}{\hbar}\left\langle \hat{\mathcal{T}}_C\left[\hat{\psi}_{\mathcal{H}}(1)\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\right]\right\rangle, \tag{17}$$

where $(1) \equiv (\boldsymbol{r}_1, t_1)$ and $(1') \equiv (\boldsymbol{r}'_1, t'_1)$ and the fermionic field operator is in the Heisenberg picture $\hat{\psi}_{\mathcal{H}}(\boldsymbol{r},t) = \hat{V}(t,-\infty)\tilde{\psi}(\boldsymbol{r},t)$. The average $\langle\cdots\rangle$ represents the thermal average over a certain initial distribution. In the following arguments, we removed the suffix "$_0$" in the thermal average $\langle\hat{O}\rangle_0$ for simplicity. It is important to notice that the Green function $G(1,1')$ is **not a function of the time difference,** $t_1 - t'_1$, but is in general depending each times.

This may be rewritten with the field operators in the interaction picture,

$$G(1,1') = -\frac{i}{\hbar}\left\langle \hat{\mathcal{T}}_C\left\{\exp\left[-\frac{i}{\hbar}\int_C d\tau \tilde{H}'(\tau)\right]\tilde{\psi}(1)\tilde{\psi}^{\dagger}(1')\right\}\right\rangle. \tag{18}$$

In the following, we use the notation that Greek letter τ represents a time on the closed-time path (C) but the Roman letter t shows the real (physical) time. The contour-ordered Green function is mapped with four different Green functions depending on the locations of the times in the two branches of the contour, $C = C_1 + C_2$:

$$G(1,1') = \begin{cases} G_c(1,1') & t_1, t'_1 \in C_1 \\ G^{>}(1,1') & t_1 \in C_2, t'_1 \in C_1 \\ G^{<}(1,1') & t_1 \in C_1, t'_1 \in C_2 \\ G_{\bar{c}}(1,1') & t_1, t'_1 \in C_2 \end{cases} \tag{19}$$

where $G^{>}(1,1'), G^{<}(1,1')$ are the greater and lesser Green functions, respectively, defined as

$$G^{>}(1,1) = -\frac{i}{\hbar}\langle\hat{\psi}_{\mathcal{H}}(1)\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\rangle, \tag{20}$$

$$G^{<}(1,1) = \frac{i}{\hbar}\langle\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\hat{\psi}_{\mathcal{H}}(1)\rangle. \tag{21}$$

$G_c, G_{\bar{c}}$ are the time-ordered and anti-time-ordered Green functions,

$$\begin{aligned} G_c(1,1') &= -\frac{i}{\hbar}\left\langle\hat{\mathcal{T}}\left[\hat{\psi}_{\mathcal{H}}(1)\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\right]\right\rangle = -\frac{i}{\hbar}\left\{\theta(t_1 - t_{1'})\langle\hat{\psi}_{\mathcal{H}}(1)\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\rangle - \theta(t_{1'} - t_1)\langle\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\hat{\psi}_{\mathcal{H}}(1)\rangle\right\} \\ &= \theta(t_1 - t_{1'})G^{>}(1,1') + \theta(t_{1'} - t_1)G^{<}(1,1'), \end{aligned} \tag{22}$$

$$\begin{aligned} G_{\bar{c}}(1,1') &= -\frac{i}{\hbar}\left\langle\tilde{\mathcal{T}}\left[\hat{\psi}_{\mathcal{H}}(1)\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\right]\right\rangle = -\frac{i}{\hbar}\left\{-\theta(t_1 - t_{1'})\langle\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\hat{\psi}_{\mathcal{H}}(1)\rangle - \theta(t_{1'} - t_1)\langle\hat{\psi}_{\mathcal{H}}(1)\hat{\psi}^{\dagger}_{\mathcal{H}}(1')\rangle\right\} \\ &= \theta(t_1 - t_{1'})G^{<}(1,1') + \theta(t_{1'} - t_1)G^{>}(1,1'). \end{aligned} \tag{23}$$

Since

$$G_c(1,1') + G_{\bar{c}}(1,1') = G^{>}(1,1') + G^{<}(1,1'), \tag{24}$$

these four Green functions are not independent.[2] We further introduce retarded/advanced Green functions, defined as

$$G^{r}(1,1') = -\frac{i}{\hbar}\theta(t_1 - t_{1'})\left\langle\left\{\hat{\psi}_{\mathcal{H}}(1), \hat{\psi}^{\dagger}_{\mathcal{H}}(1')\right\}\right\rangle = \theta(t_1 - t_{1'})\left[G^{>}(1,1') - G^{<}(1,1')\right], \tag{26}$$

$$G^{a}(1,1') = \frac{i}{\hbar}\theta(t_{1'} - t_1)\left\langle\left\{\hat{\psi}_{\mathcal{H}}(1), \hat{\psi}^{\dagger}_{\mathcal{H}}(1')\right\}\right\rangle = -\theta(t_{1'} - t_1)\left[G^{>}(1,1') - G^{<}(1,1')\right], \tag{27}$$

[2] Sometimes, another Green function, Keldysh component, is defined by

$$G^{K}(1,1') \equiv G^{>}(1,1') + G^{<}(1,1'). \tag{25}$$

hence $G^r(1,1') - G^a(1,1') = G^>(1,1') - G^<(1,1')$.

There is a strong formal connection between the contour-ordered Green function and corresponding equilibrium time-ordered Green function. This is quite useful to calculate the contour-ordered Green function in a perturbation formalism. (In the calculation of the next lecture, we explore this property to obtain the Dyson's equation.)

9.3 Langreth Theorem

In this subsection, with so-called analytic continuation (Langreth Theorem), we introduce various relations between Green functions. The derivation are based on Ref.[1]. Let us consider a Green function $A(t_1,\tau)$ with the time t_1 locates on the contour C_1, we have

$$\begin{aligned}\int_C d\tau A(t_1,\tau) &= \int_{-\infty}^{t_1} dt A^>(t_1,t) + \int_{t_1}^{-\infty} dt A^<(t_1,t) \\ &= \int_{-\infty}^{\infty} dt \theta(t_1-t)\left\{A^>(t_1,t) - A^<(t_1,t)\right\} \\ &= \int_{-\infty}^{\infty} dt G^r(t_1,t), \end{aligned} \tag{28}$$

where the same result is obtained when the time t_1 locates on the contour C_2. Similarly, for a Green function $B(\tau,t_{1'})$, we have

$$\begin{aligned}\int_C d\tau B(\tau,t_{1'}) &= \int_{-\infty}^{t_{1'}} dt B^<(t,t_{1'}) + \int_{t_{1'}}^{-\infty} dt B^>(t,t_{1'}) \\ &= \int_{-\infty}^{\infty} \theta(t_{1'}-t)\left\{B^<(t,t_{1'}) - B^>(t,t_{1'})\right\} \\ &= \int_{-\infty}^{\infty} dt B^a(t,t_{1'}). \end{aligned} \tag{29}$$

We may have the following relation between contour ordered Green functions A, B and C,

$$C(t_1,t_{1'}) = \int_C d\tau A(t_1,\tau)B(\tau,t_{1'}). \tag{30}$$

The lesser function of $C(t_1,t_{1'})$ is defined by placing the time t_1 in the contour $C_1 = (-\infty,\infty)$ and $t_{1'}$ in the contour $C_2 = (\infty,-\infty)$. We can extend the contour as $C_1' = (-\infty,\infty,-\infty)$ and $C_2' = (-\infty,\infty,-\infty)$ and hence

$$\begin{aligned}C^<(t_1,t_{1'}) &= \int_{C_1'} d\tau A(t_1,\tau)B(\tau,t_{1'}) + \int_{C_2'} d\tau A(t_1,\tau)B(\tau,t_{1'}) \\ &= \int_{-\infty}^{\infty} dt A^r(t_1,t)B^<(t,t_{1'}) + \int_{-\infty}^{\infty} dt A^<(t_1,t)B^a(t,t_{1'}) \\ &= \int_{-\infty}^{\infty} dt \left[A^r(t_1,t)B^<(t,t_{1'}) + A^<(t_1,t)B^a(t,t_{1'})\right]. \end{aligned} \tag{31}$$

The greater function of $C(t_1,t_{1'})$ is also evaluated assuming the the time t_1 in the contour C_2' and the time $t_{1'}$ in the contour C_1',

$$\begin{aligned}C^>(t_1,t_{1'}) &= \int_{C_1'} d\tau A(t_1,\tau)B(\tau,t_{1'}) + \int_{C_2'} d\tau A(t_1,\tau)B(\tau,t_{1'}) \\ &= \int_{-\infty}^{\infty} dt A^>(t_1,t)B^a(t,t_{1'}) + \int_{-\infty}^{\infty} dt A^r(t_1,t)B^>(t,t_{1'}) \\ &= \int_{-\infty}^{\infty} dt \left[A^>(t_1,t)B^a(t,t_{1'}) + A^r(t_1,t)B^>(t,t_{1'})\right]. \end{aligned} \tag{32}$$

The retarded function is evaluated from Eq. (26),

$$
\begin{aligned}
C^r(t_1,t_1') &= \theta(t_1-t_{1'})\left[C^>(t_1,t_{1'})-C^<(t_1,t_{1'})\right] \\
&= \theta(t_1-t_{1'})\int_{-\infty}^{\infty}dt\left[A^>(t_1,t)B^a(t,t_{1'})+A^r(t_1,t)B^>(t,t_1')-A^r(t_1,t)B^<(t,t_{1'})-A^<(t_1,t)B^a(t,t_{1'})\right] \\
&= \theta(t_1-t_{1'})\int_{-\infty}^{\infty}dt\left[A^r(t_1,t)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right)+\left(A^>(t_1,t)-A^<(t_1,t)\right)B^a(t,t_{1'})\right] \\
&= \theta(t_1-t_{1'})\Big[\int_{-\infty}^{t_1}dt\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right) \\
&\qquad -\int_{-\infty}^{t_{1'}}dt\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right)\Big] \\
&= \theta(t_1-t_{1'})\int_{t_{1'}}^{t_1}dt\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right) \\
&= \int_{-\infty}^{\infty}dt\theta(t_1-t)\theta(t-t_{1'})\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right) \\
&= \int_{-\infty}^{\infty}dtA^r(t_1,t)B^r(t,t_1'),
\end{aligned} \tag{33}
$$

and the advanced function is

$$
\begin{aligned}
C^a(t_1,t_1') &= -\theta(t_{1'}-t_1)\left[C^>(t_1,t_{1'})-C^<(t_1,t_{1'})\right] \\
&= -\theta(t_{1'}-t_1)\int_{-\infty}^{\infty}dt\left[A^r(t_1,t)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right)+\left(A^>(t_1,t)-A^<(t_1,t)\right)B^a(t,t_{1'})\right] \\
&= -\theta(t_{1'}-t_1)\Big[\int_{-\infty}^{t_1}dt\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right) \\
&\qquad -\int_{-\infty}^{t_{1'}}dt\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right)\Big] \\
&= \theta(t_{1'}-t_1)\int_{t_1}^{t_{1'}}dt\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right) \\
&= \int_{-\infty}^{\infty}dt\theta(t_{1'}-t)\theta(t-t_1)\left(A^>(t_1,t)-A^<(t_1,t)\right)\left(B^>(t,t_{1'})-B^<(t,t_{1'})\right) \\
&= \int_{-\infty}^{\infty}dtA^a(t_1,t)B^a(t,t_1'),
\end{aligned} \tag{34}
$$

Similarly, for the products of three functions,

$$
D(t_1,t_{1'}) = \int_C d\tau\int_{C'}d\tau' A(t,\tau)B(\tau,\tau')C(\tau',t_{1'}), \tag{35}
$$

we have

$$
\begin{aligned}
D^<(t_1,t_{1'}) &= \int_{C_1'} d\tau A(t,\tau)\int_{C'} d\tau' B(\tau,\tau')C(\tau',t_{1'}) + \int_{C_2'} d\tau A(t,\tau)\int_{C'} d\tau' B(\tau,\tau')C(\tau',t_{1'}) \\
&= \int_{-\infty}^{\infty} dt A^r(t_1,t)\left\{\int_{C'} d\tau' B(t,\tau')C(\tau',t_{1'})\right\}^< + \int_{-\infty}^{\infty} dt A^<(t_1,t)\left\{\int_{C'} d\tau' B(t,\tau')C(\tau',t_{1'})\right\}^a \\
&= \int_{-\infty}^{\infty} dt dt' \left[A^r(t_1,t)B^r(t,t')C^<(t'-t_{1'}) + A^r(t_1,t)B^<(t,t')C^a(t',t_{1'}) + A^<(t_1,t)B^a(t,t')C^a(t'-t_{1'})\right],
\end{aligned}
\tag{36}
$$

$$
\begin{aligned}
D^>(t_1,t_{1'}) &= \int_{C} d\tau A(t,\tau)\int_{C_1'} d\tau' B(\tau,\tau')C(\tau',t_{1'}) + \int_{C} d\tau A(t,\tau)\int_{C_2'} d\tau' B(\tau,\tau')C(\tau',t_{1'}) \\
&= \int_{-\infty}^{\infty} dt' \left\{\int_{C} A(t_1,\tau)B(\tau,t')\right\}^> C^a(t',t_{1'}) + \int_{-\infty}^{\infty} dt' \left\{\int_{C} A(t_1,\tau)B(\tau,t')\right\}^r C^>(t',t_{1'}) \\
&= \int_{-\infty}^{\infty} dt dt' \left[A^>(t_1,t)B^a(t,t')C^a(t'-t_{1'}) + A^r(t_1,t)B^>(t,t')C^a(t',t_{1'}) + A^r(t_1,t)B^r(t,t')C^>(t'-t_{1'})\right],
\end{aligned}
\tag{37}
$$

and

$$
\begin{aligned}
D^r(t_1,t_{1'}) &= \int_{-\infty}^{\infty} dt A^r(t_1,t)\left\{\int_{C'} d\tau' B(t,\tau')C(\tau',t_{1'})\right\}^r \\
&= \int_{-\infty}^{\infty} dt dt' A^r(t_1,t)B^r(t,t')C^r(t',t_{1'}),
\end{aligned}
\tag{38}
$$

$$
\begin{aligned}
D^a(t_1,t_{1'}) &= \int_{-\infty}^{\infty} dt A^a(t_1,t)\left\{\int_{C'} d\tau' B(t,\tau')C(\tau',t_{1'})\right\}^a \\
&= \int_{-\infty}^{\infty} dt dt' A^a(t_1,t)B^a(t,t')C^a(t',t_{1'}).
\end{aligned}
\tag{39}
$$

Next, we evaluate the product of two Green functions

$$C(\tau,\tau') \equiv A(\tau,\tau')B(\tau,\tau'). \tag{40}$$

It is obvious, the lesser and greater functions are

$$C^<(t,t') = A^<(t,t')B^<(t,t'), \tag{41}$$
$$C^>(t,t') = A^>(t,t')B^>(t,t'). \tag{42}$$

The retarded function is

$$
\begin{aligned}
C^r(t,t') &= \theta(t-t')\left[C^>(t,t') - C^<(t,t')\right] \\
&= \theta(t-t')\left[A^>(t,t')B^>(t,t') - A^<(t,t')B^<(t,t')\right] \\
&= \theta(t-t')\Big[A^<(t,t')\left(B^>(t,t') - B^<(t,t')\right) + \left(A^>(t,t') - A^<(t,t')\right)B^<(t,t') \\
&\qquad + \left(A^>(t,t') - A^<(t,t')\right)\left(B^>(t,t') - B^<(t,t')\right)\Big] \\
&= A^<(t,t')B^r(t,t') + A^r(t,t')B^<(t,t') + A^r(t,t')B^r(t,t').
\end{aligned}
\tag{43}
$$

Finally, we evaluate the another type of product of two Green functions

$$D(\tau,\tau') \equiv A(\tau,\tau')B(\tau',\tau). \tag{44}$$

It is obvious, the lesser and greater functions are

$$D^<(t,t') = A^<(t,t')B^>(t',t), \tag{45}$$
$$D^>(t,t') = A^>(t,t')B^<(t',t). \tag{46}$$

The retarded function is

$$\begin{aligned}
D^r(t,t') &= \theta(t-t')\left[D^>(t,t') - D^<t',t)\right] \\
&= \theta(t-t')\left[A^>(t,t')B^<(t',t) - A^<(t,t')B^>(t',t)\right] \\
&= \theta(t-t')\left[\left(A^>(t,t') - A^<(t,t')\right)B^<(t',t) + A^<(t,t')\left(B^<(t',t) - B^>(t',t)\right)\right] \\
&= A^r(t,t')B^<(t',t) + A^<(t,t')B^a(t',t). \qquad (47)
\end{aligned}$$

9.4 Conclusions

We have introduced Keldysh Green function defined on contour-ordered path. We had also explained basic properties of Keldysh Green function, so-called Langreth theorem.

A Linear response

When the effect of the perturbation $\hat{H}'(t)$ can be assumed small, we may focus our attention to the first order of the expansion of the exponential operator in Eq. (16), namely,

$$\left\langle \hat{O} \right\rangle(t) = \langle \hat{O} \rangle_0 + \left\langle \hat{\mathcal{T}}_c \left\{ -\frac{i}{\hbar} \int_C d\tau \tilde{\mathcal{H}}'(\tau)\tilde{O}(t) \right\} \right\rangle_0 + O((\hat{H}')^2). \qquad (48)$$

Then the first-order correction (linear response (LR)) is

$$\begin{aligned}
\delta \left\langle \hat{O} \right\rangle_{\rm LR} &\equiv \left\langle \hat{O} \right\rangle(t)\Big|_{\rm LR} - \left\langle \hat{O} \right\rangle_0 \\
&= -\frac{i}{\hbar} \left\langle \int_{-\infty}^{t} dt' \tilde{O}(t)\tilde{H}'(t') + \int_{t}^{-\infty} (-dt')\tilde{H}'(t')\tilde{O}(t) \right\rangle_0 \\
&= -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \left\langle \left\{ \tilde{O}(t), \tilde{H}'(t') \right\} \right\rangle_0 . \qquad (49)
\end{aligned}$$

Assuming that the perturbation Hamiltonian is given like

$$\hat{\mathcal{H}}'(t) = B(t)\hat{P}, \qquad (50)$$

where $B(t)$ is some time-depending function and $\tilde{\mathcal{H}}'(t) = B(t)\tilde{P}(t)$ and by changing integration variable $s = t - t'$,

$$\begin{aligned}
\delta \left\langle \hat{O} \right\rangle_{\rm LR} &= -\frac{i}{\hbar} \int_0^{\infty} ds \left\langle \left\{ \tilde{O}(t), \tilde{\mathcal{H}}'(t-s) \right\} \right\rangle_0 \\
&= -\frac{i}{\hbar} \int_{-\infty}^{\infty} ds \; B(t-s)\chi^r_{OP}(s), \qquad (51)
\end{aligned}$$

where we used the property of the thermal average that only depends on the time-difference, and we defined the *response function*

$$\chi^r_{OP}(s) \equiv -\frac{i}{\hbar}\theta(s) \langle \left\{ \tilde{O}(s), \tilde{P}(0) \right\} \rangle_0 , \qquad (52)$$

which is in fact the retarded Green function that will be introduced in the next section. This result is a standard form of the linear-response theory.

A.1 Simple example of linear response - spin susceptibility

As a simple example, we consider single electron spin driven by a time-dependent magnetic field. The free part of the Hamiltonian is

$$\hat{\mathcal{H}}_0 = \frac{\hbar\omega_0}{2}\hat{\sigma}_z, \qquad (53)$$

and the interaction Hamiltonian, which is nonzero for $t \geq t_0 = -\infty$, is

$$\hat{H}'(t) = B(t)\hat{\sigma}_x. \tag{54}$$

Obviously, at thermal equilibrium, $\langle\hat{\sigma}_x\rangle_0 = 0$. Then the linear order of the induced magnetization in the x direction is

$$\langle\hat{\sigma}_x\rangle_{\mathrm{LR}}(t) = \int_{-\infty}^{\infty} ds\ B(t-s)\chi^r_{xx}(s), \tag{55}$$

where the function

$$\chi^r_{xx}(s) \equiv -\frac{i}{\hbar}\theta(s)\left\langle\{\tilde{\sigma}_x(s), \tilde{\sigma}_x(0)\}\right\rangle_0, \tag{56}$$

is a longitudinal susceptibility function.

Explicitly, the equation of motion of $\tilde{\sigma}_x(s)$ is

$$\frac{d\tilde{\sigma}_x(s)}{ds} = e^{i\frac{\omega_0}{2}\hat{\sigma}_z s}\frac{i\omega_0}{2}\left[\hat{\sigma}_z, \hat{\sigma}_x\right]e^{-i\frac{\omega_0}{2}\hat{\sigma}_z s} = -\omega_0\tilde{\sigma}_y(s), \tag{57}$$

and similarly

$$\frac{d\tilde{\sigma}_y(s)}{ds} = e^{i\frac{\omega_0}{2}\hat{\sigma}_z s}\frac{i\omega_0}{2}\left[\hat{\sigma}_z, \hat{\sigma}_y\right]e^{-i\frac{\omega_0}{2}\hat{\sigma}_z s} = \omega_0\tilde{\sigma}_x(s). \tag{58}$$

Hence, the general solution is

$$\tilde{\sigma}_x(s) = \hat{a}\cos\omega_0 s + \hat{b}\sin\omega_0 s, \tag{59}$$

and from the initial condition, $\tilde{\sigma}_x(0) = \hat{\sigma}_x = \hat{a}$ and $\tilde{\sigma}_y(0) = \hat{\sigma}_y = -\frac{1}{\omega_0}\frac{d\tilde{\sigma}_x(s)}{ds}\Big|_{s=0} = -\frac{1}{\omega_0}\omega_0\hat{b} = -\hat{b}$, hence $\tilde{\sigma}_x(s) = \hat{\sigma}_x\cos\omega_0 s - \hat{\sigma}_y\sin\omega_0 s$. Assuming the applied field $B(t-s) = A\cos\omega(t-s)$ and introducing phenomenologically a relaxation factor $e^{-\gamma s}$ with a positive phenological parameter γ to the susceptibility function, we have

$$\begin{aligned}\langle\hat{\sigma}_x\rangle(t) &= -\frac{i}{\hbar}\int_0^{\infty} dsA\cos\omega(t-s)\left\langle\{\hat{\sigma}_x\cos\omega_0 s - \hat{\sigma}_y\sin\omega_0 s, \hat{\sigma}_x\}\right\rangle_0 e^{-\gamma s}\\ &= -\frac{iA}{\hbar}\int_0^{\infty} ds\cos\omega(t-s)(2i)\langle\hat{\sigma}_z\rangle_0\sin\omega_0 s\ e^{-\gamma s}\\ &\sim \frac{A}{\hbar\gamma}\langle\hat{\sigma}_z\rangle_0\sin\omega_0 t,\end{aligned} \tag{60}$$

where in the last, we set $\omega_0 = \omega$ and neglected the fast oscillating term. Similarly, the magnetization in the y direction is

$$\begin{aligned}\langle\hat{\sigma}_y\rangle(t) &= -\frac{iA}{\hbar}\int_0^{\infty} ds\cos\omega(t-s)(2i)\langle\hat{\sigma}_z\rangle_0\cos\omega_0 s e^{-\gamma_s}\\ &\sim \frac{A}{\hbar\gamma}\langle\hat{\sigma}_z\rangle_0\cos\omega_0 t.\end{aligned} \tag{61}$$

Hence, absolute value of the induced transverse magnetization is

$$\sqrt{\langle\hat{\sigma}_x\rangle^2(t) + \langle\hat{\sigma}_y\rangle^2(t)} \sim \frac{A}{\hbar\gamma}\langle\hat{\sigma}_z\rangle_0. \tag{62}$$

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