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Physics

DYSON EQUATIONS FOR GREEN FUNCTIONS OF ELECTRONS IN OPEN SINGLE-LEVEL QUANTUM DOT

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Abstract. The infinite system of differential equations for the nonequilibrium Green functions of electrons in a single-level quantum dot connected with two conducting leads is truncated by applying the mean-field approximation to the mean values of the products of four operators. As the result the system of Dyson equations for the two-point real-time nonequilibrium Green functions in the Keldysh formalism as well as that of the two-point imaginary-time Green functions are derived.

1. INTRODUCTION

The electrons transport through a single-level quantum dot (QD) connected with two conducting leads was the subject for the theoretical and experimental studies in many works since the early days of the nanophysics [1-19]. Two observable physical quantities which can be measured in the experiments on the electrons transport are the electron current through the QD and the time-averaged value of the electrons number in the QD. All they are expressed in terms of the single-electron Green functions. Since the electron transport is a nonequilibrium process one should work with the in Keldysh formalism of nonequilibrium complex-time Green functions [20,21]. Due to the presence of the strong Coulomb interaction between electrons in the QD the differential equations for the single-electron Green functions contain the multi-electron Green functions and all these coupled equations form an infinite system of differential equations for an infinite number of Green functions. In order to find some approximate finite closed system of equations one can either to apply the perturbation theory and retain only some appropriate chain of ladder diagrams or to assume some approximation to decouple the infinite system of equations and obtain a finite closed system. In the former case one should use the noncrossing approximation. In both cases the form of the approximate finite system of equations depends on the mechanism of the approximation and therefore the approximate systems in different works are different. In order to prepare our further study we revise the derivation of the approximate finite system of equations for the complex-time Green functions of electrons in the open single-level QD. As the mechanism for decoupling the infinite system of equations to obtain the approximate finite one we assume the mean-field approximation to the mean values of the products of four operators. The system of two Dyson equations for two complex-time two-point Green functions will be derived.

In Sec. II the Hamiltonian of the model and the equations of motion for the electron destruction and creation operators are presented. The differential equations for the Green functions are derived in Sec. III. In Sec. IV from the mean-field approximation it follows the relations between the Green functions which decouple the infinite system of equations and lead to the closed system of Dyson equations for two complex-time Green functions. The conclusion and discussions are presented in Sec. V.

2. HAMILTONIAN AND EQUATIONS OF MOTION

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 in many theoretical works [1-19]. It was assumed that the electron system in this SET has following total Hamiltonian

$$\begin{aligned} H =& E\sum_{\sigma} c_{\sigma}^{+}c_{\sigma} + Un_{\uparrow}n_{\downarrow} + \sum_{\mathbf{k}}\sum_{\sigma}\left\{E_a(\ \mathbf{k})a_{\sigma}^{+}(\ \mathbf{k})a_{\sigma}(\ \mathbf{k}) + E_b(\ \mathbf{k})b_{\sigma}^{+}(\ \mathbf{k})b_{\sigma}(\ \mathbf{k})\right\} \\ &+ \sum_{\mathbf{k}}\sum_{\sigma}\left\{V_a(\ \mathbf{k})a_{\sigma}^{+}(\ \mathbf{k})c_{\sigma} + V_a^{*}(\ \mathbf{k})c_{\sigma}^{+}a_{\sigma}(\ \mathbf{k}) + V_b(\ \mathbf{k})b_{\sigma}^{+}(\ \mathbf{k})c_{\sigma} + V_b^{*}(\ \mathbf{k})c_{\sigma}^{+}b_{\sigma}(\ \mathbf{k})\right\}, \\ n_{\sigma} =& c_{\sigma}^{+}c_{\sigma}, \quad \sigma = \uparrow, \downarrow, \\ E =& E^0 - \mu, \quad E_a(\mathbf{k}) = E_a^0(\mathbf{k}) - \mu_a, \quad E_b(\mathbf{k}) = E_b^0(\mathbf{k}) - \mu_b, \end{aligned} \tag{1}$$

where c_{σ} and c_{σ}^{+} are the destruction and creation operators for the electron at the energy level E^0 in the QD, $a_{\sigma}(\mathbf{k})$, $b_{\sigma}(\mathbf{k})$ and $a_{\sigma}^{+}(\mathbf{k})$, $b_{\sigma}^{+}(\mathbf{k})$ are those of the electrons with the kinetic energies $E_a^0(\mathbf{k})$, $E_b^0(\mathbf{k})$, resp., in the leads; μ, μ_a, μ_b are the corresponding chemical potentials, $V_a(\mathbf{k})$ and $V_b(\mathbf{k})$ are the coupling constants in the effective tunneling interaction Hamiltonian.

For the study of the Green functions we work in the Heisenberg picture and set

$$\begin{aligned} c_{\sigma}(t) &= e^{iHt}c_{\sigma}e^{-iHt}, & \bar{c}_{\sigma}(t) &= e^{iHt}c_{\sigma}^{+}e^{-iHt}, \\ a_{\sigma}(\ \mathbf{k},t) &= e^{iHt}a_{\sigma}(\ \mathbf{k})e^{-iHt}, & \bar{a}_{\sigma}(\ \mathbf{k},t) &= e^{iHt}a_{\sigma}^{+}(\ \mathbf{k})e^{-iHt}, \\ b_{\sigma}(\ \mathbf{k},t) &= e^{iHt}b_{\sigma}(\ \mathbf{k})e^{-iHt}, & \bar{b}_{\sigma}(\ \mathbf{k},t) &= e^{iHt}b_{\sigma}^{+}(\ \mathbf{k})e^{-iHt}. \end{aligned} \tag{2}$$

These formulae can be used not only for the real time t, but also for the complex time t in the Keldysh formalism. In terms of the operators in the l. h. s. of the formulae (2) we define the Green functions

$$G_{\sigma\sigma'}^{c\bar{c}}(t-t') = \delta_{\sigma\sigma'}G^{c\bar{c}}(t-t') = -i\left\langle T_C[c_{\sigma}(t)\bar{c}_{\sigma'}(t')]\right\rangle_{\beta}, \tag{3}$$

$$H_{\sigma\sigma'}^{c\bar{c}}(t-t') = \delta_{\sigma\sigma'}H^{c\bar{c}}(t-t') = -i\left\langle T_C[n_{-\sigma}(t)\,c_{\sigma}(t)\,\bar{c}_{\sigma'}\left(t'\right)]\right\rangle_{\beta}, \tag{4}$$

$$G_{\sigma\sigma'}^{a\bar{c}}(\ \mathbf{k};t-t') = \delta_{\sigma\sigma'}G^{a\bar{c}}(\ \mathbf{k};t-t') = -i\left\langle T_C[a_{\sigma}(\ \mathbf{k},t)\bar{c}_{\sigma'}(t')]\right\rangle_{\beta}, \tag{5}$$

$$H_{\sigma\sigma'}^{a\bar{c}}(\ \mathbf{k};t-t') = \delta_{\sigma\sigma'}H^{a\bar{c}}(\ \mathbf{k};t-t') = -i\left\langle T_C[n_{-\sigma}(t)a_{\sigma}(\ \mathbf{k},t)\bar{c}_{\sigma'}(t')]\right\rangle_{\beta}, \tag{6}$$

$$G_{\sigma\sigma'}^{ac\bar{c}\bar{c}}(\ \mathbf{k};t-t') = \delta_{\sigma\sigma'}G^{ac\bar{c}\bar{c}}(\ \mathbf{k};t-t') = -i\left\langle T_C[a_{-\sigma}(\ \mathbf{k},t)c_{\sigma}(t)\bar{c}_{-\sigma}(t)\bar{c}_{\sigma'}\left(t'\right)]\right\rangle_{\beta}, \tag{7}$$

$$G^{cc\bar{a}\bar{c}}_{\sigma\sigma'}(\ \mathbf{k};t-t') = \delta_{\sigma\sigma'}G^{cc\bar{a}\bar{c}}(\ \mathbf{k};t-t') = -i\left\langle T_C[c_{-\sigma}(t)c_\sigma(t)\,\bar{a}_{-\sigma}(\ \mathbf{k};t)\bar{c}_{\sigma'}\left(t'\right)]\right\rangle_\beta, \quad (8)$$

$$G^{aa\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t') = \delta_{\sigma\sigma'}G^{aa\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t') = -i\left\langle T_C[a_{-\sigma}(\mathbf{k},t)a_\sigma(\mathbf{l},t)\bar{c}_{-\sigma}(t)\,\bar{c}_{\sigma'}\left(t'\right)]\right\rangle_\beta, \quad (9)$$

$$G^{ac\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t') = \delta_{\sigma\sigma'}G^{ac\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t') = -i\left\langle T_C[a_{-\sigma}(\mathbf{k},t)c_\sigma(t)\,\bar{a}_{-\sigma}(\mathbf{l},t)\bar{c}_{\sigma'}\left(t'\right)]\right\rangle_\beta \quad (10)$$

and similarly for the others

$$G^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t'), \quad H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t'), \quad G^{bc\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t'),$$
$$G^{cc\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t'), \quad G^{ab\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t'), \quad G^{ac\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t')$$

etc., where $\langle\ldots\rangle_\beta$ denote the thermal equilibrium statistical average value

$$\langle\ldots\rangle_\beta = \frac{Tr\left\{\ldots e^{-\beta H}\right\}}{Tr\left\{e^{-\beta H}\right\}}$$

and T_C denote the ordering along the Keldysh contour C in the complex t plane presented in Fig. 1.

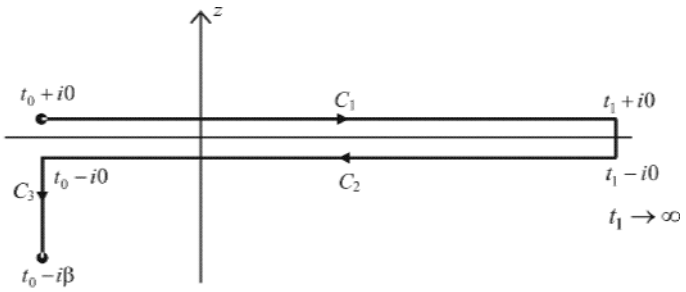

Fig. 1. Contour C consists of three parts $C = C_1 \cup C_2 \cup C_3$.

Because there is no magnetic interaction all Green functions (3)–(10) are proportional to $\delta_{\sigma\sigma'}$. From the equal-time canonical anti-commutation relations between the electron destruction and creation operators it follows the equations of motion for the operators

$$i\frac{dc_\sigma(t)}{dt} = Ec_\sigma(t) + Un_{-\sigma}(t)c_\sigma(t) + \sum_{\mathbf{k}}[V^*_a(\mathbf{k})\,a_\sigma(\mathbf{k},t) + V^*_b(\mathbf{k})\,b_\sigma(\mathbf{k},t)], \quad (11)$$

$$i\frac{d\bar{c}_\sigma(t)}{dt} = -E\bar{c}_\sigma(t) - Un_{-\sigma}(t)\,\bar{c}_\sigma(t) - \sum_{\mathbf{k}}[V_a(\mathbf{k})\bar{a}_\sigma(\mathbf{k},t) + V_b(\mathbf{k})\bar{b}_\sigma(\mathbf{k},t)], \quad (12)$$

$$i\frac{da_\sigma(\mathbf{k},t)}{dt} = E_a(\mathbf{k})a_\sigma(\mathbf{k},t) + V_a(\mathbf{k})c_\sigma(t), \quad (13)$$

$$i\frac{d\bar{a}_\sigma(\mathbf{k},t)}{dt} = -E_a(\mathbf{k})\bar{a}_\sigma(\mathbf{k},t) - V^*_a(\mathbf{k})\bar{c}_\sigma(t), \quad (14)$$

and similarly for $b_\sigma(\mathbf{k},t)$ and $\bar{b}_\sigma(\mathbf{k},t)$.

3. DIFFERENTIAL EQUATIONS FOR THE GREEN FUNCTIONS

Using the equation of motion (11) and the equal-time canonical anti-commutation relation between $c_\sigma(t)$ and $\bar{c}_{\sigma'}(t')$ it is easy to derive the differential equation for the Green function $G^{c\bar{c}}_{\sigma\sigma'}(t-t')$

$$\begin{aligned}\left[i\frac{d}{dt}-E\right]G^{c\bar{c}}_{\sigma\sigma'}(t-t') =&\delta_{\sigma\sigma'}\delta_C(t-t')+UH^{c\bar{c}}_{\sigma\sigma'}(t-t')\\ &+\sum_{\mathbf{k}}[V^*_a(\mathbf{k})G^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')+V^*_b(\mathbf{k})G^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')],\end{aligned} \tag{15}$$

which contains the Green functions $H^{c\bar{c}}_{\sigma\sigma'}(t-t')$, $G^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$ and $G^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$. These new functions must satisfy following differential equations which can be also derived by using the equations of motion (11)–(14)

$$\begin{aligned}&\left[i\frac{d}{dt}-(E+U)\right]H^{c\bar{c}}_{\sigma\sigma'}(t-t')\\ =&n\delta_C(t-t')+\sum_{\mathbf{k}}[V^*_a(\mathbf{k})H^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')+V^*_b(\mathbf{k})H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')]\\ &+\sum_{\mathbf{k}}\Big[V^*_a(\mathbf{k})G^{ac\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')+V^*_b(\mathbf{k})G^{bc\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')\\ &-V_a(\mathbf{k})G^{cc\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')-V_b(\mathbf{k})G^{cc\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')\Big],\end{aligned} \tag{16}$$

where

$$n=\left\langle c^+_\uparrow c_\uparrow\right\rangle=\left\langle c^+_\downarrow c_\downarrow\right\rangle, \tag{17}$$

$$\left[i\frac{d}{dt}-E_a(\mathbf{k})\right]G^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')=V_a(\mathbf{k})G^{c\bar{c}}_{\sigma\sigma'}(t-t'), \tag{18}$$

and similarly for $G^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$.

Introduce the complex-time Green function $S^E(t-t')$ of the free electron with a given energy E. It is the solution of the differential equation

$$\left[i\frac{d}{dt}-E\right]S^E(t-t')=\delta_C(t-t'). \tag{19}$$

Then we can write the solution of the differential equation (18) in the integral form

$$G^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')=V_a(\mathbf{k})\int_C dt''S^E(t-t'')G^{c\bar{c}}_{\sigma\sigma'}(t-t''), \tag{20}$$

and similarly for $G^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$. Substituting the expression of the form (20) for $G^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$ and $G^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$ into the r.h.s. of the differential equation (15) for $G^{c\bar{c}}_{\sigma\sigma'}(t-t')$ we rewrite this equation in the new form

$$\left[i\frac{d}{dt}-E\right]G^{c\bar{c}}_{\sigma\sigma'}(t-t')=\delta_{\sigma\sigma'}\delta_C(t-t')+UH^{c\bar{c}}_{\sigma\sigma'}(t-t')+\int_C dt''\Sigma^{(1)}(t-t'')G^{c\bar{c}}_{\sigma\sigma'}(t''-t), \tag{21}$$

where $\Sigma^{(1)}(t-t')$ is the following self-energy part

$$\Sigma^{(1)}(t-t') = \sum_{\mathbf{k}} \left\{ |V_a(\mathbf{k})|^2 \, S^{E_a(\mathbf{k})}(t-t') + |V_b(\mathbf{k})|^2 \, S^{E_b(\mathbf{k})}(t-t') \right\}. \tag{22}$$

The differential equation for the Green function $H^{c\bar{c}}_{\sigma\sigma'}(t-t')$ contains the Green function $H^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$, $H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$, $G^{ac\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$, $G^{bc\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$, $G^{cc\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$ and $G^{cc\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$ which must satisfy following differential equations

$$\left[i\frac{d}{dt} - E_a(\mathbf{k}) \right] H^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t') = V_a(\mathbf{k}) H^{c\bar{c}}_{\sigma\sigma'}(t-t'), \tag{23}$$

and similarly for $H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$,

$$\begin{aligned}
&\left[i\frac{d}{dt} - E_a(\mathbf{k}) \right] G^{ac\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t') \\
&= \left\langle \left\{ a_{-\sigma}(\mathbf{k}) c_\sigma c^+_{-\sigma}, c^+_{\sigma'} \right\} \right\rangle \delta_C(t-t') + V_a(\mathbf{k}) [H^{c\bar{c}}_{\sigma\sigma'}(t-t') - G^{c\bar{c}}_{\sigma\sigma'}(t-t')] \\
&\quad + \sum_{\mathbf{l}} [V^*_a(\mathbf{l}) G^{aa\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t') + V^*_b(\mathbf{l}) G^{ab\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t')] \\
&\quad - \sum_{\mathbf{l}} [V_a(\mathbf{l}) G^{ac\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t') + V_b(\mathbf{l}) G^{ac\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t')],
\end{aligned} \tag{24}$$

and similarly for $G^{bc\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$,

$$\begin{aligned}
&\left\{ i\frac{d}{dt} - [2E - E_a(\mathbf{k}) + U] \right\} G^{cc\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t') \\
&= \left\langle \{ c_{-\sigma} c_\sigma a^+_{-\sigma}(\mathbf{k}), c^+_{\sigma'} \} \right\rangle \delta_C(t-t') - V^*_a(\mathbf{k}) [H^{c\bar{c}}_{\sigma\sigma'}(t-t') - G^{c\bar{c}}_{\sigma\sigma'}(t-t')] \\
&\quad + \sum_{\mathbf{l}} \left\{ V^*_a(\mathbf{l}) [G^{ac\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t-t') + G^{ca\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t-t')] \right. \\
&\quad \left. + V^*_b(\mathbf{l}) [G^{bc\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t-t') + G^{cb\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t-t')] \right\},
\end{aligned} \tag{25}$$

and similarly for $G^{cc\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$. The solutions of the differential equations (23), (24) and (25) can be written in the integral form

$$H^{a\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t') = V_a(\mathbf{k}) \int\limits_C dt'' S^{E_a(\mathbf{k})}(t-t'') H^{c\bar{c}}_{\sigma\sigma'}(t''-t'), \tag{26}$$

and similarly for $H^{b\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$,

$$\begin{aligned}
&G^{ac\,\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')\\
&=\left\langle\{a_{-\sigma}(\mathbf{k})c_\sigma c^+_{-\sigma},c^+_{\sigma'}\}\right\rangle S^{E_a(\mathbf{k})}(t-t')\\
&\quad+V_a(\mathbf{k})\int\limits_C dt"\,S^{E_a(\mathbf{k})}(t-t'')\,[H^{c\bar{c}}_{\sigma\sigma'}(t-t')-G^{c\bar{c}}_{\sigma\sigma'}(t-t')]\\
&\quad+\int\limits_C dt''S^{E_a(\mathbf{k})}(t-t'')\sum_{\mathbf{l}}[V^*_a(\mathbf{l})G^{aa\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t''-t')+V^*_b(\mathbf{l})G^{ab\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t''-t')]\\
&\quad-\int\limits_C dt''S^{E_a(\mathbf{k})}(t-t'')\sum_{\mathbf{l}}[V_a(\mathbf{l})G^{ac\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t''-t')+V_b(\mathbf{l})G^{ac\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t''-t')],
\end{aligned}\tag{27}$$

and similarly for $G^{bc\bar{c}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$,

$$\begin{aligned}
&G^{cc\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')\\
&=\left\langle\{c_{-\sigma}c_\sigma a^+_{-\sigma}(\mathbf{k}),c^+_{\sigma'}\}\right\rangle S^{2E+U-E_a(\mathbf{k})}(t-t')\\
&\quad-V^*_a(\mathbf{k})\int\limits_C dt''S^{2E+U-E_a(\mathbf{k})}(t-t'')[H^{c\bar{c}}_{\sigma\sigma'}(t''-t)-G^{c\bar{c}}_{\sigma\sigma'}(t''-t)]\\
&\quad+\int\limits_C dt''S^{2E+U-E_a(\mathbf{k})}(t-t'')\sum_{\mathbf{l}}\Big\{V^*_a(\mathbf{l})[G^{ac\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t''-t')+G^{ca\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t''-t')]\\
&\qquad\qquad+V^*_b(\mathbf{l})[G^{bc\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t''-t')+G^{cb\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{l},\mathbf{k};t''-t']\Big\},
\end{aligned}\tag{28}$$

and similarly for $G^{cc\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k};t-t')$. Substituting these solutions into the r.h.s. of the differential equation for $H^{c\bar{c}}_{\sigma\sigma'}(t-t')$ we rewrite this equation in the new form

$$\begin{aligned}
&\left[i\frac{d}{dt}-(E+U)\right]H^{c\bar{c}}_{\sigma\sigma'}(t-t')\\
&=n\delta_{\sigma\sigma'}\delta_C(t-t')+\int\limits_C dt''\Sigma^{(1)}(t-t'')H^{c\bar{c}}_{\sigma\sigma'}(t''-t)\\
&\quad+\sum_{\mathbf{k}}\Bigg\{V^*_a(\mathbf{k})\left\langle\{a_{-\sigma}(\mathbf{k})c_\sigma c^+_{-\sigma},c^+_{\sigma'}\}\right\rangle S^{E_a(\mathbf{k})}(t-t')\\
&\qquad+|V_a(\mathbf{k})|^2\int\limits_C dt''S^{E_a(\mathbf{k})}(t-t'')[H^{c\bar{c}}_{\sigma\sigma'}(t-t')-G^{c\bar{c}}_{\sigma\sigma'}(t-t')]\Bigg\}
\end{aligned}$$

$$
\begin{aligned}
&+\int\limits_C dt'' \sum_{\mathbf{k}} V_a^*(\mathbf{k}) S^{E_a(\mathbf{k})}(t-t'') \sum_{\mathbf{l}} [V_a^*(\mathbf{l}) G_{\sigma\sigma'}^{aa\bar{c}\bar{c}}(\mathbf{k},\mathbf{l};t''-t') + V_b^*(\mathbf{l}) G_{\sigma\sigma'}^{ab\bar{c}\bar{c}}(\mathbf{k},\mathbf{l};t''-t')] \\
&-\int\limits_C dt" \sum_{\mathbf{k}} V_a^*(\mathbf{k}) S^{E_a(\mathbf{k})}(t-t'') \sum_{\mathbf{l}} [V_a(\mathbf{l}) G_{\sigma\sigma'}^{ac\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t''-t') + V_b(\mathbf{l}) G_{\sigma\sigma'}^{ac\bar{b}\bar{c}}(\mathbf{k},\mathbf{l};t''-t')] \\
&-\sum_{\mathbf{k}} \Bigg\{ V_a(\mathbf{k}) \left\langle \{c_{-\sigma} c_\sigma a_{-\sigma}^+(\mathbf{k}), c_{\sigma'}^+\} \right\rangle S^{2E+U-E_a(\mathbf{k})}(t-t') \\
&\qquad + |V_a(\mathbf{k})|^2 \int\limits_C dt'' S^{2E+U-E_a(\mathbf{k})}(t-t'') [H_{\sigma\sigma'}^{c\bar{c}}(t''-t) - G_{\sigma\sigma'}^{c\bar{c}}(t''-t)] \Bigg\} \\
&-\int\limits_C dt'' \sum_{\mathbf{k}} V_a(\mathbf{k}) S^{2E+U-E_a(\mathbf{k})}(t-t'') \sum_{\mathbf{l}} V_a^*(\mathbf{l}) [G_{\sigma\sigma'}^{ac\bar{a}\bar{c}}(\mathbf{l},\mathbf{k};t''-t') + G_{\sigma\sigma'}^{ca\bar{a}\bar{c}}(\mathbf{l},\mathbf{k};t''-t')] \\
&-\int\limits_C dt'' \sum_{\mathbf{k}} V_a(\mathbf{k}) S^{2E+U-E_a(\mathbf{k})}(t-t'') V_b^*(\mathbf{l}) [G_{\sigma\sigma'}^{bc\bar{a}\bar{c}}(\mathbf{l},\mathbf{k};t''-t') + G_{\sigma\sigma'}^{cb\bar{a}\bar{c}}(\mathbf{l},\mathbf{k};t''-t')] \\
&+ \text{similar terms with the interchange} (a \leftrightarrow b).
\end{aligned}
\tag{29}
$$

4. MEAN- FIELD APPROXIMATION

The r.h.s. of the equation (29) for the Green function $H_{\sigma\sigma'}^{c\bar{c}}(t-t')$ contains the multi-electron Green functions

$$
\begin{aligned}
&G_{\sigma\sigma'}^{aa\bar{c}\bar{c}}(\mathbf{k},\mathbf{l};t-t'), \quad G_{\sigma\sigma'}^{ab\bar{c}\bar{c}}(\mathbf{k},\mathbf{l};t-t'), \quad G_{\sigma\sigma'}^{ac\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t'), \quad G_{\sigma\sigma'}^{ac\bar{b}\bar{c}}(\mathbf{k};t-t'), \\
&G_{\sigma\sigma'}^{ca\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t'), \quad G_{\sigma\sigma'}^{bc\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t'), \quad G_{\sigma\sigma'}^{bc\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t')
\end{aligned}
$$

and the similarly ones with the interchange $(a \leftrightarrow b)$. In order to decouple this equation with those for the last multi-electron Green functions we apply the mean-field approximation to the products of four operators in the expressions of above-mentioned Green functions. Consider first the Green function $G_{\sigma\sigma'}^{ac\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t')$ expressing in terms of the mean value of the product $\bar{a}_{-\sigma}(\mathbf{k},t) a_{-\sigma}(\mathbf{l},t) c_\sigma(t) \bar{c}_{\sigma'}(t')$. This product is that of two pairs each of which consists of a creation operator ($\bar{a}_{-\sigma}(\mathbf{k},t)$ or $\bar{c}_{\sigma'}(t)$) and a destruction one ($a_{-\sigma}(\mathbf{l},t)$ or $c_\sigma(t)$) for the electrons of one and the same type. The mean-field approximation can be applied to the T-product of these four operators in the following manner

$$
\left\langle T_C[\bar{a}_{-\sigma}(\mathbf{l};t) a_{-\sigma}(\mathbf{k};t) c_\sigma(t) \bar{c}_{\sigma'}(t')] \right\rangle \approx \left\langle \bar{a}_{-\sigma}(\mathbf{l};t) a_{-\sigma}(\mathbf{k};t) \right\rangle \left\langle T_C[c_\sigma(t) \bar{c}_{\sigma'}(t')] \right\rangle
$$

with

$$
\begin{aligned}
&\left\langle \bar{a}_{-\sigma}(\mathbf{l};t) a_{-\sigma}(\mathbf{k};t) \right\rangle = \delta_{kl} \left\langle \bar{a}_{-\sigma}(\mathbf{k}) a_{-\sigma}(\mathbf{k}) \right\rangle = \delta_{kl} n_a(\mathbf{k}), \\
&\left\langle T_C[c_\sigma(t) \bar{c}_{\sigma'}(t')] \right\rangle = i G_{\sigma\sigma'}^{c\bar{c}}(t-t').
\end{aligned}
$$

As the result we have

$$
G_{\sigma\sigma'}^{ac\bar{a}\bar{c}}(\mathbf{k},\mathbf{l};t-t') \approx -\delta_{\mathbf{kl}} [1 - n_a(\mathbf{k})] G_{\sigma\sigma'}^{c\bar{c}}(t-t'), \tag{30}
$$

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

$$n_a(\mathbf{k}) = \frac{e^{-\beta E_a(\mathbf{k})}}{1 + e^{-\beta E_a(\mathbf{k})}},$$

and similarly for $G^{bc\bar{b}\bar{c}}_{\sigma\sigma'}(\mathbf{k}, \mathbf{l}; t - t')$. Applying the mean-field approximation to each of the others among above-mentioned multi-electron Green functions in any manner we always obtain the vanishing mean values in the lowest order the perturbation theory with respect to the effective tunneling coupling constants $V_{a,b}(\mathbf{k})$. 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 tunneling coupling constants. This means that in this second order they do not give contributions. Thus in the second order approximation the equation (29) is simplified and becomes

$$\begin{aligned}\left[i\frac{d}{dt} - (E+U)\right] H^{c\bar{c}}_{\sigma\sigma'}(t-t') =& n\delta_{\sigma\sigma'}\delta_C(t-t') + \Gamma(t-t') \\ &+ \int\limits_C dt''\Sigma^{(2)}(t-t'')H^{c\bar{c}}_{\sigma\sigma'}(t''-t) \\ &- \int\limits_C dt''\Sigma^{(3)}(t-t'')G^{c\bar{c}}_{\sigma\sigma'}(t''-t),\end{aligned} \tag{31}$$

where

$$\begin{aligned}\Gamma(t-t') = \sum_{\mathbf{k}} \Big[& V^*_a(\mathbf{k}) \left\langle \{a_{-\sigma}(\mathbf{k}) c_\sigma c^+_{-\sigma}, c^+_{\sigma'}\} \right\rangle S^{E_a(\mathbf{k})}(t-t') \\ & - V_a(\mathbf{k}) \left\langle \{c_{-\sigma} c_\sigma a^+_{-\sigma}(\mathbf{k}), c^+_{\sigma'}\} \right\rangle S^{2E+U-E_a(\mathbf{k})}(t-t') + (a \to b) \Big],\end{aligned} \tag{32}$$

$$\Sigma^{(2)}(t-t') = \sum_{\mathbf{k}} \Big\{ |V_a(\mathbf{k})|^2 \left[2S^{E_a(\mathbf{k})}(t-t') + S^{2E+U-E_a(\mathbf{k})}(t-t') \right] + (a \to b) \Big\}, \tag{33}$$

$$\Sigma^{(3)}(t-t') = \sum_{\mathbf{k}} \Big\{ n_a(\mathbf{k}) |V_a(\mathbf{k})|^2 \left[S^{E_a(\mathbf{k})}(t-t') + S^{2E+U-E_a(\mathbf{k})}(t-t') \right] + (a \to b) \Big\}. \tag{34}$$

Note that in the r. h. s. of the formulae (32)-(34) there appear the crossing terms containing $S^{2E+U-E_a(\mathbf{k})}(t-t')$. They must disappear in the noncrossing approximation.

To proceed further we note that

$$\begin{aligned}\left\langle \{a_{-\sigma}(\mathbf{k}) c_\sigma c^+_\sigma, c^+_{\sigma'}\} \right\rangle &= -\delta_{\sigma\sigma'} \left\langle a_{-\sigma}(\mathbf{k}) c^+_{-\sigma} \right\rangle, \\ \left\langle \{c_{-\sigma} c_\sigma a^+_\sigma(\mathbf{k}), c^+_{\sigma'}\} \right\rangle &= -\delta_{\sigma\sigma'} \left\langle a_{-\sigma}(\mathbf{k}) c^+_{-\sigma} \right\rangle^*,\end{aligned} \tag{35}$$

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

$$\left\langle a_{-\sigma}(\mathbf{k}) c^+_{-\sigma} \right\rangle = iG^{ac}_{-\sigma-\sigma}(\mathbf{k}; +0). \tag{36}$$

For evaluating the vertex (32) in the second order with respect to the tunneling coupling constants $V_{a,b}(\mathbf{k})$ we calculate the limiting value (36) in the first order. Introduce the

Fourier transformations of the Green functions, for example

$$\begin{aligned} G^{a\bar{c}}(\mathbf{k};t) &= \tfrac{1}{2\pi}\int\limits_{-\infty}^{+\infty} d\omega e^{-i\omega t}\tilde{G}^{a\bar{c}}(\mathbf{k};\omega), \\ S^{E_a(\mathbf{k})}(t) &= \tfrac{1}{2\pi}\int\limits_{-\infty}^{+\infty} d\omega e^{-i\omega t}\tilde{S}^{E_a(\mathbf{k})}(\omega), \\ G^{c\bar{c}}(t) &= \tfrac{1}{2\pi}\int\limits_{-\infty}^{+\infty} d\omega e^{-i\omega t}\tilde{G}^{c\bar{c}}(\omega). \end{aligned} \tag{37}$$

From the equation (18) it follows that

$$\tilde{G}^{a\bar{c}}(\mathbf{k};\omega) = V_a(\mathbf{k})\tilde{S}^{E_a(\mathbf{k})}(\omega)\tilde{G}^{c\bar{c}}(\omega). \tag{38}$$

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

$$\begin{aligned} G^{a\bar{c}}(\mathbf{k};\omega) =& V_a(\mathbf{k})\left[\frac{n_a(\mathbf{k})}{\omega - i0 - E_a(\mathbf{k})} + \frac{1-n_a(\mathbf{k})}{\omega + i0 - E_a(\mathbf{k})}\right] \\ &+ \frac{1}{Z}\left[\frac{e^{-\beta E}}{\omega - i0 - E} + \frac{e^{-\beta(2E+U)}}{\omega - i0 - E - U} + \frac{1}{\omega + i0 - E} + \frac{e^{-\beta E}}{\omega + i0 - E - U}\right], \end{aligned} \tag{39}$$

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

It is easy to calculate the limit

$$G^{a\bar{c}}(\mathbf{k};+0) = \lim_{\varepsilon\to+0}\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} d\omega e^{-i\omega\varepsilon}\tilde{G}^{a\bar{c}}(\mathbf{k},\omega). \tag{40}$$

by using the residue theorem and obtain

$$\left\langle a_{-\sigma}(\mathbf{k})c^{+}_{-\sigma}\right\rangle = -\nu_a(\mathbf{k})V_a(\mathbf{k}), \tag{41}$$

where

$$\nu_a(\mathbf{k}) = \frac{1}{Z}\left\{\frac{e^{-\beta E} - [1+e^{-\beta E}]n_a(\mathbf{k})}{E - E_a(\mathbf{k})} + e^{-\beta E}\frac{e^{-\beta(E+U)} - [1+e^{-\beta(E+U)}]n_a(\mathbf{k})}{E + U - E_a(\mathbf{k})}\right\}, \tag{42}$$

Therefore the formula (32) can be rewritten in the following manner

$$\Gamma(t-t') = \sum_{\mathbf{k}}\Big\{\,|V_a(\mathbf{k})|^2\,\nu_a(\mathbf{k})[S^{E_a(\mathbf{k})}(t-t') - S^{2E+U-E_a(\mathbf{k})}(t-t')] + (a\to b)\Big\}. \tag{43}$$

In many previous works this vertex was omitted.

5. CONCLUSION AND DISCUSSION

In the second order approximation with respect to the effective tunneling coupling constants and the mean-field approximation for the products of 4 operators in the Green function $G^{ac\bar{a}\bar{c}}_{\sigma\sigma'}(\mathbf{k},\mathbf{l};t-t')$ the system of the two Dyson equations for the complex-time non-equilibrium Green functions were derived:

$$\left[i\frac{d}{dt}-E\right]G^{c\bar{c}}(t-t')=\delta_C(t-t')+UH^{c\bar{c}}(t-t')+\int\limits_C dt''\Sigma^{(1)}(t-t'')G^{c\bar{c}}(t''-t'), \quad (44)$$

$$\left[i\frac{d}{dt}-(E+U)\right]H^{c\bar{c}}(t-t')=n\delta_C(t-t')+\Gamma(t-t')+\int\limits_C dt''\Sigma^{(2)}(t-t'')H^{c\bar{c}}(t''-t') - \int\limits_C dt''\Sigma^{(3)}(t-t'')G^{c\bar{c}}(t''-t'), \quad (45)$$

where the self-energy parts $\Sigma^{(i)}(t-t'), i=1,2,3$ and the vertex $\Gamma(t-t')$ are determined by the formulae (22), (33), (34) and (43). If t and t' are the imaginary times $t=-i\tau$, $t'=-i\tau'$ then this system of equations becomes that of two Dyson equations for the imaginary time Green functions

$$G^{c\bar{c}}(\tau-\tau')=\left\langle T_\tau[c_\sigma(\tau)\bar{c}_{\sigma'}(\tau')]\right\rangle, \quad (46)$$

$$H^{c\bar{c}}(\tau-\tau')=\left\langle T_\tau[n_{-\sigma}(\tau)c_\sigma(\tau)\bar{c}_{\sigma'}(\tau')]\right\rangle. \quad (47)$$

From the equations (44) and (45) and formulae (22), (33), (34) and (43) with the complex times it is straightforward to derive the Dyson equations for the imaginary time Green functions

$$\left(\frac{d}{d\tau}-E\right)G^{c\bar{c}}(\tau-\tau')=\delta_C(\tau-\tau')+UH^{c\bar{c}}(\tau-\tau')+\int\limits_C d\tau''\Sigma^{(1)}(\tau-\tau'')G^{c\bar{c}}(\tau''-\tau') \quad (48)$$

$$\left(\frac{d}{d\tau}+E+U\right)H^{c\bar{c}}(\tau-\tau')=n\delta_C(\tau-\tau')+\Gamma(\tau-\tau')+\int\limits_C d\tau''\Sigma^{(2)}(\tau-\tau'')H^{c\bar{c}}(\tau''-\tau') - \int\limits_C d\tau''\Sigma^{(3)}(\tau-\tau'')G^{c\bar{c}}(\tau''-\tau'), \quad (49)$$

with following self-energy parts $\Sigma^{(i)}(\tau-\tau')$ and vertex $\Gamma(\tau-\tau')$

$$\Sigma^{(1)}(\tau-\tau')=\sum_{\mathbf{k}}\Big\{\,|V_a(\mathbf{k})|^2\,S^{E_a(\mathbf{k})}(\tau-\tau')+|V_b(\mathbf{k})|^2\,S^{E_b(\mathbf{k})}(\tau-\tau')\Big\}, \quad (50)$$

$$\Sigma^{(2)}(\tau-\tau')=\sum_{\mathbf{k}}\Big\{|V_a(\,\mathbf{k})|^2\left[2S^{E_a(\,\mathbf{k})}(\tau-\tau')+S^{2E+U-E_a(\,\mathbf{k})}(\tau-\tau')\right]+(a\to b)\Big\} \quad (51)$$

$$\Sigma^{(3)}(\tau-\tau')=\sum_{\mathbf{k}}\Big\{\,n_a(\mathbf{k})\,|V_a(\mathbf{k})|^2\,[S^{E_a(\mathbf{k})}(\tau-\tau')+S^{2E+U-E_a(\mathbf{k})}(\tau-\tau')]+(a\to b)\Big\} \quad (52)$$

$$\Gamma(\tau-\tau')=\sum_{\mathbf{k}}\left\{|V_a(\ \mathbf{k})|^2\,\nu_a(\ \mathbf{k})[S^{E_a(\ \mathbf{k})}(\tau-\tau')-S^{2E+U-E_a(\ \mathbf{k})}(\tau-\tau')]+(a\to b)\right\} \tag{53}$$

For the study of the real-time Green functions one often considers the case $t_0\to-\infty$. In this limit the contribution of the imaginary-time interval $[t_0,t_0-i\beta]$ vanishes and the integral over the contour C becomes the sum of two integral on two straight lines : C_1 from $-\infty$ to $+\infty$ in the upper half plane and C_2 from $+\infty$ to $-\infty$ in the lower half plane (Fig. 1). Because each complex time t or t' can belong either to C_1 or C_2, each complex-time Green functions is a set of four functions of the real variable $t-t'$, for example

$$G\left(t-t'\right)=\begin{cases} G(t-t')_{11} & \textit{if } t,t'\in C_1,\\ G(t-t')_{12} & \textit{if } t\in C_1,t'\in C_2,\\ G(t-t')_{21} & \textit{if } t\in C_2,t'\in C_1,\\ G(t-t')_{22} & \textit{if } t,t'\in C_2. \end{cases} \tag{54}$$

Therefore the Fourier transform of each complex-time Green function is a set of four Fourier transforms of four functions of the real time $t-t'$ and can be represented as a 2×2 matrix

$$\begin{aligned}\hat{G}(\omega)&=\begin{pmatrix}\tilde{G}(\omega)_{11}\tilde{G}(\omega)_{12}\\ \tilde{G}(\omega)_{21}\tilde{G}(\omega)_{22}\end{pmatrix},\\ \hat{H}(\omega)&=\begin{pmatrix}\tilde{H}(\omega)_{11}\tilde{H}(\omega)_{12}\\ \tilde{H}(\omega)_{21}\tilde{H}(\omega)_{22}\end{pmatrix}.\end{aligned} \tag{55}$$

From the differential – integral equations (44) and (45) it follows two matrix equations for the matrices (55):

$$(\omega-E)\hat{G}(\omega)=1+U\hat{H}(\omega)+\hat{\Sigma}^{(1)}(\omega)\hat{\eta}\hat{G}(\omega), \tag{56}$$

$$(\omega-E-U)\hat{H}(\omega)=n+\hat{\Gamma}+\hat{\Sigma}^{(2)}\hat{\eta}\,\hat{H}(\omega)-\hat{\Sigma}^{(3)}(\omega)\hat{\eta}\hat{G}(\omega) \tag{57}$$

where $\hat{\eta}$ is the metric matrix

$$\hat{\eta}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \tag{58}$$

and $\hat{\Sigma}^{(1)}(\omega)$, $\hat{\Sigma}^{(2)}(\omega)$, $\hat{\Sigma}^{(3)}(\omega)$ and $\hat{\Gamma}(\omega)$ are the matrices of the Fourier transforms of the self-energy parts and the vertex.

By solving the system of equations (56) and (57) we can derive the analytical expressions of the Fourier transforms of the Green functions. They will be used for the study of the physical characters of the QD in subsequent works.

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