物性理論IV 講義ノート 6月24日 2024

Yasuhiro Tokura

June 12, 2024

10 Landauer-Büttiker formula

This is a lecture note of the theory of condensed matter IV, on Jun. 24 explaining the derivation of the Landauer-Büttiker formula, which expresses the current in terms of the transmission probability and distribution functions of the reservoirs. We use the Keldysh formula explained in the last lecture, to treat the situation far from the equilibrium. The effect of electron interaction and spin degree's of freedom is neglected. Average current is expressed with quantum dot (QD) retarded/advance Green function and line-width functions (Meir-Wingreen formula). General expression reduces to that from classical master equation in the limit of small line-width (weak couplings).

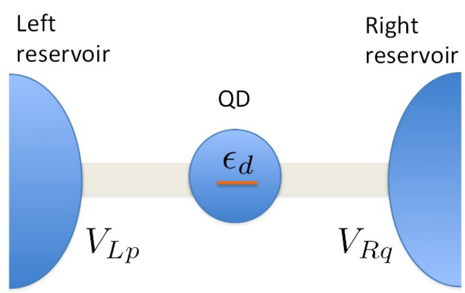

Figure 1: Schematics of the considered system.

10.1 Average current

We consider a single quantum dot (QD), which is tunnel coupled to the left and right reservoirs as shown in Fig.1. We disregard the Coulomb interaction in the QDs and in the reservoirs and the spin degrees of freedom. We take account of only single level in the QD. The total Hamiltonian is $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\rm QD} + \hat{\mathcal{H}}_{\rm Res} + \hat{\mathcal{H}}_{\rm T}$, which is time-independent (after $t > t_0 = -\infty$). The unperturbed part is $\hat{\mathcal{H}}_0 \equiv \hat{\mathcal{H}}_{\rm QD} + \hat{\mathcal{H}}_{\rm Res}$. The Hamiltonian of the QD is

$$\hat{\mathcal{H}}_{\rm QD} = \epsilon_d \hat{d}^\dagger \hat{d}, \tag{1}$$

where $\hat{d}^\dagger$ ($\hat{d}$) and ϵ_d are the creation (annihilation) operator and the level energy of the QD, respectively. The Hamiltonian of the two non-interacting reservoirs is

$$\hat{\mathcal{H}}_{\rm Res} = \sum_p \epsilon_p \hat{C}_p^\dagger \hat{C}_p + \sum_q \epsilon_q \hat{C}_q^\dagger \hat{C}_q, \tag{2}$$

where p (q) and ϵ_p (ϵ_q) are the quantum state index and its energy in the left (right) reservoir. $\hat{C}_p^\dagger$ ($\hat{C}_p$) and $\hat{C}_q^\dagger$ ($\hat{C}_q$) are the creation (annihilation) operators of the left and right reservoirs, respectively. Finally, the Hamiltonian of the tunnel coupling between the QD and reservoirs is

$$\hat{\mathcal{H}}_{\rm T} = \sum_p V_{Lp} \hat{C}_p^\dagger \hat{d} + \sum_q V_{Rq} \hat{C}_q^\dagger \hat{d} + \text{H.c.}, \tag{3}$$

where V_{Lp} (V_{Rq}) is a complex tunnel coupling parameter between the left reservoir and the QD (between the right reservoir and the QD), and H.c. means the Hermite conjugate terms.

The results of this subsection and the next (Sec. 10.2) are general and are not dependent on the details of the QDs Hamiltonian, $\mathcal{H}_{\rm QD}$, but depends through QD's Green functions which will be discussed in Sec. 10.3. We study the current flowing from the QD to the right reservoir and is defined by

$$J_R(t) = -e\left\langle \frac{d}{dt}\hat{\mathcal{N}}_R(t)\right\rangle = -\frac{ie}{\hbar}\left\langle [\hat{\mathcal{H}}, \hat{\mathcal{N}}_R(t)]\right\rangle, \tag{4}$$

where the operators are in the Heisenberg picture and the average $\langle\cdots\rangle$ means the quantum mechanical and statistical average over the reservoir states locally in thermal equilibrium and for an arbitrary initial state of the QDs. $\hat{\mathcal{N}}_R \equiv \sum_q \hat{C}_q^\dagger \hat{C}_q$ is the number operator of the right reservoir. e (> 0) is the unit charge and $-e$ is the charge of an electron. Therefore, positive J_R means current flowing from QD to the right reservoir. We used equation of motion of the Heisenberg operator $\hat{O}(t)$,

$$\frac{\partial}{\partial t}\hat{O}(t) = \frac{i}{\hbar}[\hat{\mathcal{H}}, \hat{O}(t)]. \tag{5}$$

Since $\hat{\mathcal{N}}_R$ commutes with $\hat{\mathcal{H}}_{\rm Res}$, evaluating the commutator in Eq. (4) in the Schrödinger picture,

$$[\hat{\mathcal{H}}, \hat{\mathcal{N}}_R] = \left[\hat{\mathcal{H}}_{\rm T}, \hat{\mathcal{N}}_R\right] = -\sum_q \left\{V_{Rq}\hat{C}_q^\dagger \hat{d} - V_{Rq}^* \hat{d}^\dagger \hat{C}_q\right\}, \tag{6}$$

the current becomes

$$J_R(t) = \frac{ie}{\hbar}\sum_q \left[V_{Rq}\left\langle \hat{C}_q^\dagger(t)\hat{d}(t)\right\rangle - V_{Rq}^*\left\langle \hat{d}^\dagger(t)\hat{C}_q(t)\right\rangle\right]. \tag{7}$$

Then we introduce the lesser Green function

$$G_{d,q}^<(t,t') \equiv \frac{i}{\hbar}\left\langle \hat{C}_q^\dagger(t')\hat{d}(t)\right\rangle. \tag{8}$$

The complex conjugate of the lesser Green function is

$$\left[G_{d,q}^<(t,t')\right]^* = -\frac{i}{\hbar}\left\{\left\langle \hat{C}_q^\dagger(t')\hat{d}(t)\right\rangle\right\}^* = -\frac{i}{\hbar}\left\langle \hat{d}^\dagger(t)\hat{C}_q(t')\right\rangle. \tag{9}$$

Therefore, the current reduces to

$$J_R(t) = \frac{ie}{\hbar}\sum_q \left\{V_{Rq}\frac{\hbar}{i}G_{d,q}^<(t,t) - V_{Rq}^*\left(-\frac{\hbar}{i}\right)\left[G_{d,p}^<(t,t)\right]^*\right\} = 2e\Re\left\{\sum_q V_{Rq}G_{d,p}^<(t,t)\right\}. \tag{10}$$

10.2 Equation of motion of contour-ordered Green function

In order to study the lesser Green function, Eq.(8), we consider contour-ordered Green function,

$$G_{d,q}(\tau,\tau') \equiv -\frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle \hat{d}(\tau)\hat{C}_q^\dagger(\tau')\right\rangle, \tag{11}$$

where the contour time ordering operator arranges $\hat{\mathcal{T}}_C\{\hat{O}_1(\tau)\hat{O}_2(\tau')\}$ to $\hat{O}_1(\tau)\hat{O}_2(\tau')$ for $\tau >_C \tau'$ and $-\hat{O}_2(\tau')\hat{O}_1(\tau)$ for $\tau <_C \tau'$, where $\hat{O}_1(\tau)$ and $\hat{O}_2(\tau')$ are Fermion operators and $>_C$ and $<_C$ mean the inequality along the closed time path C. The equation of motion is

$$\begin{aligned}
-i\hbar\frac{\partial}{\partial\tau'}G_{d,q}(\tau,\tau') &= -\left\{\frac{\partial\theta_C(\tau-\tau')}{\partial\tau'}\left\langle \hat{d}(\tau)\hat{C}_q^\dagger(\tau')\right\rangle - \frac{\partial\theta_C(\tau'-\tau)}{\partial\tau'}\left\langle \hat{C}_q^\dagger(\tau')\hat{d}(\tau)\right\rangle\right\} - \frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle \hat{d}(\tau)\left(-i\hbar\frac{\partial}{\partial\tau'}\hat{C}_q^\dagger(\tau')\right)\right\rangle \\
&= \delta_C(\tau-\tau')\left\langle\left\{\hat{d}(\tau), \hat{C}_q^\dagger(\tau)\right\}\right\rangle - \frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle \hat{d}(\tau)\left[\hat{\mathcal{H}}, \hat{C}_q^\dagger(\tau')\right]\right\rangle,
\end{aligned} \tag{12}$$

whtere $\theta_C(\tau)$ and $\delta_C(\tau)$ are the Heaviside step function and the Dirac delta function along the closed time path, respectively. The equal-time anti-commutator of the first term is zero and the commutator in the second term is evaluated using

$$\left[\hat{\mathcal{H}}, \hat{C}_q^\dagger\right] = \left[\hat{\mathcal{H}}_{\rm Res} + \hat{\mathcal{H}}_{\rm T}, \hat{C}_q^\dagger\right] = \epsilon_q \hat{C}_q^\dagger + V_{Rq}^* \hat{d}^\dagger. \tag{13}$$

Therefore, the equation of motion Eq. (12) becomes

$$\begin{aligned} -i\hbar \frac{\partial}{\partial \tau'} G_{d,q}(\tau,\tau') &= \epsilon_q \left\{ -\frac{i}{\hbar} \hat{\mathcal{T}}_C \left\langle \hat{d}(\tau) \hat{C}_q^\dagger(\tau') \right\rangle \right\} + V_{Rq}^* \left\{ -\frac{i}{\hbar} \hat{\mathcal{T}}_C \left\langle \hat{d}(\tau) \hat{d}^\dagger(\tau') \right\rangle \right\} \\ &= \epsilon_q G_{d,q}(\tau,\tau') + V_{Rq}^* G_d(\tau,\tau'), \end{aligned} \tag{14}$$

where we define QD's Green function

$$G_d(\tau,\tau') \equiv -\frac{i}{\hbar} \hat{\mathcal{T}}_C \left\langle \hat{d}(\tau) \hat{d}^\dagger(\tau') \right\rangle. \tag{15}$$

Then, we have

$$G_{d,q}(\tau,\tau') \overleftarrow{g}_{Rq}^{-1}(\tau') = V_{Rq}^* G_d(\tau,\tau'). \tag{16}$$

where we defined an operator operating to the left,

$$\overleftarrow{g}_{Rq}^{-1}(\tau') \equiv -i\hbar \frac{\partial}{\partial \tau'} - \epsilon_q. \tag{17}$$

We then study free Green function of the right reservoir (in the following, the Green functions with small character g are "free" Green function without the effect of the tunneling Hamiltonian $\mathcal{H}_{\rm T}$),

$$g_{Rq}(\tau,\tau') \equiv -\frac{i}{\hbar} \hat{\mathcal{T}}_C \left\langle \tilde{C}_q(\tau) \tilde{C}_q^\dagger(\tau') \right\rangle, \tag{18}$$

where the "tilde" operator is in the interaction picture,

$$\tilde{C}_q(\tau) \equiv \left\{ \hat{\mathcal{T}} e^{i\hat{\mathcal{H}}_0 \tau/\hbar} \right\} \hat{C}_q \left\{ \tilde{\mathcal{T}} e^{-i\hat{\mathcal{H}}_0 \tau/\hbar} \right\} = e^{i\hat{\mathcal{H}}_{\rm Res}\tau/\hbar} \hat{C}_q e^{-i\hat{\mathcal{H}}_{\rm Res}\tau/\hbar}. \tag{19}$$

The equation of motion of free Green function is

$$-i\hbar \frac{\partial}{\partial \tau'} g_{Rq}(\tau,\tau') = \delta_C(\tau-\tau') \left\langle \left\{ \tilde{C}_q(\tau), \tilde{C}_q^\dagger(\tau) \right\} \right\rangle - \frac{i}{\hbar} \hat{\mathcal{T}}_C \left\langle \tilde{C}_q(\tau) \left[\tilde{\mathcal{H}}_0, \tilde{C}_q^\dagger(\tau') \right] \right\rangle. \tag{20}$$

Noting the commutator $\left[\hat{\mathcal{H}}_0, \hat{C}_q^\dagger\right] = \left[\hat{\mathcal{H}}_{\rm Res}, \hat{C}_q^\dagger\right] = \epsilon_q \hat{C}_q^\dagger$, and $\left\{\hat{C}_q, \hat{C}_q^\dagger\right\} = 1$, we have

$$-i\hbar \frac{\partial}{\partial \tau'} g_{Rq}(\tau,\tau') = \delta_C(\tau-\tau') + \epsilon_q g_{Rq}(\tau,\tau'), \tag{21}$$

or equivalently,

$$g_{Rq}(\tau,\tau') \overleftarrow{g}_{Rq}^{-1}(\tau') = \delta_C(\tau-\tau'). \tag{22}$$

Then, we can express $G_{d,q}$ by G_d and g_{Rq} as follows

$$G_{d,q}(\tau,\tau') = \int_C d\tau_1 G_d(\tau,\tau_1) V_{Rq}^* g_{Rq}(\tau_1,\tau'), \tag{23}$$

which can be checked by applying $\overleftarrow{g}_{Rq}^{-1}(\tau')$ from the right.

With a procedure of the analytic continuation (Langreth formula), we obtain

$$G_{d,q}^<(t,t') = \int_{-\infty}^{\infty} dt_1 \left[G_d^r(t,t_1) V_{Rq}^* g_{Rq}^<(t_1,t') + G_d^<(t,t_1) V_{Rq}^* g_{Rq}^a(t_1,t') \right], \tag{24}$$

where we introduced the retarded and lesser Green functions of the QD system

$$G_d^r(t,t') \equiv -\frac{i}{\hbar}\theta(t-t')\left\langle\left\{\hat{d}(t),\hat{d}^\dagger(t')\right\}\right\rangle, \tag{25}$$

$$G_d^<(t,t') \equiv \frac{i}{\hbar}\left\langle\hat{d}^\dagger(t')\hat{d}(t)\right\rangle, \tag{26}$$

which will be studied in detail in the next section. The advanced Green function is also defined accordingly. Putting these relations into the expression of the current, Eq. (10), we have

$$J_R(t) = 2e\sum_q |V_{Rq}|^2 \Re\left\{\int_{-\infty}^{\infty} dt_1 \left[G_d^r(t,t_1)g_{Rq}^<(t_1-t) + G_d^<(t,t_1)g_{Rq}^a(t_1-t)\right]\right\}. \tag{27}$$

The free Green functions are discussed in Sec. 10.3.4 and is shown to be the function of only the time difference $t_1 - t$.

Now, the current is determined by calculating QD's Green functions, $G_d^r(t,t')$ and $G_d^<(t,t')$.

10.3 QD's Green functions

This section studies QD's Green functions in detail.

10.3.1 Closed time-ordered Green function

Let us start from closed time-ordered free Green function of QD:

$$g_d(\tau,\tau') \equiv -\frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle\tilde{d}(\tau)\tilde{d}^\dagger(\tau')\right\rangle, \tag{28}$$

and its equation of motion is

$$i\hbar\frac{\partial}{\partial\tau}g_d(\tau,\tau') = \delta_C(\tau-\tau')\left\langle\left\{\tilde{d}(\tau),\tilde{d}^\dagger(\tau')\right\}\right\rangle - \frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle-\left[\tilde{\mathcal{H}}_0,\tilde{d}(\tau)\right]\tilde{d}^\dagger(\tau')\right\rangle. \tag{29}$$

The commutator is

$$\left[\hat{\mathcal{H}}_0,\hat{d}\right] = -\epsilon_d\hat{d}, \tag{30}$$

then the equation of motion reduces to

$$i\hbar\frac{\partial}{\partial\tau}g_d(\tau,\tau') = \delta_C(\tau-\tau') + \epsilon_d g_d(\tau,\tau'). \tag{31}$$

We define an operator applying to the right

$$\overrightarrow{g}_d^{-1}(\tau) \equiv i\hbar\frac{\partial}{\partial\tau} - \epsilon_d \tag{32}$$

and we have

$$\overrightarrow{g}_d^{-1}(\tau)\hat{g}(\tau,\tau') = \delta_C(\tau-\tau'). \tag{33}$$

Similarly, another equation of motion of $g_d(\tau,\tau')$ is

$$-i\hbar\frac{\partial}{\partial\tau'}g_d(\tau,\tau') = \delta_C(\tau-\tau')\left\langle\left\{\tilde{d}(\tau),\tilde{d}^\dagger(\tau')\right\}\right\rangle - \frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle\tilde{d}(\tau)\left[\tilde{\mathcal{H}}_0,\tilde{d}^\dagger(\tau')\right]\right\rangle. \tag{34}$$

The commutator is

$$\left[\hat{\mathcal{H}}_0,\hat{d}^\dagger\right] = \epsilon_d\hat{d}^\dagger. \tag{35}$$

Therefore,

$$-i\hbar\frac{\partial}{\partial\tau'}g_d(\tau,\tau') = \delta_C(\tau-\tau') + \epsilon_d g_d(\tau,\tau'). \tag{36}$$

We defined an operator

$$\overleftarrow{g}_d^{-1}(\tau') \equiv -i\hbar\frac{\partial}{\partial\tau'} - \epsilon_d \tag{37}$$

where the differential operator of $\overleftarrow{g}_d^{-1}(\tau)$ applies to the function with time τ' on the left, and we have

$$\hat{g}_d(\tau,\tau')\overleftarrow{g}_d^{-1}(\tau') = \delta_C(\tau-\tau'). \tag{38}$$

With these preparations, we study full QDs' Green function, Eq.(15). The equation of motion is now

$$i\hbar\frac{\partial}{\partial\tau}G_d(\tau,\tau') = \delta_C(\tau-\tau') - \frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle -\left[\hat{\mathcal{H}},\hat{d}(\tau)\right]\hat{d}^\dagger(\tau')\right\rangle, \tag{39}$$

where the commutator is

$$\left[\hat{\mathcal{H}},\hat{d}\right] = \left[\hat{\mathcal{H}}_0,\hat{d}\right] + \left[\hat{\mathcal{H}}_\mathrm{T},\hat{d}\right], \tag{40}$$

$$\left[\hat{\mathcal{H}}_\mathrm{T},\hat{d}\right] = -\sum_p V_{Lp}^*\hat{C}_p - \sum_q V_{Rq}^*\hat{C}_q. \tag{41}$$

Therefore,

$$i\hbar\frac{\partial}{\partial\tau}G_d(\tau,\tau') = \delta_C(\tau-\tau') + \epsilon_d G_d(\tau,\tau') + \sum_p V_{Lp}^* G_{p,d}(\tau,\tau') + \sum_q V_{Rq}^* G_{q,d}(\tau,\tau'). \tag{42}$$

The new Green function

$$G_{p,d}(\tau,\tau') \equiv -\frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle \hat{C}_p(\tau)\hat{d}^\dagger(\tau')\right\rangle, \tag{43}$$

obeys following equation of motion

$$i\hbar\frac{\partial}{\partial\tau}G_{p,d}(\tau,\tau') = \delta_C(\tau-\tau')\left\langle\left\{\hat{C}_p(\tau),\hat{d}^\dagger(\tau)\right\}\right\rangle - \frac{i}{\hbar}\hat{\mathcal{T}}_C\left\langle -\left[\hat{\mathcal{H}},\hat{C}_p(\tau)\right]\hat{d}^\dagger(\tau')\right\rangle. \tag{44}$$

Using the commutator

$$\left[\hat{\mathcal{H}},\hat{C}_p\right] = -\epsilon_p\hat{C}_p - V_{Lp}\hat{d}, \tag{45}$$

we have

$$\overrightarrow{g}_{Lp}^{-1}(\tau)G_{p,d}(\tau,\tau') = V_{Lp}G_d(\tau,\tau'). \tag{46}$$

Therefore,

$$G_{p,d}(\tau,\tau') = \int_C d\tau_1 g_{Lp}(\tau,\tau_1)V_{Lp}G_d(\tau_1,\tau'), \tag{47}$$

where $g_{Lp}(\tau,\tau_1)$ is free Green function in the left reservoir satisfying $\overrightarrow{g}_{Lp}^{-1}(\tau)g_{Lp}(\tau,\tau_1) = \delta_C(\tau-\tau_1)$, which is defined similarly to the free Green function in the right reservoir $g_{Rq}(\tau,\tau')$ defined in Eq. (18). Quite similarly, we also have the relation for the right reservoir

$$G_{q,d}(\tau,\tau') = \int_C d\tau_1 g_{Rq}(\tau,\tau_1)V_{Rq}G_d(\tau_1,\tau'). \tag{48}$$

Putting these into Eq.(42), we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial\tau}G_d(\tau,\tau') &= \delta_C(\tau-\tau') + \epsilon_d G_d(\tau,\tau') \\ &\quad + \int_C d\tau_1\sum_p g_{Lp}(\tau,\tau_1)|V_{Lp}|^2 G_d(\tau_1,\tau') + \int_C d\tau_1\sum_q g_{Rq}(\tau,\tau_1)|V_{Rq}|^2 G_d(\tau_1,\tau'), \end{aligned} \tag{49}$$

which reduces to

$$\overrightarrow{g}_d^{-1}(\tau)G_d(\tau,\tau') = \delta_C(\tau-\tau') + \int_C d\tau_1 \Sigma(\tau,\tau_1)G_d(\tau_1,\tau'), \tag{50}$$

where the self-energy is defined by

$$\Sigma(\tau,\tau_1) \equiv \sum_p |V_{Lp}|^2 g_{Lp}(\tau,\tau_1) + \sum_q |V_{Rq}|^2 g_{Rq}(\tau,\tau_1). \tag{51}$$

Now we had obtained the Dyson equation

$$G_d(\tau,\tau') = g_d(\tau,\tau') + \int_C d\tau_1 g_d(\tau,\tau_1)\int_C d\tau_2 \Sigma(\tau_1,\tau_2)G_d(\tau_2,\tau'), \tag{52}$$

which can be verified by applying $\overrightarrow{g}_d^{-1}(\tau)$ from the left.

10.3.2 Application of Langreth's theorem

From the Dyson equation obtained in the previous subsection, the analytic continuation provides Keldysh Green function matrix elements of QD

$$G_d^r(t,t') = g_d^r(t,t') + \int_{-\infty}^{\infty} dt_1 dt_2 g_d^r(t,t_1)\Sigma^r(t_1,t_2)G_d^r(t_2,t'), \tag{53}$$

$$G_d^a(t,t') = g_d^a(t,t') + \int_{-\infty}^{\infty} dt_1 dt_2 g_d^a(t,t_1)\Sigma^a(t_1,t_2)G_d^a(t_2,t'), \tag{54}$$

$$\begin{aligned} G_d^<(t,t') = g_d^<(t,t') + \int_{-\infty}^{\infty} dt_1 dt_2 \Big\{ & g_d^r(t,t_1)\Sigma^r(t_1,t_2)G_d^<(t_2,t') \\ & + g_d^r(t,t_1)\Sigma^<(t_1,t_2)G_d^a(t_2,t') + g_d^<(t,t_1)\Sigma^a(t_1,t_2)G_d^a(t_2,t')\Big\}. \end{aligned} \tag{55}$$

The free QD's Green functions are defined by

$$g_d^r(t,t') \equiv -\frac{i}{\hbar}\theta(t-t')\left\langle\left\{\tilde{d}(t),\tilde{d}^\dagger(t')\right\}\right\rangle, \tag{56}$$

$$g_d^a(t,t') \equiv \frac{i}{\hbar}\theta(-t+t')\left\langle\left\{\tilde{d}(t),\tilde{d}^\dagger(t')\right\}\right\rangle, \tag{57}$$

$$g_d^<(t,t') \equiv \frac{i}{\hbar}\left\langle\tilde{d}^\dagger(t')\tilde{d}(t)\right\rangle. \tag{58}$$

The meaning of the average $\langle\cdots\rangle$ needs some consideration, especially for the lesser free Green function, since we do not know the density matrix $\rho_{QD}(t)$ at $t\to-\infty$. However, by the discussions in the next section, if we are considering the steady states far later after the initial situation, $g_d^<(-\infty,-\infty)$ does not appear in the expression of the current. Evaluating the equation of motion, it is easy to show the following relations

$$\overrightarrow{g}_d^{-1}(t)g_d^{r/a}(t,t') = \delta(t-t'), \tag{59}$$

$$g_d^{r/a}(t,t')\overleftarrow{g}_d^{-1}(t') = \delta(t-t'). \tag{60}$$

By explicit evaluation, we can show

$$\overrightarrow{g}_d^{-1}(t_1)g_d^<(t_1,t_2) = \left(i\hbar\frac{\partial}{\partial t_1}-\epsilon_d\right)i\left\langle\tilde{d}^\dagger(t_2)\tilde{d}(t_1)\right\rangle = 0, \tag{61}$$

which is checked using the relations

$$i\hbar\frac{\partial\tilde{d}(t_1)}{\partial t_1} = \epsilon_d\tilde{d}(t_1). \tag{62}$$

Similarly,

$$g_d^<(t_1,t_2)\overleftarrow{g}_d^{-1}(t_2) = 0. \tag{63}$$

The self-energies $\Sigma^{r/a/<}(t,t')$ are obtained from Eq. (51) by replacing $g_{Lp/Rq}(t,t')$ by $g_{Lp/Rq}^{r/a/<}(t,t')$. Retarded self-energy is

$$\Sigma^r(t_1,t_2) \equiv \sum_p g_{Lp}^r(t_1,t_2)|V_{Lp}|^2 + \sum_q g_{Rq}^r(t_1,t_2)|V_{Rq}|^2, \tag{64}$$

and the lesser self-energy is

$$\Sigma^<(t_1,t_2) \equiv \sum_p g_{Lp}^<(t_1,t_2)|V_{Lp}|^2 + \sum_q g_{Rq}^<(t_1,t_2)|V_{Rq}|^2. \tag{65}$$

10.3.3 Important properties of QD Green functions

In the following, in order to simplify the notation, the Green functions and self-energies without time variables are understood as matrices with indices of two times and the product of two functions is understood as employing internal time integral from $-\infty$ to $+\infty$.

Keldysh Green function matrices of QD, Eq. (53), obtained by the analytic continuation, are shown again

$$G_d^r = g_d^r + g_d^r\Sigma^r G_d^r, \tag{66}$$
$$G_d^a = g_d^a + g_d^a\Sigma^a G_d^a, \tag{67}$$
$$G_d^< = g_d^< + g_d^r\Sigma^r G_d^< + g_d^r\Sigma^< G_d^a + g_d^<\Sigma^a G_d^a. \tag{68}$$

Equation (66) is an iterative expression and we can formally expand it and resums

$$\begin{aligned}
G_d^r &= g_d^r + g_d^r\Sigma^r G_d^r,\\
&= g_d^r + g_d^r\Sigma^r g_d^r + g_d^r\Sigma^r g_d^r\Sigma^r g_d^r + \cdots\\
&= g_d^r + (g_d^r + g_d^r\Sigma^r g_d^r + \cdots)\Sigma^r g_d^r\\
&= g_d^r + G_d^r\Sigma^r g_d^r.
\end{aligned} \tag{69}$$

Applying $\overleftarrow{g}_d^{-1}(t')$ from the right and using Eq. (60), we have

$$G_d^r(t,t_1)\overleftarrow{g}_d^{-1}(t_1) = \delta(t-t_1) + \int dt_2 G_d^r(t,t_2)\Sigma^r(t_2,t_1). \tag{70}$$

where we replaced t' by t_1 and t_1 by t_2. Then we multiply $G_d^a(t_1,t')$ from the right and by integrating with t_1, we have

$$\int dt_1 G_d^r(t,t_1)\overleftarrow{g}_d^{-1}(t_1)G_d^a(t_1,t') = G_d^a(t,t') + \int dt_1 dt_2 G_d^r(t,t_2)\Sigma^r(t_2,t_1)G_d^a(t_1,t'). \tag{71}$$

The left hand side can be evaluated with partial integration,

$$\begin{aligned}
\int dt_1 G_d^r(t,t_1)\overleftarrow{g}_d^{-1}(t_1)G_d^a(t_1,t') &= \int dt_1 \left\{-i\hbar\frac{\partial}{\partial t_1}G_d^r(t,t_1)\right\} G_d^a(t_1,t') - \int dt_1 G_d^r(t,t_1)\epsilon_d G_d^a(t_1,t')\\
&= -i\hbar G_d^r(t,t_1)G_d^a(t_1,t')|_{t_1=-\infty}^{t_1=\infty} + \int dt_1 G_d^r(t,t_1)\left\{i\hbar\frac{\partial}{\partial t_1}G_d^a(t_1,t')\right\}\\
&- \int dt_1 G_d^r(t,t_1)\epsilon_d G_d^a(t_1,t')\\
&= \int dt_1 G_d^r(t,t_1)\overrightarrow{g}_d^{-1}(t_1)G_d^a(t_1,t'),
\end{aligned} \tag{72}$$

where we used the relation $G_d^r(t,\infty)G_d^a(\infty,t') = 0$, which comes from the step function of retarded/advanced Green function, and $G_d^r(t,-\infty)G_d^a(-\infty,t') = 0$, for t,t' far after the initial time $-\infty$, which comes from the exponentially dumping factor, which will be discussed explicitly in Sec. 10.3.5. Similarly, applying $\overrightarrow{g}_d^{-1}(t)$ from the left to Eq. (54), we have

$$\overrightarrow{g}_d^{-1}(t_1)G_d^a(t_1,t') = \delta(t_1-t') + \int dt_2\Sigma^a(t_1,t_2)G_d^a(t_2,t'), \tag{73}$$

where we replaced t by t_1. Then we multiply $G_d^r(t,t_1)$ from the left and by integrating with t_1, we have

$$\int dt_1 G_d^r(t,t_1)\overrightarrow{g}_d^{-1}(t_1)G_d^a(t_1,t') = G_d^r(t,t') + \int dt_1dt_2 G_d^r(t,t_1)\Sigma^a(t_1,t_2)G_d^a(t_2,t'). \tag{74}$$

Since the left hand side of Eqs. (71,74) are equal using the property Eq. (72), we arrive the following relation of the difference of retarded and advanced Green functions:

$$G_d^r(t,t') - G_d^a(t,t') = \int dt_1dt_2 G_d^r(t,t_1)\left[\Sigma^r(t_1,t_2) - \Sigma^a(t_1,t_2)\right]G_d^a(t_2,t'). \tag{75}$$

The Dyson's equation for the lesser Green function is evaluated with expanding the iterations:

$$\begin{aligned}
G_d^< &= g_d^< + g^r\Sigma^<G_d^a + g_d^<\Sigma_d^a\hat{G}^a + g_d^r\Sigma_d^rG_d^< \\
&= g_d^< + g_d^r\Sigma^<G_d^a + g_d^<\Sigma^aG_d^a + g_d^r\Sigma^r\{g_d^< + g_d^r\Sigma^<G_d^a + g_d^<\Sigma^aG_d^a + g_d^r\Sigma^rG_d^<\} \\
&= \{1+g_d^r\Sigma^r\}g_d^<\{1+\Sigma^aG_d^a\} + \{g_d^r + g_d^r\Sigma^rg_d^r\}\Sigma^<G_d^a + g_d^r\Sigma^rg_d^r\Sigma^rG_d^< \\
&= \{1+g_d^r\Sigma^r\}g_d^<\{1+\Sigma^aG_d^a\} + \{g_d^r + g_d^r\Sigma^rg_d^r\}\Sigma^<G_d^a + g_d^r\Sigma^rg_d^r\Sigma^r\{g_d^< + g_d^r\Sigma^<G_d^a + g_d^<\Sigma^aG_d^a + g_d^r\Sigma^rG_d^<\} \\
&= \{1+g_d^r\Sigma^r + g_d^r\Sigma^rg_d^r\Sigma^r\}g_d^<\{1+\Sigma^aG_d^a\} + \{g_d^r + g_d^r\Sigma^rg_d^r + g_d^r\Sigma^rg_d^r\Sigma^rg_d^r\}\Sigma^<G_d^a + g_d^r\Sigma^rg_d^r\Sigma^rg_d^r\Sigma^rG_d^< \\
&= \cdots \\
&= \{1+G_d^r\Sigma^r\}g_d^<\{1+\Sigma^aG_d^a\} + G_d^r\Sigma^<G_d^a.
\end{aligned} \tag{76}$$

We examine the first term of the last expression, which is shown to be negligible. By using Eqs. (70,73),

$$\begin{aligned}
&\int dt_1dt_2 G_d^r(t,t_1)\overleftarrow{g}_d^{-1}(t_1)g_d^<(t_1,t_2)\overrightarrow{g}_d^{-1}(t_2)G_d^a(t_2,t') \\
&= \Big[-i\hbar G_d^r(t,t_1)g_d^<(t_1,t_2)\Big|_{t_1=-\infty}^{t_1=\infty} + i\hbar\int dt_1 G_d^r(t,t_1)\frac{\partial}{\partial t_1}g_d^<(t_1,t_2) \\
&+ \int dt_1 G_d^r(t,t_1)\hat{\mathcal{H}}_{\rm QD}g_d^<(t_1,t_2)\Big]\overrightarrow{g}_d^{-1}(t_2)G_d^a(t_2,t') \\
&= \left[i\hbar G_d^r(t,-\infty)g_d^<(-\infty,t_2) + \int dt_1 G_d^r(t,t_1)\overrightarrow{g}_d^{-1}(t_1)g_d^<(t_1,t_2)\right]\overrightarrow{g}_d^{-1}(t_2)G_d^a(t_2,t') = (*),
\end{aligned} \tag{77}$$

where we used $G_d^r(t,\infty)=0$ because of the retarded property. The second term in the bracket is zero using Eq. (61). Then we execute partial integration again

$$\begin{aligned}
(*) &= i\hbar G_d^r(t,-\infty)g_d^<(-\infty,t_2)i\hbar G_d^a(t_2,t')\Big|_{t_2=-\infty}^{t_2=\infty} - i\hbar G_d^r(t,-\infty)\int dt_2 g_d^<(-\infty,t_2)\overleftarrow{g}_d^{-1}(t_2)G_d^a(t_2,t') \\
&= \hbar^2 G_d^r(t,-\infty)g_d^<(-\infty,-\infty)G_d^a(-\infty,t'),
\end{aligned} \tag{78}$$

where we used $G_d^a(\infty,t')=0$ because of the advanced property and the relation $g_d^<(-\infty,t_2)\overleftarrow{g}_d^{-1}(t_2)=0$, Eq. (63). Apparently, the last expression depends on the initial population of the QD represented by $g_d^<(t,t)$ at $t=-\infty$, but there is no contribution for the times of interest, t,t', since $G_d^r(t,-\infty), G_d^a(-\infty,t')$ are exponentially dumped as shown in Sec. 10.3.5. Therefore, we can express the lesser Green function by retarded and advanced Green functions:

$$G_d^<(t,t') = \int dt_1dt_2 G_d^r(t,t_1)\Sigma^<(t_1,t_2)G_d^a(t_2,t'). \tag{79}$$

10.3.4 Free Green functions and self-energies

The *free* Green functions for the right reservoir and QD are defined by

$$g^<_{Rq}(t,t') \equiv \frac{i}{\hbar}\left\langle \tilde{C}^\dagger_q(t')\tilde{C}_q(t)\right\rangle, \tag{80}$$

$$g^a_{Rq}(t,t') \equiv \frac{i}{\hbar}\theta(-t+t')\left\langle\left\{\hat{C}_q(t),\hat{C}^\dagger_q(t')\right\}\right\rangle, \tag{81}$$

$$g^<_{d}(t,t') \equiv \frac{i}{\hbar}\left\langle \tilde{d}^\dagger(t')\tilde{d}(t)\right\rangle, \tag{82}$$

$$g^a_{d}(t,t') \equiv \frac{i}{\hbar}\theta(-t+t')\left\langle\left\{\hat{d}(t),\hat{d}^\dagger(t')\right\}\right\rangle. \tag{83}$$

These are only the function of two times difference $t-t'$ as demonstrated as follows.

The equation of motion of $\tilde{C}^\dagger_q(t')$ is

$$\frac{d}{dt'}\tilde{C}^\dagger_q(t') = \left\{\hat{\mathcal{T}}e^{i\hat{\mathcal{H}}_0 t'/\hbar}\right\}\frac{i}{\hbar}\left[\hat{\mathcal{H}}_0,\hat{C}^\dagger_q\right]\left\{\tilde{\mathcal{T}}e^{-i\hat{\mathcal{H}}_0 t'/\hbar}\right\} = \frac{i}{\hbar}\epsilon_q\tilde{C}^\dagger_q(t'), \tag{84}$$

and noting $\tilde{C}^\dagger_q(0)=\hat{C}^\dagger_q$, we have

$$\tilde{C}^\dagger_q(t') = e^{\frac{i}{\hbar}\epsilon_q t'}\hat{C}^\dagger_q, \tag{85}$$

and similarly,

$$\tilde{C}_q(t) = e^{-\frac{i}{\hbar}\epsilon_q t}\hat{C}_q. \tag{86}$$

Therefore, the lesser free Green function is

$$g^<_{Rq}(t,t') = \frac{i}{\hbar}\left\langle\hat{C}^\dagger_q\hat{C}_q\right\rangle e^{-\frac{i}{\hbar}\epsilon_q(t-t')} = \frac{i}{\hbar}f_{Rq}e^{-\frac{i}{\hbar}\epsilon_q(t-t')}, \tag{87}$$

where f_{Rq} is the Fermi-Dirac distribution function of the right reservoir,

$$f_{Rq} \equiv \frac{1}{e^{\beta_R(\epsilon_q-\mu_R)}+1} \equiv f_R(\epsilon_q). \tag{88}$$

β_R, μ_R are the inverse temperature ($=1/(k_BT_R)$) and the chemical potential of the right reservoir, respectively. The advanced free Green function is

$$g^a_{Rq}(t,t') \equiv \frac{i}{\hbar}\theta(-t+t')\left\langle\left\{\hat{C}_q,\hat{C}^\dagger_q\right\}\right\rangle e^{-\frac{i}{\hbar}\epsilon_q(t-t')} = \frac{i}{\hbar}\theta(-t+t')e^{-\frac{i}{\hbar}\epsilon_q(t-t')}. \tag{89}$$

Similarly, the retarded free Green function is

$$g^r_{Rq}(t,t') = -\frac{i}{\hbar}\theta(t-t')e^{-\frac{i}{\hbar}\epsilon_q(t-t')}. \tag{90}$$

Therefore, $g^<_{Rq}(t,t')$, $g^a_{Rq}(t,t')$ and $g^r_{Rq}(t,t')$ are only the function of the time difference $t-t'$.

The equation of motion of $\tilde{d}^\dagger(t')$ is

$$\frac{d}{dt'}\tilde{d}^\dagger(t') = \left\{\hat{\mathcal{T}}e^{i\hat{\mathcal{H}}_0 t'/\hbar}\right\}\frac{i}{\hbar}\left[\hat{\mathcal{H}}_0,\hat{d}^\dagger\right]\left\{\tilde{\mathcal{T}}e^{-i\hat{\mathcal{H}}_0 t'/\hbar}\right\} = \frac{i}{\hbar}\epsilon_d\tilde{d}^\dagger(t'), \tag{91}$$

and noting $\tilde{d}^\dagger(0)=\hat{d}^\dagger$, we have

$$\tilde{d}^\dagger(t') = e^{\frac{i}{\hbar}\epsilon_d t'}\hat{d}^\dagger, \tag{92}$$

and similarly,

$$\tilde{d}(t) = e^{-\frac{i}{\hbar}\epsilon_d t}\hat{d}. \tag{93}$$

Therefore, the lesser free Green function is

$$g_d^<(t,t') = \frac{i}{\hbar}\left\langle \hat{d}^\dagger \hat{d} \right\rangle e^{-\frac{i}{\hbar}\epsilon_d(t-t')} = \frac{i}{\hbar} f_d e^{-\frac{i}{\hbar}\epsilon_d(t-t')}, \tag{94}$$

where $f_d \equiv \langle \hat{d}^\dagger \hat{d} \rangle$ is the initial distribution function of the QD, which does not appear in the final expression of the current as explained in the last section. The advanced free Green function is

$$g_d^a(t,t') \equiv \frac{i}{\hbar}\theta(-t+t')\left\langle \left\{ \hat{d}, \hat{d}^\dagger \right\} \right\rangle e^{-\frac{i}{\hbar}\epsilon_d(t-t')} = \frac{i}{\hbar}\theta(-t+t')e^{-\frac{i}{\hbar}\epsilon_d(t-t')}. \tag{95}$$

Similarly, the retarded free Green function is

$$g_d^r(t,t') = -\frac{i}{\hbar}\theta(t-t')e^{-\frac{i}{\hbar}\epsilon_d(t-t')}. \tag{96}$$

Therefore, $g_{Rq}^<(t,t')$, $g_{Rq}^a(t,t')$, $g_{Rq}^r(t,t')$ and $g_d^<(t,t')$, $g_d^a(t,t')$, $g_d^r(t,t')$ are only the function of the time difference $t-t'$.

Retarded self-energy is

$$\begin{aligned}
\Sigma^r(t_1,t_2) &\equiv \sum_p g_{Lp}^r(t_1,t_2)|V_{Lp}|^2 + \sum_q g_{Rq}^r(t_1,t_2)|V_{Rq}|^2 \\
&\sim -\frac{i}{\hbar}\theta(t_1-t_2)\left\{ \int d\epsilon_p \rho_L(\epsilon_p)\left|V_L(\epsilon_p)\right|^2 e^{-\frac{i}{\hbar}\epsilon_p(t_1-t_2)} + \int d\epsilon_q \rho_R(\epsilon_q)\left|V_R(\epsilon_q)\right|^2 e^{-\frac{i}{\hbar}\epsilon_q(t_1-t_2)} \right\} \\
&= -i\theta(t_1-t_2)\int \frac{d\epsilon}{2\pi} e^{-i\frac{\epsilon}{\hbar}(t_1-t_2)}\left(\Gamma_L(\epsilon)+\Gamma_R(\epsilon)\right),
\end{aligned} \tag{97}$$

where we used the expression of retarded free Green functions in the reservoirs and replace the sum over the quantum state in the reservoir by the integral of the energy $\epsilon_{p(q)}$, $\sum_{p(q)} \to \int d\epsilon_{p(q)}\rho_{L(R)}(\epsilon_{p(q)})$ where $\rho_{L(R)}(\epsilon)$ is the density of states of the left (right) reservoir. We have introduced the line-width function of left (right) reservoir

$$\Gamma_{L(R)}(\epsilon) \equiv \frac{2\pi}{\hbar}\rho_{L(R)}(\epsilon)|V_{L(R)}(\epsilon)|^2, \tag{98}$$

which is positive-definite function of energy ϵ. The lesser self-energy is similarly evaluated as

$$\Sigma^<(t_1,t_2) = i\int \frac{d\epsilon}{2\pi} e^{-i\frac{\epsilon}{\hbar}(t_1-t_2)}\left\{\Gamma_L(\epsilon)f_L(\epsilon)+\Gamma_R(\epsilon)f_R(\epsilon)\right\}. \tag{99}$$

From these analysis, we had known that the self-energies $\Sigma^r(t_1,t_2)$ and $\Sigma^<(t_1,t_2)$ are only the function of the time difference t_1-t_2. From Eq. (53) and Eq. (79), the full QD Green functions are also the function of the time difference t_1-t_2 for the long-time limit. Hence, we can make the Fourier transform of these function with the frequency $\epsilon/\hbar$, which turns out to be quite a powerful approach.

10.3.5 Fourier transform

The Fourier transforms of some function $f(t)$ is

$$F(\epsilon) = \int_{-\infty}^{\infty} dt e^{i\epsilon t/\hbar} f(t), \tag{100}$$

and its reverse transform,

$$f(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi\hbar} e^{-i\epsilon t/\hbar} F(\epsilon). \tag{101}$$

The free retarded Green function in the reservoir R is

$$\begin{aligned}
g_{Rq}^r(\epsilon) &= \int_{-\infty}^{\infty} dt e^{i\epsilon t/\hbar} g_{Rq}^r(t) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt e^{i\epsilon t/\hbar}\theta(t)e^{-\frac{i}{\hbar}\epsilon_q t - \eta t} \\
&= \frac{i}{\hbar}\int_0^{\infty} dt e^{i(\epsilon-\epsilon_q+i\eta')t/\hbar} = \frac{1}{\epsilon-\epsilon_q+i\eta'},
\end{aligned} \tag{102}$$

where we introduced an infinitesimal positive constant η (or $\eta' \equiv \hbar\eta$) to make the integral converge. The advanced Green function is

$$g^a_{Rq}(\epsilon) = \frac{1}{\epsilon - \epsilon_q - i\eta'}, \tag{103}$$

and hence $\left\{g^a_{Rq}(\epsilon)\right\}^* = g^r_{Rq}(\epsilon)$. Similarly, free lesser Green function is

$$g^<_{Rq}(\epsilon) = \int dt e^{i\epsilon t/\hbar} g^<_{Rq}(t) = \frac{i}{\hbar} f_R(\epsilon_q) \int dt e^{i(\epsilon-\epsilon_q)t/\hbar} = 2\pi i f_R(\epsilon)\delta\left(\epsilon - \epsilon_q\right), \tag{104}$$

which is pure imaginary. Fourier transform of the free retarded Green function of QD is

$$\begin{aligned} g^r_d(\epsilon) &= \int d(t-t') e^{i\epsilon(t-t')/\hbar} g^r_d(t,t') = \int d(t-t') e^{i\epsilon(t-t')/\hbar} \left(-\frac{i}{\hbar}\right) \theta(t-t') e^{i\epsilon_d(t-t')/\hbar} \\ &= -\frac{i}{\hbar}\int_0^\infty dt e^{i(\epsilon-\epsilon_d+i\eta')t/\hbar} = \frac{1}{\epsilon - \epsilon_d + i\eta'}. \end{aligned} \tag{105}$$

Since the QD's free Green function and its self-energies are only the function of the time difference $t_1 - t_2$ for the long-time limit (steady-state condition), we expect the QD's Green function is also the function of time difference. Then, the Fourier transform is

$$G^{r/a}_d(\epsilon) \equiv \int dt e^{i\epsilon(t-t')/\hbar} G^{r/a}_d(t,t'). \tag{106}$$

Fourier transform of Eq. (66) is

$$G^r_d(\epsilon) = g^r_d(\epsilon) + g^r_d(\epsilon)\Sigma^r(\epsilon)G^r_d(\epsilon), \tag{107}$$

hence

$$G^r_d(\epsilon) = \frac{g^r_d(\epsilon)}{1 - g^r_d(\epsilon)\Sigma^r(\epsilon)} = \frac{1}{\epsilon - \epsilon_d - \Sigma^r(\epsilon)}. \tag{108}$$

Similarly,

$$G^a_d(\epsilon) = \frac{1}{\epsilon - \epsilon_d - \Sigma^a(\epsilon)}. \tag{109}$$

The self-energy is

$$\Sigma^r(\epsilon) \equiv \int dt e^{i\epsilon t/\hbar}\Sigma^r(t) = \sum_p g^r_{Lp}(\epsilon)\left|V_{Lp}\right|^2 + \sum_q g^r_{Rq}(\epsilon)\left|V_{Rq}\right|^2, \tag{110}$$

and hence $(\Sigma^a(\epsilon))^* = \Sigma^r(\epsilon)$. Using the expression of Eq. (97),

$$\begin{aligned} \Sigma^r(\epsilon) &= -i\int_0^\infty dt e^{i\epsilon t/\hbar}\int \frac{d\epsilon'}{2\pi} e^{-i\frac{\epsilon'}{\hbar}t}\left(\Gamma_L(\epsilon') + \Gamma_R(\epsilon')\right) \\ &= \int \frac{d\epsilon'}{2\pi}\frac{\hbar}{\epsilon - \epsilon' + i\eta'}\left(\Gamma_L(\epsilon') + \Gamma_R(\epsilon')\right) \\ &= \left\{\Lambda_L(\epsilon) - \frac{i\hbar}{2}\Gamma_L(\epsilon)\right\} + \left\{\Lambda_R(\epsilon) - \frac{i\hbar}{2}\Gamma_R(\epsilon)\right\}. \end{aligned} \tag{111}$$

where the real part of the self-energy $\Lambda_{L/R}(\epsilon)$ is defined by the Cauchy's principle integral

$$\Lambda_{L/R}(\epsilon) = \mathrm{P}\int \frac{d\epsilon'}{2\pi}\frac{\hbar\Gamma_{L/R}(\epsilon')}{\epsilon - \epsilon'}. \tag{112}$$

We have used the relation for real a, $\frac{1}{a+i\eta} = \mathrm{P}\frac{1}{a} - i\pi\delta(a)$.

Therefore, the full retarded Green function is

$$G_d^r(\epsilon) = \frac{1}{\epsilon - \epsilon_d - \Lambda_L(\epsilon) - \Lambda_R(\epsilon) + i\frac{\hbar(\Gamma_L(\epsilon)+\Gamma_R(\epsilon))}{2}} = \frac{1}{\epsilon - \tilde{\epsilon}_d(\epsilon) + i\hbar\gamma(\epsilon)}, \tag{113}$$

where we defined renormalized effective QD energy $\tilde{\epsilon}_d(\epsilon) = \epsilon_d + \Lambda_L(\epsilon) + \Lambda_R(\epsilon)$ and effective line-width $\gamma(\epsilon) = (\Gamma_L(\epsilon) + \Gamma_R(\epsilon))/2$. This function shows a peak when $\epsilon = \epsilon_{\text{peak}}$ where ϵ_{peak} satisfies the relation $\epsilon_{\text{peak}} = \tilde{\epsilon}_d(\epsilon_{\text{peak}})$. The peak width is characterized by $\hbar\gamma_{\text{peak}} \equiv \hbar\gamma(\epsilon_{\text{peak}})$ (> 0). Near this peak, we can approximate the Green function as

$$G_d^r(\epsilon) \sim \frac{1}{\epsilon - \epsilon_{\text{peak}} + i\hbar\gamma_{\text{peak}}}. \tag{114}$$

Then, the Fourier reverse transformation provides

$$\begin{aligned} G_d^r(t) &\sim \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi\hbar} G_d^r(\epsilon) e^{-i\epsilon t/\hbar} \\ &= -\frac{i}{\hbar}\theta(t) e^{-i(\epsilon_{\text{peak}} - i\hbar\gamma_{\text{peak}})t/\hbar} \propto e^{-\gamma_{\text{peak}} t}, \end{aligned} \tag{115}$$

which dumps exponentially with time. This property is universally found in an open quantum system, and this is the reason that for a long time after the initial condition, the factor containing the retarded Green function can be neglected.

The advanced self-energy is the complex conjugate of $\Sigma^r(\epsilon)$, and hence

$$\Sigma^r(\epsilon) - \Sigma^a(\epsilon) = -i\hbar\Gamma_L(\epsilon) - i\hbar\Gamma_R(\epsilon). \tag{116}$$

The Fourier transform of Eq.(75) becomes

$$\begin{aligned} G_d^r(\epsilon) - G_d^a(\epsilon) &= G_d^r(\epsilon)\left[\Sigma^r(\epsilon) - \Sigma^a(\epsilon)\right] G_d^a(\epsilon) \\ &= -i\hbar G_d^r(\epsilon)\left[\Gamma_L(\epsilon) + \Gamma_R(\epsilon)\right] G_d^a(\epsilon). \end{aligned} \tag{117}$$

Similarly, Fourier transformed lesser self-energy is pure imaginary,

$$\begin{aligned} \Sigma^<(\epsilon) &= \int dt e^{i\epsilon t/\hbar} i \int \frac{d\epsilon'}{2\pi} e^{-i\frac{\epsilon'}{\hbar}t} \left(\Gamma_L(\epsilon') f_L(\epsilon') + \Gamma_R(\epsilon') f_R(\epsilon')\right) \\ &= i \int \frac{d\epsilon'}{2\pi} \left(\Gamma_L(\epsilon') f_L(\epsilon') + \Gamma_R(\epsilon') f_R(\epsilon')\right) \int dt e^{i(\epsilon - \epsilon')t/\hbar} \\ &= i\hbar \left(\Gamma_L(\epsilon) f_L(\epsilon) + \Gamma_R(\epsilon) f_R(\epsilon)\right). \end{aligned} \tag{118}$$

The Fourier transform of the lesser Green function is by using Eq. (79),

$$\begin{aligned} G_d^<(\epsilon) &= \int d(t-t') e^{i\frac{\epsilon(t-t')}{\hbar}} \int dt_1 dt_2 \int \frac{d\epsilon_1}{2\pi\hbar} e^{-i\frac{\epsilon_1(t-t_1)}{\hbar}} G_d^r(\epsilon_1) \int \frac{d\epsilon'}{2\pi\hbar} e^{-i\frac{\epsilon'(t_1-t_2)}{\hbar}} \Sigma^<(\epsilon') \int \frac{d\epsilon_2}{2\pi\hbar} e^{-i\frac{\epsilon_2(t_2-t')}{\hbar}} G_d^a(\epsilon_2) \\ &= \int \frac{d\epsilon_1}{2\pi\hbar} G_d^r(\epsilon_1) \int \frac{d\epsilon'}{2\pi\hbar} \Sigma^<(\epsilon') \int \frac{d\epsilon_2}{2\pi\hbar} G_d^a(\epsilon_2) \int dt_1 e^{i\frac{(\epsilon_1-\epsilon')t_1}{\hbar}} \int dt_2 e^{i\frac{(\epsilon'-\epsilon_2)t_2}{\hbar}} \int d(t-t') e^{i\frac{\epsilon(t-t')}{\hbar}} e^{-i\frac{(\epsilon_1 t - \epsilon_2 t')}{\hbar}} \\ &= G_d^r(\epsilon)\Sigma^<(\epsilon) G_d^a(\epsilon). \end{aligned} \tag{119}$$

Since $(G_d^r(\epsilon))^* = G_d^a(\epsilon)$ and $\Sigma^<(\epsilon)$ is pure imaginary, $G_d^<(\epsilon)$ is also pure imaginary.

10.4 Steady current

In the previous section, the QD's lesser Green function, needed for the calculation of the current, is expressed by QD's retarded/advanced Green function, Eq. (79). In this section, we express the current formula with the Fourier transform and obtain the Landauer-Büttiker formula.

Let us get back to the expression of the current Eq.(27), which is Fourier transformed

$$\begin{aligned}
J_R(t) &= 2e\sum_q |V_{Rq}|^2 \Re\left\{\int dt_1\left[G_d^r(t,t_1)g_{Rq}^<(t_1-t)+G_d^<(t,t_1)g_{Rq}^a(t_1-t)\right]\right\}\\
&= 2e\sum_q |V_{Rq}|^2 \Re\left\{\int dt_1\int\frac{d\epsilon}{2\pi\hbar}\frac{d\epsilon'}{2\pi\hbar}\left[G_d^r(\epsilon)e^{-i\frac{\epsilon(t-t_1)}{\hbar}}g_{Rq}^<(\epsilon')e^{-i\frac{\epsilon'(t_1-t)}{\hbar}}+G_d^<(\epsilon)e^{i\frac{\epsilon(t-t_1)}{\hbar}}g_{Rq}^a(\epsilon')e^{-i\frac{\epsilon'(t_1-t)}{\hbar}}\right]\right\}\\
&= 2e\sum_q |V_{Rq}|^2 \Re\left\{\int\frac{d\epsilon}{2\pi\hbar}\left[G_d^r(\epsilon)g_{Rq}^<(\epsilon)+G_d^<(\epsilon)g_{Rq}^a(\epsilon)\right]\right\}. \qquad (120)
\end{aligned}$$

As one can see, the current J_R is independent of time t (steady current). Since $g_{Rq}^<(\epsilon)$ and $G_d^<(\epsilon)$ are pure imaginary as shown in previous section, Eq.(104,119),

$$\begin{aligned}
J_R &= 2e\sum_q |V_R(\epsilon_q)|^2\int\frac{d\epsilon}{2\pi\hbar}\left[-\Im\left\{G_d^r(\epsilon)\right\}\Im\left\{g_{Rq}^<(\epsilon)\right\}-\Im\left\{G_d^<(\epsilon)\right\}\Im\left\{g_{Rq}^a(\epsilon)\right\}\right]\\
&= 2e\sum_q |V_R(\epsilon_q)|^2\int\frac{d\epsilon}{2\pi\hbar}\left[-\frac{1}{2i}\left\{G_d^r(\epsilon)-G_d^a(\epsilon)\right\}2\pi f_R(\epsilon_q)\delta\left(\epsilon-\epsilon_q\right)-\frac{1}{i}G_d^<(\epsilon)\pi\delta\left(\epsilon-\epsilon_q\right)\right]\\
&= \frac{2e}{\hbar}\int d\epsilon\rho_R(\epsilon)\left|V_R(\epsilon)\right|^2\Big[-\frac{1}{2i}(-i\hbar)G_d^r(\epsilon)\left\{\Gamma_L(\epsilon)+\Gamma_R(\epsilon)\right\}G_d^a(\epsilon)f_R(\epsilon)\\
&\qquad -\frac{1}{2i}G_d^r(\epsilon)\,i\hbar\left\{\Gamma_L(\epsilon)f_L(\epsilon)+\Gamma_R(\epsilon)f_R(\epsilon)\right\}G_d^a(\epsilon)\Big]\\
&= \frac{e}{h}\int d\epsilon\hbar^2\Gamma_R(\epsilon)G_d^r(\epsilon)\left[\left\{\Gamma_L(\epsilon)+\Gamma_R(\epsilon)\right\}f_R(\epsilon)-\left\{\Gamma_L(\epsilon)f_L(\epsilon)+\Gamma_R(\epsilon)f_R(\epsilon)\right\}\right]G_d^a(\epsilon)\\
&= -\frac{e}{h}\int d\epsilon\hbar^2\Gamma_L(\epsilon)\Gamma_R(\epsilon)G_d^r(\epsilon)G_d^a(\epsilon)\left(f_L(\epsilon)-f_R(\epsilon)\right), \qquad (121)
\end{aligned}$$

which is Meir-Wingreen form[1].

We define the transmission probability:

$$\mathcal{T}(\epsilon)\equiv\hbar^2\Gamma_L(\epsilon)\Gamma_R(\epsilon)\left|G_d^r(\epsilon)\right|^2. \qquad (122)$$

Then, we arrive the final expression,

$$J_R=-\frac{e}{h}\int d\epsilon(f_L(\epsilon)-f_R(\epsilon))\mathcal{T}(\epsilon), \qquad (123)$$

which is corresponding to the Landauer-Büttiker formula.

The transmission probability is by using Eq. (113),

$$\mathcal{T}(\epsilon)=\hbar^2\Gamma_L(\epsilon)\Gamma_R(\epsilon)\left|\frac{1}{\epsilon-\tilde{\epsilon}_d(\epsilon)+i\hbar\gamma(\epsilon)}\right|^2=\frac{\hbar^2\Gamma_L(\epsilon)\Gamma_R(\epsilon)}{\left(\epsilon-\tilde{\epsilon}_d(\epsilon)\right)^2+\hbar^2\gamma^2}, \qquad (124)$$

where the renormalized level energy is $\tilde{\epsilon}_d(\epsilon)\equiv\epsilon_d+\Lambda_L(\epsilon)+\Lambda_R(\epsilon)$ and the line width is $\gamma(\epsilon)=(\Gamma_L(\epsilon)+\Gamma_R(\epsilon))/2$. This form of the transmission probability is called Breit-Wigner resonance. At the resonant energy, determined by $\epsilon_{\rm peak}=\tilde{\epsilon}_d(\epsilon_{\rm peak})$, the peak transmission probability is

$$\mathcal{T}(\epsilon_{\rm peak})=\frac{4\Gamma_L(\epsilon_{\rm peak})\Gamma_R(\epsilon_{\rm peak})}{\left(\Gamma_L(\epsilon_{\rm peak})+\Gamma_R(\epsilon_{\rm peak})\right)^2}, \qquad (125)$$

which can become unity when $\Gamma_L(\epsilon_{\rm peak})=\Gamma_R(\epsilon_{\rm peak})$.

The Landauer-Büttiker formula, Eq. (123), reduces to that obtained with classical master equation, lecture note on May 13, page 6, Eq. (38) by multiplying the charge factor $-e$ in the limit of weak couplings, where the level energy becomes to the bare one, $\tilde{\epsilon}_d(\epsilon)\to\epsilon_d$ and $\gamma(\epsilon)\to 0$. Hence,

$$\mathcal{T}(\epsilon)\to\frac{\hbar^2\Gamma_L(\epsilon)\Gamma_R(\epsilon)}{\hbar\gamma(\epsilon)}\frac{\hbar\gamma(\epsilon)}{(\epsilon-\epsilon_d)^2+(\hbar\gamma(\epsilon))^2}. \qquad (126)$$

The last factor is well approximated with a Dirac's delta function in the limit of $\gamma \to 0$, [1]

$$\lim_{\gamma(\epsilon)\to 0} \frac{\hbar\gamma(\epsilon)}{(\epsilon-\epsilon_d)^2+(\hbar\gamma(\epsilon))^2} = \pi\delta(\epsilon-\epsilon_d). \tag{128}$$

Therefore, in the limit of small $\gamma(\epsilon_d)$,

$$\mathcal{T}(\epsilon) \to \frac{\hbar\Gamma_L(\epsilon_0)\Gamma_R(\epsilon_0)}{\gamma(\epsilon_0}\pi\delta(\epsilon-\epsilon_d) = h\frac{\Gamma_L(\epsilon_0)\Gamma_R(\epsilon_0)}{\Gamma_L(\epsilon_0)+\Gamma_R(\epsilon_0)}\delta(\epsilon-\epsilon_d). \tag{129}$$

By putting this into Eq. (123), we have

$$J_R = -e\frac{\Gamma_L(\epsilon_0)\Gamma_R(\epsilon_0)}{\Gamma_L(\epsilon_0)+\Gamma_R(\epsilon_0)}\left\{f_L(\epsilon_0)-f_R(\epsilon_0)\right\}. \tag{130}$$

10.5 Conclusions

We have derived the formula of the current through a quantum dot using Keldysh nonequilibrium Green function method.

References

[1] Yigal Meir and Ned S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).

[1] This could be understood since at $\epsilon = \epsilon_d$, the function is sharply peaked with a peak height $1/(\hbar\gamma(\epsilon_d)) \to \infty$ and the integral over the energy in the range including ϵ_d is (for some $\delta > 0$)

$$\int_{\epsilon_d-\delta}^{\epsilon_d+\delta} d\epsilon \lim_{\gamma(\epsilon)\to 0} \frac{\hbar\gamma(\epsilon)}{(\epsilon-\epsilon_d)^2+(\hbar\gamma(\epsilon))^2} = \int_{-\infty}^{\infty} dx \frac{\hbar\gamma(\epsilon_d)}{x^2+(\hbar\gamma(\epsilon_d))^2} = \pi, \tag{127}$$

where we had changed variable $x = \epsilon - \epsilon_d$.