非平衡グリーン関数法
～ナノスケール系の電気伝導計算への応用～
【英語版】

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Contents

Chapter 1

Tight-Binding Hamiltonian for Electron Transport

1.1 Nano-scale system

We consider a center nano-scale system (C) sandwiched between a left electrode (L) and a right electrode (R). We employ a simple tight-binding model, where electrons are spinless fermions having no Coulomb repulsive interactions and each site has a single orbital. The Hamiltonian of this nano-scale system (C) is written as

$$\hat{\mathcal{H}}^C = -\sum_{1\leq i,j\leq N} t_{ij}\hat{c}_i^\dagger \hat{c}_j + \sum_{1\leq i\leq N} V_i \hat{c}_i^\dagger \hat{c}_i, \tag{1.1}$$

where $\hat{c}_i^\dagger$ and $\hat{c}_i$ are the creation and annihilation operators of the electron at the i-th site, t_{ij} the electron transfer energy between the nearest neighboring i- and j-th sites, and N the number of sites in the nano-scale system (C). V_i describes the on-site energy of the i-th site, which represents the effects of external electric fields. We consider that the entire region of the nano-scale system (C) is attached to the gate electrode; thus, all the on-site energies are uniformly varied by applying the gate voltage. Moreover, we apply the external electric field to the nano-scale system (C), thus changing the on-site energy individually depending on its position. In this case, V_i is written as

$$V_i = V^{\mathrm{G}} + V_i^{\mathrm{E}}, \tag{1.2}$$

where V^{G} is the applied gate voltage, and V_i^{E} represents the potential due to the external electric field.

1.2 Electrodes

To study the transport properties of electrons, the edges of the nano-scale system (C) are connected to the left (L) and right (R) electrodes, as shown in Fig. 1.1. We assume that both electrodes are represented by the tight-binding models of one-dimensional lattices having a half-infinity length. Thus, the Hamiltonian of the electrode is written as

$$\hat{\mathcal{H}}^\xi = -\sum_{i,j} t^\xi \hat{c}_i^\dagger \hat{c}_j + \mu^\xi \sum_i \hat{c}_i^\dagger \hat{c}_i, \tag{1.3}$$

where ξ denotes either left (L) or right (R) electrode. When we number the sites in the electrodes, as shown in Fig. 1.1, the summation runs over the sites with $i \leq 0$ ($i \geq N+1$) for the $\xi = \mathrm{L}$ (R) electrode. t^ξ is the electron transfer energy between the i- and j-th sites in the ξ electrode, and μ^ξ is the chemical potential of electrode. In this case, the electrode is half filled with electrons because the on-site energies are equal to the chemical potential.

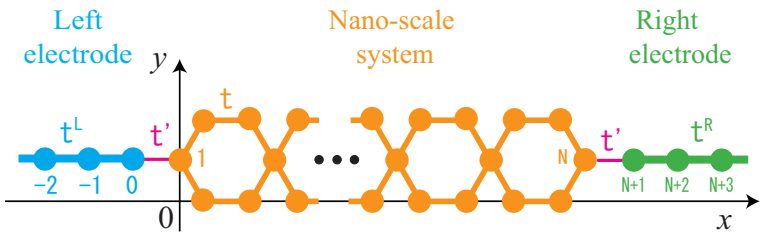

Figure 1.1: Schematic pictures of joint system of nano-scale system and half-infinite-length one-dimensional electrodes. The transfer energies are shown by various t's. We adopt the x and y axes along and perpendicular to the chain direction.

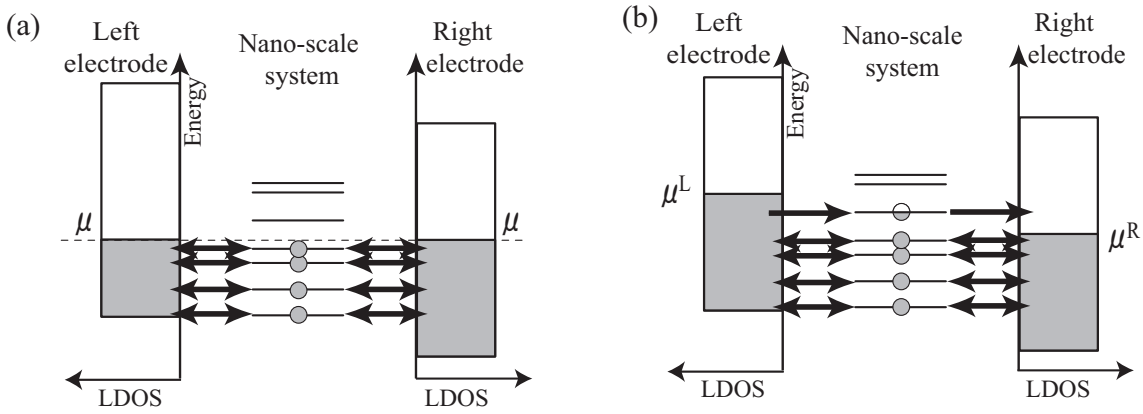

Figure 1.2: (a) Schematic energy diagram of joint system in the equilibrium state. (b) Schematic energy diagram of joint system in the nonequilibrium state. Electrons transfer from the left electrode to the right electrode passing through the energy levels of the center system, as shown by arrows.

1.3 Connection to Electrode

In order to connect the electrodes to the nano-scale system, the following Hamiltonian is introduced,

$$\hat{\mathcal{W}} = -t'(\hat{c}_0^\dagger \hat{c}_1 + \hat{c}_1^\dagger \hat{c}_0 + \hat{c}_N^\dagger \hat{c}_{N+1} + \hat{c}_{N+1}^\dagger \hat{c}_N), \tag{1.4}$$

where t' is an electron transfer energy between the nano-scale system and electrodes. The total Hamiltonian of the joint system is represented as follows using above Hamiltonians,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}^L + \hat{\mathcal{H}}^C + \hat{\mathcal{H}}^R + \hat{\mathcal{W}}. \tag{1.5}$$

When the joint system is in the equilibrium state, the electronic states are filled with electrons up to the spatially uniform chemical potential μ, as shown in Fig. 1.2(a). In this equilibrium situation, the electrons can't flow effectively through the nano-scale system from the left electrode to the right electrode. Thus, we have to employ the nonequilibrium Green's function method.

Chapter 2

Schrödinger, Heisenberg & Interaction pictures

2.1 Schrödinger picture

First, we summarize the Schrödinger, Heisenberg and interaction pictures for following Hamiltonian,

$$\begin{aligned}\hat{\mathcal{H}}(t) &= \hat{\mathcal{H}}^L + \hat{\mathcal{H}}^C + \hat{\mathcal{H}}^R + \hat{\mathcal{W}}(t) \\ &= \hat{\mathcal{H}}_0 + \hat{\mathcal{W}}(t),\end{aligned} \tag{2.1}$$

where $\hat{\mathcal{H}}_0 \equiv \hat{\mathcal{H}}^L + \hat{\mathcal{H}}^C + \hat{\mathcal{H}}^R$ and

$$\hat{\mathcal{W}}(t) \equiv \hat{\mathcal{W}}\,\theta(t-t_0) \equiv \begin{cases}\hat{\mathcal{W}} & \text{for } t > t_0, \\ 0 & \text{for } t \leq t_0.\end{cases} \tag{2.2}$$

Each Hamiltonian has been already defined in Eqs. (1.1)-(1.4). In the Schrödinger picture, well-known equation of motion

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{\mathcal{H}}(t)|\psi(t)\rangle, \tag{2.3}$$

is satisfied. Here, $|\psi(t)\rangle$ is the state vector. We write the operator in the Schödinger picture as $\hat{\mathcal{O}}$. The expectation value of the operator $\langle\mathcal{O}(t)\rangle$ in the state $|\psi(t)\rangle$ is obtained by $\langle\psi(t)|\hat{\mathcal{O}}|\psi(t)\rangle$. Let consider the time-evolution operator $\hat{S}(t,t_0)$ in the Schrödinger picture, which satisfies the relation $(t > t_0)$,

$$|\psi(t)\rangle = \hat{S}(t,t_0)|\psi(t_0)\rangle. \tag{2.4}$$

To calculate the nonequilibrium state, we need the $|\psi(t)\rangle$. However, we know only the initial equilibrium state $|\psi(t_0)\rangle$. Thus, we must calculate the time-evolution operator $\hat{S}(t,t_0)$. Inserting Eq. (2.4) to Eq. (2.3), we obtain

$$i\hbar\frac{\partial\hat{S}(t,t_0)}{\partial t} = \hat{\mathcal{H}}(t)\hat{S}(t,t_0). \tag{2.5}$$

2.2 Heisenberg picture

Using the time-evolution operator, we define the operator $\hat{\mathcal{O}}_H(t)$ and the state vector $|\psi_H\rangle$ in the Heisenberg picture as

$$\hat{\mathcal{O}}_H(t) = \hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\hat{S}(t,t_0), \tag{2.6}$$

and

$$|\psi_H\rangle = |\psi(t_0)\rangle, \tag{2.7}$$

respectively. The expectation value is obtained as

$$\langle \mathcal{O}(t) \rangle = \langle \psi_H | \hat{\mathcal{O}}_H(t) | \psi_H \rangle. \tag{2.8}$$

Using Eq. (2.4), we can confirm that the expectation value in the Schrödinger picture is equal to that in the Heisenberg picture. The operator $\hat{\mathcal{O}}_H(t)$ satisfies what we call Heisenberg equation of motion,

$$\begin{aligned} i\hbar \frac{d\hat{\mathcal{O}}_H(t)}{dt} &= i\hbar \frac{d(\hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\hat{S}(t,t_0))}{dt} \\ &= i\hbar \frac{d\hat{S}^\dagger(t,t_0)}{dt}\hat{\mathcal{O}}\hat{S}(t,t_0) + i\hbar \hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\frac{\hat{S}(t,t_0)}{dt} \\ &= -\hat{S}^\dagger(t,t_0)\hat{\mathcal{H}}(t)\hat{\mathcal{O}}\hat{S}(t,t_0) + \hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\hat{\mathcal{H}}(t)\hat{S}(t,t_0) \\ &= -\hat{S}^\dagger(t,t_0)\hat{\mathcal{H}}(t)\hat{S}(t,t_0)\hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\hat{S}(t,t_0) \\ &\quad + \hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\hat{S}(t,t_0)\hat{S}^\dagger(t,t_0)\hat{\mathcal{H}}(t)\hat{S}(t,t_0) \\ &= \left[\hat{\mathcal{O}}_H(t), \hat{\mathcal{H}}_H(t)\right] \end{aligned} \tag{2.9}$$

2.3 Interaction picture

The operator in the interaction picture $\hat{\mathcal{O}}_I(t)$ is related to that in the Schrödinger picture as a unitary transformation

$$\hat{\mathcal{O}}_I(t) = e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{\mathcal{O}}e^{-i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}. \tag{2.10}$$

On the other hand, the relation between the interaction picture and the Heisenberg picture satisfies the following equation,

$$\hat{\mathcal{O}}_H(t) = \hat{S}_I^\dagger(t,t_0)\hat{\mathcal{O}}_I(t)\hat{S}_I(t,t_0), \tag{2.11}$$

where we define the time-evolution operator $\hat{S}_I(t,t_0)$ in the interaction picture,

$$\hat{S}_I(t,t_0) = e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{S}(t,t_0). \tag{2.12}$$

The state vector in the interaction picture is defined as

$$|\psi_I(t)\rangle = e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}|\psi(t)\rangle, \tag{2.13}$$

because the expectation value has to be the same in any pictures. In other words, the expectation value can be written as follows,

$$\langle \mathcal{O}(t) \rangle = \langle \psi_I(t) | \hat{\mathcal{O}}_I(t) | \psi_I(t) \rangle = \langle \psi(t) | \hat{\mathcal{O}} | \psi(t) \rangle. \tag{2.14}$$

We note that $|\psi(t_0)\rangle = |\psi_H\rangle = |\psi_I(t_0)\rangle$. Using Eq. (2.4), we obtain the time-evolution of the state vector in the interaction picture,

$$\begin{aligned} |\psi_I(t)\rangle &= e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}|\psi(t)\rangle \\ &= e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{S}(t,t_0)|\psi(t_0)\rangle \\ &= e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{S}(t,t_0)|\psi_I(t_0)\rangle \\ &= \hat{S}_I(t,t_0)|\psi_I(t_0)\rangle. \end{aligned} \tag{2.15}$$

For the practical applications it is quite important to derive an explicit formula of $\hat{S}_I(t,t_0)$ in terms of $\hat{\mathcal{W}}_I(t)$. Let first derive an equation of motion for $\hat{S}_I(t,t_0)$ from Eq. (2.5) and Eq. (2.12),

$$
\begin{aligned}
i\hbar\frac{\partial \hat{S}_I(t,t_0)}{\partial t} &= i\hbar\Big[i\frac{\hat{\mathcal{H}}_0}{\hbar}e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{S}(t,t_0) + e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\frac{\partial \hat{S}(t,t_0)}{\partial t}\Big] && (2.16)\\
&= -\hat{\mathcal{H}}_0 e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{S}(t,t_0) + e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{\mathcal{H}}(t)\hat{S}(t,t_0) && (2.17)\\
&= e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{\mathcal{W}}(t)\hat{S}(t,t_0) && (2.18)\\
&= e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{\mathcal{W}}(t)e^{-i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}e^{i\frac{\hat{\mathcal{H}}_0}{\hbar}(t-t_0)}\hat{S}(t,t_0) && (2.19)\\
&= \hat{\mathcal{W}}_I(t)\hat{S}_I(t,t_0). && (2.20)
\end{aligned}
$$

We now convert it to an integral equation by integrating from t_0 to t and taking the initial condition $\hat{S}(t_0,t_0)=1$,

$$
\hat{S}_I(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t} d\tau \hat{\mathcal{W}}_I(\tau)\hat{S}_I(\tau,t_0). \tag{2.21}
$$

Successive iterative substitution yields

$$
\begin{aligned}
\hat{S}_I(t,t_0) &= 1 + \frac{1}{i\hbar}\int_{t_0}^{t} d\tau_1 \hat{\mathcal{W}}_I(\tau) + \frac{1}{2!}\Big(\frac{1}{i\hbar}\Big)^2\int_{t_0}^{t} d\tau_1\int_{t_0}^{t} d\tau_2 \mathrm{T}[\hat{\mathcal{W}}_I(\tau_1)\hat{\mathcal{W}}_I(\tau_2)] + \cdots \\
&= \sum_{n=0}^{+\infty}\frac{1}{n!}\Big(\frac{-i}{\hbar}\Big)^n\int_{t'}^{t} d\tau_1\cdots\int_{t'}^{t} d\tau_n\ \mathrm{T}\left[\hat{\mathcal{W}}_I(\tau_1)\cdots\hat{\mathcal{W}}_I(\tau_n)\right] && (2.22)\\
&= \mathrm{T}\exp\Big[-\frac{i}{\hbar}\int_{t_0}^{t} d\tau \hat{\mathcal{W}}_I(\tau)\Big],
\end{aligned}
$$

where T is the time-ordering operator. The Hermitian conjugate of $\hat{S}_I(t,t_0)$ is written as

$$
\hat{S}_I^{\dagger}(t,t_0) = \hat{S}_I(t_0,t) = \tilde{\mathrm{T}}\exp\Big[\frac{i}{\hbar}\int_{t'}^{t} d\tau \hat{\mathcal{W}}_I(\tau)\Big], \tag{2.23}
$$

where $\tilde{\mathrm{T}}$ represents the $\tilde{\mathrm{T}}$-product operator, which arranges the time-dependent operators in inverse chronological order.

Chapter 3

Nonequilibrium Green's Function

3.1 Expectation value in mixed state

So far we have considered the expectation value in the pure state. In order to calculate the expectation value in the mixed state, the statistical (density) operator $\hat{\rho}(t)$ is introduced,

$$\hat{\rho}(t) = \sum_n P_n |\psi_n(t)\rangle\langle\psi_n(t)|, \tag{3.1}$$

where P_n is the statistical probability that the system is to be in state $|\psi_n(t)\rangle$. We can relate $\hat{\rho}(t)$ to initial density operator $\hat{\rho}(t_0)$ in terms of $\hat{S}$,

$$\hat{\rho}(t) = \sum_n P_n \hat{S}(t,t_0)|\psi_n(t_0)\rangle\langle\psi_n(t_0)|\hat{S}^\dagger(t,t_0) = \hat{S}(t,t_0)\hat{\rho}(t_0)\hat{S}^\dagger(t,t_0). \tag{3.2}$$

By use of $\hat{\rho}(t)$ we can calculate the expectation value $\langle\mathcal{O}(t)\rangle$ in the statistical ensemble,

$$\begin{aligned}
\langle\mathcal{O}(t)\rangle &\equiv \sum_n P_n \langle\psi_n(t)|\hat{\mathcal{O}}(t)|\psi_n(t)\rangle && (3.3)\\
&= \mathrm{Tr}[\hat{\rho}(t)\hat{\mathcal{O}}] \\
&= \mathrm{Tr}[\hat{S}(t,t_0)\hat{\rho}(t_0)\hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}] \\
&= \mathrm{Tr}[\hat{\rho}(t_0)\hat{S}^\dagger(t,t_0)\hat{\mathcal{O}}\hat{S}(t,t_0)] \\
&= \mathrm{Tr}[\hat{\rho}(t_0)\hat{\mathcal{O}}_H(t)] && (3.4)\\
&= \langle\hat{\mathcal{O}}_H(t)\rangle_0, && (3.5)
\end{aligned}$$

where $\mathrm{Tr}[\hat{X}\hat{Y}] = \mathrm{Tr}[\hat{Y}\hat{X}]$ is applied and $\langle\cdots\rangle_0 \equiv \mathrm{Tr}[\hat{\rho}(t_0)\cdots]$. For the practical purpose, it is convenient to write it in the interaction picture with aid of Eq. (2.11),

$$\begin{aligned}
\langle\mathcal{O}(t)\rangle &= \langle\hat{S}_I^\dagger(t,t_0)\hat{\mathcal{O}}_I(t)\hat{S}_I(t,t_0)\rangle_0 && (3.6)\\
&= \langle(\hat{S}_I(t,+\infty)\hat{S}_I(+\infty,t_0))^\dagger\hat{\mathcal{O}}_I(t)\hat{S}_I(t,t_0)\rangle_0 && (3.7)\\
&= \langle\hat{S}_I(t_0,+\infty)\hat{S}_I(+\infty,t)\hat{\mathcal{O}}_I(t)\hat{S}_I(t,t_0)\rangle_0, && (3.8)
\end{aligned}$$

where $\hat{S}_I(t,t_0) = \hat{S}_I(t,+\infty)\hat{S}_I(+\infty,t_0)$ is used.

3.2 Path-ordered Green's function

The equation (3.8) shows that the initial equilibrium state develops to the nonequilibrium state under the operator $\hat{S}_I(t,t_0)$, and then the physical quantity $\mathcal{O}(t)$ is observed at time t , after that, the state develops

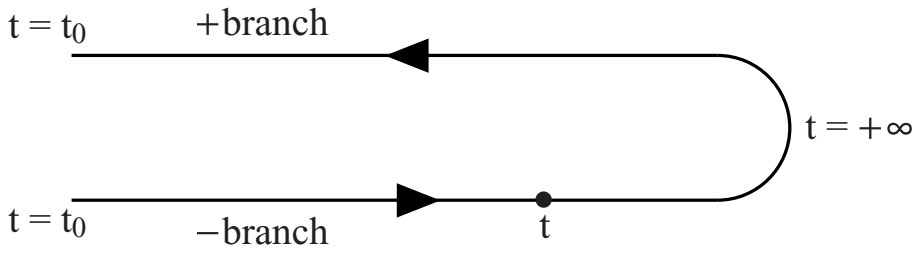

Figure 3.1: Schematic picture of the time loop. the time loop consists of the chronological-order path (- branch) and the inverse-chronological-order path (+ branch).

from time t to time $+\infty$. Finally, the state returns from time $+\infty$ to time t_0 under the $\hat{S}_I(t_0, +\infty)$. Thus, the time-evolution path consists of the chronological-order path (- branch) and the inverse-chronological-order path (+ branch). This path is called as the time loop. The time loop is shown in Fig. 3.1.

When we calculate Eq. (3.8) concretely, we need to expand the time-evolution operators $\hat{S}_I$ by using Eq. (2.22) and Eq. (2.23).

$$\langle \mathcal{O}(t) \rangle = \sum_{n=0}^{+\infty} \sum_{m=0}^{+\infty} \frac{1}{n!} \Big(\frac{i}{\hbar}\Big)^n \frac{1}{m!} \Big(\frac{-i}{\hbar}\Big)^m \int_{t_0}^{+\infty} d\tau_1' \cdots \int_{t_0}^{+\infty} d\tau_n' \int_{t_0}^{+\infty} d\tau_1 \cdots \int_{t_0}^{+\infty} d\tau_m \\ \langle \tilde{\mathrm{T}}[\hat{\mathcal{W}}_I(\tau_1') \cdots \hat{\mathcal{W}}_I(\tau_n')] \, \mathrm{T}[\hat{\mathcal{W}}_I(\tau_1) \cdots \hat{\mathcal{W}}_I(\tau_m) \hat{\mathcal{O}}_I(t)] \rangle_0. \tag{3.9}$$

We can obtain the statistical averages $\langle \mathcal{O}(t) \rangle$ by solving the Eq. (3.9). For example, when the operator $\hat{\mathcal{O}}$ is the electron number at i-th site, we set $\hat{\mathcal{O}}$ as $\hat{c}_i^\dagger \hat{c}_i$. The statistical average $\langle \cdots \rangle_0$ in Eq. (3.9) is resolved into the products of the pair-correlation functions such as $\langle \hat{c}_{Ii}^\dagger(\tau_1) \hat{c}_{Ij}(\tau_2) \rangle_0$ when we apply the Wick's theorem to the statistical average. The pair-correlation functions are classified into four types dependent on whether the operator is in the $+$ branch or in the $-$ branch of the time loop. The four nonequilibrium Green functions are defined as follows,

$$i\hbar \, G_{ij}^{--}(t_1, t_2) \equiv \langle \mathrm{T}[\hat{c}_{Hi}(t_1) \hat{c}_{Hj}^\dagger(t_2)] \rangle, \tag{3.10}$$

$$i\hbar \, G_{ij}^{++}(t_1, t_2) \equiv \langle \tilde{\mathrm{T}}[\hat{c}_{Hi}(t_1) \hat{c}_{Hj}^\dagger(t_2)] \rangle, \tag{3.11}$$

$$i\hbar \, G_{ij}^{+-}(t_1, t_2) \equiv \langle \hat{c}_{Hi}(t_1) \hat{c}_{Hj}^\dagger(t_2) \rangle, \tag{3.12}$$

$$i\hbar \, G_{ij}^{-+}(t_1, t_2) \equiv -\langle \hat{c}_{Hj}^\dagger(t_2) \hat{c}_{Hi}(t_1) \rangle. \tag{3.13}$$

Here $\hat{c}_{Hi}$ and $\hat{c}_{Hi}^\dagger$ represent the annihilation and creation operators of electron at i-th site in the Heisenberg picture, respectively. In the case of $G_{ij}^{ss'}(t_1, t_2)$, the operator $\hat{c}_{Hi}(t_1)(\hat{c}_{Hj}^\dagger(t_2))$ is in $s(s')$ branch of the time loop. For convenience, we introduce the retarded Green functions G_{ij}^r and the advanced Green functions G_{ij}^a,

$$i\hbar \, G_{ij}^r(t_1, t_2) \equiv \langle \hat{c}_{Hi}(t_1) \hat{c}_{Hj}^\dagger(t_2) + \hat{c}_{Hj}^\dagger(t_2) \hat{c}_{Hi}(t_1) \rangle \theta(t_1 - t_2), \tag{3.14}$$

$$i\hbar \, G_{ij}^a(t_1, t_2) \equiv -\langle \hat{c}_{Hi}(t_1) \hat{c}_{Hj}^\dagger(t_2) + \hat{c}_{Hj}^\dagger(t_2) \hat{c}_{Hi}(t_1) \rangle \theta(t_2 - t_1). \tag{3.15}$$

We readily have the following useful relations:

$$G_{ij}^{--}(t_1,t_2)+G_{ij}^{++}(t_1,t_2)=G_{ij}^{-+}(t_1,t_2)+G_{ij}^{+-}(t_1,t_2), \tag{3.16}$$
$$G_{ij}^{r}(t_1,t_2)=G_{ij}^{--}(t_1,t_2)-G_{ij}^{-+}(t_1,t_2), \tag{3.17}$$
$$=G_{ij}^{+-}(t_1,t_2)-G_{ij}^{++}(t_1,t_2), \tag{3.18}$$
$$G_{ij}^{a}(t_1,t_2)=G_{ij}^{--}(t_1,t_2)-G_{ij}^{+-}(t_1,t_2), \tag{3.19}$$
$$=G_{ij}^{-+}(t_1,t_2)-G_{ij}^{++}(t_1,t_2), \tag{3.20}$$
$$G_{ij}^{--}(t_1,t_2)=-(G_{ji}^{++}(t_2,t_1))^*, \tag{3.21}$$
$$G_{ij}^{-+}(t_1,t_2)=-(G_{ji}^{-+}(t_2,t_1))^*, \tag{3.22}$$
$$G_{ij}^{+-}(t_1,t_2)=-(G_{ji}^{+-}(t_2,t_1))^*, \tag{3.23}$$
$$G_{ij}^{a}(t_1,t_2)=(G_{ji}^{r}(t_2,t_1))^*, \tag{3.24}$$

where $(\cdots)^*$ means the complex conjugate.

3.3 Dyson equation

Our aim in this section is to obtain the equation of motion for the Green functions. First, we differentiate Green functions $G_{ij}^{ss'}(t_1,t_2)$ with respect to the time t_1,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_1}G_{ij}^{--}(t_1,t_2)=&-\sum_m t_{im}G_{mj}^{--}(t_1,t_2)\\ &-t'(t_1)\{\delta_{i0}G_{1j}^{--}(t_1,t_2)+\delta_{i1}G_{0j}^{--}(t_1,t_2)\}\\ &-t'(t_1)\{\delta_{iN}G_{N+1,j}^{--}(t_1,t_2)+\delta_{i,N+1}G_{0j}^{--}(t_1,t_2)\}\\ &+\delta_{ij}\delta(t_1-t_2), \end{aligned} \tag{3.25}$$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_1}G_{ij}^{++}(t_1,t_2)=&-\sum_m t_{im}G_{mj}^{++}(t_1,t_2)\\ &-t'(t_1)\{\delta_{i0}G_{1j}^{++}(t_1,t_2)+\delta_{i1}G_{0j}^{++}(t_1,t_2)\}\\ &-t'(t_1)\{\delta_{iN}G_{N+1,j}^{++}(t_1,t_2)+\delta_{i,N+1}G_{0j}^{++}(t_1,t_2)\}\\ &-\delta_{ij}\delta(t_1-t_2), \end{aligned} \tag{3.26}$$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_1}G_{ij}^{-+}(t_1,t_2)=&-\sum_m t_{im}G_{mj}^{-+}(t_1,t_2)\\ &-t'(t_1)\{\delta_{i0}G_{1j}^{-+}(t_1,t_2)+\delta_{i1}G_{0j}^{-+}(t_1,t_2)\}\\ &-t'(t_1)\{\delta_{iN}G_{N+1,j}^{-+}(t_1,t_2)+\delta_{i,N+1}G_{0j}^{-+}(t_1,t_2)\}, \end{aligned} \tag{3.27}$$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_1}G_{ij}^{+-}(t_1,t_2)=&-\sum_m t_{im}G_{mj}^{+-}(t_1,t_2)\\ &-t'(t_1)\{\delta_{i0}G_{1j}^{+-}(t_1,t_2)+\delta_{i1}G_{0j}^{+-}(t_1,t_2)\}\\ &-t'(t_1)\{\delta_{iN}G_{N+1,j}^{+-}(t_1,t_2)+\delta_{i,N+1}G_{0j}^{+-}(t_1,t_2)\}, \end{aligned} \tag{3.28}$$

where we have used the Heisenberg equation,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_1}\hat{c}_{Hi}(t_1) &= [\hat{c}_{Hi}(t_1), \hat{\mathcal{H}}(t_1)] \\ &= -\sum_m t_{im}\hat{c}_{Hm}(t_1) - t'(t_1)(\delta_{i0}\hat{c}_{H1}(t_1) + \delta_{i1}\hat{c}_{H0}(t_1)) \\ &\quad - t'(t_1)(\delta_{iN}\hat{c}_{HN+1}(t_1) + \delta_{i,N+1}\hat{c}_{HN}(t_1)). \end{aligned} \tag{3.29}$$

Here, we define $t'(t)$ as $t' \cdot \theta(t - t_0)$. If the electrodes are connected to the nano-scale system at $t_0 = -\infty$, we can suppose that the joint system has reached the steady state at any time t. Under the steady state, the Green function $G(t_1, t_2)$ depend on only time difference between t_1 and t_2. We define the Fourier transform,

$$G(\tau) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dE\, G(E)e^{-i\frac{E}{\hbar}\tau}, \tag{3.30}$$

where $\tau \equiv t_1 - t_2$. When the Fourier transform is applied to Eqs. (3.25)-(3.28), we obtain the following equations,

$$\begin{aligned} EG^{--}_{ij}(E) &= -\sum_m t_{im}G^{--}_{mj}(E) \\ &\quad - t'\{\delta_{i0}G^{--}_{1j}(E) + \delta_{i1}G^{--}_{0j}(E)\} \\ &\quad - t'\{\delta_{iN}G^{--}_{N+1,j}(E) + \delta_{i,N+1}G^{--}_{0j}(E)\} \\ &\quad + \delta_{ij}, \end{aligned} \tag{3.31}$$

$$\begin{aligned} EG^{++}_{ij}(E) &= -\sum_m t_{im}G^{++}_{mj}(E) \\ &\quad - t'\{\delta_{i0}G^{++}_{1j}(E) + \delta_{i1}G^{++}_{0j}(E)\} \\ &\quad - t'\{\delta_{iN}G^{++}_{N+1,j}(E) + \delta_{i,N+1}G^{++}_{0j}(E)\} \\ &\quad - \delta_{ij}, \end{aligned} \tag{3.32}$$

$$\begin{aligned} EG^{-+}_{ij}(E) &= -\sum_m t_{im}G^{-+}_{mj}(E) \\ &\quad - t'\{\delta_{i0}G^{-+}_{1j}(E) + \delta_{i1}G^{-+}_{0j}(E)\} \\ &\quad - t'\{\delta_{iN}G^{-+}_{N+1,j}(E) + \delta_{i,N+1}G^{-+}_{0j}(E)\}, \end{aligned} \tag{3.33}$$

$$\begin{aligned} EG^{+-}_{ij}(E) &= -\sum_m t_{im}G^{+-}_{mj}(E) \\ &\quad - t'\{\delta_{i0}G^{+-}_{1j}(E) + \delta_{i1}G^{+-}_{0j}(E)\} \\ &\quad - t'\{\delta_{iN}G^{+-}_{N+1,j}(E) + \delta_{i,N+1}G^{+-}_{0j}(E)\}. \end{aligned} \tag{3.34}$$

The matrix Green function is defined as

$$\mathbf{G}_{ij}(E) \equiv \begin{bmatrix} G^{--}_{ij}(E) & G^{-+}_{ij}(E) \\ G^{+-}_{ij}(E) & G^{++}_{ij}(E) \end{bmatrix}. \tag{3.35}$$

Using the matrix Green functions, we rewrite the equations (3.31)-(3.34) as follows,

$$\sum_m \{E\delta_{im} - (-t_{im})\}\mathbf{G}_{mj}(E) - \sum_m \Sigma_{im}\mathbf{G}_{mj}(E) = \delta_{ij}\tau_z, \tag{3.36}$$

where

$$\Sigma_{im} \equiv -t'\{\delta_{i0}\delta_{m1} + \delta_{i1}\delta_{m0}\} - t'\{\delta_{iN}\delta_{mN+1} + \delta_{iN+1}\delta_{mN}\}, \tag{3.37}$$

and

$$\tau_z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{3.38}$$

When the perturbation term $\hat{\mathcal{W}}$ becomes zero, we rewrite the Green functions $\mathbf{G}(E)$ to the nonperturbative Green functions $\mathbf{g}(E)$. Thus, we obtain the following equation from Eq. (3.36),

$$\sum_m g_{im}^{-1}(E)\mathbf{g}_{mj}(E) = \delta_{ij}\tau_z, \tag{3.39}$$

where $g_{im}^{-1}(E)$ is defined as

$$g_{im}^{-1}(E) \equiv E\delta_{im} - (-t_{im}). \tag{3.40}$$

Using Eq. (3.40), the equation (3.36) is rewritten as

$$\sum_m g_{im}^{-1}(E)\mathbf{G}_{mj}(E) - \sum_m \Sigma_{im}\mathbf{G}_{mj}(E) = \delta_{ij}\tau_z. \tag{3.41}$$

Then we use the relation $\tau_z\tau_z = 1$, and we have

$$\sum_m g_{im}^{-1}(E)\mathbf{G}_{mj}(E) - \sum_m \tau_z\mathbf{\Sigma}_{im}\mathbf{G}_{mj}(E) = \delta_{ij}\tau_z, \tag{3.42}$$

where $\mathbf{\Sigma}_{im}$ called the matrix self-energy is defined as follows,

$$\mathbf{\Sigma}_{im} \equiv \begin{bmatrix} \Sigma_{im}^{--} & \Sigma_{im}^{-+} \\ \Sigma_{im}^{+-} & \Sigma_{im}^{++} \end{bmatrix} \equiv \tau_z\Sigma_{im} = \begin{bmatrix} \Sigma_{im} & 0 \\ 0 & -\Sigma_{im} \end{bmatrix}. \tag{3.43}$$

Furthermore, equation (3.42) is rewritten as

$$\sum_m g_{im}^{-1}(E)\mathbf{G}_{mj}(E) - \sum_{lm} \tau_z\delta_{il}\mathbf{\Sigma}_{lm}\mathbf{G}_{mj}(E) = \delta_{ij}\tau_z, \tag{3.44}$$

where we have used the relation $\mathbf{\Sigma}_{im} = \sum_l \delta_{il}\mathbf{\Sigma}_{lm}$. Inserting Eq. (3.39) to Eq. (3.44), we obtain

$$\sum_n g_{in}^{-1}(E)\Big\{\mathbf{G}_{nj}(E) - \sum_{lm} \mathbf{g}_{nl}(E)\mathbf{\Sigma}_{lm}\mathbf{G}_{mj}(E)\Big\} = \sum_n g_{in}^{-1}(E)\mathbf{g}_{nj}(E). \tag{3.45}$$

Thus we yield the equation of motion for the nonequilibrium Green functions

$$\mathbf{G}_{ij}(E) = \mathbf{g}_{ij}(E) + \sum_{lm} \mathbf{g}_{il}(E)\mathbf{\Sigma}_{lm}\mathbf{G}_{mj}(E), \tag{3.46}$$

where

$$\mathbf{G}_{ij}(E) \equiv \begin{bmatrix} G_{ij}^{--}(E) & G_{ij}^{-+}(E) \\ G_{ij}^{+-}(E) & G_{ij}^{++}(E) \end{bmatrix}, \tag{3.47}$$

$$\mathbf{g}_{ij}(E) \equiv \begin{bmatrix} g_{ij}^{--}(E) & g_{ij}^{-+}(E) \\ g_{ij}^{+-}(E) & g_{ij}^{++}(E) \end{bmatrix}, \tag{3.48}$$

$$\mathbf{\Sigma}_{lm} \equiv \begin{bmatrix} \Sigma_{lm}^{--} & 0 \\ 0 & \Sigma_{lm}^{++} \end{bmatrix}. \tag{3.49}$$

As you know, Equation (3.16) shows that the four Green functions, G^{--}, G^{++}, G^{-+}, and G^{+-}, are not independent each other. Thus, we can transform the four Green functions into the three Green functions, G^a, G^r, and G^k with aid of the transform matrix $\mathbf{P}$,

$$\mathbf{P} \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}. \tag{3.50}$$

We introduce the Keldysh Green function, G^k, which is defined as

$$G^k_{ij}(E) \equiv G^{--}_{ij}(E) + G^{++}_{ij}(E). \tag{3.51}$$

Actually, using Eq. (3.50), the matrix Green function $\mathbf{G}_{ij}$ is transformed as follows,

$$\begin{aligned}\mathbf{P}^{-1}\mathbf{G}_{ij}\mathbf{P} &= \frac{1}{2}\begin{bmatrix} G^{--}_{ij} - G^{+-}_{ij} - G^{-+}_{ij} + G^{++}_{ij} & G^{--}_{ij} - G^{+-}_{ij} + G^{-+}_{ij} - G^{++}_{ij} \\ G^{--}_{ij} + G^{+-}_{ij} - G^{-+}_{ij} - G^{++}_{ij} & G^{--}_{ij} + G^{+-}_{ij} + G^{-+}_{ij} + G^{++}_{ij} \end{bmatrix} \\ &= \begin{bmatrix} 0 & G^a_{ij} \\ G^r_{ij} & G^k_{ij} \end{bmatrix},\end{aligned} \tag{3.52}$$

where we have used the equations (3.16)-(3.20). The matrix self-energy is transformed similarly,

$$\begin{aligned}\mathbf{P}^{-1}\mathbf{\Sigma}_{ij}\mathbf{P} &= \frac{1}{2}\begin{bmatrix} \Sigma^{--}_{ij} + \Sigma^{++}_{ij} & \Sigma^{--}_{ij} - \Sigma^{++}_{ij} \\ \Sigma^{--}_{ij} - \Sigma^{++}_{ij} & \Sigma^{--}_{ij} + \Sigma^{++}_{ij} \end{bmatrix} \\ &= \begin{bmatrix} 0 & \Sigma^r_{ij} \\ \Sigma^a_{ij} & 0 \end{bmatrix},\end{aligned} \tag{3.53}$$

where the retarded self-energy and the advanced self-energy are defined respectively as follows,

$$\Sigma^r_{ij} \equiv \frac{1}{2}(\Sigma^{--}_{ij} - \Sigma^{++}_{ij}), \tag{3.54}$$

$$\Sigma^a_{ij} \equiv \frac{1}{2}(\Sigma^{--}_{ij} - \Sigma^{++}_{ij}). \tag{3.55}$$

Using Eqs. (3.52) and (3.53), the transformed equation of motion for $\mathbf{G}_{ij}$ is written as

$$\mathbf{P}^{-1}\mathbf{G}_{ij}\mathbf{P} = \mathbf{P}^{-1}\mathbf{g}_{ij}\mathbf{P} + \sum_{lm}\mathbf{P}^{-1}\mathbf{g}_{il}\mathbf{P}\mathbf{P}^{-1}\mathbf{\Sigma}_{lm}\mathbf{P}\mathbf{P}^{-1}\mathbf{G}_{mj}\mathbf{P}, \tag{3.56}$$

$$\begin{bmatrix} 0 & G^a_{ij} \\ G^r_{ij} & G^k_{ij} \end{bmatrix} = \begin{bmatrix} 0 & g^a_{ij} \\ g^r_{ij} & g^k_{ij} \end{bmatrix} + \sum_{lm}\begin{bmatrix} 0 & g^a_{il} \\ g^r_{il} & g^k_{il} \end{bmatrix}\begin{bmatrix} 0 & \Sigma^r_{lm} \\ \Sigma^a_{lm} & 0 \end{bmatrix}\begin{bmatrix} 0 & G^a_{mj} \\ G^r_{mj} & G^k_{mj} \end{bmatrix}. \tag{3.57}$$

As a result, we obtain the following equation of motion for the nonequilibrium Green functions,

$$G^a_{ij}(E) = g^a_{ij}(E) + \sum_{lm} g^a_{il}(E)\Sigma^a_{lm}G^a_{mj}(E), \tag{3.58}$$

$$G^r_{ij}(E) = g^r_{ij}(E) + \sum_{lm} g^r_{il}(E)\Sigma^r_{lm}G^r_{mj}(E), \tag{3.59}$$

$$G^k_{ij}(E) = g^k_{ij}(E) + \sum_{lm}\Big\{g^r_{il}(E)\Sigma^r_{lm}G^k_{mj}(E) + g^k_{il}(E)\Sigma^a_{lm}G^a_{mj}(E)\Big\}. \tag{3.60}$$

We introduce the following Green functions and self-energies of the matrix form,

$$\mathbf{G}^a = \begin{bmatrix} \ddots & \vdots & \vdots & & \vdots & \vdots & \ddots \\ \cdots & G^a_{00} & G^a_{01} & \cdots & G^a_{0N} & G^a_{0\ N+1} & \cdots \\ \cdots & G^a_{10} & G^a_{11} & \cdots & G^a_{1N} & G^a_{1\ N+1} & \cdots \\ & \vdots & \vdots & \ddots & \vdots & \vdots & \\ \cdots & G^a_{N0} & G^a_{N1} & \cdots & G^a_{NN} & G^a_{N\ N+1} & \cdots \\ \cdots & G^a_{N+1\ 0} & G^a_{N+1\ 1} & \cdots & G^a_{N+1\ N} & G^a_{N+1\ N+1} & \cdots \\ \ddots & \vdots & \vdots & & \vdots & \vdots & \ddots \end{bmatrix}, \tag{3.61}$$

$$\mathbf{g}^a = \begin{bmatrix} \ddots & \vdots & \vdots & & \vdots & \vdots & \ddots \\ \cdots & g^a_{00} & 0 & \cdots & 0 & 0 & \cdots \\ \cdots & 0 & g^a_{11} & \cdots & g^a_{1N} & 0 & \cdots \\ & \vdots & \vdots & \ddots & \vdots & \vdots & \\ \cdots & 0 & g^a_{N1} & \cdots & g^a_{NN} & 0 & \cdots \\ \cdots & 0 & 0 & \cdots & 0 & g^a_{N+1\ N+1} & \cdots \\ \ddots & \vdots & \vdots & & \vdots & \vdots & \ddots \end{bmatrix}, \tag{3.62}$$

$$\mathbf{\Sigma}^a = \begin{bmatrix} \ddots & \vdots & \vdots & & \vdots & \vdots & \ddots \\ \cdots & 0 & -t' & \cdots & 0 & 0 & \cdots \\ \cdots & -t' & 0 & \cdots & 0 & 0 & \cdots \\ & \vdots & \vdots & \ddots & \vdots & \vdots & \\ \cdots & 0 & 0 & \cdots & 0 & -t' & \cdots \\ \cdots & 0 & 0 & \cdots & -t' & 0 & \cdots \\ \ddots & \vdots & \vdots & & \vdots & \vdots & \ddots \end{bmatrix}. \tag{3.63}$$

The matrix forms of the other Green functions and self-energies are similarly introduced, and then we can rewrite the Dyson equations as follows,

$$\mathbf{G}^a = \mathbf{g}^a + \mathbf{g}^a\mathbf{\Sigma}^a\mathbf{G}^a, \tag{3.64}$$

$$\mathbf{G}^r = \mathbf{g}^r + \mathbf{g}^r\mathbf{\Sigma}^r\mathbf{G}^r, \tag{3.65}$$

$$\mathbf{G}^k = \mathbf{g}^k + \mathbf{g}^r\mathbf{\Sigma}^r\mathbf{G}^k + \mathbf{g}^k\mathbf{\Sigma}^a\mathbf{G}^a. \tag{3.66}$$

Chapter 4

Electronic Current Formulation

In this chapter, we express the electronic current using the Green's functions.

4.1 Equation of electronic current

We consider the electronic current through the i-th site as shown in Fig. 4.1. We assume that the electronic current between $(i-1)$-th site and i-th site is represented by $\hat{I}_l$. Similarly, the current between i-th site and $(i+1)$-th site is written by $\hat{I}_r$. We write the continuity equation around i-th site under the tight-binding approximation,

$$\hat{I}_{rH}(t) - \hat{I}_{lH}(t) = -\frac{\partial \hat{\rho}_{Hi}(t)}{\partial t}, \tag{4.1}$$

where the electron charge at i-th site is written as

$$\hat{\rho}_{Hi}(t) = -e\hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hi}(t). \tag{4.2}$$

The electronic current between i-th site and $(i+1)$-th site is the difference between the flow of electrons from left to right and right to left. We thus expect the current operator $\hat{I}_r$ of the form

$$\hat{I}_{rH}(t) = A_{i+1,i}\hat{c}^{\dagger}_{Hi+1}(t)\hat{c}_{Hi}(t) - A_{i,i+1}\hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hi+1}(t). \tag{4.3}$$

The electronic current operator $\hat{I}_l$ between $(i-1)$-th site and i-th site is similarly written,

$$\hat{I}_{lH}(t) = A_{i,i-1}\hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hi-1}(t) - A_{i-1,i}\hat{c}^{\dagger}_{Hi-1}(t)\hat{c}_{Hi}(t). \tag{4.4}$$

Using the Heisenberg equation, we find

$$\frac{\partial \hat{\rho}_{Hi}(t)}{\partial t} = \frac{1}{i\hbar}[\hat{\rho}_{Hi}(t), \hat{\mathcal{H}}_H(t)] \tag{4.5}$$

$$= \frac{1}{i\hbar}\Big\{\hat{\rho}_{Hi}(t)\hat{\mathcal{H}}_H(t) - \hat{\mathcal{H}}_H(t)\hat{\rho}_{Hi}(t)\Big\} \tag{4.6}$$

$$= \frac{e}{i\hbar}\Big\{\sum_m t_{im}\hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hm}(t) - \sum_l t_{li}\hat{c}^{\dagger}_{Hl}(t)\hat{c}_{Hi}(t)\Big\} \tag{4.7}$$

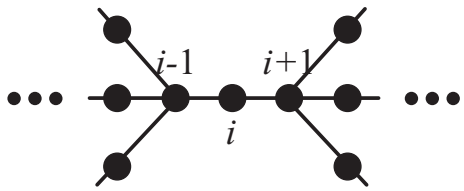

Figure 4.1: Schematic picture of the system.

As shown in Fig. 4.1, i-th site is connected to only both $(i-1)$-th site and $(i+1)$-th site. Therefore, we have

$$\frac{\partial \hat{\rho}_{Hi}(t)}{\partial t} = \frac{e}{i\hbar}\Big\{ t_{i,i-1}\hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hi-1}(t) + t_{i,i+1}\hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hi+1}(t) \\ -t_{i-1,i}\hat{c}^{\dagger}_{Hi-1}(t)\hat{c}_{Hi}(t) - t_{i+1,i}\hat{c}^{\dagger}_{Hi+1}(t)\hat{c}_{Hi}(t)\Big\}. \tag{4.8}$$

A comparison of equations (4.1) and (4.8) yields

$$A_{lm} = \frac{e}{i\hbar}t_{lm}. \tag{4.9}$$

When we assume $t_{lm} = t_{ml}$, the electronic current is written as follows

$$\langle I_r(t)\rangle = \frac{e}{i\hbar}t_{i,i+1}\langle \hat{c}^{\dagger}_{Hi+1}(t)\hat{c}_{Hi}(t) - \hat{c}^{\dagger}_{Hi}(t)\hat{c}_{Hi+1}(t)\rangle \tag{4.10}$$

$$= et_{i,i+1}\{G^{-+}_{i+1,i}(t,t) - G^{-+}_{i,i+1}(t,t)\}, \tag{4.11}$$

where Eq. (3.13) has been used. In a steady state, using the Fourier transform (3.30), we have

$$\langle I_r\rangle = \frac{et_{i,i+1}}{2\pi\hbar}\int_{-\infty}^{+\infty} dE\Big\{G^{-+}_{i+1,i}(E) - G^{-+}_{i,i+1}(E)\Big\} \tag{4.12}$$

$$= \frac{e}{2h}t_{i,i+1}\int_{-\infty}^{+\infty} dE\Big\{G^{k}_{i+1,i}(E) - G^{k}_{i,i+1}(E)\Big\}. \tag{4.13}$$

Here, to obtain Eq. (4.13) we have used the following relations,

$$G^{-+}_{ij} = \frac{1}{2}(-G^{r}_{ij} + G^{a}_{ij} + G^{k}_{ij}). \tag{4.14}$$

In case of the joint system shown in Fig. 1.1, the electronic current can be written using the Green's functions, as follows,

$$\langle I\rangle = \frac{e}{2h}t'\int_{-\infty}^{+\infty} dE\Big\{G^{k}_{10}(E) - G^{k}_{01}(E)\Big\}. \tag{4.15}$$

Similarly, we can obtain the electron number density at i-th site,

$$\langle n_i\rangle = -e\langle \hat{c}^{\dagger}_{i}\hat{c}_{i}\rangle \tag{4.16}$$

$$= \frac{e}{2\pi}\int_{-\infty}^{+\infty} dE G^{-+}_{ii}(E) \tag{4.17}$$

$$= \frac{e}{4\pi}\int_{-\infty}^{+\infty} dE(-G^{r}_{ii}(E) + G^{a}_{ij}(E) + G^{k}_{ij}(E)). \tag{4.18}$$

4.2 Green's functions for the isolated systems

In this section, we produce the Green's functions $\mathrm{g}(E)$ of the isolated electrodes and the nano-scale system.

4.2.1 Green's functions for the isolated electrodes

We assume that both source and drain electrodes are represented by the tight-binding models of one-dimensional lattices having a half-infinity length as shown in Fig. 4.2(a). The Hamiltonian of an electrode is written as follows,

$$\hat{\mathcal{H}^{L}} = -\sum_{ij\leq 0} t^{L}\hat{c}^{\dagger}_{i}\hat{c}_{j}. \tag{4.19}$$

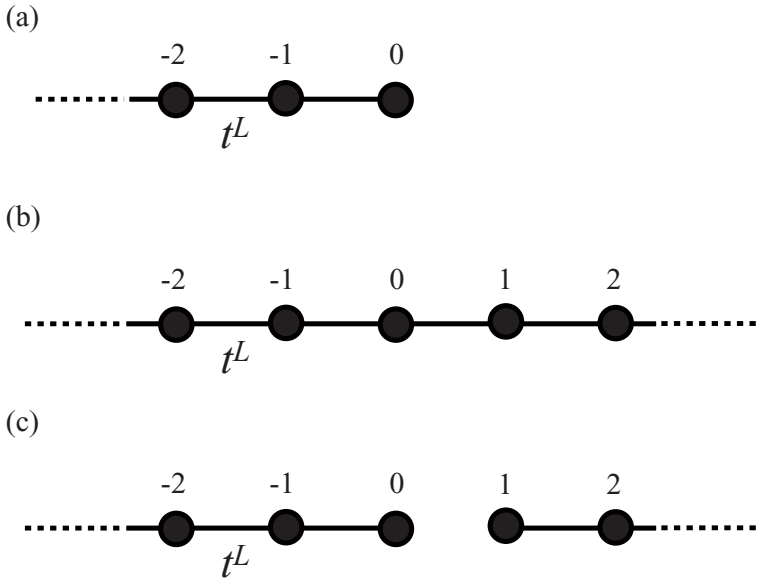

Figure 4.2: (a) One-dimensional lattices having a half-infinity length under the tight-binding approximation. (b) Infinite length one-dimensional lattice. (c) Half-infinite-length one-dimensional lattices produced by removing the electron transfer between 0-th site and 1-st site.

To produce the half-infinity length one-dimensional lattice, we remove the transfer between 0-th site and 1-st site from the infinite length one-dimensional lattice. The situation is shown in Figs. 4.2(b) and 4.2(c). Therefore, we rewrite the Hamiltonian of the electrode as follows,

$$\hat{\mathcal{H}}^L = \hat{\mathcal{H}}_0^L + \hat{\mathcal{H}}_1^L, \tag{4.20}$$

where

$$\hat{\mathcal{H}}_0^L = -\sum_{ij} t^L \hat{c}_i^\dagger \hat{c}_j, \tag{4.21}$$

$$\hat{\mathcal{H}}_1^L = +t^L(\hat{c}_0^\dagger \hat{c}_1 + \hat{c}_1^\dagger \hat{c}_0). \tag{4.22}$$

$\mathcal{H}_0^L$ represents the Hamiltonian of the infinite length one-dimensional lattice. In the previous chapter, we have already obtained the Dyson equations (3.58)-(3.60) from the Hamiltonian (2.1). In the similar way with this process, we obtain the following Dyson equations from the Hamiltonian (4.20),

$$g_{ij}^a(E) = g_{ij}^{0a}(E) + \sum_{lm} g_{il}^{0a}(E)\sigma_{lm}^a g_{mj}^a(E), \tag{4.23}$$

$$g_{ij}^r(E) = g_{ij}^{0r}(E) + \sum_{lm} g_{il}^{0r}(E)\sigma_{lm}^r g_{mj}^r(E), \tag{4.24}$$

$$g_{ij}^k(E) = g_{ij}^{0k}(E) + \sum_{lm} \Big\{ g_{il}^{0r}(E)\sigma_{lm}^r g_{mj}^k(E) + g_{il}^{0k}(E)\sigma_{lm}^a g_{mj}^a(E) \Big\}, \tag{4.25}$$

where the self-energies are defined as

$$\sigma_{lm}^a = \sigma_{lm}^r = t^L(\delta_{l0}\delta_{m1} + \delta_{l1}\delta_{m0}). \tag{4.26}$$

Here $g_{ij}(E)$ and $g_{ij}^0(E)$ are the Green's functions for the half-infinite length electrode and the infinite length one-dimensional lattice, respectively. Inserting Eq. (4.26) to Eq. (4.23), we obtain

$$\begin{aligned} g_{ij}^a(E) &= g_{ij}^{0a}(E) + t^L \sum_{lm} g_{il}^{0a}(E)(\delta_{l0}\delta_{m1} + \delta_{l1}\delta_{m0}) g_{mj}^a(E) \\ &= g_{ij}^{0a}(E) + t^L g_{i0}^{0a}(E) g_{1j}^a(E) + t^L g_{i1}^{0a}(E) g_{0j}^a(E). \end{aligned} \tag{4.27}$$

Both i and j are zero or less, because g^a_{ij} is the Green's function of the left-side half infinite length one-dimensional lattice shown in Fig. 4.2(c). Thus, the Green function g^a_{1j} becomes zero, because electrons in the left-side lattice can not transfer to the right-side lattice. Thus, we yield following equation from Eq. (4.27),

$$g^a_{ij}(E) = g^{0a}_{ij}(E) + t^L g^{0a}_{i1}(E) g^a_{0j}(E). \tag{4.28}$$

When $i = 0$, we obtain the Green's function g^a_{0j} as follows,

$$g^a_{0j}(E) = \frac{g^{0a}_{0j(E)}}{1 - t^L g^{0a}_{01}(E)}. \tag{4.29}$$

Inserting Eq. (4.29) to Eq. (4.28), we have advanced Green's functions for electrodes,

$$g^a_{ij}(E) = g^{0a}_{ij}(E) + t^L \frac{g^{0a}_{i1}(E) g^{0a}_{0j}(E)}{1 - t^L g^{0a}_{01}(E)}. \tag{4.30}$$

In the same way, we obtain the retarded Green's functions,

$$g^r_{ij}(E) = g^{0r}_{ij}(E) + t^L \frac{g^{0r}_{i1}(E) g^{0r}_{0j}(E)}{1 - t^L g^{0r}_{01}(E)}. \tag{4.31}$$

The Green's functions for the infinite length one-dimensional lattice $g^{0a}_{ij}(g^{0r}_{ij})$ are necessary to calculate the Green functions $g^a_{ij}(g^r_{ij})$.

The Green's function $g^{0--}_{ij}(t_1, t_2)$ for the infinite length one-dimensional lattice is defined as

$$\begin{aligned} g^{0--}_{ij}(t_1, t_2) &= \frac{1}{i\hbar} \langle \mathrm{T}[\hat{c}_{Hi}(t_1) \hat{c}^\dagger_{Hj}(t_2)] \rangle \\ &= \frac{1}{i\hbar} \Big\{ \langle \hat{c}_{Hi}(t_1) \hat{c}^\dagger_{Hj}(t_2) \rangle \theta(t_1 - t_2) - \langle \hat{c}^\dagger_{Hj}(t_2) \hat{c}_{Hi}(t_1) \rangle \theta(t_2 - t_1) \Big\}, \end{aligned} \tag{4.32}$$

where $\hat{c}_{Hi}(t) = \exp[-\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t] \hat{c}_i \exp[\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t]$. When there is no interaction between electrons in the periodic system, we can develop the operator $\hat{c}_i$ in the plane wave,

$$\hat{c}_{Hi}(t) = \exp\left[-\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right] \hat{c}_i \exp\left[+\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right] \tag{4.33}$$

$$= \frac{1}{\sqrt{N}} \sum_k \exp[ik \cdot (ia)] \exp\left[-\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right] \hat{c}_k \exp\left[+\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right], \tag{4.34}$$

where k is the wavevector and $\hat{c}_k$ represents the annihilation operator of an electron with a wavevector k. Here we put the distance between nearest neighbor sites with a. Applying the operator $\hat{c}_{Hi}(t)$ to the state $|I\rangle$, we obtain

$$\hat{c}_{Hi}(t)|I\rangle = \frac{1}{\sqrt{N}} \sum_k \exp[ik \cdot (ia)] \exp\left[-\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right] \hat{c}_k \exp\left[+\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right] |I\rangle, \tag{4.35}$$

$$= \frac{1}{\sqrt{N}} \sum_k \exp[ik \cdot (ia)] \exp\left[-\frac{\hat{\mathcal{H}}^L_0}{i\hbar} t\right] \hat{c}_k \exp\left[+\frac{\mathcal{E}^L_{0I}}{i\hbar} t\right] |I\rangle, \tag{4.36}$$

$$= \frac{1}{\sqrt{N}} \sum_k \exp[ik \cdot (ia)] \exp\left[-\frac{\mathcal{E}^L_{0F}}{i\hbar} t\right] \exp\left[+\frac{\mathcal{E}^L_{0I}}{i\hbar} t\right] |F\rangle, \tag{4.37}$$

$$= \frac{1}{\sqrt{N}} \sum_k \exp[ik \cdot (ia)] \exp\left[+\frac{\mathcal{E}^L_{0I} - \mathcal{E}^L_{0F}}{i\hbar} t\right] \hat{c}_k |I\rangle, \tag{4.38}$$

where we have defined $|F\rangle = \hat{c}_k|I\rangle$. $\mathcal{E}_{0I}^L$ and $\mathcal{E}_{0F}^L$ are represent the eigenenergies of $\hat{\mathcal{H}}_0^L$ for the states $|I\rangle$ and $|F\rangle$, respectively. The energy difference $\mathcal{E}_{0I}^L - \mathcal{E}_{0F}^L$ corresponds to the energy of an electron with wavevector k, thus we define

$$\mathcal{E}_k \equiv \mathcal{E}_{0I}^L - \mathcal{E}_{0F}^L. \tag{4.39}$$

Therefore, we have the following equation,

$$\hat{c}_{Hi}(t_1) = \frac{1}{\sqrt{N}} \sum_k \exp\left[ik \cdot (ia)\right] \exp\left[-i\frac{\mathcal{E}_k}{\hbar} t_1\right] \hat{c}_k, \tag{4.40}$$

$$\hat{c}_{Hj}^\dagger(t_2) = \frac{1}{\sqrt{N}} \sum_k \exp\left[-ik \cdot (ja)\right] \exp\left[+i\frac{\mathcal{E}_k}{\hbar} t_2\right] \hat{c}_k^\dagger. \tag{4.41}$$

Inserting Eqs. (4.40) and (4.41) to Eq. (4.32), the Green function $g_{ij}^{0--}(t_1, t_2)$ is rewritten as

$$\begin{aligned} g_{ij}^{0--}(t_1, t_2) = \frac{1}{i\hbar}\frac{1}{N}\Big\{ &\sum_{kk'} \langle \hat{c}_k \hat{c}_{k'}^\dagger \rangle e^{ik(ia) - i\frac{\mathcal{E}_k}{\hbar}t_1} e^{-ik'(ja) + i\frac{\mathcal{E}_{k'}}{\hbar}t_2} \theta(t_1 - t_2) \\ &- \sum_{kk'} \langle \hat{c}_{k'}^\dagger \hat{c}_k \rangle e^{-ik'(ja) + i\frac{\mathcal{E}_{k'}}{\hbar}t_2} e^{ik(ia) - i\frac{\mathcal{E}_k}{\hbar}t_1} \theta(t_2 - t_1) \Big\}. \end{aligned} \tag{4.42}$$

To calculate the pair-correlation functions, we introduce the Fermi distribution function f_k.

$$\langle \hat{c}_{k'}^\dagger \hat{c}_k \rangle = \delta_{kk'} f_k, \tag{4.43}$$

$$\langle \hat{c}_k \hat{c}_{k'}^\dagger \rangle = \langle \delta_{kk'} - \hat{c}_{k'}^\dagger \hat{c}_k \rangle = \delta_{kk'} - \langle \hat{c}_{k'}^\dagger \hat{c}_k \rangle = \delta_{kk'}(1 - f_k). \tag{4.44}$$

Using Eqs. (4.43) and (4.44), we have

$$\begin{aligned} g_{ij}^{0--}(t_1, t_2) = \frac{1}{i\hbar}\frac{1}{N}\Big\{ &\sum_k e^{ik(i-j)a} e^{-i\frac{\mathcal{E}_k}{\hbar}(t_1 - t_2)} (1 - f_k) \theta(t_1 - t_2) \\ &- \sum_k e^{ik(i-j)a} e^{-i\frac{\mathcal{E}_k}{\hbar}(t_1 - t_2)} f_k \theta(t_2 - t_1) \Big\}. \end{aligned} \tag{4.45}$$

This equation depends on only time deference $\tau \equiv (t_1 - t_2)$. Therefore we obtain the following equation by performing the Fourier transform,

$$\begin{aligned} g_{ij}^{0--}(E) &= \int_{-\infty}^{+\infty} d\tau \; g_{ij}^{0--}(\tau) e^{+i\frac{E}{\hbar}\tau} \\ &= \frac{1}{i\hbar}\frac{1}{N}\Big\{ \sum_k e^{ik(i-j)a}(1 - f_k) \int_0^{+\infty} d\tau \; e^{i\frac{E - \mathcal{E}_k}{\hbar}\tau} \\ &\quad - \sum_k e^{ik(i-j)a} f_k \int_{-\infty}^{0} d\tau \; e^{i\frac{E - \mathcal{E}_k}{\hbar}\tau} \Big\} \\ &= \frac{1}{i\hbar}\frac{1}{N}\Bigg\{ \sum_k e^{ik(i-j)a}(1 - f_k) \left[\frac{e^{i(\frac{E - \mathcal{E}_k}{\hbar} + i\delta)\tau}}{i(\frac{E - \mathcal{E}_k}{\hbar} + i\delta)} \right]_{\tau=0}^{\tau=+\infty} \\ &\quad - \sum_k e^{ik(i-j)a} f_k \left[\frac{e^{i(\frac{E - \mathcal{E}_k}{\hbar} - i\delta)\tau}}{i(\frac{E - \mathcal{E}_k}{\hbar} - i\delta)} \right]_{\tau=-\infty}^{\tau=0} \Bigg\} \\ &= \frac{1}{N} \sum_k e^{ik(i-j)a} \left\{ \frac{1 - f_k}{E - \mathcal{E}_k + i\delta} + \frac{f_k}{E - \mathcal{E}_k - i\delta} \right\}. \end{aligned} \tag{4.46}$$

We have the other Green's functions similarly,

$$g_{ij}^{0++}(E) = \frac{1}{N}\sum_k e^{ik(i-j)a}\left\{\frac{-1+f_k}{E-\mathcal{E}_k+i\delta}+\frac{-f_k}{E-\mathcal{E}_k-i\delta}\right\}, \tag{4.47}$$

$$g_{ij}^{0+-}(E) = \frac{1}{i\hbar}\frac{1}{N}\sum_k e^{ik(i-j)a}(1-f_k)2\pi\delta(\mathcal{E}_k-E), \tag{4.48}$$

$$g_{ij}^{0-+}(E) = -\frac{1}{i\hbar}\frac{1}{N}\sum_k e^{ik(i-j)a}f_k 2\pi\delta(\mathcal{E}_k-E). \tag{4.49}$$

Using Eqs. (4.46)-(4.49), we obtain the Green's functions $g_{ij}^{0r}(E)$, $g_{ij}^{0a}(E)$, and $g_{ij}^{0k}(E)$, as follows,

$$g_{ij}^{0r}(E) = g_{ij}^{0--}(E) - g_{ij}^{0-+}(E) \tag{4.50}$$

$$= \frac{1}{N}\sum_k \frac{e^{ik(i-j)a}}{E-\mathcal{E}_k+i\delta}, \tag{4.51}$$

$$g_{ij}^{0a}(E) = g_{ij}^{0--}(E) - g_{ij}^{0+-}(E) \tag{4.52}$$

$$= \frac{1}{N}\sum_k \frac{e^{ik(i-j)a}}{E-\mathcal{E}_k-i\delta}, \tag{4.53}$$

$$g_{ij}^{0k}(E) = g_{ij}^{0-+}(E) + g_{ij}^{0+-}(E) \tag{4.54}$$

$$= (1-2f(E))(g_{ij}^{0r}(E) - g_{ij}^{0a}(E)), \tag{4.55}$$

where the relation $\frac{1}{x-i\delta} = \mathrm{P}\frac{1}{x} + i\pi\delta(x)$ has been used. Note that the electron distribution function $f(E)$ is included in only the Keldysh Green's function. Because $\mathcal{E}_k$ is the eigenenergy of the infinite length one-dimensional lattice, $\mathcal{E}_k$ is written as

$$\mathcal{E}_k = -2t^L\cos ka. \tag{4.56}$$

Thus, we obtain the following retarded Green's function $g_{ij}^{0r}(E)$,

$$g_{ij}^{0r}(E) = \frac{1}{N}\sum_k \frac{e^{ik(i-j)a}}{E+2t^L\cos ka+i\delta} \tag{4.57}$$

$$= \frac{1}{N}\frac{Na}{2\pi}\int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} dk \frac{e^{ik(i-j)a}}{E+2t^L\cos ka+i\delta}. \tag{4.58}$$

The Green's function g_{ij}^{0r} depends on only site difference $m \equiv i-j$. We can rewrite Eq. (4.58) as follows,

$$g_{|m|}^{0r}(E) = \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} dk\ \frac{e^{ik|m|a}}{E+2t^L\cos ka+i\delta} \tag{4.59}$$

$$= \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta\ \frac{(e^{i\theta})^{|m|}}{E+2t^L\cos\theta+i\delta} \qquad (\theta = ka) \tag{4.60}$$

$$= \frac{1}{2\pi}\oint_{|z|=1} dz\ \frac{1}{iz}\ \frac{z^{|m|}}{E+t^L(z+z^{-1})+i\delta} \qquad (z = e^{i\theta}) \tag{4.61}$$

$$= \frac{1}{2\pi i}\oint_{|z|=1} dz\ \frac{z^{|m|}}{t^L\{z^2-\frac{E+i\delta}{t^L}z+1\}}. \tag{4.62}$$

The integrand has the following poles.

$$z_{pole} = \frac{E \pm \sqrt{E^2-4(t^L)^2}+i\delta\cdot\left(1\pm E\frac{\sqrt{E^2-4(t^L)^2}}{E^2-4(t^L)^2}\right)}{2t^L} \tag{4.63}$$

Using the residue theorem, the Green's function $g^{0r}_{|m|}$ is obtained as follows.

- For $-2t^L < E < 2t^L$,

  we have

$$g^{0r}_{|m|}(E) = -\frac{i}{\sqrt{4(t^L)^2 - E^2}}\left(\frac{E - i\sqrt{4(t^L)^2 - E^2}}{2t^L}\right)^{|m|}. \tag{4.64}$$

  In the same way, we have

$$g^{0a}_{|m|}(E) = +\frac{i}{\sqrt{4(t^L)^2 - E^2}}\left(\frac{E + i\sqrt{4(t^L)^2 - E^2}}{2t^L}\right)^{|m|}. \tag{4.65}$$

  The absolute values of Green's functions, $|g^{0r}_{|m|}|$ and $|g^{0a}_{|m|}|$, are independent of the distance $|m|$. It means that electrons in the energy band of the one-dimensional lattice can propagate without damping.

- For $E < -2t^L$,

  we have following form,

$$g^{0r}_{|m|}(E) = -\frac{1}{\sqrt{E^2 - 4(t^L)^2}}\left(\frac{E + \sqrt{E^2 - 4(t^L)^2}}{2t^L}\right)^{|m|}, \tag{4.66}$$

$$g^{0a}_{|m|}(E) = -\frac{1}{\sqrt{E^2 - 4(t^L)^2}}\left(\frac{E + \sqrt{E^2 - 4(t^L)^2}}{2t^L}\right)^{|m|}. \tag{4.67}$$

- For $E > 2t^L$,

  we have following form,

$$g^{0r}_{|m|}(E) = \frac{1}{\sqrt{E^2 - 4(t^L)^2}}\left(\frac{E - \sqrt{E^2 - 4(t^L)^2}}{2t^L}\right)^{|m|}, \tag{4.68}$$

$$g^{0a}_{|m|}(E) = \frac{1}{\sqrt{E^2 - 4(t^L)^2}}\left(\frac{E - \sqrt{E^2 - 4(t^L)^2}}{2t^L}\right)^{|m|}. \tag{4.69}$$

  When electrons are in the outside of the energy band of the one-dimensional lattice, the absolute values of Green's functions, $|g^{0r}_{|m|}|$ and $|g^{0a}_{|m|}|$, decrease proportional to the distance $|m|$. It means that electrons can not propagate without damping.

Inserting Eqs. (4.64)-(4.69) to Eqs. (4.30) and (4.31), we can obtain the Green's functions for electrodes. Especially, the Green's function at the edge (0-th site) of the electrode is written as

$$g^a_{00}(E) = \frac{g^{0a}_{|0|}(E)}{1 - t^L g^{0a}_{|1|}(E)} = \begin{cases} \frac{2}{E+\sqrt{E^2-4(t^L)^2}} & \text{for } E > 2t^L, \\ \frac{E+i\sqrt{4(t^L)^2-E^2}}{2(t^L)^2} & \text{for } -2t^L < E < 2t^L, \\ \frac{2}{E-\sqrt{E^2-4(t^L)^2}} & \text{for } E < -2t^L. \end{cases} \tag{4.70}$$

4.2.2 Green's functions for the isolated nano-scale system

The statistical average of operator $\hat{\mathcal{O}}$ is given by Eq. (3.4),

$$\langle \mathcal{O}(t) \rangle = \mathrm{Tr}[\hat{\rho}(t_0)\hat{\mathcal{O}}_H(t)] \tag{4.71}$$

$$= \sum_{lm} \langle N,l|\hat{\rho}(t_0)|N,m\rangle\langle N,m|\hat{\mathcal{O}}_H(t)|N,l\rangle \tag{4.72}$$

$$= \sum_{l} \langle N,l|\hat{\rho}(t_0)|N,l\rangle\langle N,l|\hat{\mathcal{O}}_H(t)|N,l\rangle. \tag{4.73}$$

Here, $|N,l\rangle$ is the N-electron eigenstate of the Hamiltonian $\hat{\mathcal{H}^C}$ and has the eigenenergy $\mathcal{E}_l$. To obtain the Green's function $g_{ij}^{--}(E)$, we calculate $(\rho(t_0))_{ll} \equiv \langle N,l|\hat{\rho}(t_0)|N,l\rangle$ and $(g_{ij}^{--}(t_1,t_2))_{ll} \equiv \langle N,l|\mathrm{T}[\hat{c}_{Hi}\hat{c}_{Hj}^{\dagger}]|N,l\rangle$, and then we obtain the Green's function by using Eq. (4.73). The density matrix is obtained as follows,

$$(\hat{\rho}(t_0))_{ll} \equiv \langle N,l|\hat{\rho}(t_0)|N,l\rangle \tag{4.74}$$

$$= \frac{\langle N,l|e^{-\beta(\hat{\mathcal{H}^C}-\mu^C\hat{\mathcal{N}^C})}|N,l\rangle}{\mathrm{Tr}[e^{-\beta(\hat{\mathcal{H}^C}-\mu^C\hat{\mathcal{N}^C})}]}, \tag{4.75}$$

where μ^C is the Fermi energy of the isolated nano-scale system. Then, we obtain $(g_{ij}^{--}(t_1,t_2))_{ll}$ as follows,

$$\begin{aligned} i\hbar(g_{ij}^{--}(t_1,t_2))_{ll} &\equiv \langle N,l|\mathrm{T}[\hat{c}_{Hi}(t_1)\hat{c}_{Hj}^{\dagger}(t_2)]|N,l\rangle \\ &= \sum_m \Big\{ \langle N,l|\hat{c}_{Hi}(t_1)|N+1,m\rangle\langle N+1,m|\hat{c}_{Hj}^{\dagger}(t_2)|N,l\rangle\theta(t_1-t_2) \\ &\quad - \langle N,l|\hat{c}_{Hj}^{\dagger}(t_2)|N-1,m\rangle\langle N-1,m|\hat{c}_{Hi}(t_1)|N,l\rangle\theta(t_2-t_1)\Big\}. \end{aligned} \tag{4.76}$$

Using the relation $\hat{c}_{Hi}(t_1) = \exp\big[+i\frac{\hat{\mathcal{H}^C}}{\hbar}t_1\big]\hat{c}_{Hi}\exp\big[-i\frac{\hat{\mathcal{H}^C}}{\hbar}t_1\big]$, equation (4.76) is rewritten as follows,

$$\begin{aligned} i\hbar(g_{ij}^{--}(\tau))_{ll} = \sum_m \Big\{ & e^{+i\frac{\mathcal{E}_l-\mathcal{E}_m}{\hbar}\tau}\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^{\dagger}|N,l\rangle\theta(\tau) \\ & - e^{-i\frac{\mathcal{E}_l-\mathcal{E}_m}{\hbar}\tau}\langle N,l|\hat{c}_j^{\dagger}|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle\theta(-\tau)\Big\}, \end{aligned} \tag{4.77}$$

where $\tau = t_1 - t_2$. We perform the Fourier transform for Eq. (4.77) and obtain,

$$\begin{aligned} i\hbar(g_{ij}^{--}(E))_{ll} &= \sum_m \int_{-\infty}^{+\infty} d\tau e^{i\frac{E}{\hbar}\tau}\Big\{ e^{+i\frac{\mathcal{E}_l-\mathcal{E}_m}{\hbar}\tau}\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^{\dagger}|N,l\rangle\theta(\tau) \\ &\qquad - e^{-i\frac{\mathcal{E}_l-\mathcal{E}_m}{\hbar}\tau}\langle N,l|\hat{c}_j^{\dagger}|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle\theta(-\tau)\Big\} \\ &= \sum_m \Big\{ \int_0^{+\infty} d\tau e^{+i\frac{E+\mathcal{E}_l-\mathcal{E}_m}{\hbar}\tau-\delta\tau}\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^{\dagger}|N,l\rangle \\ &\quad - \int_{-\infty}^{0} d\tau e^{+i\frac{E-\mathcal{E}_l+\mathcal{E}_m}{\hbar}\tau+\delta\tau}\langle N,l|\hat{c}_j^{\dagger}|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle\Big\}. \end{aligned} \tag{4.78}$$

Carrying out the integration, we have

$$\begin{aligned} (g_{ij}^{--}(E))_{ll} = \sum_m \Big\{ & \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^{\dagger}|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m+i\delta} \\ & + \frac{\langle N,l|\hat{c}_j^{\dagger}|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta}\Big\}. \end{aligned} \tag{4.79}$$

Other functions are obtained similarly,

$$(g_{ij}^{++}(E))_{ll} = -\sum_m \Big\{ \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^\dagger|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} + \frac{\langle N,l|\hat{c}_j^\dagger|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m+i\delta}\Big\}, \tag{4.80}$$

$$(g_{ij}^{+-}(E))_{ll} = -i\sum_m 2\pi\delta(E+\mathcal{E}_l-\mathcal{E}_m)\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^\dagger|N,l\rangle, \tag{4.81}$$

$$(g_{ij}^{-+}(E))_{ll} = i\sum_m 2\pi\delta(E+\mathcal{E}_l-\mathcal{E}_m)\langle N,l|\hat{c}_j^\dagger|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle. \tag{4.82}$$

We can produce the following functions using Eqs. (4.79)-(4.82).

$$\begin{aligned}(g_{ij}^{r}(E))_{ll} &= (g_{ij}^{--}(E))_{ll} - (g_{ij}^{-+}(E))_{ll} \\ &= \sum_m \Big\{ \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^\dagger|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m+i\delta} \\ &\quad + \frac{\langle N,l|\hat{c}_j^\dagger|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m+i\delta}\Big\},\end{aligned} \tag{4.83}$$

$$\begin{aligned}(g_{ij}^{a}(E))_{ll} &= (g_{ij}^{--}(E))_{ll} - (g_{ij}^{+-}(E))_{ll} \\ &= \sum_m \Big\{ \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^\dagger|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} \\ &\quad + \frac{\langle N,l|\hat{c}_j^\dagger|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta}\Big\},\end{aligned} \tag{4.84}$$

$$\begin{aligned}(g_{ij}^{k}(E))_{ll} &= (g_{ij}^{-+}(E))_{ll} - (g_{ij}^{+-}(E))_{ll} \\ &= \sum_m \Big\{ \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^\dagger|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m+i\delta} \\ &\quad - \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}_j^\dagger|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} \\ &\quad + \frac{\langle N,l|\hat{c}_j^\dagger|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta} \\ &\quad - \frac{\langle N,l|\hat{c}_j^\dagger|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m+i\delta}\Big\}.\end{aligned} \tag{4.85}$$

Using Eqs. (4.73), (4.75) and (4.83), the advanced Green's function for the nano-scale system is given by,

$$g^a_{ij}(E) = \sum_l (\rho(t_0))_{ll} (g^a_{ij}(E))_{ll} \tag{4.86}$$

$$= \sum_l \frac{\langle N,l|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N,l\rangle}{\mathrm{Tr}[e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}]} \sum_m \Big\{ \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}^\dagger_j|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} + \frac{\langle N,l|\hat{c}^\dagger_j|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta} \Big\} \tag{4.87}$$

$$= \frac{1}{\mathrm{Tr}[e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}]} \sum_{lm} \Big\{ \langle N,l|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N,l\rangle \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}^\dagger_j|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} + \langle N,l|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N,l\rangle \frac{\langle N,l|\hat{c}^\dagger_j|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta} \Big\}. \tag{4.88}$$

We consider the only first term,

$$\begin{aligned}
&\sum_{lm} \langle N,l|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N,l\rangle \frac{\langle N,l|\hat{c}_i|N+1,m\rangle\langle N+1,m|\hat{c}^\dagger_j|N,l\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} \\
&= \sum_{lm} \langle N,l|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N,l\rangle \frac{\langle N+1,m|\hat{c}^\dagger_j|N,l\rangle\langle N,l|\hat{c}_i|N+1,m\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} \\
&= \sum_{lm} \langle N-1,l|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N-1,l\rangle \frac{\langle N,m|\hat{c}^\dagger_j|N-1,l\rangle\langle N-1,l|\hat{c}_i|N,m\rangle}{E+\mathcal{E}_l-\mathcal{E}_m-i\delta} \\
&= \sum_{lm} \langle N-1,m|e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}|N-1,m\rangle \frac{\langle N,l|\hat{c}^\dagger_j|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta}.
\end{aligned} \tag{4.89}$$

Inserting Eq. (4.89) to Eq. (4.88) we have

$$g^a_{ij}(E) = \frac{1}{\mathrm{Tr}[e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}]} \sum_{lm} \Big\{ \big(e^{-\beta(\mathcal{E}_m-\mu^C(N-1))} + e^{-\beta(\mathcal{E}_l-\mu^C N)}\big) \frac{\langle N,l|\hat{c}^\dagger_j|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m-i\delta} \Big\}. \tag{4.90}$$

In the similar way, we obtain

$$g^r_{ij}(E) = \frac{1}{\mathrm{Tr}[e^{-\beta(\hat{\mathcal{H}}^C-\mu^C\hat{\mathcal{N}}^C)}]} \sum_{lm} \Big\{ \big(e^{-\beta(\mathcal{E}_m-\mu^C(N-1))} + e^{-\beta(\mathcal{E}_l-\mu^C N)}\big) \frac{\langle N,l|\hat{c}^\dagger_j|N-1,m\rangle\langle N-1,m|\hat{c}_i|N,l\rangle}{E-\mathcal{E}_l+\mathcal{E}_m+i\delta} \Big\}, \tag{4.91}$$

$$g^k_{ij}(E) = (1-2f(E))(g^r_{ij}(E) - g^a_{ij}(E)), \tag{4.92}$$

where the relation $1-e^{-\beta(E-\mu^C)} = (1-2f(E))(1+e^{-\beta(E-\mu^C)})$ has been used.

When we assume that there is no Coulomb interaction between electrons, the Green functions become more simple form. For example, the eigenstate $|N=3,l\rangle$ where the α-th, β-th, and γ-th energy levels are filled with electrons is written as follows,

$$|3,l\rangle = \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}^\dagger_\gamma |0\rangle, \qquad (\alpha<\beta<\gamma) \tag{4.93}$$

where the operator $\hat{a}_m^\dagger$ creates an electron at m-th energy level with energy ε_m, and $|0\rangle$ is a vacuum state. The eigenenergy $\mathcal{E}_l$ for the state becomes $\varepsilon_\alpha + \varepsilon_\beta + \varepsilon_\gamma$. The orbital for the α-th energy level is written in the energy picture as follows,

$$|\alpha\rangle \equiv \hat{a}_\alpha^\dagger |0\rangle. \tag{4.94}$$

On the other hand, the orbital is also written in the site picture as follows,

$$|\alpha\rangle \equiv \sum_n \chi_n^\alpha \hat{c}_n^\dagger |0\rangle, \tag{4.95}$$

where χ_n^α is the amplitude of the α-th wavefunction at n-th site. A comparison of Eqs. (4.94) and (4.95) yields

$$\hat{a}_\alpha^\dagger = \sum_n \chi_n^\alpha \hat{c}_n^\dagger. \tag{4.96}$$

We can carry out $\langle 2, m|\hat{c}_i|3, l\rangle$ with aid of Eq. (4.96),

$$\begin{aligned}
\langle 2, m|\hat{c}_i|3, l\rangle &= \langle 0|\hat{a}_\eta \hat{a}_\xi \hat{c}_i \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\gamma^\dagger|0\rangle \\
&= \langle \hat{a}_\eta \hat{a}_\beta^\dagger\rangle\langle \hat{a}_\xi \hat{a}_\alpha^\dagger\rangle\langle \hat{c}_i \hat{a}_\gamma^\dagger\rangle - \langle \hat{a}_\eta \hat{a}_\gamma^\dagger\rangle\langle \hat{a}_\xi \hat{a}_\alpha^\dagger\rangle\langle \hat{c}_i \hat{a}_\beta^\dagger\rangle + \langle \hat{a}_\eta \hat{a}_\gamma^\dagger\rangle\langle \hat{a}_\xi \hat{a}_\beta^\dagger\rangle\langle \hat{c}_i \hat{a}_\alpha^\dagger\rangle \\
&= \delta_{\eta\beta}\delta_{\xi\alpha}\langle \hat{c}_i \hat{a}_\gamma^\dagger\rangle - \delta_{\eta\gamma}\delta_{\xi\alpha}\langle \hat{c}_i \hat{a}_\beta^\dagger\rangle + \delta_{\eta\gamma}\delta_{\xi\beta}\langle \hat{c}_i \hat{a}_\alpha^\dagger\rangle \\
&= \delta_{\eta\beta}\delta_{\xi\alpha}\chi_i^\gamma - \delta_{\eta\gamma}\delta_{\xi\alpha}\chi_i^\beta + \delta_{\eta\gamma}\delta_{\xi\beta}\chi_i^\alpha.
\end{aligned} \tag{4.97}$$

We do similar calculations about all eigenstates and obtain the following simple form of Green's functions,

$$g_{ij}^a(E) = \sum_n \frac{\chi_j^{n*}\chi_i^n}{E - \varepsilon_n - i\delta}, \tag{4.98}$$

$$g_{ij}^r(E) = \sum_n \frac{\chi_j^{n*}\chi_i^n}{E - \varepsilon_n + i\delta}, \tag{4.99}$$

$$g_{ij}^k(E) = (1 - 2f(E))(g_{ij}^r(E) - g_{ij}^a(E)), \tag{4.100}$$

where the summation runs over the all energy levels.

4.3 Green's functions for the joint system

We have already obtained the Green's functions for the isolated electrodes and nano-scale system in the previous section. To calculate the electronic current through the nano-scale system by using Eq. (4.15), we must obtain the Keldysh Green's functions G_{01}^k and G_{10}^k for the joint system which consists of the electrodes and the chain. Then the Dyson equations show that it is necessary to obtain the Green's functions G_{mn}^l in order to calculate G_{01}^k and G_{10}^k ($l = a, r, k$; $m(n) = 0, 1, N, N+1$). Therefore, the following contracted matrix forms of the Green's functions and the self-energies should be considered instead of Eqs. (3.61)-

(3.63),

$$\mathbf{G}^a = \begin{bmatrix} G^a_{00} & G^a_{01} & G^a_{0N} & G^a_{0\ N+1} \\ G^a_{10} & G^a_{11} & G^a_{1N} & G^a_{1\ N+1} \\ G^a_{N0} & G^a_{N1} & G^a_{NN} & G^a_{N\ N+1} \\ G^a_{N+1\ 0} & G^a_{N+1\ 1} & G^a_{N+1\ N} & G^a_{N+1\ N+1} \end{bmatrix}, \tag{4.101}$$

$$\mathbf{g}^a = \begin{bmatrix} g^a_{00} & 0 & 0 & 0 \\ 0 & g^a_{11} & g^a_{1N} & 0 \\ 0 & g^a_{N1} & g^a_{NN} & 0 \\ 0 & 0 & 0 & g^a_{N+1\ N+1} \end{bmatrix}, \tag{4.102}$$

$$\mathbf{\Sigma}^a = \begin{bmatrix} 0 & -t' & 0 & 0 \\ -t' & 0 & 0 & 0 \\ 0 & 0 & 0 & -t' \\ 0 & 0 & -t' & 0 \end{bmatrix}. \tag{4.103}$$

The retarded Green's functions and the self-energies are obtained similarly. Furthermore, using the Dyson equations (3.64) and (3.65), we have the advanced and the retarded Green's functions of the joint system as follows,

$$\mathbf{G}^a = (\mathbf{I} - \mathbf{g}^a\mathbf{\Sigma}^a)^{-1}\mathbf{g}^a, \tag{4.104}$$

$$\mathbf{G}^r = (\mathbf{I} - \mathbf{g}^r\mathbf{\Sigma}^r)^{-1}\mathbf{g}^r, \tag{4.105}$$

where $\mathbf{I}$ is the 4×4 unit matrix. The Keldysh Green's functions obey the Dyson equation (3.66). We have the following equation from Eq. (3.66),

$$\mathbf{G}^k = (\mathbf{I} - \mathbf{g}^r\mathbf{\Sigma}^r)^{-1}\mathbf{g}^k(\mathbf{I} + \mathbf{g}^a\mathbf{\Sigma}^a). \tag{4.106}$$

Furthermore, using Eqs. (4.104) and (4.105), we obtain

$$\mathbf{G}^k = \mathbf{G}^r\mathbf{g}^{r-1}\mathbf{g}^k\mathbf{g}^{a-1}\mathbf{G}^a. \tag{4.107}$$

When the i- and j-th sites are included in the nano-scale system, the (i,j)-component of $\mathbf{g}^{r-1}\mathbf{g}^k\mathbf{g}^{a-1}$ is written with aid of Eq. (4.100) as follows,

$$\begin{aligned} \{\mathbf{g}^{r-1}\mathbf{g}^k\mathbf{g}^{a-1}\}_{ij} &= (1-2f)\{\mathbf{g}^{r-1}(\mathbf{g}^r - \mathbf{g}^a)\mathbf{g}^{a-1})\}_{ij} \\ &= (1-2f)(\{\mathbf{g}^{a-1}\}_{ij} - \{\mathbf{g}^{r-1}\}_{ij}). \end{aligned} \tag{4.108}$$

Equation (4.108) is calculated as follows, by using Eqs. (4.98) and (4.99),

$$\{\mathbf{g}^{r-1}\mathbf{g}^k\mathbf{g}^{a-1}\}_{ij} = (1-2f)(\{\mathbf{g}^{a-1}\}_{ij} - \{\mathbf{g}^{r-1}\}_{ij}) \propto (1-2f)\ \delta \to 0. \tag{4.109}$$

It means that the Fermi energy of the isolated nano-scale system doesn't contribute the electronic current. On the other hand, When the $i\ (= j)$-th sites are included in the left or the right electrode, equation (4.108) is calculated as follows,

$$\begin{aligned} \{\mathbf{g}^{r-1}\mathbf{g}^k\mathbf{g}^{a-1}\}_{ii} &= (1-2f)(\{\mathbf{g}^{a-1}\}_{ij} - \{\mathbf{g}^{r-1}\}_{ii}) \\ &= \begin{cases} (1-2f^L)((g^a_{00})^{-1} - (g^r_{00})^{-1}) & \text{for } i = 0, \\ (1-2f^R)((g^a_{N+1\ N+1})^{-1} - (g^r_{N+1\ N+1})^{-1}) & \text{for } i = N+1. \end{cases} \end{aligned} \tag{4.110}$$

Thus, we obtain the Keldysh Green functions for the joint system,

$$
\begin{aligned}
G^k_{01} &= (1-2f^L)G^r_{00}((g^a_{00})^{-1}-(g^r_{00})^{-1})G^a_{01} \\
&\quad + (1-2f^R)G^r_{0\ N+1}((g^a_{N+1\ N+1})^{-1}-(g^r_{N+1\ N+1})^{-1})G^a_{N+1\ 1}, \qquad (4.111)\\
G^k_{10} &= (1-2f^L)G^r_{10}((g^a_{00})^{-1}-(g^r_{00})^{-1})G^a_{00} \\
&\quad + (1-2f^R)G^r_{1\ N+1}((g^a_{N+1\ N+1})^{-1}-(g^r_{N+1\ N+1})^{-1})G^a_{N+1\ 0}. \qquad (4.112)
\end{aligned}
$$

In this paper, first, we calculated numerically Eqs. (4.104)-(4.105) and obtained the G^a and G^r, and then we calculated numerically the G^k using Eqs. (4.111) and (4.112). Finally, the electronic currents are calculated using Eq. (4.15)