QUANTUM THEORY OF ELECTRON TRANSPORT THRU
SINGLE-LEVEL QUANTUM DOT

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Abstract. A new approach in the quantum theory of few-electron nanoelectronic devices – the S-matrix approach – is presented in a simple example: a single-electron transistor consisting of a single-level quantum dot connected with two metallic leads through the corresponding potential barriers. The electron transport through the quantum dot due to the electron tunneling between the dot and the leads is studied. The strong Coulomb repulsion between the electrons in the dot is taken into account exactly, while the tunneling between the dot and the leads, considered as a small perturbation, is studied by means of the perturbation theory. For summing up the infinite perturbation theory series we apply the Green function technique and the Heisenberg equation of motion of the electron annihilation and creation operators. The matrix elements of the transition processes include both the direct and crossing terms, so that there is no need to use the non-crossing approximation (NCA). The explicit expression of the electron transport current is derived.

I. INTRODUCTION

The transport of electrons through the single-electron transistor (SET) consisting of a quantum dot and two (metallic or ferromagnetic) leads under some bias voltage between two leads was studied in many theoretical and experimental works. Following Meir, Wingreen and Lee [1] for the study of the electron transport many authors [2-11] used the Landauer formula [12] expressing the conductance in terms of the Green function of the electron in the dot, while Izumida et al. [13-15] applied the Kubo linear response theory [16] to express the electrical current (or the conductivity tensor) in terms of the Green functions. The calculation of the Green functions has been done by means of different approximate methods: the truncation of the system of equations for many-point Green functions derived from the Heisenberg equation of motion [1,3], the perturbation theory with respect to the strong Coulomb repulsion potential [2,8,9], the non-crossing approximation (NCA) [7], the numerical renormalization group method [10,13,15] and the Quantum Monte Carlo technique [14].

In a recent work [17] for the study of the electron transport through a single-level quantum dot one of the authors has proposed another method based on the use of the S-matrix in the perturbation theory with respect to the Hamiltonian of the tunneling between the dot and the leads considered as the interaction Hamiltonian $H_{int}$, the strong Coulomb repulsion potential between two electrons in the dot being included into the part $H_0$ with exactly determined eigenvalues and eigenvectors of the total Hamiltonian

$$H = H_0 + H_{int}. \quad (1)$$
As in earlier works [1 - 11, 13 - 15] we consider the single-electron transistor consisting of a single-level quantum dot connected with two metallic leads “a” and “b” through two potential barriers. The dot and the leads are assumed to be kept in the quasi-equilibrium states at a fixed temperature and with given chemical potentials being under control. We use the unit system with $\hbar = c = 1$.

Denote $c_\sigma$ and $c_\sigma^+$ the annihilation and creation operators of the electron with the spin projection $\sigma = \uparrow, \downarrow$ at the single energy level $E$ in the quantum dot, $a_\sigma(k)$, $b_\sigma(k)$ and $a_\sigma^+(k)$, $b_\sigma^+(k)$ those of electrons with the spin projection $\sigma$ and the momentum $k$ in the leads “a” and “b”, resp. Following earlier works [1 - 11, 13 - 15] we assume that

$$H_0 = E \sum_\sigma c_\sigma^+ c_\sigma + U n_\uparrow n_\downarrow + \sum_k \sum_\sigma \{ E_a(k) a_\sigma^+(k) a_\sigma(k) + E_b(k) b_\sigma^+(k) b_\sigma(k) \}, \quad (2)$$

$$n_\sigma = c_\sigma^+ c_\sigma, \quad (3)$$

$$H_{\text{int}} = \sum_k \sum_\sigma \{ V_a(k) a_\sigma^+(k) c_\sigma + V_a(k) c_\sigma^+ a_\sigma(k) + V_b(k) b_\sigma^+(k) c_\sigma + V_b(k) c_\sigma^+ b_\sigma(k) \}. \quad (4)$$

In the previous report [17] the electron current from one lead to another one in the presence of some bias voltage between two leads was calculated in the second order of the perturbation theory with respect to the interaction Hamiltonian (4). In this work the sums of the series of high order terms of the perturbation theory in the ladder approximation are calculated by means of the Green function technique with the use of the Heisenberg equation of motion for the electron annihilation and creation operators. As we shall see, the matrix elements of the S-matrix contain both the “direct” and “crossing” terms, so that in the framework of the present S-matrix approach there is no need to assume the non-crossing approximation. The “crossing” terms describe the co-tunneling processes. In many cases their contributions are significant.

**II. PERTURBATION THEORY IN THE SECOND ORDER**

In order to apply the perturbation theory we introduce the electron annihilation and creation operators as well as the interaction Hamiltonian in the interaction representation

$$c_\sigma^+(t) = e^{iH_0 t} c_\sigma^+ e^{-iH_0 t}, \quad c_\sigma(t) = e^{iH_0 t} c_\sigma e^{-iH_0 t},$$

$$a_\sigma^+(k, t) = e^{iH_0 t} a_\sigma^+(k) e^{-iH_0 t}, \quad a_\sigma(k, t) = e^{iH_0 t} a_\sigma(k) e^{-iH_0 t},$$

$$b_\sigma^+(k, t) = e^{iH_0 t} b_\sigma^+(k) e^{-iH_0 t}, \quad b_\sigma(k, t) = e^{iH_0 t} b_\sigma(k) e^{-iH_0 t}, \quad \quad (5)$$

$$H_{\text{int}}(t) = e^{iH_0 t} H_{\text{int}} e^{-iH_0 t}. $$
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The S-matrix in the perturbation theory with respect to the interaction Hamiltonian (4) equals

\[ S = T \left\{ \exp \left( -i \int_{-\infty}^{\infty} H_{\text{int}}(t) \, dt \right) \right\} = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} T \{ H_{\text{int}}(t_1) \cdots H_{\text{int}}(t_n) \}. \] (6)

We set

\[ S = 1 - iR, \] (7)

and write

\[ R = \sum_{n=1}^{\infty} R^{(n)}, \] (8)

where \( R^{(n)} \) denotes the contribution of all \( n \)-th order terms. In the first order of the perturbation theory we have

\[ R^{(1)} = \sum_{\sigma} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} dt \left\{ V_\sigma(\mathbf{k}) a_\sigma^+(\mathbf{k}, t) c_\sigma(t) + V_\sigma(\mathbf{k})^* c_\sigma^+(t) a_\sigma(\mathbf{k}, t) + V_\sigma(\mathbf{k}) b_\sigma^+(\mathbf{k}, t) c_\sigma(t) + V_\sigma(\mathbf{k})^* c_\sigma^+(t) b_\sigma(\mathbf{k}, t) \right\}, \] (9)

while in the second order

\[ R^{(2)} = \frac{i}{2} \sum_{\sigma_1} \sum_{\sigma_2} \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 T \left\{ \left[ V_\sigma(\mathbf{k}_1) a_{\sigma_1}^+(\mathbf{k}_1, t_1) c_{\sigma_1}(t_1) + V_\sigma(\mathbf{k}_1) a_{\sigma_1}^+(t_1) c_{\sigma_1}(t_1) + \right. \right. \] \[ \left. \left. + V_\sigma(\mathbf{k}_1) b_{\sigma_1}^+(\mathbf{k}_1, t_1) c_{\sigma_1}(t_1) + V_\sigma(\mathbf{k}_1) b_{\sigma_1}^+(t_1) c_{\sigma_1}(t_1) \right] \right. \] \[ \left. \left. \left. \left. a_{\sigma_1}(\mathbf{k}_1, t_1) + V_\sigma(\mathbf{k}_2) a_{\sigma_2}^+(\mathbf{k}_2, t_2) c_{\sigma_2}(t_2) + V_\sigma(\mathbf{k}_2) a_{\sigma_2}^+(t_2) c_{\sigma_2}(t_2) + V_\sigma(\mathbf{k}_2) b_{\sigma_2}^+(\mathbf{k}_2, t_2) c_{\sigma_2}(t_2) + V_\sigma(\mathbf{k}_2) b_{\sigma_2}^+(t_2) c_{\sigma_2}(t_2) \right) \right) \right) \right) \right) \right) \] (10)

If the initial and final states \(|i\rangle \) and \(|f\rangle \) in some matrix element \( \langle f \mid R \mid i \rangle \) of the scattering operator \( R \) contain one and the same subsystem of \( n \) particles \( a_\sigma(\mathbf{k}) \) and \( m \) particles \( b_\sigma(\mathbf{k}) \), \((n, m=0,1,2,\ldots)\) which do not participate in the interaction process, then this matrix element can be written in the form

\[ \langle f \mid R \mid i \rangle = \sum_{P} (-1)^P \langle a_{\sigma_1'}(\mathbf{k}_1') \mid a_{\sigma_1}(\mathbf{k}_1) \rangle \cdots \langle a_{\sigma_n'}(\mathbf{k}_n') \mid a_{\sigma_n}(\mathbf{k}_n) \rangle \times \] \[ \times \langle b_{\sigma_{n+1}'}(\mathbf{k}_{n+1}') \mid b_{\sigma_{n+1}}(\mathbf{k}_{n+1}) \rangle \cdots \langle b_{\sigma_{n+m}'}(\mathbf{k}_{n+m}') \mid b_{\sigma_{n+m}}(\mathbf{k}_{n+m}) \rangle \langle \tilde{f} \mid R \mid \tilde{i} \rangle, \] (11)

where \( \{ \tilde{i} \} \) and \( \{ \tilde{f} \} \) are the subsystems complementary to those of the non-interacting particles \( a_{\sigma_1}(\mathbf{k}_1), \ldots a_{\sigma_n}(\mathbf{k}_n), b_{\sigma_{n+1}}(\mathbf{k}_{n+1}), \ldots b_{\sigma_{n+m}}(\mathbf{k}_{n+m}) \) in the initial and final states, resp., \( P \) denotes the antisymmetrization with respect to the identical particles of each kind \( a_\sigma(\mathbf{k}) \) and \( b_\sigma(\mathbf{k}) \). The matrix elements in this factorized and antisymmetrized form
are called reducible ones contrary to the irreducible matrix elements which cannot be expressed in the above-mentioned form \((11)\). In the study of the observable physical quantities of the system it is necessary and sufficient to derive the explicit expressions of the irreducible matrix elements of the scattering operator \(R\).

Consider now in detail the transport of the electron through the quantum dot – the transition of the electron from one lead into another one \((a_\sigma(k) \rightarrow b_\sigma(k'), \text{for example})\) via the intermediate states of the electron in the quantum dot (virtual particles \(c_\sigma\)) by means of the tunneling of the electrons between the leads and the dot. In the second order of the perturbation theory we have following irreducible matrix elements:

\[
\langle b_\sigma'(k') \mid R^{(2)} \mid a_\sigma(k) \rangle = -i V_a(k)^* V_b(k') \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 e^{i[E_b(k') t_1 - E_a(k) t_2]} \langle 0 \mid T\{c_{\sigma'}(t_1) c_{\sigma}^+(t_2)\} \mid 0 \rangle, \tag{12}
\]

\[
\langle c_{\sigma'} b_{\sigma'}(k') \mid R^{(2)} \mid a_{\sigma_1}(k) c_{\sigma_2} \rangle = -i V_a(k)^* V_b(k') \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 e^{i[E_b(k') t_1 - E_a(k) t_2]} \langle c_{\sigma_2} \mid T\{c_{\sigma_1'}(t_1) c_{\sigma_1}^+(t_2)\} \mid c_{\sigma_2} \rangle, \tag{13}
\]

\[
\langle c_{\sigma_1} c_{\sigma} b_{\sigma'}(k') \mid R^{(2)} \mid a_\sigma(k) c_{\sigma_1'} \rangle = -i V_a(k)^* V_b(k') \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 e^{i[E_b(k') t_1 - E_a(k) t_2]} \langle c_{\sigma_1} \mid T\{c_{\sigma'}(t_1) c_{\sigma}^+(t_2)\} \mid c_{\sigma_1'} \rangle. \tag{14}
\]

The problem is now reduced to the calculation of the matrix elements of the chronological product of two operators \(c_{\sigma'}(t')\) and \(c_{\sigma}^+(t)\) between different electronic states of the quantum dot: the empty state \(\ket{0}\), the singly occupied states \(\ket{c_\sigma}\) and the doubly occupied one \(\ket{c_{\sigma} c_{\sigma}}\).

The matrix element

\[
G^{(0)}_{\sigma'\sigma}(t' - t) = -i \langle 0 \mid T\{c_{\sigma'}(t') c_{\sigma}^+(t)\} \mid 0 \rangle \tag{15}
\]

is the usual Green function of the electron in the quantum dot, while two other matrix elements

\[
G^{(2)}_{\sigma_1\sigma_1'\sigma_2\sigma_{2'}}(t' - t) = -i \langle c_{\sigma_2'} \mid T\{c_{\sigma_1'}(t') c_{\sigma_1}^+(t)\} \mid c_{\sigma_2} \rangle \tag{16}
\]

and

\[
G^{(2)}_{\sigma\sigma'}(t' - t) = -i \langle c_{\sigma} c_{\sigma}^+ \mid T\{c_{\sigma'}(t') c_{\sigma}^+(t)\} \mid c_{\sigma} c_{\sigma} \rangle \tag{17}
\]

are only similar to the usual Green function and might be called the generalized Green functions. They can be exactly calculated without any approximation with respect to the large Coulomb repulsion potential \(U\).

The chronological product of two operators \(c_{\sigma'}(t')\) and \(c_{\sigma}^+(t)\) has the explicit form

\[
T\{c_{\sigma'}(t') c_{\sigma}^+(t)\} = \theta(t' - t) c_{\sigma'}(t') c_{\sigma}^+(t) - \theta(t - t') c_{\sigma}^+(t) c_{\sigma'}(t'). \tag{18}
\]
The first term in the r. h. s. of the relation (18) describes the creation of an electron in the quantum dot at the moment \( t \) (due to the tunneling of this electron from the lead “a”) and then the subsequent annihilation of this electron (\( \sigma = \sigma' \)) or another electron (\( \sigma \neq \sigma' \)) in the quantum dot at a later moment \( t' > t \) (due to its tunneling to the lead “b”), while the second term describes the annihilation of an electron in the quantum dot at the moment \( t' \) (due to its tunneling to the lead “b”) and the subsequent creation of another electron in the quantum dot at a later moment \( t' > t \) (due to the tunneling of this electron from the lead “a”). The first term is called the direct one, while the second one is called the crossing term. They are represented by the diagrams in Fig. 1a and Fig. 1b.

\[
\begin{align*}
\text{Fig. 1a} & \quad \text{Fig. 1b}
\end{align*}
\]

The ability to take into account the contributions of the crossing terms is an advantage of the present S-matrix method. If the initial state is the empty one \( |0\rangle \), then there is no electron in the quantum dot to be annihilated and the crossing term does not appear:

\[
\langle 0 | T\{c_\sigma'(t') c_\sigma^\dagger(t)\} | 0 \rangle = \theta(t' - t) e^{-iE(t'-t)} \delta_{\sigma \sigma'} . \tag{19}
\]

On the contrary, if the initial state is the doubly occupied one \( |c_\uparrow c_\uparrow\rangle \), then it is impossible to add one more electron into the quantum dot and only the crossing term gives the contribution:

\[
\langle c_\downarrow c_\uparrow | T\{c_\sigma'(t') c_\sigma^\dagger(t)\} | c_\uparrow c_\uparrow \rangle = -\theta(t - t') e^{-i(E+U)(t'-t)} \delta_{\sigma \sigma'} . \tag{20}
\]

In the case of the singly occupied initial states \( |c_\sigma\rangle \) both the direct and crossing terms can give non-vanishing contributions depending on the spin configuration of the electron system:

\[
\langle c_{\sigma_2} | T\{c_{\sigma_1}(t') c_{\sigma_1}^\dagger(t)\} | c_{\sigma_2} \rangle = \theta(t' - t) e^{-i(E+U)(t'-t)} \delta_{\sigma_1 \sigma_2} \delta_{\sigma_1' \sigma_2'} \left[ \delta_{\sigma_1' \sigma_1} - \delta_{\sigma_1' \sigma_2} \right] - \theta(t - t') e^{-iE(t'-t)} \delta_{\sigma_1' \sigma_1} \delta_{\sigma_1' \sigma_2} \delta_{\sigma_1' \sigma_2} . \tag{21}
\]

Introduce the Fourier transformations of the usual and generalized Green functions

\[
G^{(0)}_{\sigma'\sigma}(t' - t) = \frac{1}{2\pi} \int d\omega e^{-i\omega(t'-t)} \tilde{G}^{(0)}_{\sigma'\sigma}(\omega) , \tag{22}
\]
\[ G_{\sigma_2'\sigma_1\sigma_2}(t' - t) = \frac{1}{2\pi} \int d\omega \, e^{-i\omega(t' - t)} \tilde{G}_{\sigma_2'\sigma_1\sigma_2}(\omega), \] (23)

\[ G_{\sigma_\sigma}^{(2)}(t' - t) = \frac{1}{2\pi} \int d\omega \, e^{-i\omega(t_1 - t_2)} \tilde{G}_{\sigma_\sigma}^{(2)}(\omega). \] (24)

From the expressions (19) - (21) of the Green functions it follows that their Fourier transforms equal

\[ \tilde{G}_{\sigma_\sigma}^{(0)}(\omega) = \frac{\delta_{\sigma_\sigma}}{\omega - E + io}, \] (25)

\[ \tilde{G}_{\sigma_\sigma}(\omega) = \frac{\delta_{\sigma_\sigma}}{\omega - E - U + io}, \] (26)

\[ \tilde{G}_{\sigma_\sigma}^{(2)}(\omega) = \frac{\delta_{\sigma_\sigma}}{\omega - E - U - io}. \] (27)

It is easy to express the matrix elements (13) - (14) in terms of these Fourier transforms. Finally we obtain following relevant non-vanishing irreducible matrix elements contributing to the transitions of a particle \( a_\sigma(k) \) into a particle \( b_{\sigma'}(k') \) via the intermediate virtual particle \( c_{\sigma''} \) in the second order of the perturbation theory:

\[ \langle b_\uparrow(k') | R^{(2)} | a_\uparrow(k) \rangle = \frac{1}{2\pi} \delta[E_a(k) - E_b(k')] V_a(k)' V_b(k) \cdot \frac{1}{E_a(k) - E + io}, \] (28)

\[ \langle c_\downarrow b_\uparrow(k') | R^{(2)} | a_\downarrow(k) c_\uparrow \rangle = \frac{1}{2\pi} \delta[E_a(k) - E_b(k')] V_a(k)' V_b(k) \cdot \frac{1}{E_a(k) - E - U + io}, \] (29)

\[ \langle c_\uparrow b_\downarrow(k') | R^{(2)} | a_\uparrow(k) c_\downarrow \rangle = \frac{1}{2\pi} \delta[E_a(k) - E_b(k')] V_a(k)' V_b(k) \cdot \frac{1}{E_a(k) - E - io}, \] (30)

\[ \langle c_\downarrow c_\uparrow b_\uparrow(k') | R^{(2)} | a_\downarrow(k) c_\uparrow c_\downarrow \rangle = \frac{1}{2\pi} \delta[E_a(k) - E_b(k')] V_a(k)' V_b(k) \cdot \frac{1}{E_a(k) - E - U + io} + \frac{1}{E_a(k) - E - io}, \] (31)

\[ \langle c_\uparrow c_\downarrow b_\uparrow(k') | R^{(2)} | a_\uparrow(k) c_\downarrow c_\uparrow \rangle = \frac{1}{2\pi} \delta[E_a(k) - E_b(k')] V_a(k)' V_b(k) \cdot \frac{1}{E_a(k) - E - U - io}. \] (32)

Note that the matrix element (31) describes the spin-flip scattering process inside the dot while other matrix elements are those of the non-spin-flip ones.

Using the expressions (28) - (32) of the matrix elements of the scattering operator it is easy to calculate the transition rate. If the matrix element of the transition from an initial pure state \( |i\rangle \) to a final one \( |f\rangle \) has the form

\[ \langle f | R | i \rangle = 2\pi \delta[E_i - E_f] \, M_{i\rightarrow f}, \] (33)

then the transition rate in an unit time interval equals

\[ W_{i\rightarrow f} = 2\pi \delta[E_i - E_f] \, |M_{i\rightarrow f}|^2. \]

If the initial state is a mixed equilibrium state \( I \) containing the pure state \( |i\rangle \) with a weight
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Let us apply this formula to the transitions between the initial and final states presented in the matrix elements (28) - (32). The statistical weights of these pure states in the initial mixed equilibrium state are given in the Table I with

$$W_{I \rightarrow F} = \sum_{i \in I} \sum_{f \in F} 2\pi \delta[E_i - E_f] |M_{i \rightarrow f}|^2 w_i.$$  \hspace{1cm} (34)

Table I

| State | Weight |
|-------|--------|
| $|a_\sigma(k)\rangle$ | $e^{-\beta E'_\sigma(k)}/Z$ |
| $|a_\sigma(k) a_\perp(k)\rangle$ | $e^{-\beta 2E'_\sigma(k)}/Z$ |
| $|a_\sigma(k) b_\sigma(k')\rangle$ | $e^{-\beta [E'_\sigma(k) + E'_\sigma(k')]/Z}$ |
| $|a_\perp(k) b_\sigma(k') a_\perp(k)\rangle$ | $e^{-\beta [2E'_\sigma(k) + E'_\sigma(k')]/Z}$ |
| $|a_\sigma(k) c_\sigma\rangle$ | $e^{-\beta E'_\sigma(k) + E'}/Z$ |
| $|a_\perp(k) c_\sigma a_\perp(k)\rangle$ | $e^{-\beta [2E'_\sigma(k) + E']/Z}$ |
| $|a_\sigma(k) c_\sigma b_\sigma(k')\rangle$ | $e^{-\beta [E'_\sigma(k) + E'_\sigma(k') + E']/Z}$ |
| $|a_\perp(k) c_\sigma c_\perp a_\perp(k)\rangle$ | $e^{-\beta [2E'_\sigma(k) + E' + U]/Z}$ |
| $|a_\sigma(k) c_\perp c_\perp\rangle$ | $e^{-\beta [E'_\sigma(k) + 2E' + U]/Z}$ |
| $|a_\perp(k) c_\perp c_\perp a_\perp(k)\rangle$ | $e^{-\beta [2E'_\sigma(k) + 2E' + U]/Z}$ |
| $|a_\sigma(k) c_\perp c_\perp b_\sigma(k')\rangle$ | $e^{-\beta [E'_\sigma(k) + E'_\sigma(k') + 2E' + U]/Z}$ |
| $|a_\perp(k) c_\perp c_\perp b_\sigma(k') a_\perp(k)\rangle$ | $e^{-\beta [2E'_\sigma(k) + E'_\sigma(k') + 2E' + U]/Z}$ |
where
\[ E'_a(k) = E_a(k) - \mu_a , \]
\[ E'_b(k) = E_b(k) - \mu_b , \]
\[ E' = E - \mu_c , \]
\[ (36) \]
\[ \mu_a, \mu_b \text{ and } \mu_c \text{ being the chemical potentials in the leads “a”, “b” and in the quantum dot, resp.} \]

Substituting the expressions of the matrix elements (28) - (32) and the statistical weights in the Table I to the r. h. s. of the formula (34) we obtain following expression of the probability of the transition of electrons from the lead “a” to the lead “b” through its intermediate states in the quantum dot:
\[ W_{a \rightarrow b} = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f_a(\omega) \left[ 1 - f_b(\omega) \right] W(\omega) , \]
\[ (37) \]
\[ W(\omega) = \sum_k 2\pi \delta [\omega - E_a(k)] \ |V_a(k)|^2 \sum_{k'} 2\pi \delta [\omega - E_b(k')] \ |V_b(k')|^2 . \]
\[ (38) \]
\[ \frac{1}{Z_c} \left\{ \left| \frac{1}{\omega - E + i\omega} \right|^2 + e^{-\beta E'_a} \left( \left| \frac{1}{\omega - E - U + i\omega} \right|^2 + \left| \frac{1}{\omega - E - i\omega} \right|^2 \right) + e^{-\beta(2E'_a + U)} \left| \frac{1}{\omega - E - U - i\omega} \right|^2 \right\} . \]
\[ \]
Here \( f_a(\omega) \) and \( f_b(\omega) \) are the Fermi distribution functions of the electrons in the leads “a” and “b”, resp.,
\[ f_b(\omega) = \frac{e^{-\beta(\omega - \mu_b)}}{1 + e^{-\beta(\omega - \mu_b)}} . \]
\[ f_a(\omega) = \frac{e^{-\beta(\omega - \mu_a)}}{1 + e^{-\beta(\omega - \mu_a)}} . \]
\[ (39) \]

For the reverse transition of electrons from the lead “b” to the lead “a” we have a similar expression of the transition rate
\[ W_{b \rightarrow a} = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f_b(\omega) \left[ 1 - f_a(\omega) \right] W(\omega) . \]
\[ (40) \]

If \( \mu_a > \mu_b \), then \( W_{a \rightarrow b} > W_{b \rightarrow a} \) and the effective transition of electrons from the lead “a” to the lead “b” generates the electrical current
\[ J_e = e \left[ W_{a \rightarrow b} - W_{b \rightarrow a} \right] = e \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \left[ f_a(\omega) - f_b(\omega) \right] W(\omega) \]
\[ (41) \]
from the lead “b” to the lead “a”, where \( e \) is the absolute value of the electron charge.

In the expression (38) there are the contributions of both direct and crossing terms of the chronological product (21). If we neglect the crossing terms, then we have the non-crossing approximation (NCA). In this approximation \( W(\omega) \) is replaced by the following
expression

\[ W_{NCA}(\omega) = \sum_k 2\pi \delta[\omega - E_a(k)] |V_a(k)|^2 \sum_{k'} 2\pi \delta[\omega - E_b(k')] |V_b(k')|^2 \times \]

\[
\times \frac{1}{Z_c} \left\{ \left| \frac{1}{\omega - E + i\alpha} \right|^2 + 2e^{-\beta E'} \left| \frac{1}{\omega - E - U + i\alpha} \right|^2 \right\}.
\]

Obviously, if \( e^{-\beta E'} \) is not very small, then the contribution of the crossing terms might be comparable to that of the direct ones.

III. HIGH ORDER APPROXIMATIONS OF THE PERTURBATION THEORY. GREEN FUNCTION TECHNIQUE

The expression in the r. h. s. of the formula (38) exhibits the sharp resonances at the values of \( \omega \) near the energy levels of the electron in the dot \( \omega \approx E \) and \( \omega \approx E + U \). However, at these values of \( \omega \) the broadening of the energy levels due to the tunneling of the electrons from (to) the dot to (from) the leads must be taken into account. This can be done by summing up the contributions of the high order terms in the ladder approximation. The most convenient way to do that is the application of the Green function technique.

As an example consider again the transport of the electrons from the lead “a” to the lead “b” due to the single-electron tunneling through the quantum dot. Instead of the annihilation and creation operators \( a_\sigma(k), b_\sigma(k) \) and \( a_\sigma^+(k), b_\sigma^+(k) \) for the electrons in the leads in the Schrödinger representation the S-matrix (6) is expressed in terms of the corresponding operators \( a_\sigma(k,t), b_\sigma(k,t) \) and \( a_\sigma^+(k,t), b_\sigma^+(k,t) \) in the interaction representation defined according to the formula (5) with the expression (2) of the operator \( H_0 \). It is easy to verify that

\[
\begin{align*}
a_\sigma^+(k,t) &= e^{iE_a(k)t} a_\sigma^+(k), & a_\sigma(k,t) &= e^{-iE_a(k)t} a_\sigma(k), \\
b_\sigma^+(k',t') &= e^{iE_b(k')t'} b_\sigma^+(k'), & b_\sigma(k',t') &= e^{-iE_b(k')t'} b_\sigma(k),
\end{align*}
\]

From the expression (6) of the S-matrix

\[
S = T\left\{ \exp \left( -i \int_{-\infty}^{\infty} H_{\text{int}}(t) dt \right) \right\}
\]

with \( H_{\text{int}}(t) \) being determined by the formulae (4), (5) and (43)

\[
H_{\text{int}}(t) = \sum_k \sum_\sigma \left\{ V_a(k) e^{iE_a(k)t} a_\sigma^+(k) c_\sigma(t) + V_a(k)^* e^{-iE_a(k)t} c_\sigma^+(t) a_\sigma(k) \right. \\
+ V_b(k) e^{iE_b(k)t} b_\sigma^+(k) c_\sigma(t) + V_b(k)^* e^{-iE_b(k)t} c_\sigma^+(t) b_\sigma(k) \}
\]

it follows that

\[
\langle b_\sigma^+(k') | R | a_\sigma(k) \rangle =
- iV_a(k)^* V_b(k') \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dt e^{i[E_b(k')t' - E_a(k)t]} \langle 0 | T \{ c_\sigma(t') c_\sigma^+(t) S \} | 0 \rangle,
\]

\[
(45)
\]
with the interaction Hamiltonian $H$ quantities The calculation of these matrix elements (45) - (47) requires the determination of following one is performed with the use of the operator $S$ (generalized) Green functions may be derived by means of the Green functions technique. the presence of the tunneling transitions to and from the leads. The expressions of these which might be called the (generalized) Green functions of the electrons in the dot in and the initial condition
\[ \langle c_{\sigma_2} b_{\sigma_1} (k') | R | a_{\sigma_1} (k) c_{\sigma_2} \rangle = - i V_{\alpha}(k)^* V_b(k') \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dt e^{it[H_b(k') + E_a(k) - E_a(k)]t} \langle c_{\sigma_2}' | T \{ c_{\sigma_1}'(t') c_{\sigma_1}^+(t) S \} | c_{\sigma_2} \rangle, \] (46)
\[ \langle c_{\sigma_1} c_{\sigma_1} b_{\sigma_1} (k') | R | a_{\sigma_1} (k) c_{\sigma_1} c_{\sigma_1} \rangle = - i V_{\alpha}(k)^* V_b(k') \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dt e^{it[H_b(k') + E_a(k) - E_a(k)]t} \langle c_{\sigma_1} c_{\sigma_1} | T \{ c_{\sigma_1}(t') c_{\sigma_1}^+(t) S \} | c_{\sigma_1} c_{\sigma_1} \rangle. \] (47)

The calculation of these matrix elements (45) - (47) requires the determination of following quantities
\[ G^{(0)cc \sigma \sigma}_{\sigma_\sigma} (t' - t) = - i \langle 0 | T \{ c_{\sigma}(t') c_{\sigma}^+(t) S \} | 0 \rangle, \] (48)
\[ G^{(1)cc}_{\sigma_\sigma, \sigma_1, \sigma_2} (t' - t) = - i \langle c_{\sigma_2}' | T \{ c_{\sigma_1}'(t') c_{\sigma_1}^+(t) S \} | c_{\sigma_2} \rangle, \] (49)
\[ G^{(2)cc}_{\sigma_\sigma, \sigma_1, \sigma_2} (t' - t) = - i \langle c_{\sigma_1} c_{\sigma_1} | T \{ c_{\sigma_1}(t') c_{\sigma_1}^+(t) S \} | c_{\sigma_1} c_{\sigma_1} \rangle. \] (50)
which might be called the (generalized) Green functions of the electrons in the dot in the presence of the tunneling transitions to and from the leads. The expressions of these (generalized) Green functions may be derived by means of the Green functions technique.

In order to apply the Green function technique we must work in the Heisenberg representation. The transformation from the interaction representation to the Heisenberg one is performed with the use of the operator $S(t, t_0)$ satisfying the Schrödinger equation with the interaction Hamiltonian $H_{\text{int}}(t)$,
\[ i \frac{dS(t, t_0)}{dt} = H_{\text{int}}(t) S(t, t_0), \] (51)
and the initial condition
\[ S(t_0, t_0) = 1. \] (52)
The solution of the equation (51) with the initial condition (52) can be represented in the form similar to the formula (6) for the S-matrix:
\[ S(t', t_0) = T \left\{ \exp \left( - i \int_{t_0}^{t'} H_{\text{int}}(t) dt \right) \right\}. \] (53)
It is obvious that
\[ S = S(\infty, -\infty). \] (54)
From the expression (53) it follows the group property of the operators $S(t, t_0)$:
\[ S(t, t_0) = S(t', t_0) S(t', t_0). \] (55)

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From this property and the initial condition \( (52) \) we obtain the relation
\[
S(t_0, t) = S(t, t_0)^{-1}.
\]  
(56)
Moreover, the operator \( (53) \) is unitary
\[
S(t, t_0)^+ = S(t, t_0)^{-1} = S(t_0, t).
\]  
(57)
Now we derive the explicit expression of the chronological product \( T \{ c_{\sigma'} (t') \ c_{\sigma}^+ (t) \ S \} \) in the matrix elements \( (48) - (50) \). In the case \( t' > t \) we write
\[
S = S(\infty, -\infty) = S(\infty, t') S(t', t) S(t, -\infty)
\]
and have
\[
T \{ c_{\sigma'} (t') \ c_{\sigma}^+ (t) \ S \} = S(\infty, t') \ c_{\sigma'} (t') S(t', -\infty) S(\infty, -\infty) S(-\infty, t') c_{\sigma'} (t') S(t', -\infty) S(-\infty, t) c_{\sigma}^+ (t) S(t, -\infty).
\]
Introducing new operators
\[
C_{\sigma'} (t') = S(-\infty, t') c_{\sigma'} (t') S(t', -\infty),
\]
\[
C_{\sigma}^+ (t) = S(-\infty, t) c_{\sigma}^+ (t) S(t, -\infty)
\]  
(58)
we rewrite
\[
T \{ c_{\sigma'} (t') \ c_{\sigma}^+ (t) \ S \} = S C_{\sigma'} (t') C_{\sigma}^+ (t), \quad t' > t.
\]  
(59)
Similarly, in the case \( t > t' \) we have
\[
T \{ c_{\sigma'} (t') \ c_{\sigma}^+ (t) \ S \} = -S C_{\sigma}^+ (t) C_{\sigma'} (t'), \quad t > t'.
\]  
(60)
Combining both expressions \( (59) \) and \( (60) \) finally we obtain the formula
\[
T \{ c_{\sigma'} (t') \ c_{\sigma}^+ (t) \ S \} = ST \{ C_{\sigma'} (t') C_{\sigma}^+ (t) \}.
\]  
(61)
Now the (generalized) Green functions \( (48) - (50) \) are expressed in terms of the new operators \( (59) \):
\[
G_{\sigma\sigma}^{(0)} (t' - t) = -i \langle 0 \mid ST \{ C_{\sigma'} (t') C_{\sigma}^+ (t) \} \mid 0 \rangle,
\]
(62)
\[
G_{\sigma_2\sigma_1\sigma_1\sigma_2}^{(1)} (t' - t) = -i \langle c_{\sigma_2} \mid ST \{ C_{\sigma_2'} (t') C_{\sigma_2}^+ (t) \} \mid c_{\sigma_2} \rangle,
\]
(63)
\[
G_{\sigma\sigma}^{(2)} (t' - t) = -i \langle c_{\sigma} \mid ST \{ C_{\sigma'} (t') C_{\sigma}^+ (t) \} \mid c_{\sigma} \rangle.
\]
(64)
In order to derive the differential equations for the (generalized) Green functions \( (62) - (64) \) we must use the Heisenberg equations of motion for the new operators \( (59) \). Denoting
\[
H(t) = S(\infty, t) [H_0 + H_{\text{int}}(t)] S(t, -\infty)
\]  
(65)
the total Hamiltonian in the new representation we obtain the Heisenberg equations of motion with the total Hamiltonian $H(t)$:

$$i \frac{dC_\sigma(t)}{dt} = [C_\sigma(t), H(t)] , \quad i \frac{dC_\sigma^+(t)}{dt} = [C_\sigma^+(t), H(t)] .$$

(66)

This means that $C_\sigma(t)$ and $C_\sigma^+(t)$ are the annihilation and creation operators in the Heisenberg representation.

Together with the operators $C_\sigma(t)$ and $C_\sigma^+(t)$ determined by the formula (58) introduce also the annihilation and creation operators for the electrons in the leads in the Heisenberg representation

$$A_\sigma(k, t) = S(-\infty, t) a_\sigma(k, t) S(t, -\infty) ,$$

$$A_\sigma^+(k, t) = S(-\infty, t) a_\sigma^+(k, t) S(t, -\infty) ,$$

$$B_\sigma(k, t) = S(-\infty, t) b_\sigma(k, t) S(t, -\infty) ,$$

$$B_\sigma^+(k, t) = S(-\infty, t) b_\sigma^+(k, t) S(t, -\infty) .$$

(67)

They satisfy also the Heisenberg equations of motion with the total Hamiltonian $H(t)$:

$$i \frac{dA_\sigma(k, t)}{dt} = [A_\sigma(k, t), H(t)] , \quad i \frac{dA_\sigma^+(k, t)}{dt} = [A_\sigma^+(k, t), H(t)] ,$$

$$i \frac{dB_\sigma(k, t)}{dt} = [B_\sigma(k, t), H(t)] , \quad i \frac{dB_\sigma^+(k, t)}{dt} = [B_\sigma^+(k, t), H(t)] .$$

(68)

The total Hamiltonian in the Heisenberg representation is expressed directly in terms of the new operators (58) and (67):

$$H(t) = E \sum_\sigma C_\sigma^+(t) C_\sigma(t) + U N_\uparrow(t) N_\downarrow(t) +$$

$$+ \sum_k \sum_\sigma \{ E_a(k) A_\sigma^+(k, t) A_\sigma(k, t) + E_b(k) B_\sigma^+(k, t) B_\sigma(k, t) \} +$$

$$+ \sum_k \sum_\sigma \{ V_a(k) A_\sigma^+(k, t) C_\sigma(t) + V_a(k)^* C_\sigma^+(t) A_\sigma(k, t) +$$

$$+ V_b(k) B_\sigma^+(k, t) C_\sigma(t) + V_b(k)^* C_\sigma^+(t) B_\sigma(k, t) \} ,$$

$$N_\sigma(t) = C_\sigma^+(t) C_\sigma(t) .$$

(69)

The operators (58) and (67) satisfy the canonical equal-time anticommutation relations

$$\{ C_\sigma(t) , C_\sigma^+(t) \} = \delta_{\sigma\sigma'} ,$$

$$\{ A_\sigma(k, t) , A_{\sigma'}^+(k', t) \} = \delta_{\sigma\sigma'} \delta_{kk'} ,$$

$$\{ B_\sigma(k, t) , B_{\sigma'}^+(k', t) \} = \delta_{\sigma\sigma'} \delta_{kk'} ,$$

(70)

other equal-time anticommutators between these operators being equal to zero.

From the Heisenberg equations of motion (66) and (68), the expression (69) of the total Hamiltonian, the equal-time canonical anticommutation relations (70) and other ones with the vanishing r. h. s. we derive following differential equations for the operators (58) and (67):

$$i \frac{dC_\sigma(t)}{dt} = EC_\sigma(t) + U N_\downarrow(t) C_\sigma(t) + \sum_k \{ V_a(k) A_\sigma(k, t) + V_b(k)^* B_\sigma(k, t) \} ,$$

(71)
functions multiplied with small functions systems of equations, but belong to some infinite systems. In order to find their approx-

cised differential equations do not form closed finite

functions into two functions according to the definition of the chronol ogical product Fourier transforms of the (generalized) Green functions (62)–(64) we divide each of them we can derive the systems of equations for the (generalized) Green functions.

IV. CALCULATION OF THE (GENERALIZED) GREEN FUNCTIONS

For the convenience in the determination of the real and imaginary parts of the Fourier transforms of the (generalized) Green functions we (62)–(64) we divide each of them into two functions according to the definition of the chronological product

\[
T \left\{ C_{\sigma'}(t') C_{\sigma}^+(t) \right\} = \theta(t' - t) C_{\sigma'}(t') C_{\sigma}^+(t) - \theta(t - t') C_{\sigma}^+(t) C_{\sigma'}(t')
\]

We have

\[
G_{\sigma'\sigma}^{(0)cc}(t' - t) = G_{\sigma'\sigma}^{(0)cc(+)}(t' - t) + G_{\sigma'\sigma}^{(0)cc(-)}(t' - t),
\]

\[
G_{\sigma_2'\sigma_1'\sigma_1\sigma_2}^{cc}(t' - t) = G_{\sigma_2'\sigma_1'\sigma_1\sigma_2}^{cc(+)}(t' - t) + G_{\sigma_2'\sigma_1'\sigma_1\sigma_2}^{cc(-)}(t' - t),
\]

\[
G_{\sigma'\sigma}^{(2)cc}(t' - t) = G_{\sigma'\sigma}^{(2)cc(+)}(t' - t) + G_{\sigma'\sigma}^{(2)cc(-)}(t' - t)
\]

with

\[
G_{\sigma'\sigma}^{(0)cc(+)}(t' - t) = -i\theta(t' - t) \langle 0 | S C_{\sigma'}(t') C_{\sigma}^+(t) | 0 \rangle,
\]

\[
G_{\sigma'\sigma}^{(0)cc(-)}(t' - t) = i\theta(t - t') \langle 0 | S C_{\sigma}^+(t') C_{\sigma'}(t) | 0 \rangle,
\]

\[
G_{\sigma_2'\sigma_1'\sigma_1\sigma_2}^{cc(+)}(t' - t) = -i\theta(t' - t) \langle c_{\sigma_2'} | S C_{\sigma_1'}(t') C_{\sigma}^+(t) | c_{\sigma_2} \rangle,
\]

\[
G_{\sigma_2'\sigma_1'\sigma_1\sigma_2}^{cc(-)}(t' - t) = i\theta(t - t') \langle c_{\sigma_2'} | S C_{\sigma_1'}(t) C_{\sigma'}(t') | c_{\sigma_2} \rangle,
\]

\[
G_{\sigma'\sigma}^{(2)cc(+)}(t' - t) = -i\theta(t' - t) \langle c_{\sigma_1} c_{\gamma} | S C_{\sigma'}(t') C_{\sigma}^+(t) | c_{\gamma} c_{\sigma} \rangle,
\]

\[
G_{\sigma'\sigma}^{(2)cc(-)}(t' - t) = i\theta(t - t') \langle c_{\sigma_1} c_{\gamma} | S C_{\sigma}^+(t) C_{\sigma'}(t') | c_{\gamma} c_{\sigma} \rangle.
\]

Using the equation (71) for \( C_{\sigma'}(t') \) we can derive the differential equations for the functions \( G_{\sigma'\sigma}^{(0)cc(\pm)}(t' - t) \), \( G_{\sigma_2'\sigma_1'\sigma_1\sigma_2}^{(1)cc(\pm)}(t' - t) \) and \( G_{\sigma'\sigma}^{(2)cc(\pm)}(t' - t) \) which contain many other (generalized) Green functions. The derived differential equations do not form closed finite systems of equations, but belong to some infinite systems. In order to find their approximate solutions we might truncate them at a corresponding order and obtain the closed systems of approximate differential equations which can be solved exactly. Let us now truncate the infinite systems of equations by neglecting the 4-point (generalized) Green functions multiplied with small functions \( V_a(\mathbf{k}) \), \( V_b(\mathbf{k}) \), \( V_a(\mathbf{k})^* \), \( V_b(\mathbf{k})^* \) and all \( n \)-point
(generalized) Green functions with $n > 4$. Then we obtain closed systems of approximate
equations containing following time-independent matrix elements (constants):

\[
\begin{align*}
\langle c_{\sigma_2}' | S\sigma_1'(t)C_{\sigma_1'}(t) | c_{\sigma_2} \rangle &= g_{\sigma_1'\sigma_2}, \\
\langle c_{\sigma_2}' | S\sigma_1'(t)C_{\sigma_1'}(t) | c_{\sigma_2} \rangle &= g_{\sigma_1'\sigma_1\sigma_2}, \\
(0) | S\sigma_1(t)C_{\sigma_1}^+(t) | 0 \rangle &= g_{\sigma_1\sigma}(0)^{(cc)}(+) , \\
(0) | S\sigma_1^+(t)C_{\sigma_1}(t) | 0 \rangle &= g_{\sigma_1\sigma}(0)^{(cc)}(-) , \\
(0) | S\sigma_1'(t)C_{\sigma_1'}(t) | 0 \rangle &= g_{\sigma_1'\sigma}(0)^{(cc)}(+) , \\
(0) | S\sigma_1'(t)C_{\sigma_1'}(t) | 0 \rangle &= g_{\sigma_1'\sigma}(0)^{(cc)}(-) , \\
(0) | S\sigma_1'(t)A_{\sigma_1'}(k, t) | 0 \rangle &= g_{\sigma_1'\sigma}(0)^{(bc)}(+) (k) , \\
(0) | S\sigma_1'(t)A_{\sigma_1'}(k, t) | 0 \rangle &= g_{\sigma_1'\sigma}(0)^{(bc)}(-) (k) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= g_{\sigma_1'\sigma}(0)^{(bc)}(+) (k) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= g_{\sigma_1'\sigma}(0)^{(bc)}(-) (k) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= f_{\sigma_1'\sigma}(0)^{(cc)}(+) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= f_{\sigma_1'\sigma}(0)^{(cc)}(-) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= f_{\sigma_1'\sigma}(0)^{(bc)}(+) (k) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= f_{\sigma_1'\sigma}(0)^{(bc)}(-) (k) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= f_{\sigma_1'\sigma}(0)^{(bc)}(+) (k) , \\
(0) | S\sigma_1'(t)B_{\sigma_1'}(k, t) | 0 \rangle &= f_{\sigma_1'\sigma}(0)^{(bc)}(-) (k) , \\
\langle c_{\sigma_2}' | S\sigma_1'(t)C_{\sigma_1'}(t) | c_{\sigma_2} \rangle &= g_{\sigma_1'\sigma_1\sigma_2}(0)^{(ac)}(-) , \\
\langle c_{\sigma_2}' | S\sigma_1'(t)C_{\sigma_1'}(t) | c_{\sigma_2} \rangle &= g_{\sigma_1'\sigma_1\sigma_2}(0)^{(ac)}(+) .
\end{align*}
\]
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Performing the Fourier transformation of the differential equations we derive a system of algebraic equations which can be solved easily and obtain following results:

$$\tilde{G}_{\sigma'\sigma}^{(0)cc(\pm)}(\omega) = \{\omega - E - \Sigma(\omega \pm i\alpha)^{-1}\},$$

$$\{g_{\sigma'\sigma}^{(0)cc(\pm)}(k) + \sum_k \left[ g_{\sigma'\sigma}^{(0)ac(\pm)}(k) \right] \} + U \tilde{F}_{\sigma'\sigma}^{(0)cc(\pm)}(\omega),$$

$$\tilde{G}_{\sigma_1\sigma_2'\sigma_1\sigma_2}^{(1)cc(\pm)}(\omega) = \{\omega - E - \Sigma(\omega \pm i\alpha)^{-1}\},$$

$$\{g_{\sigma_1\sigma_2'}^{(1)cc(\pm)}(k) + \sum_k \left[ g_{\sigma_1\sigma_2'}^{(1)ac(\pm)}(k) \right] \} + U \tilde{F}_{\sigma_1\sigma_2'}^{(1)cc(\pm)}(\omega),$$

$$\tilde{F}_{\sigma_1\sigma_2'}^{(0)cc(\pm)}(\omega) = \{\omega - E - U - \Sigma(\omega \pm i\alpha)^{-1}\},$$

$$\{f_{\sigma_1\sigma_2'}^{(0)cc(\pm)}(k) + \sum_k \left[ f_{\sigma_1\sigma_2'}^{(0)ac(\pm)}(k) \right] \} ,$$

$$\tilde{F}_{\sigma_1\sigma_2'}^{(1)cc(\pm)}(\omega) = \{\omega - E - U - \Sigma(\omega \pm i\alpha)^{-1}\},$$

$$\{f_{\sigma_1\sigma_2'}^{(1)cc(\pm)}(k) + \sum_k \left[ f_{\sigma_1\sigma_2'}^{(1)ac(\pm)}(k) \right] \} ,$$
Substituting these values of the constants into the r. h. s. of the relations (84) - (89) we obtain

\[
\tilde{F}_{\sigma'\sigma}^{(2)cc}(\omega) = \{\omega - E - U - \Sigma(\omega \pm io)\}^{-1}.
\]

\[
\left\{ f_{\sigma'\sigma}^{(2)cc}(\pm) + \sum_{\mathbf{k}} \left[ \frac{f_{\sigma'\sigma}^{(2)ac}(\pm)(\mathbf{k})}{\omega - E_a(\mathbf{k}) \pm io} + \frac{f_{\sigma'\sigma}^{(2)bc}(\pm)(\mathbf{k})}{\omega - E_b(\mathbf{k}) \pm io} \right] \right\},
\]

where

\[
\Sigma(\omega \pm io) = \sum_{\mathbf{k}} \left( \frac{|V_a(\mathbf{k})|^2}{\omega - E_a(\mathbf{k}) \pm io} \right)
\]

is the self-energy part of the electron in the dot due to its tunneling from and to the leads. The self-energy part \(\Sigma(\omega)\) in the denominators of the (generalized) Green functions describes the broadening of the energy levels of the electron in the dot.

The constants (83) can be calculated in the perturbation theory with respect to the tunnelling Hamiltonian \(H_{\text{int}}\). In the lowest (zero) order we have following values:

\[
\begin{align*}
    f_{\sigma'\sigma}^{(0)cc}(\pm)(\mathbf{k}) &= f_{\sigma'\sigma}^{(0)ac}(\pm)(\mathbf{k}) = f_{\sigma'\sigma}^{(0)bc}(\pm)(\mathbf{k}) = 0, \\
    f_{\sigma'\sigma}^{(2)cc}(\pm)(\mathbf{k}) &= f_{\sigma'\sigma}^{(2)ac}(\pm)(\mathbf{k}) = f_{\sigma'\sigma}^{(2)bc}(\pm)(\mathbf{k}) = 0, \\
    f_{\sigma'\sigma}^{(0)cc}(\pm)(\mathbf{k}) &= f_{\sigma'\sigma}^{(0)ac}(\pm)(\mathbf{k}) = f_{\sigma'\sigma}^{(0)bc}(\pm)(\mathbf{k}) = 0, \\
    g_{\sigma'\sigma}^{(0)ac}(\pm)(\mathbf{k}) &= g_{\sigma'\sigma}^{(0)bc}(\pm)(\mathbf{k}) = 0, \\
    g_{\sigma'\sigma}^{(2)cc}(\pm)(\mathbf{k}) &= g_{\sigma'\sigma}^{(2)ac}(\pm)(\mathbf{k}) = g_{\sigma'\sigma}^{(2)bc}(\pm)(\mathbf{k}) = 0.
\end{align*}
\]

Substituting these values of the constants into the r. h. s. of the relations (84) - (89) we obtain

\[
\tilde{F}_{\sigma'\sigma}^{(0)cc}(\omega) = 0,
\]

\[
\tilde{F}_{\sigma'\sigma}^{(2)cc}(\omega) = \frac{\delta_{\sigma'\sigma}}{\omega - E - U - \Sigma(\omega + io)}.
\]

\[
\tilde{F}_{\sigma'\sigma}^{(2)ac}(\omega) = \frac{\delta_{\sigma'\sigma}}{\omega - E - U - \Sigma(\omega - io)},
\]

\[
\tilde{F}_{\sigma'\sigma}^{(2)bc}(\omega) = 0,
\]

\[
\tilde{F}_{\sigma'\sigma}^{(2)ac}(\omega) = 0,
\]

\[
\tilde{F}_{\sigma'\sigma}^{(2)bc}(\omega) = 0.
\]

(Question: Do you have any specific questions or topics you would like to discuss further about this content?)
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\begin{align}
\tilde{G}^{(0)cc(+)}_{\sigma'\sigma}(\omega) &= \frac{\delta_{\sigma'\sigma}}{\omega - E - \Sigma(\omega + i\delta)}, \\
\tilde{G}^{(0)cc(-)}_{\sigma'\sigma}(\omega) &= 0, \\
\tilde{G}^{(1)cc(+)}_{\sigma'\sigma_1\sigma_2}(\omega) &= \frac{\delta_{\sigma_1\sigma_2}\delta_{\sigma'\sigma_1}\delta_{\sigma'\sigma_2}}{\omega - E - U - \Sigma(\omega + i\delta)}, \\
\tilde{G}^{(1)cc(-)}_{\sigma'\sigma_1\sigma_2}(\omega) &= \frac{\delta_{\sigma_1\sigma_2}\delta_{\sigma'\sigma_1}}{\omega - E - \Sigma(\omega - i\delta)}, \\
\tilde{G}^{(2)cc(+)}_{\sigma'\sigma}(\omega) &= 0, \\
\tilde{G}^{(2)cc(-)}_{\sigma'\sigma}(\omega) &= \frac{\delta_{\sigma'\sigma}}{\omega - E - U - \Sigma(\omega - i\delta)}.
\end{align}

Summing up the two parts of each (generalized) Green functions \( \tilde{G}^{(0)cc}_{\sigma'\sigma}(\omega) \), \( \tilde{G}^{(1)cc}_{\sigma'\sigma_1\sigma_2}(\omega) \) and \( \tilde{G}^{(2)cc}_{\sigma'\sigma}(\omega) \) finally we have

\begin{align}
\tilde{G}^{(0)cc}_{\sigma'\sigma}(\omega) &= \frac{\delta_{\sigma'\sigma}}{\omega - E - \Sigma(\omega + i\delta)}, \\
\tilde{G}^{(1)cc}_{\sigma'\sigma_1\sigma_2}(\omega) &= \frac{\delta_{\sigma_1\sigma_2}\delta_{\sigma'\sigma_1}\delta_{\sigma'\sigma_2}}{\omega - E - U - \Sigma(\omega + i\delta)} + \frac{\delta_{\sigma_1\sigma_2}\delta_{\sigma'\sigma_1}}{\omega - E - \Sigma(\omega - i\delta)}, \\
\tilde{G}^{(2)cc}_{\sigma'\sigma}(\omega) &= \frac{\delta_{\sigma'\sigma}}{\omega - E - U - \Sigma(\omega - i\delta)}.
\end{align}

VI. CONCLUSION

The expressions (103) - (105) of the (generalized) Green functions with the contributions of the high order approximations are similar to the expression (25) - (27) of these functions in the lowest order of the perturbation theory. The appearance of the self-energy part \( \Sigma(\omega) \) in the denominators of the (generalized) Green functions is the consequence of the tunneling of electrons between the dot and the leads which takes place in high order approximations. Instead of the expression (38) of the function \( W(\omega) \) determining the transport current now we have

\begin{align}
W(\omega) &= \sum_{k} 2\pi \delta [\omega - E_a(k)] \ |V_a(k)|^2 \sum_{k'} 2\pi \delta [\omega - E_b(k')] \ |V_b(k')|^2, \\
\frac{1}{Z_c} \left\{ \frac{1}{\omega - E - \Sigma(\omega + i\delta)} \right\}^2 &+ e^{-\beta E'} \left( \frac{1}{\omega - E - U - \Sigma(\omega + i\delta)} \right)^2 \\
&\quad + \left( \frac{1}{\omega - E - \Sigma(\omega - i\delta)} \right)^2 + \left( \frac{1}{\omega - E - U - \Sigma(\omega + i\delta)} - \frac{1}{\omega - E - \Sigma(\omega - i\delta)} \right)^2 \right) \\
&\quad + e^{-\beta(2E'+U)} \left( \frac{1}{\omega - E - U - \Sigma(\omega - i\delta)} \right)^2.
\end{align}

In comparison with other methods the S-matrix approach presented in this work has several advantages. The strong Coulomb interaction between the electrons in the dot was
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taken into account exactly without the use of the perturbation theory. All crossing terms
describing the co-tunneling are included automatically so that there is no need to assume
the non-crossing approximation (NCA). We have derived the expression of the electrical
current generated by the single-electron tunneling between the dot and the leads. The
role of the multi-electron co-tunneling will be studied in a subsequent work. Moreover, it
is easy to extend the presented method to the study of the multi-level quantum dots as
well as to other nanosystems.

Since the electron spin projections are explicitly indicated in the expressions of the
matrix elements, it is convenient to apply the presented method to the study of the spin-
dependent transition (transport) processes in the spintronic materials and devices. By
including the interactions of the electrons with the electromagnetic field it is straight-
forward to extend the presented method to the study of the photon-assisted transition
(transport) processes and develop the S-matrix approach in the theory of nanophotonic
materials and devices.

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