Chapter 4

Nonequilibrium Green’s function (NEGF) formalism

Study of quantum transport through mesoscopic and nanoscale systems is one of the most interesting and active areas of present research. Quantum transport through such low-dimensional systems is divided into stationary and time-dependent phenomena. The nonequilibrium Green’s function (NEGF) formalism [126, 127, 128] also known as the Keldysh formalism is widely used to describe transport phenomena in these systems. The NEGF formalism allows one to solve the time-dependent Schrodinger equation for an interacting many-body system exactly, from which one can calculate the time-dependent current by solving equations-of-motion for specific time-dependent single-particle Green’s functions [163]. The NEGF technique is somewhat delicate, and needs a rigorous treatment as given in [123, 132, 133, 161, 162, 163]. This chapter presents a brief discussion on the nonequilibrium Green’s function (NEGF) formalism to give a birds eye view of this technique and the notation used in the following chapters. To illustrate the usefulness of this theory, the formalism is applied to study the (a) static and (b) time-dependent electronic transport in mesoscopic systems. For the detailed description of this formalism readers are referred to Refs. [123, 132, 133,
The main difference between the NEGF formalism and ordinary equilibrium theory is that all time-dependent functions are defined for time-arguments on a contour, called the Keldysh contour. To construct equilibrium perturbation theory one considers that the system returns to its initial state (or a thermodynamic equilibrium state at finite temperature) as $t \to +\infty$, but in nonequilibrium theory this may not be true as the initial state at $t = -\infty$ can be different from the final state $t = +\infty$. Therefore, in the nonequilibrium theory any reference to large times should be avoided [132]. To formulate the nonequilibrium problem, a system is exposed to a time-dependent perturbation $H'(t)$ at time $t_0$ so that the total Hamiltonian is given by

$$H(t) = h + H'(t) = H_0 + H_i + H'(t),$$

(4.1)

where $H_0$ is the Hamiltonian which represents free particles and $H_i$ is the Hamiltonian which represents interaction between the particles. The perturbation $H'(t)$ can be of any form such as a time varying electric field or a coupling to contacts maintained at distinct chemical potentials. For time $t < t_0$, where $t_0$ is the time prior to which the system is in thermal equilibrium with contacts, the perturbation $H'(t)$ is zero and the system is described by the thermal equilibrium density operator given by

$$\rho(h) = \frac{e^{-\beta h}}{\text{Tr}[e^{-\beta h}]}, \quad \beta = 1/k_BT.$$

(4.2)

For a given density operator $\rho(h)$, the average value of an observable for $t \geq t_0$ is defined as

$$< O(t) > = \text{Tr}[\rho(h)O_H(t)],$$

(4.3)

where $O_H(t)$ is an observable in the Heisenberg picture*. 

*Heisenberg, Schrodinger, and Interaction representation pictures of quantum mechanics can
4.1 Contour-ordered Green’s function

The task is to transform the time dependence of \( O_H \) to a simpler form \( O_h \) using the relation

\[
O_H(t) = u_h(t, t_0) O_h(t) u_h(t, t_0), \tag{4.4}
\]

where \( u_h(t, t_0) \) is the time evolution operator which satisfies the equation-of-motion

\[
i \frac{\partial u_h(t, t_0)}{\partial t} = H'_h(t) u_h(t, t_0). \tag{4.5}
\]

The solution of Eq. (4.5) is given as

\[
u_h(t, t_0) = T \left\{ \exp \left[ -i \int_{t_0}^t dt' H'_h(t') \right] \right\}, \tag{4.6}
\]

with

\[
H'_h(t) = e^{i h(t-t_0)} H'(t) e^{-i h(t-t_0)}, \tag{4.7}
\]

the interaction representation of \( H'(t) \) [132, 162] and \( T \) is the time-ordering operator which always orders the operator with the latest time argument to the left:

\[
T \{ A(t) B(t') \} = \theta(t - t') A(t) B(t') \mp \theta(t' - t) B(t') A(t), \tag{4.8}
\]

where the negative and positive signs stand for fermions and bosons, respectively.

The operator \( O_H(t) \) in Eq. (4.4) can be expressed in another equivalent form as

\[
O_H(t) = T_{C_1} \left\{ \exp \left[ -i \int_{C_1} d\tau H'_h(\tau) \right] O_h(t) \right\}, \tag{4.9}
\]

where the contour \( C_1 \) is shown in Fig. 4.1 which runs on the real axis from time \( t_0 \) to \( t \), and back to the initial time \( t_0 \). The contour-ordering operator \( T_{C_1} \) orders be found in Ref. [132].
the time arguments such that the operators with time arguments that occur later on the contour appear to the left of operators with earlier time arguments.

![Contour](image)

**Figure 4.1:** Contour $C_t$. Reproduced from [162].

The contour-ordering operator allows the development of the nonequilibrium theory along lines parallel to the equilibrium theory [132].

The contour-ordered Green’s function is defined as

\[ G(1; 1') = -i < T_C[\psi_H(1)\psi_H^\dagger(1')] >. \]  (4.10)

The compact notation $(1; 1')$ means $(x_1, t_1; x'_1, t'_1)$ or $(x_1, \tau_1; x'_1, \tau'_1)$, where $\tau$ is the time variable defined on the contour. The contour $C$ starts and ends at $t_0$ passing through $t_1$ and $t'_1$ just once. The contour-ordering operator $T_C$ is defined as

\[ T_C[\psi_H(1)\psi_H^\dagger(1')] = \begin{cases} 
\psi_H(1)\psi_H^\dagger(1'), & t_1 > t'_1, \\
\pm\psi_H^\dagger(1')\psi_H(1), & t_1 < t'_1.
\end{cases} \]  (4.11)

Here $t_1 > t'_1$ indicates that $t_1$ is further along the contour than $t'_1$. From Eqs. (4.10) and (4.11) one can define
The contour $C$ is shown in Fig. 4.2 for $t_1 > t'_1$. 

Using Eq. (4.9) the contour-ordered Green’s function can be expressed in the interaction picture with respect to the Hamiltonian $h$ as

$$G(1; 1') = \begin{cases} G^>(1; 1') & t_1 > t'_1 \\ G^<(1; 1') & t_1 < t'_1. \end{cases} \quad (4.12)$$

The contour $C$ is as shown in Fig. 4.2. A perturbation expansion of the contour-ordered Green’s function can be obtained using Wick’s theorem which allows decomposition of many particle Green’s functions into sum and products of single-particle Green’s functions. Wick’s theorem is applicable only when the field operators and the density operator are represented in the interaction picture with their time evolution governed by the noninteracting Hamiltonian $H_0$ [132]. To
employ Wick’s theorem one must transform to the interaction picture with respect to $H_0$. Using the relationship [162]

$$e^{-\beta h} = e^{-\beta H_0} v(t_0 - i\beta, t_0), \quad (4.15)$$

where

$$v(t, t_0) = T \exp \left[ -i \int_{t_0}^{t} dt' H_{H_0}^i(t') \right], \quad (4.16)$$

with $H_{H_0}^i(t')$ the operator $H_i$ in the interaction picture with respect to the Hamiltonian $H_0$. The Green’s function becomes

$$G(1; 1') = -i \frac{\langle S_{C_u}^i S_C^i \psi_{H_0}^i(1) \psi_{H_0}^i(1') \rangle > 0}{\langle S_{C_u}^i S_C^i \rangle > 0} \frac{\text{Tr} \left\{ \rho_0 T_{C_u} [S_{C_u}^i S_C^i \psi_{H_0}^i(1) \psi_{H_0}^i(1')] \right\} \right)}{\text{Tr} \left[ \rho_0 T_{C_u} (S_{C_u}^i S_C^i) \right]} = -i \frac{\text{Tr} \left\{ e^{-\beta H_0} T_{C_u} [S_{C_u}^i S_C^i \psi_{H_0}^i(1) \psi_{H_0}^i(1')] \right\} \right)}{\text{Tr} \left[ e^{-\beta H_0} T_{C_u} (S_{C_u}^i S_C^i) \right]}, \quad (4.17)$$

where

$$\rho_0 = \frac{e^{-\beta H_0}}{\text{Tr}[e^{-\beta H_0}]}, \quad (4.18)$$

is the density matrix operator and

$$S_C^i = \exp \left[ -i \int_{C} d\tau H_{H_0}^i(\tau) \right],$$

$$S_{C_u}^i = \exp \left[ -i \int_{C_u} d\tau H_{H_0}^i(\tau) \right]. \quad (4.19)$$

The contour $C_u$ is shown in Fig. 4.3. Now Wick’s theorem can be used to obtain a perturbation expansion for the Green’s function and Feynman diagrams can be constructed just like in equilibrium theory. The equilibrium and nonequi-
librium theories are structurally similar with the only formal difference of appearance of contour integrals instead of real axis integrals.

4.2 Keldysh contour

For the Keldysh contour, initial correlations are neglected and \( t_0 \to -\infty \). Since it is assumed that the Green’s function falls off rapidly as a function of its time difference, the part of the contour \( C_v \) running from \( t_0 \) to \( t_0 - i\beta \) can be neglected and the contour \( C_v \) and \( C \) become identical both starting and ending at \(-\infty\).

These can be extend beyond the largest time by considering that the time evolution operator is a unitary and the resulting contour is the Keldysh contour [162]. Keldysh contour consists of two branches \( C_1 \) running from \(-\infty\) to \(+\infty\) and \( C_2 \) going from \(+\infty\) to \(-\infty\) as represented in Fig. 4.4. Each of the time arguments of the Green’s function can reside on both parts \( C_1 \) and \( C_2 \) of the contour. Any time residing on first part \( C_1 \) is earlier to any time residing on the latter part \( C_2 \) (in the contour sense) [132]. Therefore, the contour-ordered Green’s function consists of
four different forms as follows:

\[
G(1; 1') = \begin{cases} 
G_c(1; 1') & t_1, t'_1 \in C_1 \\
G^>(1; 1') & t_1 \in C_2, t'_1 \in C_1, \quad t_1 > t'_1 \\
G^<(1; 1') & t_1 \in C_1, t'_1 \in C_2, \quad t_1 < t'_1 \\
G_\tilde{c}(1; 1') & t_1, t'_1 \in C_2
\end{cases}, \tag{4.20}
\]

where \(G_c(1; 1')\), \(G^>(1; 1')\), \(G^<(1; 1')\), and \(G_{\tilde{c}}(1; 1')\) are the time-ordered, greater, lesser, and antitime-ordered Green’s functions.

The causal or time-ordered Green’s function \(G_c(1; 1')\) is defined as

\[
G_c(1; 1') = -i < \tilde{T} [\psi_H(1) \psi_H^\dagger(1')] > \\
= -i \theta(t_1 - t'_1) < \psi_H(1) \psi_H^\dagger(1') > + i \theta(t'_1 - t_1) < \psi_H^\dagger(1') \psi_H(1) > \tag{4.21}
\]

The greater function \(G^>(1; 1')\) is

\[
G^>(1; 1') = -i < \psi_H(1) \psi_H^\dagger(1') >, \tag{4.22}
\]

the lesser function \(G^<(1; 1')\) is

\[
G^<(1; 1') = +i < \psi_H^\dagger(1') \psi_H(1) >, \tag{4.23}
\]

and the antitime-ordered Green’s function \(G_{\tilde{c}}(1; 1')\) is

\[
G_{\tilde{c}}(1; 1') = -i < \tilde{T} [\psi_H(1) \psi_H^\dagger(1')] > \\
= -i \theta(t'_1 - t_1) < \psi_H(1) \psi_H^\dagger(1') > + i \theta(t_1 - t'_1) < \psi_H^\dagger(1') \psi_H(1) > \tag{4.24}
\]

where \(G^>\) and \(G^<\) are the correlation functions and called the hole and electron
propagators. These correlation functions are key quantities in the nonequilibrium problem as they are directly related to the particle densities and currents [123, 132, 133, 163]. The other two retarded and advanced Green’s functions are also defined. The retarded Green’s function is given as

\[ G^r(1; 1') = -i\theta(t_1 - t_1') \langle \psi_H(1), \psi^\dagger_H(1') \rangle > \]

\[ = \theta(t_1 - t_1')[G^>(1; 1') - G^<(1; 1')], \quad (4.25) \]

where \( G^r(1; 1') \) is non-zero for times \( t_1 > t_1' \). Therefore this function can be used to calculate the response at time \( t_1 \) to an earlier perturbation of the system at time \( t_1' \) and the advanced Green’s function is expressed as

\[ G^a(1; 1') = i\theta(t_1' - t_1) \langle \psi_H(1), \psi^\dagger_H(1') \rangle > \]

\[ = \theta(t_1' - t_1)[G^<(1; 1') - G^>(1; 1')], \quad (4.26) \]

which is non-zero only for \( t_1 < t_1' \). The curly brackets are used for the anticommutator. It is also clear from Eqs. (4.20), (4.25) and (4.26) that

\[ G^r - G^a = G^> - G^< \quad (4.27) \]

The contour-ordered Green’s function satisfies the Dyson equation given as

\[ G(1; 1') = G_0(1; 1') + \int d^3x_2 \int_{C_u} d\tau_2 G_0(1, 2)U(2)G(2, 1') \]

\[ + \int d^3x_2 \int d^3x_3 \int_{C_u} d\tau_2 \int_{C_u} d\tau_3 G_0(1, 2)\Sigma(2, 3)G(3, 1'), \quad (4.28) \]

with the notation \((i) = (r_i, t_i)\), where the times may be complex. In the Dyson equation the time-dependent external perturbation \( H'(t) \) is represented by a one-body potential \( U \) and all possible interactions are incorporated in the self energy.
denoted by the symbol $\Sigma[G]$ which is a function of the single-particle Green’s function $G$. The technical detail of the derivation of the Dyson equation is given in [132, 163] and for the systems considered in the thesis in Chapter 5.

### 4.3 Analytic continuation: Langreth theorem

Contour representation is impractical in calculations so one has to replace the contour-integrals with real time integral in the Dyson equation using the analytic continuation method as given in [132]. In order to make this replacement one considers a contour integral of the form (from Dyson equation)

$$C(t_1, t'_1) = \int_C d\tau A(t_1, \tau) B(\tau, t'_1),$$

where only temporal variables are considered. To evaluate Eq. (4.29) it is assumed that $t_1$ lies on the first half of the contour and $t'_1$ on the later half as shown in Fig. 4.5(a). This placement of $t_1$ and $t'_1$ ($t_1 < t'_1$) leads to the definition of the lesser function $C^<(t_1, t'_1)$. The contour shown in Fig. 4.5(a) can be deformed to give two contours $C_1$ and $C_2$ as shown in Fig. 4.5 (b). Thus Eq. (4.29) becomes
\begin{equation}
C^<(t_1, t'_1) = \int_{C_1} d\tau A(t_1, \tau) B^<(\tau, t'_1) + \int_{C_2} d\tau A^<(t_1, \tau) B^>(\tau, t'_1). \tag{4.30}
\end{equation}

The label \'< on \(B\) in the first term indicates that as long as the integration variable \(\tau\) is confined on the contour \(C_1\) it is less than \(t'_1\) in the contour sense. The same argument holds for \(A^<(t_1, \tau)\) in the second term with \(\tau\) on \(C_2\).

Now to solve the first contour the integration can be divided into two parts as follows

\begin{equation}
\int_{C_1} d\tau A(t_1, \tau) B^<(\tau, t'_1) = \int_{-\infty}^{t_1} dt A^>(t_1, t) B^<(t, t'_1) + \int_{t_1}^{-\infty} dt A^<(t_1, t) B^<(t, t'_1) = \int_{-\infty}^{t_1} dt (A^>(t_1, t) - A^<(t_1, t)) B^<(t, t'_1). \tag{4.31}
\end{equation}

In the first term, \(A(t_1, t)\) becomes \(A^>(t_1, t)\) for \(-\infty < t < t_1\) as \(t_1\) is later than \(t\) in this case. The same reason is true for \(A^<(t_1, t))\). Using the definition of the retarded Green’s function from Eq.(4.25), Eq. (4.31) can be further written as

\begin{equation}
\int_{C_1} d\tau A(t_1, \tau) B^<(\tau, t'_1) = \int_{-\infty}^{t_1} dt A^>(t_1, t) B^<(t, t'_1). \tag{4.32}
\end{equation}

Similarly using the definition of the advanced Green’s function (Eq. (4.26)) the second contour can be solved which gives rise to

\begin{equation}
\int_{C_2} d\tau A^<(t_1, \tau) B^>(\tau, t'_1) = \int_{-\infty}^{t_1} dt A^<(t_1, t) B^a(t, t'_1). \tag{4.33}
\end{equation}

Substituting Eq. (4.32) and (4.33) in Eq. (4.30) one gets

\begin{equation}
C^<(t_1, t'_1) = \int_{-\infty}^{t_1} dt [A^>(t_1, t) B^<(t, t'_1) + A^<(t_1, t) B^a(t, t'_1)]. \tag{4.34}
\end{equation}

This result can be generalized for a product of three functions of the form
\( D = ABC \) then the lesser function

\[
D^< = A^r B^r C^< + A^r B^< C^a + A^< B^a C^a.
\] (4.35)

In a similar manner the greater function is derived as

\[
C^>(t_1, t_1') = \int_{-\infty}^{\infty} dt [A^r(t_1, t)B^>(t, t_1') + A^>(t_1, t)B^a(t, t_1')].
\] (4.36)

The retarded or advanced component of a product of functions defined on the contour can also be derived [132] using various definition in Eq. (4.21) to Eq. (4.26) and Eqs. (4.34) and Eq. (4.36), and is given as

\[
C^r(t_1, t_1') = \theta(t_1 - t_1') [C^>(t_1, t_1') - C^<(t_1, t_1')] \\
= \theta(t_1 - t_1') \left[ \int_{-\infty}^{t_1} dt [A^>(B^> - B^<) + (A^> - A^<)B^a] \right] \\
= \theta(t_1 - t_1') \left[ \int_{-\infty}^{t_1} dt (A^> - A^<)(B^> - B^<) \right. \\
+ \left. \int_{t_1'}^{t_1} dt (A^> - A^<)(B^< - B^>) \right] \\
= \int_{t_1'}^{t_1} dt A^r(t_1, t)B^r(t, t_1')
\] (4.37)

In compact form: \( C^r = A^r B^r \).

### 4.3.1 Keldysh formulation

Applying Eq. (4.35) on Eq. (4.28) the lesser function becomes

\[
G^< = G^<_0 + G^<_0 \Sigma^r G^< + G^r \Sigma^< G^a + G^<_0 \Sigma^a G^a.
\] (4.38)
Iterating Eq. (4.38) with respect to $G^<$ and regrouping of the terms lead to the Keldysh equation for the lesser Green’s function

$$G^< = (1 + G^r \Sigma^r)G^<_0(1 + \Sigma^aG^a) + G^r\Sigma^<G^a,$$ (4.39)

where the retarded and advanced Green’s functions satisfy the Dyson equation

$$G^{r,a} = G^{r,a}_0 + G^{r,a}_0\Sigma^{r,a}G^{r,a}.$$ (4.40)

Using the Dyson equation for the retarded Green’s function, it can be shown that the first term in Eq. (4.39) vanishes for steady-state systems, if the system was in a non-interacting state in infinite past because $(1+G^r\Sigma^r)G^<_0 = G^r(G^r_0)^{-1}G^<_0 = 0$ [132, 150]. Therefore, in many applications it is sufficient to write only the second term.

$$G^< = G^r\Sigma^<G^a.$$ (4.41)
4.4 Application to Steady-state transport

4.4.1 Interacting case:

This section discusses the steady-state transport problem addressed in [132, 144, 163] where a general formulation of the current is presented using the nonequilibrium Green’s function formalism. The system under study consists of an interacting central region and the two non-interacting left and right leads. The approach used in this study works as follows: in the infinite past (at $t = -\infty$) the system is unperturbed and the leads are at thermal equilibrium at their own electrochemical potentials, $\mu_L$ and $\mu_R$ for the left and right leads, respectively. The central region is also at its own equilibrium and no current is allowed to flow through the system. When the coupling between the central region and the two leads is turned on the current flows from the left lead to the right lead through the central region if $\mu_L > \mu_R$. After this the system attains a steady-state. In this study [132, 144, 163], an exact formula for this steady-state current is derived in terms of the Fermi distribution functions of the left and right leads, that is $f_L(\varepsilon)$ and $f_R(\varepsilon)$, and local properties of the interacting region.

To study the transport in the system, the total Hamiltonian of the complete system, lead-central region-lead is divided into three Hamiltonian as

$$H = H_{\text{lead}} + H_{\text{central}} + H_{\text{tunneling}}.$$  \hfill (4.42)

Each of these Hamiltonian is defined as

- The Hamiltonian of the left and right lead is given as

$$H_{\text{lead}} = \sum_{k, \alpha L, R} \varepsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha},$$  \hfill (4.43)
where \( c^\dagger_{k\alpha} \) and \( c_{k\alpha} \) are the operators that create and destroy an electron with momentum \( k \) in channel \( \alpha \) with energy \( \epsilon_{k\alpha} \) in either the left (L) or the right (R) lead [132, 144]. The Green’s functions for the isolated leads are defined as

\[
\begin{align*}
    g_{k\alpha}^{r,a}(t, t') &= \mp i\theta(\pm t \mp t') \langle \{ c_{k\alpha}(t), c^\dagger_{k\alpha}(t') \} \rangle = \mp i\theta(\pm t \mp t') \exp[-i\epsilon_{k\alpha}(t - t')] \\
    g_{k\alpha}^{<}(t, t') &= i \langle c^\dagger_{k\alpha}(t') c_{k\alpha}(t) \rangle = i f(\epsilon_{k\alpha}) \exp[-i\epsilon_{k\alpha}(t - t')],
\end{align*}
\]

where \( f(\epsilon_{k\alpha}) = \left[ \exp[(\epsilon_{k\alpha} - \mu_{\alpha})/k_B T] + 1 \right]^{-1} \) is the equilibrium distribution function in a given lead. The lead Green’s functions are derived in Appendix C for a time-dependent problem. In steady-state, the Green’s functions depend only on time difference.

- The Hamiltonian of the central interacting region is

\[
    H_{\text{central}} = \sum_m \epsilon_m d^\dagger_m d_m.
\]

The form of this Hamiltonian depends on the model system chosen to describe interactions. If the electrons interact only with each other and not with some other excitation such as phonons then it can be assumed that the Hamiltonian is a function of a complete set of single-electron creation \( d^\dagger_m \) and annihilation \( d_m \) operators in the interacting region.

- The tunneling Hamiltonian which describes the coupling between leads and the interacting region is expressed as

\[
    H_{\text{tunneling}} = H_T = \sum_{n,k,\alpha L,R} (V_{k\alpha,n} c^\dagger_{k\alpha} d_n + \text{h.c.}),
\]

where \( d^\dagger_n (d_n) \) is the single-electron creation (annihilation) operator for the
complete and orthonormal set of the states $|n\rangle$ in the interacting region and $V_{kα,n}$ is some complex number.

Hence the total Hamiltonian is

$$H = \sum_{k,α\in L,R} \varepsilon_{kα} c_{kα}^\dagger c_{kα} + \sum_m \varepsilon_m d_m^\dagger d_m + \sum_{n,k,α\in L,R} (V_{kα,n} c_{kα}^\dagger d_n + \text{h.c.}). \quad (4.47)$$

Guided by the experimental geometry in which the leads rapidly broaden into large metallic contacts [132], an assumption is made that the interaction between electrons in the leads and the interaction between electrons in the central interacting region and in the leads are strongly screened and can be neglected [144].

4.4.1.1 Expression for the current

The current flowing from the left lead into the central region can be calculated by taking the expectation value of the rate of change of the occupation number operator of the left lead as

$$J_L = -e \left\langle \frac{N_L}{dt} \right\rangle = -\frac{i e}{\hbar} < [H, N_L] >,$$  \quad (4.48)

where $N_L = \sum_{k,α\in L} c_{kα}^\dagger c_{kα}$ and $H$ is the total Hamiltonian. The Hamiltonian $H_{\text{central}}$ and $H_{\text{contact}}$ commute with $N_L$, therefore the current is calculated from $H_{\text{tunneling}}$ (using $[c, c^\dagger]$=1).

$$[H_{\text{tunneling}}, N_L] = \left\{ \sum_{n,k,α\in L} V_{kα,n} c_{kα}^\dagger d_n + V_{kα,n}^* d_n^\dagger c_{kα}, \sum_{k,α\in L} c_{kα}^\dagger c_{kα} \right\}$$

$$= \sum_{n,k,α\in L} \left[ V_{kα,n}^* d_n^\dagger c_{kα} - V_{kα,n} c_{kα}^\dagger d_n \right]. \quad (4.49)$$
Substituting Eq. (4.49) in Eq. (4.48) the expression for the current becomes

\[
J_L = -\frac{ie}{\hbar} < [H_{\text{tunneling}}, N_L] >
= -\frac{ie}{\hbar} \sum_{n,k,\alpha \in L} \left[ V_{k\alpha,n}^* < d_n^\dagger c_{k\alpha} > - V_{k\alpha,n} < c_{k\alpha}^\dagger d_n > \right]
= -\frac{ie}{\hbar} \sum_{n,k,\alpha \in L} \left[ V_{k\alpha,n} < c_{k\alpha}^\dagger d_n > - V_{k\alpha,n}^* < d_n^\dagger c_{k\alpha} > \right]
\tag{4.50}
\]

Equation (4.50) can be simplified further by defining the two lesser Green’s functions with \( \hbar = 1 \):

\[
G_{n,k\alpha}^<(t - t') = i < c_{k\alpha}(t')d_n(t) >,
G_{k\alpha,n}^<(t - t') = i < d_n^\dagger(t')c_{k\alpha}(t) >.
\tag{4.51}
\]

The time-diagonal components of these Green’s functions give rise to the current. These Green’s functions satisfy the property \( G_{k\alpha,n}^<(t,t) = -[G_{n,k\alpha}^<(t,t)]^* \) or \( G_{k\alpha,n}^<(\epsilon) = -[G_{n,k\alpha}^<(\epsilon)]^* \) after taking the Fourier transform. Making use of this property in Fourier space the current becomes

\[
J_L = \frac{2e}{\hbar} \text{Re} \left\{ \sum_{n,k,\alpha \in L} V_{k\alpha,n} G_{n,k\alpha}^<(t,t) \right\}
= \frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} \text{Re} \left\{ \sum_{n,k,\alpha \in L} V_{k\alpha,n} G_{n,k\alpha}^<(\epsilon) \right\}.
\tag{4.52}
\]

Now one needs to calculate the lesser Green’s function \( G_{n,k\alpha}^< \). For the noninteracting leads, an expression for \( G_{n,k\alpha}^< \) can be derived from the equation-of-motion for the time-ordered Green’s function \( G_{n,k\alpha}(t - t') \) which is defined as

\[
G_{n,k\alpha}(t - t') = -i \left< T[ d_n(t)c_{k\alpha}^\dagger (t') \right>.
\tag{4.53}
\]
Here $T$ is the time-ordering operator. The equation-of-motion for $G_{n,k\alpha}(t - t')$ is

$$\left[ -i \frac{\partial}{\partial t'} - \varepsilon_{k\alpha} \right] G_{n,k\alpha}(t - t') = \sum_m V_{k\alpha,m}^* G_{nm}(t - t'), \quad (4.54)$$

where $G_{nm}(t - t')$ is the time-ordered Green’s function of the central interacting region defined as

$$G_{nm}(t - t') = -i < T[d_n(t)d_m^\dagger(t')] > \quad (4.55)$$

The lesser Green’s function $G_{n,k\alpha}^<$ can be calculated by first defining the contour-ordered version of the Green’s function $G_{n,k\alpha}$ (Eq. (4.10)) and then obtaining the lesser Green’s function from the correct segments on the contour (Eq. (4.20)) [163].

Here, only the final key results are presented as a complete derivation of the Green’s functions and the time-dependent current through a system based on the carbon nanotube is presented in the next chapter and appendix C. For the full derivation of the steady-state current readers are referred to [132, 163].

After following the steps given in [132, 163] one gets the lesser Green’s functions as

$$G_{n,k\alpha}^<(t - t') = \sum_m \int dt_1 V_{k\alpha,m}^*[G_{nm}^r(t-t_1)g_{k\alpha}^<(t_1-t') + G_{nm}^<(t-t_1)g_{k\alpha}^a(t_1-t')] \quad (4.56)$$

where $g_{k\alpha}^{<,a}(t_1 - t')$ are the Green’s functions of the lead defined in Eq. (4.44). The lesser Green’s function $G_{n,m}^<(t - t_1)$ and the retarded $G_{n,m}^r(t - t_1)$ Green’s function of the central region are defined as

$$G_{nm}^<(t - t_1) = i < d_m^\dagger(t_1)d_n(t) >, \quad (4.57)$$

and

$$G_{nm}^r(t - t_1) = -i\theta(t - t_1) < \{d_n(t), d_m^\dagger(t_1)\} > . \quad (4.58)$$
Taking the Fourier transform of Eq. (4.56) the lesser Green’s function becomes

\[ G_{n,k\alpha}(\epsilon) = \sum_m V^*_{k\alpha,m}[G^r_{nm}(\epsilon)g^<_{ka}(\epsilon) + G^<_{nm}(\epsilon)g^a_{ka}(\epsilon)]. \]  

(4.59)

Using Eq. (4.59) the current becomes

\[ J_L = \frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} \text{Re} \left\{ \sum_{n,m:k\alpha L} V_{k\alpha,n}V^*_{k\alpha,m}[G^r_{nm}(\epsilon)g^<_{ka}(\epsilon) + G^<_{nm}(\epsilon)g^a_{ka}(\epsilon)] \right\}. \]  

(4.60)

Here it is convenient to convert the sum over the momentum states \( k \) in the leads into an integral over energies by defining the elastic coupling between the left lead and the interacting region as

\[ [\Gamma_L(\epsilon_k)]_{mn} = 2\pi \sum_{\alpha L} \rho_{\alpha}(\epsilon_k)V_{\alpha,n}(\epsilon_k)V^*_{\alpha,m}(\epsilon_k), \]  

(4.61)

where \( \rho_{\alpha}(\epsilon) \) is the density of states. Therefore, Eq. (4.60) can be expressed as

\[ J_L = \frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} \int d\epsilon_k[\Gamma_L(\epsilon_k)]_{mn} \text{Re} \left\{ G^r_{nm}(\epsilon) i \delta(\epsilon - \epsilon_k) f_L(\epsilon) + i \theta(\epsilon - \epsilon_k) G^<_{nm}(\epsilon) \right\}. \]  

(4.62)

In matrix form

\[ J_L = \frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} d\epsilon_k \Gamma_L(\epsilon_k) \text{ReTr} \left\{ G^r(\epsilon) i \delta(\epsilon - \epsilon_k) f_L(\epsilon) + i \theta(\epsilon - \epsilon_k) G^<(\epsilon) \right\}. \]  

(4.63)

Solving the first term containing \( G^r(\epsilon) \) and using \( G^a = [G^r]^* \)

\[ J_L = \frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} \int d\epsilon_k \Gamma_L(\epsilon_k) \text{ReTr} \left\{ G^r(\epsilon) i \delta(\epsilon - \epsilon_k) f_L(\epsilon) \right\} \]

\[ = \frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} \text{Tr} \left\{ \Gamma_L(\epsilon)f_L(\epsilon) \text{Re[iG^r(\epsilon)]]} \right\} \]

\[ = -\frac{2e}{\hbar} \int \frac{d\epsilon}{2\pi} \text{Tr} \left\{ \Gamma_L(\epsilon)f_L(\epsilon) \text{Im[G^r(\epsilon)]} \right\} \]

\[ = \frac{ie}{\hbar} \int \frac{d\epsilon}{2\pi} \text{Tr} \left\{ \Gamma_L(\epsilon)f_L(\epsilon) [G^r(\epsilon) - G^a(\epsilon)] \right\}. \]  

(4.64)
Similarly the second term can be solved [132]. A similar derivation is given in chapter 5. Therefore, the current from left lead to central region can be written as

\[ J_L = \frac{i e}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \Gamma_L(\varepsilon) \left\{ G^< (\varepsilon) + f_L(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)] \right\} \right). \]  

(4.65)

An analogous expression can also be derived for the current flowing from the right lead to the central interacting region, and is given as

\[ J_R = \frac{i e}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \Gamma_R(\varepsilon) \left\{ G^< (\varepsilon) + f_R(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)] \right\} \right). \]  

(4.66)

In steady state, the current is uniform, hence \( J = J_L = -J_R \), and the total current can be symmetrized as \( J = (J_L - J_R)/2 \). Using Eqs.(4.65) and (4.66) the expression for the total current is given by:

\[ J = \frac{i e}{2\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left\{ [\Gamma_L(\varepsilon) - \Gamma_R(\varepsilon)] G^< (\varepsilon) + [f_L(\varepsilon) \Gamma_L(\varepsilon) - f_R(\varepsilon) \Gamma_R(\varepsilon)] [G^r (\varepsilon) - G^a (\varepsilon)] \right\}. \]  

(4.67)

Using the relationship between the left and right coupling functions, i.e. \( \Gamma_L(\varepsilon) = \lambda \Gamma_R(\varepsilon) \) and \( J = x J_L - (1 - x) J_R \), where \( x = 1/(1 + \lambda) \) is an arbitrary parameter, a simpler expression for the total current can be obtained

\[
J = \frac{i e}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( x \Gamma_L(\varepsilon) \left\{ G^< (\varepsilon) + f_L(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)] \right\}
- \Gamma_R(\varepsilon) \left\{ G^< (\varepsilon) + f_R(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)] \right\}
+ x \Gamma_R(\varepsilon) \left\{ G^< (\varepsilon) + f_R(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)] \right\}\right)
\]

\[
= \frac{i e}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( x \Gamma_L(\varepsilon) G^< (\varepsilon) - \Gamma_R(\varepsilon) G^< (\varepsilon) + x \Gamma_R(\varepsilon) G^< (\varepsilon)
+ x \Gamma_L(\varepsilon) f_L(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)] - \Gamma_R(\varepsilon) f_R(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)]
+ x \Gamma_R(\varepsilon) f_R(\varepsilon) [G^r (\varepsilon) - G^a (\varepsilon)]\right)\]
\]
\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \left\{ x\Gamma_L(\varepsilon) - (1 - x)\Gamma_R(\varepsilon) \right\} [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

substituting \( \Gamma_L(\varepsilon) = \lambda \Gamma_R(\varepsilon) \)

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \left\{ x\lambda - (1 - x) \right\} \Gamma_R(\varepsilon) G^r(\varepsilon) + \left\{ x\lambda f_L(\varepsilon) - (1 - x)f_R(\varepsilon) \right\} \Gamma_R(\varepsilon) \right. \\
\left. \times [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

and putting \( x = 1/(1 + \lambda) \) the current becomes

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \Gamma_R(\varepsilon) \left\{ [\lambda x - (1 - x)]G^r(\varepsilon) + [\lambda x f_L(\varepsilon) - (1 - x)f_R(\varepsilon)] \right\} \times [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \frac{\lambda x}{1 + \lambda} [f_L(\varepsilon) - f_R(\varepsilon)] \right) \left( \frac{\lambda}{1 + \lambda} [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \frac{\lambda x}{1 + \lambda} [f_L(\varepsilon) - f_R(\varepsilon)] \right) \left( \frac{\lambda}{1 + \lambda} [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \frac{\lambda x}{1 + \lambda} [f_L(\varepsilon) - f_R(\varepsilon)] \right) \left( \frac{\lambda}{1 + \lambda} [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \frac{\lambda x}{1 + \lambda} [f_L(\varepsilon) - f_R(\varepsilon)] \right) \left( \frac{\lambda}{1 + \lambda} [G^r(\varepsilon) - G^a(\varepsilon)] \right) \]

\[ J = \frac{ie}{\hbar} \int \frac{d\varepsilon}{2\pi} [f_L(\varepsilon) - f_R(\varepsilon)] \mathbf{T}(\varepsilon), \]
where $T(\epsilon)$ is given as\footnote{Equation (4.70) can be multiplied by a factor of 2 to include the spin degeneracy.}

$$T(\epsilon) = \text{Tr} \left( \frac{\Gamma_L(\epsilon)\Gamma_R(\epsilon)}{\Gamma_L(\epsilon) + \Gamma_R(\epsilon)} \left[ G^r(\epsilon) - G^a(\epsilon) \right] \right). \quad (4.71)$$

The difference between the retarded and advanced Green’s functions is the density of states. The quantity $T(\epsilon)$ looks similar to the transmission coefficient $T(\epsilon)$ of the Landauer formula, but there is no connection between these two quantities. In particular, when inelastic scattering is involved, no such connection is present. In the next section, a non-interacting central region is discussed where a connection between $T(\epsilon)$ and the transmission coefficient can be seen.

### 4.4.2 Non-interacting case:

In this case, the electrons in the central region also also non-interacting and the central Hamiltonian has the form: $H_{\text{central}} = \sum_n \epsilon_n d_n^\dagger d_n$. From Eq. (4.40) the Dyson equation for the retarded Green’s function is given as

$$G^r(\epsilon) = G^r_0(\epsilon) + G^r_0(\epsilon)\Sigma^r(\epsilon)G^r(\epsilon), \quad (4.72)$$

where the retarded self-energy is given, following similar steps as in chapter 5 (Eq. (5.41), as

$$\Sigma^r_{nn'}(\epsilon) = \sum_{k\alpha L,R} V^r_{k\alpha,n} g^r_{k\alpha}(\epsilon) V_{k\alpha,n'}. \quad (4.73)$$

In the non-interacting case, the lesser Green’s function from Eq. (4.41) is written as

$$G^<(\epsilon) = G^r(\epsilon)\Sigma^<(\epsilon)G^a(\epsilon), \quad (4.74)$$
with the lesser self-energy \([132]\) given as

\[
\Sigma^<(\varepsilon) = \sum_{k\alpha,n,L,R} V_{k\alpha,n}^* g_{k\alpha}^<(\varepsilon) V_{k\alpha,n'} = i[\Gamma_L(\varepsilon) f_L(\varepsilon) + \Gamma_R(\varepsilon) f_R(\varepsilon)].
\] (4.75)

The Dyson equation for the retarded Green’s function requires matrix inversion. Therefore, the retarded (advanced) self-energy \([132]\) is given by

\[
\Sigma^{r,a}(\varepsilon) = \sum_{k\alpha,L,R} \frac{|V_{k\alpha}|^2}{\varepsilon - \varepsilon_{k\alpha} \pm i\eta} = \Lambda(\varepsilon) \mp \frac{i}{2} \Gamma(\varepsilon),
\] (4.76)

where the real and imaginary parts are \(\Lambda(\varepsilon) = \Lambda_L(\varepsilon) + \Lambda_R(\varepsilon)\) and \(\Gamma(\varepsilon) = \Gamma_L(\varepsilon) + \Gamma_R(\varepsilon)\).

Using the identity \([132]\)

\[
G^r G^a = \frac{G^r - G^a}{(G^s - 1)^{-1}} = A(\varepsilon) \Gamma(\varepsilon)^{-1},
\] (4.77)

where \(A(\varepsilon) = i[G^r(\varepsilon) - G^a(\varepsilon)]\) is the spectral function, \(G^<\) can be written as

\[
G^<(\varepsilon) = G^r \Sigma^< G^a = iG^r [f_L(\varepsilon) \Gamma_L(\varepsilon) + f_R(\varepsilon) \Gamma_R(\varepsilon)] G^a \\
= \frac{iA(\varepsilon)[f_L(\varepsilon) \Gamma_L + f_R(\varepsilon) \Gamma_R]}{\Gamma(\varepsilon)}
\]

\[
G^<(\varepsilon) = iA(\varepsilon) \bar{f}(\varepsilon),
\] (4.78)

where

\[
\bar{f}(\varepsilon) = \frac{\Gamma_L(\varepsilon) f_L(\varepsilon) + \Gamma_R(\varepsilon) f_R(\varepsilon)}{\Gamma(\varepsilon)}.
\] (4.79)

From Eqs. (4.72) and (4.76) the retarded and advanced Green’s functions can be written as

\[
G^{r,a}(\varepsilon) = [\varepsilon - \varepsilon_0 - \Lambda(\varepsilon) \pm i\Gamma(\varepsilon)/2]^{-1},
\] (4.80)
the spectral function becomes

\[ A(\varepsilon) = \frac{\Gamma(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + [\Gamma(\varepsilon)/2]^2}. \]  

(4.81)

Using these expressions in Eq. (4.67) the expression for the current becomes

\[ J = \frac{ie}{2\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( iA(\varepsilon)[\Gamma_L(\varepsilon) - \Gamma_R(\varepsilon)]f(\varepsilon) + [f_L(\varepsilon)\Gamma_L(\varepsilon) - f_R(\varepsilon)\Gamma_R(\varepsilon)](-i)A(\varepsilon) \right) \]

\[ J = -\frac{e}{2\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( A(\varepsilon) \left\{ [\Gamma_L(\varepsilon) - \Gamma_R(\varepsilon)]f(\varepsilon) - [f_L(\varepsilon)\Gamma_L(\varepsilon) - f_R(\varepsilon)\Gamma_R(\varepsilon)] \right\} \right) \]

\[ = -\frac{e}{2\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( \frac{\Gamma(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + [\Gamma(\varepsilon)/2]^2} \left\{ [\Gamma_L(\varepsilon) - \Gamma_R(\varepsilon)] \right\} \right) \]

\[ \times \frac{\Gamma_L(\varepsilon)f_L(\varepsilon) + \Gamma_R(\varepsilon)f_R(\varepsilon)}{\Gamma(\varepsilon)} - [f_L(\varepsilon)\Gamma_L(\varepsilon) - f_R(\varepsilon)\Gamma_R(\varepsilon)] \right\} \right) \]

\[ = \frac{e}{\hbar} \int \frac{d\varepsilon}{2\pi} T(\varepsilon)[f_L(\varepsilon) - f_R(\varepsilon)], \]  

(4.82)

where

\[ T(\varepsilon) = \text{Tr} \left( \frac{\Gamma_L(\varepsilon)\Gamma_R(\varepsilon)}{[\varepsilon - \varepsilon_0 - \Lambda(\varepsilon)]^2 + [\Gamma(\varepsilon)/2]^2} \right). \]  

(4.83)

is the elastic transmission coefficient. The result obtained in Eq. (4.70) is the current for an interacting central region. In that case, calculation of the retarded and advanced Green’s functions requires a consideration of interactions such as electron-electron, electron-phonon etc. in addition to tunneling to the contacts. The difference between this result (Eq. (4.82)) and the result given by Eq. (4.70) can be further seen assuming that the Green’s function for the interacting central region can be solved as \( G^{r,a}(\varepsilon) = [\varepsilon - \varepsilon_0 - \lambda(\varepsilon) \pm i\gamma(\varepsilon)/2] \) where \( \lambda \) and \( \gamma/2 \) are the real and imaginary parts of the self-energy which includes interactions and
tunneling. Then the result for the interacting system Eq. (4.70) becomes

\[ J = \frac{e}{\hbar} \int \frac{d\varepsilon}{2\pi} \text{Tr} \left( [f_L(\varepsilon) - f_R(\varepsilon)] \frac{\Gamma_L(\varepsilon)\Gamma_R(\varepsilon)}{\Gamma_L(\varepsilon) + \Gamma_R(\varepsilon)} \frac{\gamma(\varepsilon)}{\varepsilon - \varepsilon_0 - \lambda(\varepsilon)^2 + [\gamma(\varepsilon)/2]^2} \right) \]  

(4.84)

This result matches with the result for the non-interacting system Eq. (4.82) if \( \lambda(\varepsilon) \to \Lambda(\varepsilon) \) and \( \gamma(\varepsilon) \to \Gamma(\varepsilon) = \Gamma_L(\varepsilon) + \Gamma_R(\varepsilon) \).

4.5 Time-dependent transport

The time-dependent current is calculated for a small interacting system connected to two non-interacting leads [149, 150]. In this case, the formalism is similar to that used for the steady-state current and the total Hamiltonian of the system is given as

\[ H(t) = \sum_{k,\alpha L,R} \varepsilon_{k\alpha}(t) c_{k\alpha}^\dagger c_{k\alpha} + \sum_{m} \varepsilon_m(t) d_m^\dagger d_m + \sum_{k,\alpha L,R}^{\nu} [V_{k,\alpha,n}(t)c_{k\alpha}^\dagger d_n + H.c.] \]  

(4.85)

Here, time-dependence due to external driving is explicitly incorporated in the energies of states in the interacting central region, in the leads, and in the coupling matrix elements [149]. The application of a time-dependent bias between the two leads causes a change in the energies of states in the leads from \( \varepsilon_{k\alpha}^0 \) to \( \varepsilon_{k\alpha}(t) = \varepsilon_{k\alpha}^0 + \Delta_{k\alpha}(\varepsilon, t) \) without changing their occupations. The coupling between the central interacting region and the leads can be modified with time-dependent gate voltages.

Following the same procedure of steady-state transport, the time-dependent current flowing from the left lead into the central interacting region is expressed as

\[ J_L(t) = \frac{2e}{\hbar} \text{Re} \left\{ \sum_{n,k,\alpha L} V_{k,\alpha,n}(t) G_{n,k\alpha}^\neq(t, t) \right\} \]  

(4.86)
where the lesser Green’s function is

\[
G^<_{n,ka}(t,t') = \sum_m \int dt_1 V^*_{ka,m}(t_1)[G^r_{nm}(t,t_1)g^<_{ka,ka}(t_1,t') + G^<_{nm}(t,t_1)g^a_{ka,ka}(t_1,t')],
\]

(4.87)

with the time-dependent Green’s functions in the leads

\[
g^<_{ka,ka}(t,t') = if(\epsilon^0_{ka})\exp \left[ -i \int_{t'}^{t} dt_1 \epsilon_{ka}(t_1) \right],
\]

\[
g^a_{ka,ka}(t,t') = i\theta(t' - t)\exp \left[ -i \int_{t'}^{t} dt_1 \epsilon_{ka}(t_1) \right],
\]

(4.88)

From Eq. (4.87) the lesser function \(G^<_{n,ka}(t,t)\) with \(t' = t\) and \(t_1 = t'\) is given as

\[
G^<_{n,ka}(t,t) = \sum_m \int dt' V^*_{ka,m}(t')\left[G^r_{nm}(t,t')g^<_{ka,ka}(t',t) + G^<_{nm}(t,t')g^a_{ka,ka}(t',t)\right].
\]

(4.89)

Hence the time-dependent Green’s functions in the leads become

\[
g^<_{ka,ka}(t',t) = if(\epsilon^0_{ka})\exp \left[ -i \int_{t}^{t'} dt_1 \epsilon_{ka}(t_1) \right],
\]

\[
g^<_{ka,ka}(t',t) = if(\epsilon^0_{ka})\exp \left[ +i \int_{t'}^{t} dt_1 \epsilon_{ka}(t_1) \right],
\]

(4.90)

and

\[
g^a_{ka,ka}(t',t) = i\theta(t - t')\exp \left[ -i \int_{t}^{t'} dt_1 \epsilon_{ka}(t_1) \right],
\]

\[
g^a_{ka,ka}(t',t) = i\theta(t - t')\exp \left[ +i \int_{t'}^{t} dt_1 \epsilon_{ka}(t_1) \right].
\]

(4.91)
Substituting Eqs. (4.90) and (4.91) in Eq. (4.89)

\[
G_{n,k\alpha}^<(t,t') = \sum_m \int dt' V^*_{k\alpha,m}(t') \left\{ G_{nm}^r(t,t')i f(\varepsilon_{k\alpha}^0) \exp \left[ i \int_{t'}^t dt_1 (\varepsilon_{k\alpha}^0 + \Delta_{\alpha}(\varepsilon,t_1)) \right] \right. \\
+ G_{nm}^<(t,t')i \theta(t - t') \exp \left[ i \int_{t'}^t dt_1 (\varepsilon_{k\alpha}^0 + \Delta_{\alpha}(\varepsilon,t_1)) \right] \} \\
= \sum_m \int dt' V^*_{k\alpha,m}(t') \left[ i \int_{t'}^t dt_1 \varepsilon \exp \left[ i \int_{t'}^t dt_1 \Delta_{\alpha}(\varepsilon,t_1) \right] \right] \left\{ G_{nm}^r(t,t')i f(\varepsilon) \\
+ i \theta(t - t')G_{nm}^<(t,t') \right\} \\
= \sum_m \int dt' V^*_{k\alpha,m}(t')e^{i\varepsilon(t-t')} \exp \left[ i \int_{t'}^t dt_1 \Delta_{\alpha}(\varepsilon,t_1) \right] \left\{ G_{nm}^r(t,t')i f(\varepsilon) \\
+ i \theta(t - t')G_{nm}^<(t,t') \right\},
\] (4.92)

where the constant part of the energy \( \varepsilon_{k\alpha}^0 \) is set equivalent to \( \varepsilon \).

Now converting the sum over momentum states \( k \) in the leads in Eq. (4.86) into an integral over energies and defining the elastic coupling between the leads and the states in the interacting region as

\[
[\Gamma_L(\varepsilon,t',t)]_{mn} = 2\pi \sum_{\alpha L} \rho_{\alpha}(\varepsilon)V_{\alpha,n}(\varepsilon,t)V^*_{\alpha,m}(\varepsilon,t') \exp \left[ i \int_{t'}^t dt_1 \Delta_{\alpha}(\varepsilon,t_1) \right],
\] (4.93)

the expression for the current using Eq. (4.92) is

\[
J_L(t) = \frac{2e}{\hbar} \int dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left( e^{i\varepsilon(t-t')}[\Gamma_L(\varepsilon,t',t)]_{mn} \left\{ i f_L(\varepsilon)G_{nm}^r(t,t') + i \theta(t-t')G_{nm}^<(t,t') \right\} \right).
\] (4.94)

Solving the first term containing \( G_{nm}^r(t,t') \) by splitting the time limit one gets

\[
J_L(t) = \frac{2e}{\hbar} \left\{ \int_{-\infty}^t dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left[ e^{i\varepsilon(t-t')}[\Gamma_L(\varepsilon,t',t)]_{mn}i f_L(\varepsilon)G_{nm}^r(t,t') \right] \right. \\
+ \int_t^\infty dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left[ e^{i\varepsilon(t-t')}[\Gamma_L(\varepsilon,t',t)]_{mn}i f_L(\varepsilon)G_{nm}^r(t,t') \right] \right\},
\]

from Eq. (4.58) \( G_{nm}^r(t,t') = -i \theta(t - t') < \{d_n(t), d^\dagger_m(t') \} >, \) where \( \theta(t - t') = 1 \) if
\[ t \geq t' \text{ otherwise it is zero. This gives rise to the current} \]

\[
J_L(t) = \frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left[ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} i f_L(\varepsilon) G_{nm}^r(t, t') \right] 
\]

\[
= -\frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{Im} \left[ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} f_L(\varepsilon) G_{nm}^r(t, t') \right].
\] (4.95)

Solving the second term containing \( G_{nm}^<(t, t') \)

\[
J_L(t) = \frac{2e}{\hbar} \left\{ \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left[ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} i \theta(t - t') G_{nm}^<(t, t') \right] 
\]

\[
+ \int_{t}^{\infty} dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left[ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} i \theta(t - t') G_{nm}^<(t, t') \right] \right\} 
\]

\[
= \frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{Re} \left[ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} i \theta(t - t') G_{nm}^<(t, t') \right] 
\]

\[
= -\frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{Im} \left[ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} G_{nm}^<(t, t') \right].
\] (4.96)

Combing Eqs. (4.95) and (4.96) the current from the left lead to the interacting region becomes

\[
J_L(t) = -\frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{Im} \left\{ e^{i(t-t')} [\Gamma_L(\varepsilon, t', t)]_{mn} G_{nm}^<(t, t') + f_L(\varepsilon) G_{nm}^r(t, t') \right\}.
\] (4.97)

In matrix form

\[
J_L(t) = -\frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{ImTr} \left\{ e^{i(t-t')} \Gamma_L(\varepsilon, t', t) \left[ G_{nm}^<(t, t') + f_L(\varepsilon) G_{nm}^r(t, t') \right] \right\}.
\] (4.98)

Similarly, the equation for the time-dependent current flowing in from the right lead is

\[
J_R(t) = -\frac{2e}{\hbar} \int_{-\infty}^{t} dt' \int \frac{d\varepsilon}{2\pi} \text{ImTr} \left\{ e^{i(t-t')} \Gamma_R(\varepsilon, t', t) \left[ G_{nm}^<(t, t') + f_R(\varepsilon) G_{nm}^r(t, t') \right] \right\}.
\] (4.99)
4.6 Summary

This chapter presented a brief discussion of the nonequilibrium Green’s function (NEGF) formalism and reviews the steady-state and time-dependent quantum transport through a mesoscopic system using this formalism. First the steady-state transport was discussed for (i) an interacting and (ii) a non-interacting central region connected to two non-interacting left and right leads. Then the time-dependent transport was discussed for an interacting system. While the steady-state formula for the current is useful for a range of mesoscopic systems, the time-dependent current formula is useful to study dynamics of these systems. The expressions for the current shown in this chapter form the basis of many calculations. A formula for the time-dependent current will be derived in the proceeding chapters for carbon nanotubes and graphene sensors.