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Non-Equilibrium Green Functions of Electrons in Single-Level Quantum Dots at Finite Temperature

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1. Introduction

In the quantum field theory with the vacuum being the ground state the Green functions are the vacuum expectation values of the chronological, retarded or advanced products of the field operators (Bjoken & Drell, 1964; Itzykson & Zuber, 1985; Peskin & Schroeder, 1995). They are the generalized functions of the real time variables t_i (and also other spatial coordinates). For the application of the Green function technique to the study of the time-independent phenomena in equilibrium many-body systems at a finite temperature, the Matsubara imaginary time Green functions were introduced and widely used (Abrikosov et al., 1975; Bruuns & Flensberg, 2004; Haken, 1976). They are the mean values over a statistical ensemble at a finite temperature of the chronological products of the imaginary time-dependent operators. Both these types of Green functions are inadequate for the application to the study of the time-dependent phenomena in the many-body systems with a finite density and at a finite temperature, in particular the non-equilibrium systems. For the application to the study of the time-dependent dynamical processes in non-equilibrium many-body systems Keldysh (Keldysh, 1965) has introduced a more general class of time-dependent Green functions at finite temperature and density. They are the mean values of the time-ordered products of quantum operators in the Heisenberg picture over statistical ensembles of many-body systems with finite densities and at finite temperatures (which may be non-vanishing). The simplest example is the two-point Green function

$$G_{ab}(t) = -i\langle T[a(t)b(0)]\rangle = -i\frac{Tr\{e^{-\beta H}T[a(t)b(0)]\}}{Tr\{e^{-\beta H}\}} \ , \tag{1.1}$$

where $a(t)$ and $b(t)$ are two quantum operators in the Heisenberg picture, H is the total Hamiltonian of the system, β and T are the Boltzmann constant and the temperature.

Having shown that the Green functions at finite density and temperature of the form (1.1) can be analytically continued with respect to the time variable t to become the functions of a complex variable z analytical in the stripe $-\beta <$ Im $z < 0$ parallel to the real axis, Keldysh (Keldysh, 1965) has proposed to consider these functions as the quantum statistical averages of the linear combinations of the products of ordered operators depending on complex variables

as complex times. For the definition of the ordering of the complex variables z, z' it was proposed to use some contour C in above-mentioned stripe with some initial point t_0 on the real axis and the final point $t_0 - i\beta$ such that all the complex numbers z, z'... belong to this contour. Then the "chronological" ordering T_C of the complex times z, z' ... is defined as the ordering along the contour C. The complex time-dependent operators $a(z)$, $b(z)$ and $\bar{a}(z), \bar{b}(z)$, for example, are defined in the analogy with the operators in the Heisenberg picture

$$
\begin{aligned}
a(z) &= e^{iHz}a(0)e^{-iHz}, \\
b(z) &= e^{iHz}b(0)e^{-iHz}, \\
\bar{a}(z) &= e^{iHz}a^+(0)e^{-iHz}, \\
\bar{b}(z) &= e^{iHz}b^+(0)e^{-iHz}.
\end{aligned}
\tag{1.2}
$$

As the generalization of formula (1.1) one defines the two-point Green function of two operators $a(z)$ and $b(z')$, for example, depending on two complex times $z, z' \in C$, as follows:

$$
G_{ab}(z - z')_C = -i\langle T_C[a(z)b(z')]\rangle = -i\frac{Tr\{e^{-\beta H}T_C[a(z)b(z')]\}}{Tr\{e^{-\beta H}\}}, \tag{1.3}
$$

T_C denoting the "chronological" ordering along the contour C. The Green functions of the form (1.3), usually called the Keldysh complex time-dependent Green functions at finite density and temperature, some time also simply called non-equilibrium Green functions, are widely used in quantum statistical physics and many-body theories (Chou et al., 1985; Kapusta, 1989; Le Bellac, 1996).

In practice we need to know the Green functions at the real values of the time variables. For the convenience we chose the contour C to consists of four parts $C = C_1 \cup C_2 \cup C_3 \cup C_\infty$, C_1 being the part of the straight line over and infinitely close to the real axis from some point $t_0 + io$ to infinity $+\infty + io$, C_2 being the part of the straight line under and infinitely close to the real axis from infinity $+\infty - io$ to the point $t_0 - io$, C_3 and C_∞ being the segments $[t_0, t_0 - i\beta]$ and $[+\infty + io, +\infty - io]$ parallel to the axis Oy (figure 1).

The contributions of the segment $[+\infty + io, +\infty - io]$ to all physical observables are negligibly small, because of its vanishing length. Therefore this segment plays no role, and the contour C can be considered to consist of only three parts C_1, C_2 and C_3. Then the function $G_{ab}(z - z')_C$ with the complex time variables z and z' on the contour C effectively becomes a set of nine functions of two variables, each of which has the values on one among three segments C_1, C_2 and C_3. When both variables z and z' belong to the line C_1, the function (1.3) is the quantum statistical average of the usual chronological product of two quantum operators $a(t)$ and $b(t')$ in the Heisenberg picture over a statistical ensemble of a many-body system at finite density and temperature, and can be denoted by $G_{ab}(t - t')_{11}$. When both variables z and z' belong to the line C_3, the function (1.3) is reduced to the Matsubara imaginary time Green function and can be denoted $G_{ab}(-i\tau + i\tau')_{33}$.

In the study of stationary physical processes one often uses the complex time Green functions of the form (1.3) in the limit $t_0 \rightarrow -\infty$. Because the interaction must satisfy the "adiabatic hypothesis" and therefore vanishes at this limit, the segment C_3 also gives no contribution to the stationary physical processes. In this case the contour C can be considered to consist of

only two segments C_1 and C_2, and the complex time Green function (1.3) effectively becomes a set of four functions of real variables $G_{ab}(t - t')_{11}$, $G_{ab}(t - t')_{12}$, $G_{ab}(t - t')_{21}$, $G_{ab}(t - t')_{22}$.
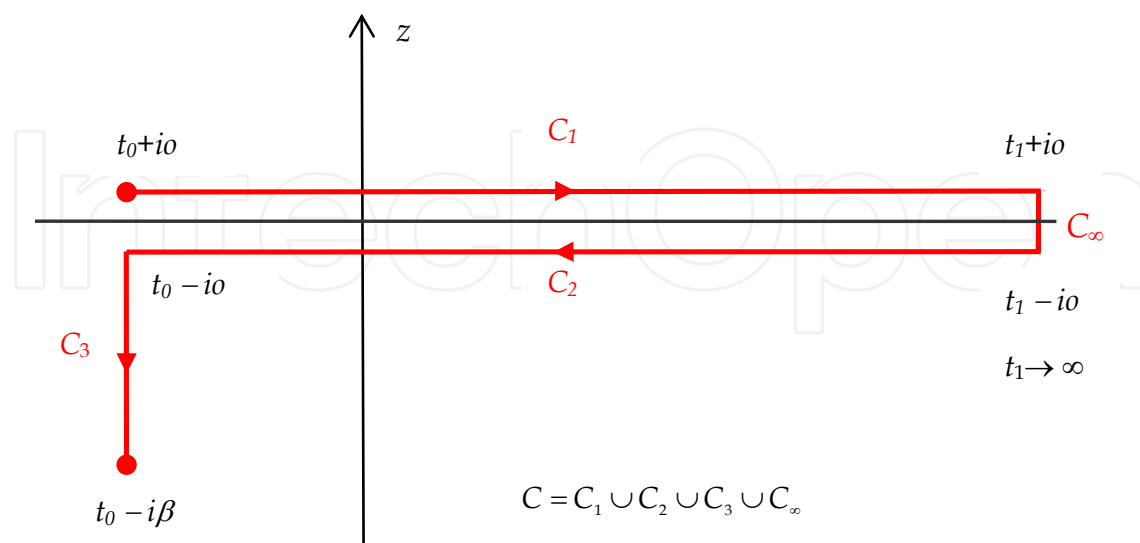

Fig. 1. Contour C consists of four parts $C = C_1 \cup C_2 \cup C_3 \cup C_\infty$.

The electrons transport through a single-level quantum dot (QD) connected with two conducting leads has been the subject for theoretical and experimental studies in many works since the early days of nanophysics (Choi et al., 2004; Costi et al., 1994; Craco & Kang, 1999; Fujii & Ueda, 2003; Hershfield et al., 1991; Inoshita et al., 1993; Izumida et al., 1997, 1998, 2001; Konig & Gefen, 2005; Meir et al., 1991, 1993; Ng, 1993; Nguyen Van Hieu & Nguyen Bich Ha, 2005, 2006; Nguyen Van Hieu et al., 2006a, 2006b; Pustilnik & Glasman, 2004; Sakai et al., 1999; Swirkowicz et al., 2003, 2006; Takagi & Saso, 1999a, 1999b; Torio et al., 2002; Wingreen & Meir, 1994; Yeyati et al., 1993). Two observable physical quantities, which can be measured in experiments on electron transport, are the electron current through the QD and the time-averaged value of the electron number in the QD. Both can be expressed in terms of the single-electron Green functions. In the pioneering theoretical works (Meir et al., 1991, 1993) on the electron transport through a single-level QD, the differential equations for the non-equilibrium Green functions were derived with the use of the Heisenberg equations of motion for the electron destruction and creation operators. Due to the presence of the strong Coulomb interaction between electrons in the QD, the differential equations for the single-electron Green functions contain multi-electron Green functions, and all the coupled equations for these Green functions form an infinite system of differential equations. In order to have a finite closed system of equations, one can assume some approximation to decouple the infinite system of equations. Moreover, since the electron transport is a non-equilibrium process, one should work with the Keldysh formalism of non-equilibrium complex time Green functions.

As the simplest explanation of the calculation methods for establishing the differential equations of non-equilibrium Green functions and deriving their exact solutions, in Section 2 we present the theory of non-equilibrium Green functions of free electron in a single-level quantum system. In Section 3 we study non-equilibrium Green functions of interacting electron in an isolated single-level QD. The elaborated calculation methods are then applied in Section 4 to the study of non-equilibrium Green functions of electrons in a single-level QD

connected with two conducting leads. Due to the electron tunneling between QD and conducting leads there does not exist a closed finite system of differential equations for some finite number of Green functions. In order to truncate the infinite system of differential equations for the infinite number of Green functions we can apply some suitable approximation. In Section 5 the mean-field approximation was used to truncate the infinite system of differential equations for the Green functions. As the result we establish a closed system of Dyson equations for a finite number of Green functions. This system of differential equations can be exactly solved. The asymptotic analytical expressions of these Green functions at the resonances, Kondo and Fano resonances, are derived in Section 6. Section 7 is the Conclusion.

2. Non-equilibrium Green function of free electrons in a single-level quantum system

For the demonstration of the calculation methods to derive the differential equations and the expressions of the non-equilibrium Green functions let us consider a simplest quantum system – that of free electrons at a single energy level E. Denote by c_σ and c_σ^+ the destruction and creation operators of the electron with the spin projection $\sigma = \uparrow, \downarrow$ in the Schrödinger picture and by H_0 the Hamiltonian of this system. We have

$$H_0 = E \sum_\sigma c_\sigma^+ c_\sigma \ . \tag{2.1}$$

The non-equilibrium Green function of electron system with Hamiltonian (2.1) is defined as follows:

$$S_{\sigma\sigma'}^E(z - z')_C = -i \langle T_C[c_\sigma(z)\overline{c}_{\sigma'}(z')] \rangle = -i \frac{Tr\{e^{-\beta H_0} T_C[c_\sigma(z)\overline{c}_{\sigma'}(z')]\}}{Tr\{e^{-\beta H_0}\}} \ , \tag{2.2}$$

where

$$\begin{aligned} c_\sigma(z) &= e^{iH_0 z} c_\sigma e^{-iH_0 z}, \\ \overline{c}_\sigma(z') &= e^{iH_0 z'} c_\sigma^+ e^{-iH_0 z'}. \end{aligned} \tag{2.3}$$

Note that at the real values t of the time variable we have $\overline{c}_\sigma(t) = c_\sigma^+(t) = c_\sigma(t)^+$. Complex time-dependent operators $c_\sigma(z)$ and $\overline{c}_\sigma(z)$ satisfy Heisenberg quantum equation of motion

$$\begin{aligned} i \frac{dc_\sigma(z)}{dz} &= -[H_0, c_\sigma(z)] \ , \\ i \frac{d\overline{c}_\sigma(z)}{dz} &= -[H_0, \overline{c}_\sigma(z)] \ . \end{aligned} \tag{2.4}$$

From the canonical anti-commutation relations

$$\begin{aligned} \{c_\sigma, c_{\sigma'}^+\} &= \delta_{\sigma\sigma'} \ , \\ \{c_\sigma, c_{\sigma'}\} &= \{c_\sigma^+, c_{\sigma'}^+\} = 0 \end{aligned} \tag{2.5}$$

it follows that

$$i\frac{dc_\sigma(z)}{dz} = Ec_\sigma(z) \,,$$

$$i\frac{d\overline{c}_\sigma(z)}{dz} = -E\overline{c}_\sigma(z) \,. \tag{2.6}$$

Green function $S^E_{\sigma\sigma'}(z-z')_C$ with both variables z and z' ranging over contour C is a set of nine functions $S^E_{\sigma\sigma'}(z-z')_{ij}$ with the variable $z(z')$ ranging over the segment $C_i(C_j)$. All they have the form

$$S^E_{\sigma\sigma'}(z-z')_C = \delta_{\sigma\sigma'}S^E(z-z')_C \,,$$

$$S^E_{\sigma\sigma'}(z-z')_{ij} = \delta_{\sigma\sigma'}S^E(z-z')_{ij} \,. \tag{2.7}$$

First consider three cases when both variables z and z' belong to one and the same segment C_i, $i = 1, 2, 3$. For $z,z' \in C_1$, $z = t + io$, $z' = t' + io$, T_C is the usual chronological ordering T of the real times t and t':

$$T[c_\sigma(t)c^+_{\sigma'}(t')] = \theta(t-t')c_\sigma(t)c^+_{\sigma'}(t') - \theta(t'-t)c^+_{\sigma'}(t')c_\sigma(t).$$

Using one of equations (2.6) and one of anti-commutation relations (2.5), we derive the differential equation for $S^E_{\sigma\sigma'}(z-z')_{11} = S^E_{\sigma\sigma'}(t-t')_{11}$ and obtain

$$\left[i\frac{d}{dt} - E\right]S^E(t-t')_{11} = \delta(t-t'). \tag{2.8.1}$$

For $z,z' \in C_2$, $z = t - io$, $z' = t' - io$, T_C is the anti-chronological ordering T^{-1} reverse to the usual chronological ordering T of the real times t and t':

$$T^{-1}[c_\sigma(t)c^+_{\sigma'}(t')] = \theta(t'-t)c_\sigma(t)c^+_{\sigma'}(t') - \theta(t-t')c^+_{\sigma'}(t')c_\sigma(t).$$

In this case we have the differential equation

$$\left[i\frac{d}{dt} - E\right]S^E(t-t')_{22} = -\delta(t-t'). \tag{2.8.2}$$

For $z,z' \in C_3$, $z = t_0 - i\tau$, $z' = t_0 - i\tau'$, T_C becomes the usual chronological ordering T_τ of the real values τ and τ' in the imaginary times $i\tau$ and $i\tau'$, $0 \le \tau,\tau' \le \beta$, and we have

$$S^E_{\sigma\sigma'}(z-z')_{33} = S^E_{\sigma\sigma'}(-i\tau + i\tau')_{33} = -i\mathbb{S}^E_{\sigma\sigma'}(\tau-\tau'), \tag{2.9}$$

where $\mathbb{S}^E_{\sigma\sigma'}(\tau-\tau')$ is the Matsubara imaginary time-dependent two-point Green function in statistical physics

$$\mathbb{S}^E_{\sigma\sigma'}(\tau-\tau') = \delta_{\sigma\sigma'}\mathbb{S}^E(\tau-\tau') = \left\langle T_\tau[\gamma_\sigma(\tau)\overline{\gamma}_{\sigma'}(\tau')]\right\rangle, \tag{2.10}$$

where

$$\gamma_\sigma(\tau) = e^{H_0\tau}c_\sigma e^{-H_0\tau} \,,$$

$$\overline{\gamma}_\sigma(\tau) = e^{H_0\tau}c^+_\sigma e^{-H_0\tau} \tag{2.11}$$

and

$$T_\tau\left[\gamma_\sigma(\tau)\overline{\gamma}_{\sigma'}(\tau')\right] = \theta(\tau - \tau')\gamma_\sigma(\tau)\overline{\gamma}_{\sigma'}(\tau') - \theta(\tau' - \tau)\overline{\gamma}_{\sigma'}(\tau')\gamma_\sigma(\tau).\tag{2.12}$$

The Heisenberg quantum equation of motion for imaginary time-dependent operators (2.11) has the form

$$\frac{d\gamma_\sigma(\tau)}{d\tau} = [H_0, \gamma_\sigma(\tau)],$$

$$\frac{d\overline{\gamma}_\sigma(\tau)}{d\tau} = [H_0, \overline{\gamma}_\sigma(\tau)].\tag{2.13}$$

From the anti-commutation relations (2.5) it follows that

$$\frac{d\gamma_\sigma(\tau)}{d\tau} = -E\gamma_\sigma(\tau),$$

$$\frac{d\overline{\gamma}_\sigma(\tau)}{d\tau} = E\overline{\gamma}_\sigma(\tau),\tag{2.14}$$

and therefore

$$\left[\frac{d}{d\tau} + E\right]\mathbb{S}^E(\tau - \tau') = \delta(\tau - \tau').\tag{2.15}$$

In the analogy with relations (2.9) we set

$$S^E(-i\tau + i\tau')_{33} = -i\mathbb{S}^E(\tau - \tau')\tag{2.16}$$

and rewrite equation (2.15) in the form similar to equations (2.8.1) and (2.8.2):

$$\left[i\frac{d}{d(-i\tau)} - E\right]S^E(-i\tau + i\tau')_{33} = i\delta(\tau - \tau').\tag{2.17}$$

Now consider six other cases when two variables z and z' belong to different segments C_i and C_j with $i \neq j$. For $z = t + io \in C_1$ and $z' = t' - io \in C_2$ the values of z always precede those of z' with respect to the ordering along the contour C and therefore

$$T_C[c_\sigma(t + io)\overline{c}_{\sigma'}(t' - io)] = -\overline{c}_{\sigma'}(t' - io)c_\sigma(t + io).$$

Similarly, for $z = t + io \in C_1$ or $z = t - io \in C_2$ and $z' = t_0 - i\tau \in C_3$ we have

$$T_C[c_\sigma(t \pm io)\overline{c}_{\sigma'}(t_0 - i\tau)] = -\overline{c}_{\sigma'}(t_0 - i\tau)c_\sigma(t \pm io).$$

On the contrary, for $z = t - io \in C_2$ and $z' = t' + io \in C_1$ the values of z' always precede those of z with respect to the ordering along the contour C and therefore

$$T_C[c_\sigma(t - io)\overline{c}_{\sigma'}(t' + io)] = c_\sigma(t - io)\overline{c}_{\sigma'}(t' + io).$$

Similarly, for $z = t_0 - i\tau \in C_3$ and $z' = t' + io \in C_1$ or $z' = t' - io \in C_2$ we have

$$T_C[c_\sigma(t_0 - i\tau)\overline{c}_{\sigma'}(t' \pm io)] = c_\sigma(t_0 - i\tau)\overline{c}_{\sigma'}(t' \pm io).$$

In all six later cases the differential equations for corresponding functions $S^E(z - z')_{ij}$, $i \neq j$, are six homogeneous ones:

$$
\begin{aligned}
\left[i\frac{d}{dt} - E\right]S^E(t - t')_{12} &= \left[i\frac{d}{dt} - E\right]S^E(t - t')_{21} \\
&= \left[i\frac{d}{dt} - E\right]S^E(t - t_0 + i\tau)_{13} = \left[i\frac{d}{dt} - E\right]S^E(t - t_0 + i\tau)_{23} \\
&= \left[i\frac{d}{d(-i\tau)} - E\right]S^E(t_0 - i\tau - t)_{31} = \left[i\frac{d}{d(-i\tau)} - E\right]S^E(t_0 - i\tau - t)_{32} = 0.
\end{aligned}
\tag{2.18}
$$

By introducing a new notation

$$
\delta(z - z')_C = \begin{cases}
\delta(t - t') & \text{for } z, z' \in C_1, \\
-\delta(t - t') & \text{for } z, z' \in C_2, \\
i\delta(\tau - \tau') & \text{for } z, z' \in C_3, \\
0 & \text{for } z \in C_i, z' \in C_j, i \neq j
\end{cases}
\tag{2.19}
$$

we rewrite equations (2.8.1), (2.8.2), (2.17) and (2.18) in the unified form

$$\left[i\frac{d}{dz} - E\right]S^E(z - z')_C = \delta(z - z')_C.\tag{2.20}$$

From above presented reasonnings and relations determining nine functions $S^E(z - z')_{ij}$, and formula (2.1) for total Hamiltonian, it is straightforward to derive explicit expressions of these functions. They depend on the average electron number with a definite spin projection

$$n = \langle n_\sigma \rangle = \langle c_\sigma^+ c_\sigma \rangle = \frac{e^{-\beta H_0}}{1 + e^{-\beta H_0}}.\tag{2.21}$$

We obtain following results:

$$S^E(z - z')_{11} = -i[\theta(t - t') - n]e^{-iE(t-t')},\tag{2.22.1}$$

$$S^E(z - z')_{22} = -i[\theta(t' - t) - n]e^{-iE(t-t')},\tag{2.22.2}$$

$$S^E(z - z')_{33} = -i[\theta(\tau - \tau') - n]e^{-E(\tau-\tau')},\tag{2.22.3}$$

$$S^E(z - z')_{12} = ine^{-iE(t-t')},\tag{2.22.4}$$

$$S^E(z - z')_{21} = -i(1 - n)e^{-iE(t-t')},\tag{2.22.5}$$

$$S^E(z - z')_{13} = S^E(z - z')_{23} = ine^{E\tau}e^{-iE(t-t_0)},\tag{2.22.6}$$

$$S^E(z - z')_{31} = S^E(z - z')_{32} = -i(1 - n)e^{-E\tau}e^{-iE(t_0-t)}.\tag{2.22.7}$$

They satisfy above presented differential equations (2.8.1), (2.8.2), (2.17) and (2.18), respectively.

For concluding this Section we consider the Fourier transformation of the functions $S^E(z-z')_{ij}$:

$$S^E(z-z')_{ij} = \frac{1}{2\pi}\int d\omega \, e^{-i\omega(t-t')}\tilde{S}^E(\omega)_{ij}, \qquad i,j=1,2, \tag{2.23.1}$$

$$S^E(z-z')_{i3} = \frac{1}{2\pi}\int d\omega \, e^{-i\omega(t-t_0+i\tau)}\tilde{S}^E(\omega)_{i3}, \qquad i=1,2, \tag{2.23.2}$$

$$S^E(z-z')_{3i} = \frac{1}{2\pi}\int d\omega \, e^{-i\omega(t_0-t-i\tau)}\tilde{S}^E(\omega)_{3i}, \qquad i=1,2, \tag{2.23.3}$$

$$S^E(z-z')_{33} = -i\frac{1}{\beta}\sum_\nu e^{i\varepsilon_\nu(\tau-\tau')}\tilde{S}^E_\nu, \tag{2.23.4}$$

$$\varepsilon_\nu = (2\nu+1)\frac{\pi}{\beta}, \qquad \nu=0,\pm1,\pm2,\dots$$

From the expressions (2.22.1)-(2.22.7) of the functions $S^E(z-z')_{ij}$ it follows that

$$\begin{aligned}\tilde{S}^E(\omega)_{11} &= \frac{1}{\omega-E+io}+i2\pi n\delta(\omega-E)\\ &= P\frac{1}{\omega-E}-i\pi\frac{1-e^{-\beta E}}{1+e^{-\beta E}}\delta(\omega-E),\end{aligned} \tag{2.24.1}$$

$$\begin{aligned}\tilde{S}^E(\omega)_{22} &= -\frac{1}{\omega-E-io}+i2\pi n\delta(\omega-E)\\ &= -P\frac{1}{\omega-E}-i\pi\frac{1-e^{-\beta E}}{1+e^{-\beta E}}\delta(\omega-E),\end{aligned} \tag{2.24.2}$$

where P means the principal value,

$$\tilde{S}^E(\omega)_{12} = i2\pi n\delta(\omega-E), \tag{2.24.3}$$

$$\tilde{S}^E(\omega)_{21} = -i2\pi(1-n)\delta(\omega-E), \tag{2.24.4}$$

$$\tilde{S}^E(\omega)_{i3} = i2\pi n\delta(\omega-E), \qquad i=1,2, \tag{2.24.5}$$

$$\tilde{S}^E(\omega)_{3i} = -i2\pi(1-n)\delta(\omega-E), \qquad i=1,2, \tag{2.24.6}$$

$$\tilde{S}^E_\nu = \frac{1}{i\varepsilon_\nu+E}. \tag{2.24.7}$$

The explicit expressions of Green functions of free electrons presented in this Section are often used in the theoretical studies of non-equilibrium processes by means of the perturbation theory.

3. Non-equilibrium Green functions of electrons in isolated single-level quantum dot

The calculation methods and reasonnings presented in the preceding Section are now applied to the study of the Keldysh non-equilibrium Green functions of interacting electrons in the simplest nanosystem – the isolated single-level quantum dot (QD) with total Hamiltonian

$$H = E\sum_{\sigma} c_{\sigma}^{+}c_{\sigma} + UN_{\uparrow}N_{\downarrow} , \qquad (3.1)$$

where U is the value of a potential energy, $\sigma = \uparrow, \downarrow$ denotes the spin projection (if $\sigma = \uparrow$ then $-\sigma = \downarrow$ and vice versa) and

$$N_{\sigma} = c_{\sigma}^{+}c_{\sigma} \qquad (3.2)$$

is the number of electrons with the spin projection σ. The second term in Hamiltonian (3.1) is the potential energy of the Coulomb electron-electron interaction (two electrons with different spin projections in one and the same energy level). The interacting nanosystem with total Hamiltonian (3.1) is an exactly solvable model. There are four exactly determined eigenstates and eigenvalues of H: the vacuum with vanishing energy, two degenerate single-electron states with two different spin projections and the same energy E, and a two-electron state with total energy $2E+U$. The Keldysh complex time-dependent two-point Green function of two operators $c(z)$ and $\overline{c}(z')$ is defined as follows

$$G_{\sigma\sigma'}(z-z')_{C} = -i\left\langle T_{C}[c_{\sigma}(z)\overline{c}_{\sigma'}(z')]\right\rangle = -i\frac{Tr\{e^{-\beta H}T_{C}[c_{\sigma}(z)\overline{c}_{\sigma'}(z')]\}}{Tr\{e^{-\beta H}\}} \qquad (3.3)$$

with total Hamiltonian (3.1). They have the form

$$G_{\sigma\sigma'}(z-z')_{C} = \delta_{\sigma\sigma'}G(z-z')_{C}. \qquad (3.4)$$

As in the preceding Section, we choose the contour C to consist of three segments C_1, C_2 and C_3. Then $G(z-z')_{C}$ becomes the set of nine functions $G(z-z')_{ij}$, $i,j = 1,2,3$. The calculations of these functions are straightforward, as they have been done in the preceding Section for free electrons at a single energy level. We obtain following results:

$$G(z-z')_{11} = \frac{i}{Z}\Big\{-\theta(t-t')[e^{-iE(t-t')} + e^{-\beta E}e^{-i(E+U)(t-t')}]$$
$$+\theta(t'-t)[e^{-\beta E}e^{-iE(t-t')} + e^{-\beta(2E+U)}e^{-i(E+U)(t-t')}]\Big\} , \qquad (3.5.1)$$

$$G(z-z')_{22} = \frac{i}{Z}\Big\{-\theta(t'-t)[e^{-iE(t-t')} + e^{-\beta E}e^{-i(E+U)(t-t')}]$$
$$+\theta(t-t')[e^{-\beta E}e^{-iE(t-t')} + e^{-\beta(2E+U)}e^{-i(E+U)(t-t')}]\Big\} , \qquad (3.5.2)$$

$$G(z - z')_{33} = i\mathbb{G}(\tau - \tau'),$$

$$\mathbb{G}(\tau) = \frac{1}{Z}\left\{[\theta(\tau)e^{-\tau E} - \theta(-\tau)e^{-(\tau+\beta)E}]\right.$$
$$\left. + e^{-\beta E}[\theta(\tau)e^{-\tau(E+U)} - \theta(-\tau)e^{-(\tau+\beta)(E+U)}]\right\},$$ (3.5.3)

$$G(z - z')_{12} = \frac{i}{Z}\left\{e^{-\beta E}e^{-iE(t-t')} + e^{-\beta(2E+U)}e^{-i(E+U)(t-t')}\right\},$$ (3.5.4)

$$G(z - z')_{21} = \frac{i}{Z}\left\{-e^{-iE(t-t')} - e^{-\beta E}e^{-i(E+U)(t-t')}\right\},$$ (3.5.5)

$$G(z - z')_{13} = G(z - z')_{23}$$
$$= \frac{i}{Z}\left\{e^{-\beta E}e^{\tau E}e^{-iE(t-t_0)} + e^{-\beta(2E+U)}e^{\tau(E+U)}e^{-i(E+U)(t-t_0)}\right\},$$ (3.5.6)

and

$$G(z - z')_{31} = G(z - z')_{32}$$
$$= \frac{i}{Z}\left\{-e^{-\tau E}e^{-iE(t_0-t')} + e^{-\beta E}e^{-\tau(E+U)}e^{-i(E+U)(t_0-t')}\right\}.$$ (3.5.7)

In the study of non-equilibrium dynamical processes by means of the perturbation theory one often needs to use the Fourier transformation of four functions $G(z - z')_{ij}$ with i, j =1,2:

$$G(z - z')_{ij} = G(t - t')_{ij} = \frac{1}{2\pi}\int d\omega e^{-i\omega(t-t')}\tilde{G}(\omega)_{ij}.$$ (3.6)

We have following exact expressions of their Fourier transforms:

$$\tilde{G}(\omega)_{11} = \frac{1}{Z}\left\{\frac{1}{\omega - E + io} + \frac{e^{-\beta E}}{\omega - E - io} + \frac{e^{-\beta E}}{\omega - E - U + io} + \frac{e^{-\beta(2E+U)}}{\omega - E - U - io}\right\}$$
$$= \frac{1}{Z}\left\{[1 + e^{-\beta E}]P\frac{1}{\omega - E} - i\pi[1 - e^{-\beta E}]\delta(\omega - E)\right.$$ (3.7.1)
$$\left. + e^{-\beta E}[1 + e^{-\beta(E+U)}]P\frac{1}{\omega - E - U} - i\pi e^{-\beta E}[1 - e^{-\beta(E+U)}]\delta(\omega - E - U)\right\},$$

$$\tilde{G}(\omega)_{22} = \frac{1}{Z}\left\{-\frac{1}{\omega - E + io} - \frac{e^{-\beta E}}{\omega - E - io} - \frac{e^{-\beta E}}{\omega - E - U - io} - \frac{e^{-\beta(2E+U)}}{\omega - E - U + io}\right\}$$
$$= -\frac{1}{Z}\left\{[1 + e^{-\beta E}]P\frac{1}{\omega - E} + i\pi[1 - e^{-\beta E}]\delta(\omega - E)\right.$$ (3.7.2)
$$\left. + e^{-\beta E}[1 + e^{-\beta(E+U)}]P\frac{1}{\omega - E - U} + i\pi e^{-\beta E}[1 - e^{-\beta(E+U)}]\delta(\omega - E - U)\right\},$$

$$\tilde{G}(\omega)_{12} = \frac{2\pi i}{Z}\left\{\delta(\omega - E) + e^{-\beta E}\delta(\omega - E - U)\right\},$$ (3.7.3)

$$\tilde{G}(\omega)_{21} = -\frac{2\pi i}{Z} \left\{ e^{-\beta E} \delta(\omega - E) + e^{-\beta(2E+U)} \delta(\omega - E - U) \right\} \tag{3.7.4}$$

with

$$Z = 1 + 2e^{-\beta E} + e^{-\beta(2E+U)}.$$

Now we derive the system of differential equations for two-point Green functions $G_{\sigma\sigma'}(t - t')_{ij}$. Consider first the function with $i = j = 1$:

$$G_{\sigma\sigma'}(t - t')_{11} = -i\left\langle T[c_\sigma(t)\overline{c}_{\sigma'}(t')]\right\rangle. \tag{3.8}$$

We have

$$i\frac{dG_{\sigma\sigma'}(t - t')_{11}}{dt} = \delta_{\sigma\sigma'}\delta(t - t') - i\left\langle T\left[i\frac{dc_\sigma(t)}{dt}\overline{c}_{\sigma'}(t')\right]\right\rangle. \tag{3.9}$$

From the Heisenberg quantum equation of motion

$$i\frac{dc_\sigma(t)}{dt} = -[H, c_\sigma(t)] \tag{3.10}$$

with total Hamiltonian (3.1) it follows that

$$i\frac{dc_\sigma(t)}{dt} = Ec_\sigma(t) + UN_{-\sigma}c_\sigma(t). \tag{3.11}$$

Substituting this expression of $i\frac{dc_\sigma(t)}{dt}$ into the r.h.s. of equation (3.9), we obtain

$$\left[i\frac{d}{dt} - E\right]G_{\sigma\sigma'}(t - t') = \delta_{\sigma\sigma'}\delta(t - t') + UH_{\sigma\sigma'}(t - t')_{11}, \tag{3.12}$$

where

$$H_{\sigma\sigma'}(t - t')_{11} = -i\left\langle T[N_{-\sigma}c_\sigma(t)\overline{c}_{\sigma'}(t')]\right\rangle = -i\theta(t - t')\left\langle [N_{-\sigma}c_\sigma(t)\overline{c}_{\sigma'}(t')]\right\rangle + i\theta(t' - t)\left\langle [\overline{c}_{\sigma'}(t')N_{-\sigma}c_\sigma(t)]\right\rangle. \tag{3.13}$$

Thus the differential equation for $G_{\sigma\sigma'}(t - t')_{11}$ contains a new Green function $H_{\sigma\sigma'}(t - t')_{11}$. In order to derive the differential equation for this new Green function it is necessary to calculate the time derivatives of both sides of equation (3.13). Note that $N_{-\sigma}$ commutes with H and therefore does not depend on t. Moreover, it has following property

$$N_{-\sigma}^2 = N_{-\sigma}.$$

Multiplying both sides of relation (3.11) with $N_{-\sigma}$ and using these two above-mentioned properties of $N_{-\sigma}$, we obtain

$$i\frac{d}{dt}[N_{-\sigma}c_\sigma(t)] = (E + U)[N_{-\sigma}c_\sigma(t)]. \tag{3.14}$$

Differentiating both sides of equation (3.13) and using relation (3.14), we derive following differential equation for the new Green function $H_{\sigma\sigma'}(t-t')_{11}$:

$$\left[i\frac{d}{dt}-(E+U)\right]H_{\sigma\sigma'}(t-t')=n\delta_{\sigma\sigma'}\delta(t-t').\tag{3.15}$$

Thus both $G_{\sigma\sigma'}(t-t')_{11}$ and $H_{\sigma\sigma'}(t-t')_{11}$ have the common form

$$\begin{aligned}G_{\sigma\sigma'}(t-t')_{11}&=\delta_{\sigma\sigma'}G(t-t')_{11},\\ H_{\sigma\sigma'}(t-t')_{11}&=\delta_{\sigma\sigma'}H(t-t')_{11},\end{aligned}\tag{3.16}$$

where $G(t-t')_{11}$ and $H(t-t')_{11}$ must satisfy differential equations

$$\left[i\frac{d}{dt}-E\right]G(t-t')_{11}=\delta(t-t')+UH(t-t')_{11},\tag{3.17}$$

$$\left[i\frac{d}{dt}-(E+U)\right]H(t-t')_{11}=n\delta(t-t').\tag{3.18}$$

In preceding Section we have shown that

$$\left[i\frac{d}{dt}-E\right]S^{E}(t-t')_{11}=\delta(t-t')$$

(equation (2.8.1)). Therefore

$$\left[i\frac{d}{dt}-(E+U)\right]S^{E+U}(t-t')_{11}=\delta(t-t').\tag{3.19}$$

Equations (3.18) and (3.19) show that $\frac{1}{n}H(t-t')_{11}$ satisfies the same inhomogeneous differential equation as $S^{E+U}(t-t')$ does. It follows that

$$H(t-t')_{11}=nS^{E+U}(t-t')_{11},\tag{3.20}$$

and the differential equation for $G(t-t')_{11}$ becomes

$$\left[i\frac{d}{dt}-E\right]G(t-t')_{11}=\delta(t-t')+nS^{E+U}(t-t')_{11}.\tag{3.21}$$

Similarly, it can be shown that the Green function

$$G_{\sigma\sigma'}(t-t')_{22}=-i\left\{\theta(t'-t)\left\langle c_{\sigma}(t)\overline{c}_{\sigma'}(t')\right\rangle-\theta(t-t')\left\langle\overline{c}_{\sigma'}(t')c_{\sigma}(t)\right\rangle\right\}\tag{3.22}$$

has the form

$$G_{\sigma\sigma'}(t-t')_{22}=\delta_{\sigma\sigma'}G(t-t')_{22},\tag{3.23}$$

and $G(t - t')_{22}$ satisfies differential equation

$$\left[i\frac{d}{dt} - E \right] G(t - t')_{22} = -\delta(t - t') + nUS^{E+U}(t - t')_{22} \tag{3.24}$$

etc. In general, Keldysh complex time Green function

$$G_{\sigma\sigma'}(z - z')_C = -i\left\langle T_C[c_\sigma(z)\overline{c}_\sigma(z')]\right\rangle \tag{3.25}$$

has the form

$$G_{\sigma\sigma'}(z - z')_C = \delta_{\sigma\sigma'}G(z - z')_C, \tag{3.26}$$

and $G(z - z')_C$ satisfies differential equation

$$\left[i\frac{d}{dt} - E \right] G(z - z')_C = \delta(z - z')_C + nUS^{E+U}(z - z')_C. \tag{3.27}$$

4. Non-equilibrium Green functions of electrons in single-level quantum dot connected with two conducting leads

Consider the single-electron transistor (SET) consisting of a single-level quantum dot (QD) connected with two conducting leads through two potential barriers. The electron transport through this SET was investigated experimentally and studied theoretically in many works (Choi et al., 2004; Costi et al., 1994; Craco & Kang, 1999; Fujii & Ueda, 2003; Hershfield et al., 1991; Inoshita et al., 1993; Izumida et al., 1997, 1998, 2001; Meir et al., 1991, 1993; Ng, 1993; Pustilnik & Glasman, 2004; Sakai et al., 1999; Swirkowicz et al., 2003, 2006; Takagi & Saso, 1999a, 1999b; Torio et al., 2002; Wingreen & Meir, 1994; Yeyati et al., 1993). It was assumed that the electron system in this SET has following total Hamiltonian

$$\begin{aligned}
H = E\sum_\sigma c_\sigma^+ c_\sigma + UN_\uparrow N_\downarrow + \sum_k \sum_\sigma \left\{ E_a(\mathbf{k})a_\sigma^+(\mathbf{k})a_\sigma(\mathbf{k}) + E_b(\mathbf{k})b_\sigma^+(\mathbf{k})b_\sigma(\mathbf{k}) \right\} \\
+ \sum_k \sum_\sigma \left\{ V_a(\mathbf{k})a_\sigma^+(\mathbf{k})c_\sigma + V_a(\mathbf{k})^* c_\sigma^+ a_\sigma(\mathbf{k}) + V_b(\mathbf{k})b_\sigma^+(\mathbf{k})c_\sigma + V_b(\mathbf{k})^* c_\sigma^+ b_\sigma(\mathbf{k}) \right\}.
\end{aligned} \tag{4.1}$$

In order to define the complex time-dependent Green functions we introduce the complex time-dependent quantum operators

$$c_\sigma(z) = e^{iHz}c_\sigma e^{-iHz}, \quad \overline{c}_\sigma(z) = e^{iHz}c_\sigma^+ e^{-iHz},$$

$$a_\sigma(\mathbf{k}, z) = e^{iHz}a_\sigma(\mathbf{k})e^{-iHz}, \quad \overline{a}_\sigma(\mathbf{k}, z) = e^{iHz}a_\sigma^+(\mathbf{k})e^{-iHz}, \tag{4.2}$$

$$b_\sigma(\mathbf{k}, z) = e^{iHz}b_\sigma(\mathbf{k})e^{-iHz}, \quad \overline{b}_\sigma(\mathbf{k}, z) = e^{iHz}b_\sigma^+(\mathbf{k})e^{-iHz}.$$

The Keldysh non-equilibrium Green functions of electrons are defined as follows:

$$G_{\sigma\sigma'}^{c\overline{c}}(z - z')_C = \delta_{\sigma\sigma'}G^{c\overline{c}}(z - z')_C = -i\left\langle T_C[c_\sigma(z)\overline{c}_\sigma(z')]\right\rangle, \tag{4.3}$$

$$H_{\sigma\sigma'}^{c\overline{c}}(z - z')_C = \delta_{\sigma\sigma'}H^{c\overline{c}}(z - z')_C = -i\left\langle T_C[N_{-\sigma}(z)c_\sigma(z)\overline{c}_\sigma(z')]\right\rangle, \tag{4.4}$$

$$G_{\sigma\sigma'}^{a\overline{c}}(\mathbf{k};z-z')_C = \delta_{\sigma\sigma'}G^{a\overline{c}}(\mathbf{k};z-z')_C = -i\left\langle T_C[a_\sigma(\mathbf{k};z)\overline{c}_{\sigma'}(z')]\right\rangle, \qquad (4.5)$$

$$H_{\sigma\sigma'}^{a\overline{c}}(\mathbf{k};z-z')_C = \delta_{\sigma\sigma'}H^{a\overline{c}}(\mathbf{k};z-z')_C = -i\left\langle T_C[N_{-\sigma}(z)a_\sigma(\mathbf{k};z)\overline{c}_{\sigma'}(z')]\right\rangle, \qquad (4.6)$$

$$\begin{aligned}
G_{\sigma\sigma'}^{ac\overline{c}\,\overline{c}}(\mathbf{k};z-z')_C &= \delta_{\sigma\sigma'}G^{ac\overline{c}\,\overline{c}}(\mathbf{k};z-z')_C \\
&= -i\left\langle T_C[a_{-\sigma}(\mathbf{k};z)c_\sigma(z)\overline{c}_{-\sigma}(z)\overline{c}_{\sigma'}(z')]\right\rangle,
\end{aligned} \qquad (4.7)$$

$$\begin{aligned}
G_{\sigma\sigma'}^{cc\overline{a}\,\overline{c}}(\mathbf{k};z-z')_C &= \delta_{\sigma\sigma'}G^{cc\overline{a}\,\overline{c}}(\mathbf{k};z-z')_C \\
&= -i\left\langle T_C[c_{-\sigma}(z)c_\sigma(z)\overline{a}_{-\sigma}(\mathbf{k};z)\overline{c}_{\sigma'}(z')]\right\rangle,
\end{aligned} \qquad (4.8)$$

$$\begin{aligned}
G_{\sigma\sigma'}^{aa\overline{c}\,\overline{c}}(\mathbf{k},\mathbf{l};z-z')_C &= \delta_{\sigma\sigma'}G^{aa\overline{c}\,\overline{c}}(\mathbf{k},\mathbf{l};z-z')_C \\
&= -i\left\langle T_C[a_{-\sigma}(\mathbf{k};z)a_\sigma(\mathbf{l};z)\overline{c}_{-\sigma}(z)\overline{c}_{\sigma'}(z')]\right\rangle,
\end{aligned} \qquad (4.9)$$

$$\begin{aligned}
G_{\sigma\sigma'}^{ac\overline{a}\,\overline{c}}(\mathbf{k},\mathbf{l};z-z')_C &= \delta_{\sigma\sigma'}G^{ac\overline{a}\,\overline{c}}(\mathbf{k},\mathbf{l};z-z')_C \\
&= -i\left\langle T_C[a_{-\sigma}(\mathbf{k};z)c_\sigma(z)\overline{a}_{-\sigma}(\mathbf{l};z)\overline{c}_{\sigma'}(z')]\right\rangle,
\end{aligned} \qquad (4.10)$$

and similarly for the others $G_{\sigma\sigma'}^{b\overline{c}}(\mathbf{k};z-z')_C$, $H_{\sigma\sigma'}^{b\overline{c}}(\mathbf{k};z-z')_C$, $G_{\sigma\sigma'}^{bc\overline{c}\,\overline{c}}(\mathbf{k};z-z')_C$, $G_{\sigma\sigma'}^{cc\overline{b}\,\overline{c}}(\mathbf{k};z-z')_C$, $G_{\sigma\sigma'}^{ab\overline{c}\,\overline{c}}(\mathbf{k},\mathbf{l};z-z')_C$, $G_{\sigma\sigma'}^{ac\overline{b}\,\overline{c}}(\mathbf{k},\mathbf{l};z-z')_C$ etc.

Because there is no magnetic interaction, all Green functions (4.3)-(4.10) and other ones are proportional to $\delta_{\sigma\sigma'}$. From Heisenberg quantum equations of motion and equal-time canonical anti-commutation relations for the electron destruction and creation operators it follows the differential equations for these operators:

$$i\frac{dc_\sigma(z)}{dz} = Ec_\sigma(z) + UN_{-\sigma}(z)c_\sigma(z) + \sum_{\mathbf{k}}\left[V_a^*(\mathbf{k})a_\sigma(\mathbf{k};z) + V_b^*(\mathbf{k})b_\sigma(\mathbf{k};z)\right], \qquad (4.11)$$

$$i\frac{d\overline{c}_\sigma(z)}{dz} = -E c_\sigma(z) - UN_{-\sigma}(z)\overline{c}_\sigma(z) - \sum_{\mathbf{k}}\left[V_a(\mathbf{k})\overline{a}_\sigma(\mathbf{k};z) + V_b(\mathbf{k})\overline{b}_\sigma(\mathbf{k};z)\right], \qquad (4.12)$$

$$i\frac{da_\sigma(\mathbf{k};z)}{dz} = E_a(\mathbf{k})a_\sigma(\mathbf{k};z) + V_a(\mathbf{k})c_\sigma(z), \qquad (4.13)$$

$$i\frac{d\overline{a}_\sigma(\mathbf{k};z)}{dz} = -E_a(\mathbf{k})\overline{a}_\sigma(\mathbf{k};z) - V_a^*(\mathbf{k})\overline{c}_\sigma(z) \qquad (4.14)$$

and similarly for $b_\sigma(\mathbf{k};z)$ and $\overline{b}_\sigma(\mathbf{k};z)$.

By using differential equation (4.11) and the equal-time canonical anti-commutation relation between $c_\sigma(z)$ and $\overline{c}_{\sigma'}(z)$, it is easy to derive the differential equation for the Green function $G_{\sigma\sigma'}^{c\overline{c}}(z-z')_C$

$$\begin{aligned}
\left[i\frac{d}{dz} - E\right]G_{\sigma\sigma'}^{c\overline{c}}(z-z')_C &= \delta_{\sigma\sigma'}\delta(z-z')_C + UH_{\sigma\sigma'}^{c\overline{c}}(z-z') \\
&+ \sum_{\mathbf{k}}\left[V_a^*(\mathbf{k})G_{\sigma\sigma'}^{a\overline{c}}(\mathbf{k};z-z')_C + V_b^*(\mathbf{k})G_{\sigma\sigma'}^{b\overline{c}}(\mathbf{k};z-z')_C\right],
\end{aligned} \qquad (4.15)$$

which contains Green functions $H_{\sigma\sigma'}^{c\bar{c}}(z-z')_C$, $G_{\sigma\sigma'}^{a\bar{c}}(\mathbf{k};z-z')_C$ and $G_{\sigma\sigma'}^{b\bar{c}}(\mathbf{k};z-z')_C$. These new functions must satisfy following differential equations which can be also derived by using differential equations (4.11)-(4.14):

$$\left[i\frac{d}{dz}-(E+U)\right]H_{\sigma\sigma'}^{c\bar{c}}(z-z')_C = n\delta_{\sigma\sigma'}\delta(z-z')_C$$
$$+\sum_{\mathbf{k}}\left[V_a^*(\mathbf{k})H_{\sigma\sigma'}^{a\bar{c}}(\mathbf{k};z-z')_C + V_b^*(\mathbf{k})H_{\sigma\sigma'}^{b\bar{c}}(\mathbf{k};z-z')_C\right. \tag{4.16}$$
$$\left.-V_a(\mathbf{k})G_{\sigma\sigma'}^{cc\bar{a}\bar{c}}(\mathbf{k};z-z')_C - V_b(\mathbf{k})G_{\sigma\sigma'}^{cc\bar{b}\bar{c}}(\mathbf{k};z-z')_C\right],$$

where

$$n = \left\langle c_\uparrow^+ c_\uparrow\right\rangle = \left\langle c_\downarrow^+ c_\downarrow\right\rangle, \tag{4.17}$$

$$\left[i\frac{d}{dz}-E_a(\mathbf{k})\right]G_{\sigma\sigma'}^{a\bar{c}}(\mathbf{k};z-z')_C = V_a(\mathbf{k})G_{\sigma\sigma'}^{c\bar{c}}(z-z')_C \tag{4.18}$$

and similarly for $G_{\sigma\sigma'}^{b\bar{c}}(\mathbf{k};z-z')_C$.

In Section 2 we have established the differential equation (2.20) for the Keldysh non-equilibrium Green function of a free electron. If the free electron has energy $E_a(\mathbf{k})$, then it is denoted by $S^{Ea(\mathbf{k})}(z-z')_C$ and must satisfy differential equation

$$\left[i\frac{d}{dz}-E_a(\mathbf{k})\right]S^{Ea(\mathbf{k})}(z-z')_C = \delta(z-z')_C. \tag{4.19}$$

Using this function, we obtain following expression of the solution of equation (4.18)

$$G_{\sigma\sigma'}^{a\bar{c}}(\mathbf{k};z-z')_C = V_a(\mathbf{k})\int dz'' S^{Ea(\mathbf{k})}(z-z'')_C G_{\sigma\sigma'}^{c\bar{c}}(z''-z')_C \tag{4.20}$$

and similarly for $G_{\sigma\sigma'}^{b\bar{c}}(\mathbf{k};z-z')_C$. Substituting the expression of the form (4.20) for $G_{\sigma\sigma'}^{a\bar{c}}(\mathbf{k};z-z')_C$ and $G_{\sigma\sigma'}^{b\bar{c}}(\mathbf{k};z-z')_C$ into the r.h.s. of differential equation (4.15) for $G_{\sigma\sigma'}^{c\bar{c}}(z-z')_C$, we rewrite this equation in a new form

$$\left[i\frac{d}{dz}-E\right]G_{\sigma\sigma'}^{c\bar{c}}(z-z')_C = \delta_{\sigma\sigma'}\delta(z-z')_C + UH_{\sigma\sigma'}^{c\bar{c}}(z-z')_C$$
$$+\int_C dz''\Sigma^{(1)}(z-z'')_C G_{\sigma\sigma'}^{c\bar{c}}(z''-z')_C, \tag{4.21}$$

where $\Sigma^{(1)}(z-z')_C$ is following self-energy part

$$\Sigma^{(1)}(z-z')_C = \sum_{\mathbf{k}}\left[\left|V_a(\mathbf{k})\right|^2 S^{Ea(\mathbf{k})}(z-z')_C + \left|V_b(\mathbf{k})\right|^2 S^{Eb(\mathbf{k})}(z-z')_C\right]. \tag{4.22}$$

The differential equation for $H_{\sigma\sigma'}^{c\bar{c}}(z-z')_C$ contains new functions $H_{\sigma\sigma'}^{a\bar{c}}(\mathbf{k};z-z')_C$, $H_{\sigma\sigma'}^{b\bar{c}}(\mathbf{k};z-z')_C$, $G_{\sigma\sigma'}^{ac\bar{c}}(\mathbf{k};z-z')_C$, $G_{\sigma\sigma'}^{bc\bar{c}}(\mathbf{k};z-z')_C$, $G_{\sigma\sigma'}^{cc\bar{a}\bar{c}}(\mathbf{k};z-z')_C$ and $G_{\sigma\sigma'}^{cc\bar{b}\bar{c}}(\mathbf{k};z-z')_C$, which must satisfy following differential equations

$$\left[i\frac{d}{dz}-E_a(\mathbf{k})\right]H^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};z-z')_C = V_a(\mathbf{k})H^{c\bar{c}}_{\sigma\sigma'}(z-z')_C \tag{4.23}$$

and similarly for $H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};z-z')_C$,

$$
\begin{aligned}
\left[i\frac{d}{dt}-E_a(\mathbf{k})\right]G^{ac\bar{c}c}_{\sigma\sigma'}(\mathbf{k};z-z')_C &= \left\langle\left\{a_{-\sigma}(\mathbf{k})c_\sigma c^+_{-\sigma},c^+_{\sigma'}\right\}\right\rangle\delta(z-z')_C \\
&+V_a(\mathbf{k})\left[H^{c\bar{c}}_{\sigma\sigma'}(z-z')_C-G^{c\bar{c}}_{\sigma\sigma'}(z-z')_C\right] \\
&+\sum_{\mathbf{l}}\left[V^*_a(\mathbf{l})G^{aa\bar{c}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z-z')_C+V^*_b(\mathbf{l})G^{ab\bar{c}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z-z')_C\right] \\
&-\sum_{\mathbf{l}}\left[V_a(\mathbf{l})G^{ac\bar{a}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z-z')_C+V_b(\mathbf{l})G^{ac\bar{b}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z-z')_C\right],
\end{aligned}
\tag{4.24}
$$

and similarly for $G^{bc\bar{c}c}_{\sigma\sigma'}(\mathbf{k};z-z')$,

$$
\begin{aligned}
\left\{i\frac{d}{dt}-\left[2E-E_a(\mathbf{k})+U\right]\right\}G^{cc\bar{a}c}_{\sigma\sigma'}(\mathbf{k};z-z')_C &= \left\langle\left\{c_{-\sigma}c_\sigma a^+_{-\sigma}(\mathbf{k}),c^+_{\sigma'}\right\}\right\rangle\delta(z-z')_C \\
&-V^*_a(\mathbf{k})\left[H^{c\bar{c}}_{\sigma\sigma'}(z-z')_C-G^{c\bar{c}}_{\sigma\sigma'}(z-z')_C\right]+ \\
&+\sum_{\mathbf{l}}\left\{V^*_a(\mathbf{l})\left[G^{ac\bar{a}c}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};z-z')_C+G^{ca\bar{a}c}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};z-z')_C\right]\right. \\
&\left.+V^*_b(\mathbf{l})\left[G^{bc\bar{a}c}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};z-z')_C+G^{cb\bar{a}c}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};z-z')_C\right]\right\}
\end{aligned}
\tag{4.25}
$$

and similarly for $G^{cc\bar{b}c}_{\sigma\sigma'}(\mathbf{k};z-z')_C$.

The presented calculations for deriving differential equations of Green function showed that there does not exist a closed system of a finite number of differential equations for a finite number of Green functions. Some approximation should be used for truncating the infinite system of all differential equations at some step. The mean-field approximation is the most appropriate one. In order to apply this approximation we rewrite equations (4.23)-(4.25) in the form of integral equations:

$$H^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};z-z')_C = V_a(\mathbf{k})\int_C dz'' S^{Ea(\mathbf{k})}(z-z'')_C H^{c\bar{c}}_{\sigma\sigma'}(z-z'')_C \tag{4.26}$$

and similarly for $H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};z-z')_C$,

$$
\begin{aligned}
G^{ac\bar{c}c}_{\sigma\sigma'}(\mathbf{k};z-z')_C &= \left\langle\left\{a_{-\sigma}(\mathbf{k})c_\sigma c^+_{-\sigma},c^+_{\sigma'}\right\}\right\rangle S^{Ea(\mathbf{k})}(z-z')_C \\
&+V_a(\mathbf{k})\int_C dz'' S^{Ea(\mathbf{k})}(z-z'')_C\left[H^{c\bar{c}}_{\sigma\sigma'}(z''-z')_C-G^{c\bar{c}}_{\sigma\sigma'}(z''-z')_C\right] \\
&+\int_C dz'' S^{Ea(\mathbf{k})}(z-z'')_C\sum_{\mathbf{l}}\left[V^*_a(\mathbf{l})G^{aa\bar{c}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z''-z')_C+V^*_b(\mathbf{l})G^{ab\bar{c}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z''-z')_C\right] \\
&-\int_C dz'' S^{Ea(\mathbf{k})}(z-z'')_C\sum_{\mathbf{l}}\left[V_a(\mathbf{l})G^{ac\bar{a}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z''-z')_C+V_b(\mathbf{l})G^{ac\bar{b}c}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};z''-z')_C\right],
\end{aligned}
\tag{4.27}
$$

and similarly for $G^{bc\bar{c}c}_{\sigma\sigma'}(\mathbf{k};z-z')_C$,

$$G_{\sigma\sigma'}^{cc\overline{ac}}\left(\mathbf{k};z-z'\right)_C = \left\langle \left\{ c_{-\sigma}c_{\sigma}a_{-\sigma}^+\left(\mathbf{k}\right),c_{\sigma'}^+ \right\} \right\rangle S^{2E+U-Ea(\mathbf{k})}\left(z-z'\right)_C$$

$$-V_a^*\left(\mathbf{k}\right)\int_C dz'' S^{2E+U-Ea(\mathbf{k})}\left(z-z'\right)_C \left[H_{\sigma\sigma'}^{c\overline{c}}\left(z''-z'\right)_C - G_{\sigma\sigma'}^{c\overline{c}}\left(z''-z'\right)_C \right]$$

$$+\int_C dz'' S^{2E+U-Ea(\mathbf{k})}\left(z''-z'\right)_C \sum_{\mathbf{l}} \left\{ V_a^*\left(\mathbf{l}\right)\left[G_{\sigma\sigma'}^{ac\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C + G_{\sigma\sigma'}^{ca\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C \right] \right.$$

$$\left. + V_b^*\left(\mathbf{l}\right)\left[G_{\sigma\sigma'}^{bc\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C + G_{\sigma\sigma'}^{cb\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C \right] \right\}, \tag{4.28}$$

and similarly for $G_{\sigma\sigma'}^{cc\overline{bc}}\left(\mathbf{k};z-z'\right)_C$. Substituting these solutions into the r.h.s. of the differential equation (4.16) for $H_{\sigma\sigma'}^{c\overline{c}}\left(z-z'\right)_C$, we rewrite this equation in the new form

$$\left[i\frac{d}{dz}-\left(E+U\right) \right]H_{\sigma\sigma'}^{c\overline{c}}\left(z-z'\right)_C = n\delta_{\sigma\sigma'}\delta\left(z-z'\right)_C + \int_C dz''\Sigma^{(1)}\left(z-z''\right)_C H_{\sigma\sigma'}^{c\overline{c}}\left(z''-z'\right)_C$$

$$+\sum_{\mathbf{k}}\left\{ V_a^*\left(\mathbf{k}\right)\left\langle \left\{ a_{-\sigma}\left(\mathbf{k}\right)c_{\sigma}c_{-\sigma}^+,c_{\sigma'}^+ \right\} \right\rangle S^{Ea(\mathbf{k})}\left(z-z'\right)_C \right.$$

$$\left. + \left|V_a\left(\mathbf{k}\right)\right|^2 \int_C dz'' S^{Ea(\mathbf{k})}\left(z-z''\right)_C \left[H_{\sigma\sigma'}^{c\overline{c}}\left(z''-z'\right)_C - G_{\sigma\sigma'}^{c\overline{c}}\left(z''-z'\right)_C \right] \right\}$$

$$+\int_C dz''\sum_{\mathbf{k}} V_a^*\left(\mathbf{k}\right)S^{Ea(\mathbf{k})}\left(z-z''\right)_C \sum_{\mathbf{l}}\left[V_a^*\left(\mathbf{l}\right)G_{\sigma\sigma'}^{aa\overline{cc}}\left(\mathbf{k},\mathbf{l};z''-z'\right)_C + V_b^*\left(\mathbf{l}\right)G_{\sigma\sigma'}^{ab\overline{cc}}\left(\mathbf{k},\mathbf{l};z''-z'\right)_C \right]$$

$$-\int_C dz''\sum_{\mathbf{k}} V_a^*\left(\mathbf{k}\right)S^{Ea(\mathbf{k})}\left(z-z''\right)_C \sum_{\mathbf{l}}\left[V_a\left(\mathbf{l}\right)G_{\sigma\sigma'}^{ac\overline{ac}}\left(\mathbf{k},\mathbf{l};z''-z'\right)_C + V_b\left(\mathbf{l}\right)G_{\sigma\sigma'}^{ac\overline{bc}}\left(\mathbf{k},\mathbf{l};z''-z'\right)_C \right] \tag{4.29}$$

$$-\sum_{\mathbf{k}}\left\{ V_a\left(\mathbf{k}\right)\left\langle \left\{ c_{-\sigma}c_{\sigma}a_{-\sigma}^+\left(\mathbf{k}\right),c_{\sigma'}^+ \right\} \right\rangle S^{2E+U-Ea(\mathbf{k})}\left(z-z''\right)_C \right.$$

$$\left. + \left|V_a\left(\mathbf{k}\right)\right|^2 \int_C dz'' S^{2E+U-Ea(\mathbf{k})}\left(z-z''\right)_C \left[H_{\sigma\sigma'}^{c\overline{c}}\left(z''-z'\right)_C - G_{\sigma\sigma'}^{c\overline{c}}\left(t''-t\right) \right] \right\}$$

$$-\int_C dz''\sum_{\mathbf{k}} V_a\left(\mathbf{k}\right)S^{2E+U-Ea(\mathbf{k})}\left(z-z''\right)_C \sum_{\mathbf{l}}\left\{ V_a^*\left(\mathbf{l}\right)\left[G_{\sigma\sigma'}^{ac\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C + G_{\sigma\sigma'}^{ca\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C \right] \right\}$$

$$-\int_C dz''\sum_{\mathbf{k}} V_a\left(\mathbf{k}\right)S^{2E+U-Ea(\mathbf{k})}\left(z-z''\right)_C \sum_{\mathbf{l}} V_b^*\left(\mathbf{l}\right)\left[G_{\sigma\sigma'}^{bc\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C + G_{\sigma\sigma'}^{cb\overline{ac}}\left(\mathbf{l},\mathbf{k};z''-z'\right)_C \right]$$

+ similar terms with suitable interchange $\left(a \leftrightarrow b\right)$.

5. Dyson equations for non-equilibrium Green functions of electrons in single-level quantum dot connected with two conducting leads and their solutions

The r.h.s. of equation (4.29) for Green function $H_{\sigma\sigma'}^{c\overline{c}}\left(z-z'\right)_C$ contains multi-electron Green functions $G_{\sigma\sigma'}^{aa\overline{cc}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$, $G_{\sigma\sigma'}^{ab\overline{cc}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$, $G_{\sigma\sigma'}^{ac\overline{ac}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$, $G_{\sigma\sigma'}^{ac\overline{bc}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$, $G_{\sigma\sigma'}^{ca\overline{ac}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$, $G_{\sigma\sigma'}^{bc\overline{ac}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$, $G_{\sigma\sigma'}^{bc\overline{ac}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$ and similar ones with suitable interchange (a ↔ b). In order to decouple this equation from those for other multi-electron Green functions we apply the mean-field approximation to the products of four operators. For example

$$\left\langle T_C\left[\overline{a}_{-\sigma}\left(\mathbf{l};z\right)a_{-\sigma}\left(\mathbf{k};z\right)c_{\sigma}\left(z\right)\overline{c}_{\sigma'}\left(z'\right) \right] \right\rangle \approx \left\langle \overline{a}_{-\sigma}\left(\mathbf{l};z\right)a_{-\sigma}\left(\mathbf{k};z\right) \right\rangle \left\langle T_C\left[c_{\sigma}\left(z\right)\overline{c}_{\sigma'}\left(z'\right) \right] \right\rangle \tag{5.1}$$

with

$$\left\langle \bar{a}_{-\sigma}\left(\mathbf{l};z\right)a_{-\sigma}\left(\mathbf{k};z\right)\right\rangle = \delta_{\mathbf{kl}}\left\langle \bar{a}_{-\sigma}\left(\mathbf{k}\right)a_{-\sigma}\left(\mathbf{k}\right)\right\rangle = \delta_{\mathbf{kl}}n_a\left(\mathbf{k}\right),\tag{5.2}$$

where $n_a\left(\mathbf{k}\right)$ is the density of electrons with momentum $\mathbf{k}$ and spin projection σ or $-\sigma$ in the lead "a" at the given temperature

$$n_a\left(\mathbf{k}\right) = \frac{e^{-\beta E_a(\mathbf{k})}}{1 + e^{-\beta E_a(\mathbf{k})}}.\tag{5.3}$$

Note that

$$\left\langle T_C\left[c_\sigma\left(z\right)\bar{c}_{\sigma'}\left(z'\right)\right]\right\rangle = iG_{\sigma\sigma'}^{c\bar{c}}\left(z-z'\right)_C.$$

As the result we have

$$G_{\sigma\sigma'}^{ac\bar{a}\bar{c}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C \approx -\delta_{\mathbf{kl}}\left[1-n_a\left(\mathbf{k}\right)\right]G_{\sigma\sigma'}^{c\bar{c}}\left(z-z'\right)_C\tag{5.4}$$

and similarly for $G_{\sigma\sigma'}^{bc\bar{b}\bar{c}}\left(\mathbf{k},\mathbf{l};z-z'\right)_C$. Applying the mean-field approximation to each of others above-mentioned multi-electron Green functions in any manner, we always obtain the vanishing mean value in the lowest order the perturbation theory with respect to the effective tunnelling coupling constants $V_{a,b}\left(\mathbf{k}\right)$. Note that these functions enter the r. h. s. of the equation (29) with the coefficients of the second order with respect to the effective tunnelling coupling constants. This means that in this second order they do not give contributions. Thus in the second order approximation the equation (4.29) is simplified and becomes

$$\begin{aligned}\left[i\frac{d}{dz}-\left(E+U\right)\right]H_{\sigma\sigma'}^{c\bar{c}}\left(z-z'\right)_C &= n\delta_{\sigma\sigma'}\delta\left(z-z'\right)_C + \Delta\left(z-z'\right)_C\\ &+ \int_C dz''\Sigma^{(2)}\left(z-z'\right)_C H_{\sigma\sigma'}^{c\bar{c}}\left(z''-z'\right)_C - \int_C dz''\Sigma^{(3)}\left(z-z''\right)_C G_{\sigma\sigma'}^{c\bar{c}}\left(z''-z'\right)_C,\end{aligned}\tag{5.5}$$

where

$$\begin{aligned}\Delta\left(z-z'\right)_C &= \sum_{\mathbf{k}}\Big[V_a^*\left(\mathbf{k}\right)\left\langle\left\{a_{-\sigma}\left(\mathbf{k}\right)c_\sigma c_{-\sigma}^+,c_{\sigma'}^+\right\}\right\rangle S^{E_a(\mathbf{k})}\left(z-z'\right)_C\\ &\quad -V_a\left(\mathbf{k}\right)\left\langle\left\{c_{-\sigma}c_\sigma a_{-\sigma}^+\left(\mathbf{k}\right),c_{\sigma'}^+\right\}\right\rangle S^{2E+U-E_a(\mathbf{k})}\left(z-z'\right)_C + \left(a\rightarrow b\right)\Big],\end{aligned}\tag{5.6}$$

$$\Sigma^{(2)}\left(z-z'\right)_C = \sum_{\mathbf{k}}\left\{\left|V_a\left(\mathbf{k}\right)\right|^2\left[2S^{E_a(\mathbf{k})}\left(z-z'\right)_C + S^{2E+U-E_a(\mathbf{k})}\left(z-z'\right)_C\right] + \left(a\rightarrow b\right)\right\},\tag{5.7}$$

$$\Sigma^{(3)}\left(z-z'\right)_C = \sum_{\mathbf{k}}\left\{n_a\left(\mathbf{k}\right)\left|V_a\left(\mathbf{k}\right)\right|^2\left[S^{E_a(\mathbf{k})}\left(z-z'\right)_C + S^{2E+U-E_a(\mathbf{k})}\left(z-z'\right)_C\right] + \left(a\rightarrow b\right)\right\}.\tag{5.8}$$

Note that in the r.h.s. of equations (5.6)-(5.8), there appear the crossing terms containing $S^{2E+U-E_a(\mathbf{k})}\left(z-z'\right)_C$. They must disappear in the non-crossing approximation. Two equations (4.21) and (5.5) form the closed system of Dyson equations for two Green functions $G_{\sigma\sigma'}^{c\bar{c}}\left(z-z'\right)_C$ and $H_{\sigma\sigma'}^{c\bar{c}}\left(z-z'\right)_C$.

To proceed further we note that

$$\left\langle \left\{ a_{-\sigma}(\mathbf{k}) c_{\sigma} c_{-\sigma}^{+}, c_{\sigma'}^{+} \right\} \right\rangle = -\delta_{\sigma\sigma'} \left\langle a_{-\sigma}(\mathbf{k}) c_{-\sigma}^{+} \right\rangle,$$
$$\left\langle \left\{ c_{-\sigma} c_{\sigma} a_{-\sigma}^{+}(\mathbf{k}), c_{\sigma'}^{+} \right\} \right\rangle = -\delta_{\sigma\sigma'} \left\langle a_{-\sigma}(\mathbf{k}) c_{-\sigma}^{+} \right\rangle^{*}, \tag{5.9}$$

where $\left\langle a_{-\sigma}(\mathbf{k}) c_{-\sigma}^{+} \right\rangle$ is a limiting value of the Green function $G_{-\sigma-\sigma}^{ac}(\mathbf{k};t)_{11}$:

$$\left\langle a_{-\sigma}(\mathbf{k}) c_{-\sigma}^{+} \right\rangle = iG_{-\sigma-\sigma}^{ac}(\mathbf{k}; +0)_{11}. \tag{5.10}$$

For evaluating the vertex (5.6) in the second order with respect to the tunnelling coupling constants $V_{a,b}(\mathbf{k})$ we calculate the limiting value (5.10) in the first order. Introduce the Fourier transformations of the Green functions, for example

$$G^{a\bar{c}}(\mathbf{k};t)_{ij} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega t} \tilde{G}^{a\bar{c}}(\mathbf{k};\omega)_{ij},$$

$$S^{Ea(\mathbf{k})}(t)_{ij} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega t} \tilde{S}^{Ea(\mathbf{k})}(\omega)_{ij}, \tag{5.11}$$

$$G^{c\bar{c}}(t)_{ij} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega t} \tilde{G}^{c\bar{c}}(\omega)_{ij} \text{ for } i, j = 1, 2.$$

From the equation (4.20) it follows that

$$\tilde{G}^{a\bar{c}}(\mathbf{k};\omega)_{11} = V_{a}(\mathbf{k}) \tilde{S}^{Ea(\mathbf{k})}(\omega)_{11} \tilde{G}^{c\bar{c}}(\omega)_{11}. \tag{5.12}$$

For deriving $\tilde{G}^{a\bar{c}}(\mathbf{k};\omega)_{11}$ in the first order with respect to the constant $V_{a}(\mathbf{k})$ it is enough to use the expression of $\tilde{G}^{c\bar{c}}(\omega)_{11}$ in the case of the vanishing tunnelling coupling constant and have

$$\tilde{G}^{a\bar{c}}(\mathbf{k};\omega)_{11} = \frac{1}{Z} V_{a}(\mathbf{k}) \left[\frac{n_{a}(\mathbf{k})}{\omega - io - E_{a}(\mathbf{k})} + \frac{1 - n_{a}(\mathbf{k})}{\omega + io - E_{a}(\mathbf{k})} \right]$$
$$\times \left[\frac{e^{-\beta E}}{\omega - io - E} + \frac{e^{-\beta(2E+U)}}{\omega - io - E - U} + \frac{1}{\omega + io - E} + \frac{e^{-\beta E}}{\omega + io - E - U} \right], \tag{5.13}$$
$$Z = 1 + 2e^{-\beta E} + e^{-\beta(2E+U)}.$$

It is easy to calculate the limit

$$G^{a\bar{c}}(\mathbf{k};+0)_{11} = \lim_{\varepsilon \to +0} \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega\, e^{-i\omega\varepsilon} \tilde{G}^{a\bar{c}}(\mathbf{k};\omega)_{11} \tag{5.14}$$

by using the residue theorem and obtain

$$\left\langle a_{-\sigma}(\mathbf{k}) c_{-\sigma}^{+} \right\rangle = -\nu_{a}(\mathbf{k}) V_{a}(\mathbf{k}), \tag{5.15}$$

where

$$\nu_a(\mathbf{k}) = \frac{1}{Z} \left\{ \frac{e^{-\beta E} - \left[1 + e^{-\beta E}\right] n_a(\mathbf{k})}{E - E_a(\mathbf{k})} + e^{-\beta E} \frac{e^{-\beta(E+U)} - \left[1 + e^{-\beta(E+U)}\right] n_a(\mathbf{k})}{E + U - E_a(\mathbf{k})} \right\}. \tag{5.16}$$

The formula (5.6) becomes

$$\Delta(z - z')_C = \sum_{\mathbf{k}} \left\{ |V_a(\mathbf{k})|^2 \nu_a(\mathbf{k}) \left[S^{Ea(\mathbf{k})}(z - z')_C - S^{2E+U-Ea(\mathbf{k})}(z - z')_C \right] + (a \to b) \right\}. \tag{5.17}$$

The system of Dyson equations (4.21) and (5.5) is the mathematical tool for the study of the electron transport through a single-level QD. Since this is a stationary process one can apply the Keldysh non-equilibrium Green function formalism in the limit $t_0 \to -\infty$. Because the interaction vanishes at this limit, the contour C can be considered to consist of only two segment $C_1 = [-\infty + io, +\infty + io]$ and $C_2 = [\infty - io, -\infty + io]$. In this case each complex time-dependent Green function $S^E(z - z')_C$, $G^{c\bar{c}}(z - z')_C$, $H^{c\bar{c}}(z - z')_C$, $\Sigma^{(\alpha)}(z - z')_C$, $\alpha = 1,2,3$ or $\Delta(z - z')_C$ becomes a set of four real time-dependent functions $S^E(t - t')_{ij}$, $G^{c\bar{c}}(t - t')_{ij}$, $H^{c\bar{c}}(t - t')_{ij}$, $\Sigma^{(\alpha)}(t - t')_{ij}$, $\alpha = 1,2,3$ or $\Delta(t - t')_{ij}$ with their Fourier transforms $\tilde{S}^E(\omega)_{ij}$, $\tilde{G}^{c\bar{c}}(\omega)_{ij}$, $\tilde{H}^{c\bar{c}}(\omega)_{ij}$, $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}$, $\alpha = 1,2,3$ or $\tilde{\Delta}(\omega)_{ij}$ with $i, j = 1,2$. Considering them as the elements of corresponding 2×2 matrices $\hat{S}^E(\omega)$, $\hat{G}^{c\bar{c}}(\omega)$, $\hat{H}^{c\bar{c}}(\omega)$, $\hat{\Sigma}^{(\alpha)}(\omega)$, $\alpha = 1,2,3$ or $\hat{\Delta}(\omega)$, and setting

$$\hat{\eta} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.18}$$

we rewrite the system of Dyson equations (4.21) and (5.5) in the matrix form

$$\hat{G}(\omega) = \hat{S}^E(\omega) + U\hat{S}^E(\omega)\hat{\eta}\hat{H}(\omega) + \hat{S}^E(\omega)\hat{\eta}\hat{\Sigma}^{(1)}(\omega)\hat{\eta}\hat{G}(\omega), \tag{5.19}$$

$$\hat{H}(\omega) = n\hat{S}^{E+U}(\omega) + \hat{S}^{E+U}(\omega)\hat{\eta}\hat{\Delta}(\omega) + \hat{S}^{E+U}(\omega)\hat{\eta}\hat{\Sigma}^{(2)}(\omega)\hat{\eta}\hat{H}(\omega) \\ - \hat{S}^{E+U}(\omega)\hat{\eta}\hat{\Sigma}^{(3)}(\omega)\hat{\eta}\hat{G}(\omega). \tag{5.20}$$

From these matrix equations we derive two systems of algebraic equations, each of which consists of four equations for four functions $\tilde{G}(\omega)_{i1}$ and $\tilde{H}(\omega)_{i1}$ or $\tilde{G}(\omega)_{i2}$ and $\tilde{H}(\omega)_{i2}$, $i = 1,2$. The observable physical quantities are expressed in terms of these functions.

For the application let us calculate the Green function $\tilde{G}(\omega)_{11}$. By solving the system of equation (5.19) and (5.20) we obtain following result:

$$\tilde{G}(\omega)_{11} = \frac{Z(\omega)}{Y(\omega)}, \tag{5.21}$$

$$Z(\omega) = \left\{ B(\omega)[1 + \Omega_{22}^{(1)}(\omega)] - UD_{22}(\omega) \right\} \left\{ B(\omega)\tilde{S}^E(\omega)_{11} + UC_1(\omega) \right\} \\ - \left\{ B(\omega)\Omega_{12}^{(1)}(\omega) - UD_{12}(\omega) \right\} \left\{ B(\omega)\tilde{S}^E(\omega)_{21} + UC_2(\omega) \right\}, \tag{5.22}$$

$$Y(\omega) = \left\{ B(\omega)[1 - \Omega_{11}^{(1)}(\omega)] + UD_{11}(\omega) \right\} \left\{ B(\omega)[1 + \Omega_{22}^{(1)}(\omega)] - UD_{22}(\omega) \right\} \\ + \left\{ B(\omega)\Omega_{12}^{(1)}(\omega) - UD_{12}(\omega) \right\} \left\{ B(\omega)\Omega_{21}^{(1)}(\omega) - UD_{21}(\omega) \right\}, \tag{5.23}$$

$$B(\omega) = [1 + \Omega_{22}^{(2)}(\omega)][1 - \Omega_{11}^{(2)}(\omega)] + \Omega_{12}^{(2)}(\omega)\Omega_{21}^{(2)}(\omega), \tag{5.24}$$

$$C_i(\omega) = \left\{ \tilde{S}^E(\omega)_{i1}[1 + \Omega_{22}^{(2)}(\omega)] - \tilde{S}^E(\omega)_{i2}\Omega_{21}^{(2)}(\omega) \right\} \lambda_{11}(\omega)$$
$$- \left\{ \tilde{S}^E(\omega)_{i1}\Omega_{12}^{(2)}(\omega) + \tilde{S}^E(\omega)_{i2}[1 - \Omega_{11}^{(2)}(\omega)] \right\} \lambda_{21}(\omega), \tag{5.25}$$

$$i = 1, 2$$

$$D_{ij}(\omega) = \left\{ \tilde{S}^E(\omega)_{i1}[1 + \Omega_{22}^{(2)}(\omega)] - \tilde{S}^E(\omega)_{i2}\Omega_{21}^{(2)}(\omega) \right\} \Omega_{1j}^{(3)}(\omega) -$$
$$- \left\{ \tilde{S}^E(\omega)_{i1}\Omega_{12}^{(2)}(\omega) + \tilde{S}^E(\omega)_{i2}[1 - \Omega_{11}^{(2)}(\omega)] \right\} \Omega_{2j}^{(3)}(\omega), \tag{5.26}$$

$$\Omega_{ij}^{(1)}(\omega) = \tilde{S}^E(\omega)_{i1}\tilde{\Sigma}^{(1)}(\omega)_{1j} - \tilde{S}^E(\omega)_{i2}\tilde{\Sigma}^{(1)}(\omega)_{2j} ,$$
$$\Omega_{ij}^{(2)}(\omega) = \tilde{S}^{E+U}(\omega)_{i1}\tilde{\Sigma}^{(2)}(\omega)_{1j} - \tilde{S}^{E+U}(\omega)_{i2}\tilde{\Sigma}^{(2)}(\omega)_{2j} , \tag{5.27}$$
$$\Omega_{ij}^{(3)}(\omega) = \tilde{S}^{E+U}(\omega)_{i1}\tilde{\Sigma}^{(3)}(\omega)_{1j} - \tilde{S}^{E+U}(\omega)_{i2}\tilde{\Sigma}^{(3)}(\omega)_{2j} ,$$

$$\lambda_{ij}(\omega) = n\tilde{S}^{E+U}(\omega)_{ij} + \tilde{S}^{E+U}(\omega)_{i1}\tilde{\Delta}(\omega)_{1j} - \tilde{S}^{E+U}(\omega)_{i2}\tilde{\Delta}(\omega)_{2j} , \tag{5.28}$$

$$i = 1, 2, \quad j = 1, 2.$$

The expressions (5.21)-(5.28) of $\tilde{G}(\omega)_{11}$ and similar ones for the Fourier transforms of other Green functions contain the self-energies $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}, \alpha = 1, 2, 3$. Because the tunnelling coupling constants $V_a(\mathbf{k})$ and $V_b(\mathbf{k})$ have small values, the contributions of these self-energies, in general, give small corrections to the Green functions. However, the self-energies may be divergent at some special values of ω. At some points near these special values the denominator $Y(\omega)$ may vanish and the Green functions have the resonances. The formulae (5.23)-(5.28) would be used for the rigorous study of the behaviour of $\tilde{G}(\omega)_{11}$ at the resonances. This will be done in the subsequent Section.

6. Kondo and Fano resonances in electron transport through single-level quantum dot

In this Section we study the appearance of the resonances in the expressions of the Fourier transforms of the Green functions when the denominator $Y(\omega)$ is vanishing. The expression of $Y(\omega)$ consists of the terms of two types: the finite terms which do not depend on the Fourier transforms $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}$ of the self-energies and those proportional to $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}, \alpha = 1, 2, 3$. The functions $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}$ contain the small tunnelling coupling constants $V_a(\mathbf{k})$ and $V_b(\mathbf{k})$. They are determined by following formulae:

$$\tilde{\Sigma}^{(1)}(\omega)_{ij} = \sum_{\mathbf{k}} \left\{ \left| V_a(\mathbf{k}) \right|^2 \tilde{S}^{Ea(\mathbf{k})}(\omega)_{ij} + (a \to b) \right\} , \tag{6.1}$$

$$\tilde{\Sigma}^{(2)}(\omega)_{ij} = \sum_{\mathbf{k}} \left\{ \left| V_a(\mathbf{k}) \right|^2 [2\tilde{S}^{Ea(\mathbf{k})}(\omega)_{ij} + \tilde{S}^{2E+U-Ea(\mathbf{k})}(\omega)_{ij}] + (a \to b) \right\} , \tag{6.2}$$

$$\tilde{\Sigma}^{(3)}(\omega) = \sum_{\mathbf{k}} \left\{ n_a(\mathbf{k}) \left| V_a(\mathbf{k}) \right|^2 [\tilde{S}^{Ea(\mathbf{k})}(\omega)_{ij} + \tilde{S}^{2E+U-Ea(\mathbf{k})}(\omega)_{ij}] + (a \to b) \right\} , \tag{6.3}$$

Introducing the spectral functions

$$\Gamma_{a,b}^{(\alpha)}(\omega) = \pi \sum_{\mathbf{k}} \left[\frac{e^{-\beta E_{a,b(\mathbf{k})}}}{1 + e^{-\beta E_{a,b(\mathbf{k})}}} \right]^{\alpha} \left| V_{a,b}(\mathbf{k}) \right|^2 \delta[\omega - E_{a,b}(\mathbf{k})] , \tag{6.4}$$

$$a = 0, 1, 2,$$

we rewrite them in the new form convenient for the study of their divergence:

$$\tilde{\Sigma}^{(1)}(\omega)_{11} = \frac{1}{\pi} P \int d\omega' \frac{1}{\omega - \omega'} \left[\Gamma_a^{(0)}(\omega') + \Gamma_b^{(0)}(\omega') \right]$$
$$-i \left[\Gamma_a^{(0)}(\omega) + \Gamma_b^{(0)}(\omega) - 2\Gamma_a^{(1)}(\omega) - 2\Gamma_b^{(1)}(\omega) \right] , \tag{6.5}$$

$$\tilde{\Sigma}^{(1)}(\omega)_{12} = 2i \left[\Gamma_a^{(1)}(\omega) + \Gamma_b^{(1)}(\omega) \right] ,$$

$$\tilde{\Sigma}^{(1)}(\omega)_{21} = -2i \left[\Gamma_a^{(0)}(\omega) + \Gamma_b^{(0)}(\omega) - \Gamma_a^{(1)}(\omega) - \Gamma_b^{(1)}(\omega) \right] ,$$

$$\tilde{\Sigma}^{(1)}(\omega)_{22} = -\frac{1}{\pi} P \int d\omega' \frac{1}{\omega - \omega'} \left[\Gamma_a^{(0)}(\omega') + \Gamma_b^{(0)}(\omega') \right]$$
$$-i \left[\Gamma_a^{(0)}(\omega) + \Gamma_b^{(0)}(\omega) - 2\Gamma_a^{(1)}(\omega) - 2\Gamma_b^{(1)}(\omega) \right] .$$

$$\tilde{\Sigma}^{(2)}(\omega)_{11} = \frac{1}{\pi} P \int d\omega' \left[\frac{2}{\omega - \omega'} + \frac{1}{\omega - 2E - U + \omega'} \right] \left[\Gamma_a^{(0)}(\omega') + \Gamma_b^{(0)}(\omega') \right] -$$
$$- 2i \left[\Gamma_a^{(0)}(\omega) + \Gamma_b^{(0)}(\omega) - 2\Gamma_a^{(1)}(\omega) - 2\Gamma_b^{(1)}(\omega) \right] - \tag{6.6}$$
$$- i \left[\Gamma_a^{(0)}(2E + U - \omega) + \Gamma_b^{(0)}(2E + U - \omega) \right.$$
$$\left. -2\Gamma_a^{(1)}(2E + U - \omega) - 2\Gamma_b^{(1)}(2E + U - \omega) \right] ,$$

$$\tilde{\Sigma}^{(2)}(\omega)_{12} = 4i \left[\Gamma_a^{(1)}(\omega) + \Gamma_b^{(1)}(\omega) \right] + 2i \left[\Gamma_a^{(1)}(2E + U - \omega) + \Gamma_b^{(1)}(2E + U - \omega) \right] ,$$

$$\tilde{\Sigma}^{(2)}(\omega)_{21} = -4i \left[\Gamma_a^{(0)}(\omega) + \Gamma_b^{(0)}(\omega) - \Gamma_a^{(1)}(\omega) - \Gamma_b^{(1)}(\omega) \right] -$$
$$-2i \left[\Gamma_a^{(0)}(2E + U - \omega) + \Gamma_b^{(0)}(2E + U - \omega) \right.$$
$$\left. -\Gamma_a^{(1)}(2E + U - \omega) - \Gamma_b^{(1)}(2E + U - \omega) \right] ,$$

$$\tilde{\Sigma}^{(2)}(\omega)_{22} = -\frac{1}{\pi} P \int d\omega' \left[\frac{2}{\omega - \omega'} + \frac{1}{\omega - 2E - U + \omega'} \right] \left[\Gamma_a^{(0)}(\omega') + \Gamma_b^{(0)}(\omega') \right] -$$
$$-2i \left[\Gamma_a^{(0)}(\omega) + \Gamma_b^{(0)}(\omega) - 2\Gamma_a^{(1)}(\omega) - 2\Gamma_b^{(1)}(\omega) \right] -$$
$$- i \left[\Gamma_a^{(0)}(2E + U - \omega) + \Gamma_b^{(0)}(2E + U - \omega) \right.$$
$$\left. -2\Gamma_a^{(1)}(2E + U - \omega) - 2\Gamma_b^{(1)}(2E + U - \omega) \right] .$$

$$\tilde{\Sigma}^{(3)}(\omega)_{11} = \frac{1}{\pi} P \int d\omega' \left[\frac{1}{\omega - \omega'} + \frac{1}{\omega - 2E - U + \omega'} \right] \left[\Gamma_a^{(1)}(\omega') + \Gamma_b^{(1)}(\omega') \right] -$$
$$- i \left[\Gamma_a^{(1)}(\omega) + \Gamma_b^{(1)}(\omega) - 2\Gamma_a^{(2)}(\omega) - 2\Gamma_b^{(2)}(\omega) + \Gamma_a^{(1)}(2E + U - \omega) \right.$$
$$\left. + \Gamma_b^{(1)}(2E + U - \omega) - 2\Gamma_a^{(2)}(2E + U - \omega) - 2\Gamma_b^{(2)}(2E + U - \omega) \right], \quad (6.7)$$

$$\tilde{\Sigma}^{(3)}(\omega)_{12} = 2i \left[\Gamma_a^{(2)}(\omega) + \Gamma_b^{(2)}(\omega) \right] + 2i \left[\Gamma_a^{(2)}(2E + U - \omega) + \Gamma_b^{(2)}(2E + U - \omega) \right],$$

$$\tilde{\Sigma}^{(3)}(\omega)_{21} = -2i \left[\Gamma_a^{(1)}(\omega) + \Gamma_b^{(1)}(\omega) - \Gamma_a^{(2)}(\omega) - \Gamma_b^{(2)}(\omega) + \Gamma_a^{(1)}(2E + U - \omega) \right.$$
$$\left. + \Gamma_b^{(1)}(2E + U - \omega) - \Gamma_a^{(2)}(2E + U - \omega) - \Gamma_b^{(2)}(2E + U - \omega) \right],$$

$$\tilde{\Sigma}^{(3)}(\omega)_{22} = -\frac{1}{\pi} P \int d\omega' \left[\frac{1}{\omega - \omega'} + \frac{1}{\omega - 2E - U + \omega'} \right] \left[\Gamma_a^{(1)}(\omega') + \Gamma_b^{(1)}(\omega') \right] -$$
$$- i \left[\Gamma_a^{(1)}(\omega) + \Gamma_b^{(1)}(\omega) - 2\Gamma_a^{(2)}(\omega) - 2\Gamma_b^{(2)}(\omega) + \Gamma_a^{(1)}(2E + U - \omega) \right.$$
$$\left. + \Gamma_b^{(1)}(2E + U - \omega) - 2\Gamma_a^{(2)}(2E + U - \omega) - 2\Gamma_b^{(2)}(2E + U - \omega) \right].$$

The integrals in the r.h.s. of formulae (6.5)–(6.7) may be divergent at definite values of the frequency ω which will be called the divergence points. Although the functions $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}$, i, $j = 1, 2$, contain the small tunnelling coupling constants $V_a(\mathbf{k})$ and $V_b(\mathbf{k})$, near each divergence point some of them may become comparable with the finite terms in $Y(\omega)$. When $Y(\omega)$ vanishes due to the cancellation between the finite terms and those containing divergent integrals, there appear the resonances. Therefore in order to study the resonances it is necessary to investigate the divergence of the integrals in the r.h.s. of the formulae (6.5)–(6.7).

The functions $\tilde{\Sigma}^{(\alpha)}(\omega)_{11}$ and $\tilde{\Sigma}^{(\alpha)}(\omega)_{22}$ contain the dispersion integrals with the spectral functions $\Gamma_{a,b}^{(\alpha)}(\omega)$. Denote μ_a and μ_b the chemical potentials of the systems of conducting electrons in the leads "a" and "b". From the definition (6.4) with

$$E_{a,b}(\mathbf{k}) = E_{a,b}^{(0)}(\mathbf{k}) - \mu_{a,b} ,$$

where $E_{a,b}^{(0)}(\mathbf{k})$ are the kinetic energies of the conducting electrons in the leads, $E_{a,b}^{(0)}(\mathbf{k}) \geq 0$, it follows that $\Gamma_a^{(\alpha)}(\omega)$ vanishes at $\omega < -\mu_a$ and similarly for $\Gamma_b^{(n)}(\omega)$. Therefore the dispersion integrals in formulae (6.5)-(6.7) have the form

$$K_{a,b}^{(n)} = P \int_{-\mu_{a,b}}^{\Omega_{a,b}} d\omega' \frac{\Gamma_{a,b}^{(n)}(\omega')}{\omega' - \omega} \quad (6.8)$$

and

$$L_{a,b}^{(n)} = P \int_{-\mu_{a,b}}^{\Omega_{a,b}} d\omega' \frac{\Gamma_{a,b}^{(n)}(\omega')}{\omega' - 2E - U + \omega} \quad , \quad (6.9)$$

where Ω_a is the top of the energy band of the conducting electrons in the leads "*a*" and similarly for Ω_b. For the study of the divergence of the integrals we replace approximately the values of $\Gamma_a^{(\alpha)}(\omega)$ in the interval $-\mu < \omega < \Omega_a$ by a constant Γ_a and similarly for $\Gamma_b^{(n)}(\omega)$. Then at zero temperature

$$
\begin{aligned}
K_{a,b}^{(0)} &= \Gamma_{a,b} I_{a,b} \; , \\
K_{a,b}^{(1)} &= K_{a,b}^{(2)} = \Gamma_{a,b} I_{a,b}' \; , \\
L_{a,b}^{(0)} &= \Gamma_{a,b} J_{a,b} \; , \\
L_{a,b}^{(1)} &= L_{a,b}^{(2)} = \Gamma_{a,b} J_{a,b}' \; ,
\end{aligned}
\tag{6.10}
$$

with

$$
I_{a,b} = P \int_{-\mu_{a,b}}^{\Omega_{a,b}} d\omega' \frac{1}{\omega - \omega'} \; ,
\tag{6.11}
$$

$$
I_{a,b}' = P \int_{-\mu_{a,b}}^{0} d\omega' \frac{1}{\omega - \omega'} \; ,
\tag{6.12}
$$

$$
J_{a,b} = P \int_{-\mu_{a,b}}^{\Omega_{a,b}} d\omega' \frac{1}{\omega - 2E - U + \omega'} \; ,
\tag{6.13}
$$

$$
J_{a,b}' = P \int_{-\mu_{a,b}}^{0} d\omega' \frac{1}{\omega - 2E - U + \omega'} \; .
\tag{6.14}
$$

Usually $\Omega_a(\Omega_b)$ is very large in comparison with $\mu_a(\mu_b)$ and ω. Therefore we have

$$
I_{a,b} \approx \ln \left| \frac{\omega + \mu_{a,b}}{\Omega_{a,b} - \mu_{a,b}} \right| \; ,
\tag{6.15}
$$

$$
I_{a,b}' \approx \ln \left| \frac{\omega + \mu_{a,b}}{\omega} \right| \; ,
\tag{6.16}
$$

$$
J_{a,b} \approx \ln \left| \frac{\Omega_{a,b} - \mu_{a,b}}{\omega - 2E - U - \mu_{a,b}} \right| \; ,
\tag{6.17}
$$

$$
J_{a,b}' \approx \ln \left| \frac{\omega - 2E - U}{\omega - 2E - U - \mu_{a,b}} \right| \; .
\tag{6.18}
$$

It is obvious that I_a is divergent at $\omega \to -\mu_a$, I_a' is divergent at $\omega \to -\mu_a$ and $\omega \to 0$, J_a is divergent at $\omega \to 2E + U + \mu_a$ and J_a' is divergent at $\omega \to 2E + U + \mu_a$ and $\omega \to 2E + U$. For I_b, I_b', J_b and J_b' we have similar results.

If the temperature T of the system is low enough, but does not vanish,

$$\mu_{a,b} \gg kT > 0,$$

then instead of the divergence of $I'_{a,b}$ at the Fermi surface $\omega \to 0$ we have the limit

$$\lim_{\omega \to 0} I'_{a,b} = \ln \frac{2e\mu_{a,b}}{kT}, \tag{6.19}$$

and, similarly, instead of the divergence of $J'_{a,b}$ at $\omega \to 2E+U$ we have the limit

$$\lim_{\omega \to 2E+U} J'_{a,b} = -\ln \frac{2e\mu_{a,b}}{kT}. \tag{6.20}$$

For the simplicity we set $\mu_a = \mu_a = \mu$.

From the results of the study of resonances of Green function $\tilde{G}^{c\bar{c}}(\omega)_{11}$ and the explicit expressions (5.21)-(5.28) determining this function we obtain its asymptotic behavious at the divergence points of $\tilde{\Sigma}^{(\alpha)}(\omega)_{ij}$:

a. As $\omega \to -\mu$ and at low temperature $T \approx 0$, the Green function in equation (5.21) has asymptotic form:

$$\begin{aligned}
\tilde{G}^{c\bar{c}}(\omega)_{11} \approx &-\frac{\left[1-n+\frac{1}{2}(E+\mu)\frac{\lambda}{\Gamma}\right]U}{E+2U+\mu} \frac{1}{\frac{1}{2}(E+\mu)+\frac{2\Gamma}{\pi}\ln\left|\frac{\omega+\mu}{\Omega}\right|+2i\Gamma} \\
&-\frac{E+\mu+\left[1+n-(E+U+\mu)\frac{\lambda}{\Gamma}\right]U}{E+2U+\mu} \frac{1}{(E+U+\mu)+\frac{2\Gamma}{\pi}\ln\left|\frac{\omega+\mu}{\Omega}\right|+2i\Gamma}.
\end{aligned} \tag{6.21}$$

If $E+\mu > 0$, then $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has two resonances at two points

$$\omega_1^{(\pm)} = -\mu \pm \Omega e^{-\frac{\pi}{4\Gamma}(E+\mu)} \tag{6.22}$$

and two resonances at two points

$$\omega_2^{(\pm)} = -\mu \pm \Omega e^{-\frac{\pi}{2\Gamma}(E+U+\mu)}. \tag{6.23}$$

Between these four resonances there are the dips. If $E+\mu < 0$ but $E+U+\mu > 0$, then $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has only two resonances at the points $\omega_2^{(\pm)}$. If $E+U+\mu < 0$, then in the neighbourhood of the point $\omega = -\mu$, the Green function $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has no resonance. All four points $\omega_1^{(\pm)}$ and $\omega_2^{(\pm)}$ are very close to the point $\omega = -\mu$ and the resonances at $\omega_1^{(\pm)}$ and $\omega_2^{(\pm)}$ look like a resonance at $\omega = -\mu$. The origin of these resonances is the presence of the Fano quasi-bound state at the lower edge of the energy band of the conducting electrons. If they exist, they would be called the Fano resonances.

b.   As $\omega \to 0$ and at $T = 0$, the Green functions $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has asymptotic form

$$\tilde{G}^{c\bar{c}}(\omega)_{11} \approx -\frac{E + (1-n)U}{E(E+U) + \dfrac{2\Gamma U}{\pi}\ln\left|\dfrac{\mu}{\omega}\right| + 2i(3E+2U)\Gamma}. \tag{6.24}$$

If $E(E+U) < 0$, then $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has two resonances at the points

$$\omega_3^{(\pm)} = \pm\mu\exp\left\{-\frac{\pi}{2\Gamma}\frac{|E(E+U)|}{U}\right\}, \tag{6.25}$$

which are very close to the point $\omega = 0$. At $\omega = 0$ and $0 < T < T_K$,

$$T_K = \frac{1}{k}\mu\exp\left\{-\frac{\pi}{2}\frac{|E(E+U)|}{\Gamma U}\right\}, \tag{6.26}$$

where k is the Boltzmann constant, instead of formula (6.24) we have

$$\tilde{G}^{c\bar{c}}(0)_{11} \approx \frac{\pi}{2}\frac{E+(1-n)U}{\Gamma U}\frac{1}{\ln|T/T_K| - i\pi(3E+2U)\Gamma}. \tag{6.27}$$

The resonances in the neighbourhood of the point $\omega = 0$ have the same physical origin as the Kondo effect due to the scattering of electrons by a magnetic impurity. They are the Kondo resonances.

c.   As $\omega \to 2E+U$ and at $T = 0$, the Green function $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has asymptotic form:

$$\tilde{G}^{c\bar{c}}(\omega)_{11} \approx \frac{E+nU}{E(E+U) - \dfrac{2\Gamma U}{\pi}\ln\left|\dfrac{\mu}{\omega - 2E - U}\right| - 2iE\Gamma}. \tag{6.28}$$

Therefore if $E(E+U) > 0$, then $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has also two resonances at the points

$$\omega_4^{(\pm)} = 2E+U \pm \mu e^{\frac{\pi}{2\Gamma}\frac{E(E+U)}{U}} \tag{6.29}$$

which are very close to the point $\omega = 2E+U$. At $\omega = 2E+U$ and $0 < T < T_K'$,

$$T_K' = \frac{1}{k}\mu\exp\left\{-\frac{\pi}{2}\frac{E(E+U)}{\Gamma U}\right\}, \tag{6.30}$$

instead of formula (6.28) we have

$$\tilde{G}^{c\bar{c}}(2E+U)_{11} \approx \frac{\pi}{2}\frac{E+nU}{\Gamma U}\frac{1}{\ln|T/T_K'| - i\pi E\Gamma}. \tag{6.31}$$

The resonances in the neighbourhood of the point $\omega = 2E+U$ are the Kondo resonances of the crossing terms.

d.   As $\omega \to 2E + U + \mu$ and at low temperature $T \approx 0$, the Green functions $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has asymptotic form:

$$\tilde{G}^{c\bar{c}}(\omega)_{11} \approx \frac{1 - n + (E + U + \mu)\dfrac{\lambda}{\Gamma}}{(E + U + \mu) + \dfrac{2\Gamma}{\pi}\ln\left|\dfrac{\omega - 2E - U - \mu}{\Omega}\right| - 2i\Gamma}\frac{U}{E + \mu} \, . \tag{6.32}$$

If $E + U + \mu > 0$, then $\tilde{G}^{c\bar{c}}(\omega)_{11}$ has two resonances at the points

$$\omega_5^{(\pm)} = 2E + U + \mu \pm \Omega e^{-\frac{\pi}{2}\frac{E+U+\mu}{\Gamma}} \, , \tag{6.33}$$

which are very close to the point $\omega = 2E + U + \mu$. They are the Fano resonances of the crossing terms.

7. Conclusion

The present Chapter is an introductory review of the Keldysh non-equilibrium Green functions of electrons in simplest nanosystems: isolated single-level QD and single-level QD connected with two conducting leads. In the case of an isolated single-level QD the closed system of a finite number of differential equations for a finite number of Green functions was established by using the Heisenberg quantum equations of motion for the electron destruction and creation operators. The exact expressions of the Green functions were derived. In the case of the nanosystem consisting of a single-level QD connected with two conducting leads there does not exist a finite closed system of differential equations for some finite number of Green functions. In the differential equations for n-point Green functions there appear the contributions from (n+2)-point Green functions. Therefore, the exact system of differential equations contains an infinite number of equations for an infinite number of Green functions. In order to truncate this infinite system of differential equations we have applied the mean-field approximation to the products of four electron quantum operators and limited at the terms of the second order with respect to the effective tunnelling coupling constants. As the result we have derived a closed system of Dyson equations for two types of 2-point Green functions. All the crossing terms are included into the equations. The exact solution of the system of Dyson equations may have the resonances of four types in the dependence on the physical parameters of the system: the Kondo resonances at the Fermi surface, whose origin is similar to that of the Kondo effect in the scattering of electrons on magnetic impurities, the Fano resonances due to the presence of the electron quasi-bound state at the lower edge of the energy band of the conducting electrons, the Kondo resonances in the crossing terms and the Fano resonances in the crossing terms. The analytical asymptotic expressions of the single-electron Green function at these resonances were derived. These results agree well with the numerical calculations in references on the electron Green functions in QD (Yeyati et al., 1993; Costi et al., 1994; Izumida et al., 1997, 1998, 2001; Sakai et al., 1999; Torio et al., 2002).

The theoretical study of the non-equilibrium Green functions of electrons in QDs would signify the beginning of the development of the quantum dynamics of physical processes in QD-based nanodevices. The next step would be the elaboration of the theory of non-

equilibrium Green functions of phonons in QDs as well as of electrons and phonons of interacting electron-phonon systems in QDs. The quantum dynamical theory of QD-based optoelectronic and photonic nanodevices necessitates also the study of non-equilibrium Green functions of electrons and phonons confined in QDs in the presence of the electron-phonon interactions as well as the interaction of photons with confined electron-phonon systems. The methods and reasonnings presented in this Chapter could be generalized for the application to the study of all above-mentioned non-equilibrium Green functions.

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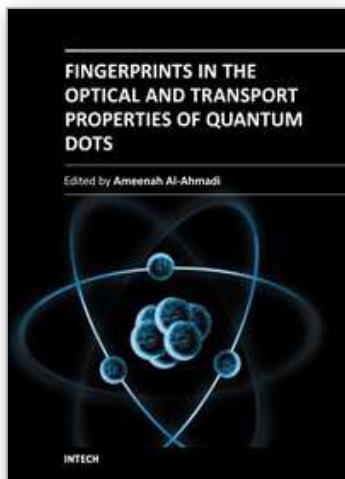
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Edited by Dr. Ameenah Al-Ahmadi

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