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Analytical Asymptotic Expressions for the Green's Function of the Electron in a Single-Level Quantum Dot at the Kondo and the Fano Resonances

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The Kondo and the Fano resonances in the two-point Green's function of the single-level quantum dot were found and investigated in many previous works by means of different numerical calculation methods. In this report, we present a derivation of the analytical forms of the resonance terms in the expression of the two-point Green's function. For that purpose, the system of Dyson equations for the two-point nonequilibrium Green's functions in the complex-time Keldysh formalism was established to the second order in the tunneling coupling constants with the mean field approximation for the statistical averages of the products of four electron creation and destruction operators. This system of Dyson equations was solved exactly by means of the computer algebra and the analytical expressions for the resonance terms are derived. The conditions for the existence of the Kondo or the Fano resonances were found.

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I. INTRODUCTION

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 [1–22]. 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's functions. In the pioneering theoretical works [1, 3] on the electron transport through a single-level QD, the differential equations for the real-time Green's 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's functions contain multi-electron Green's functions and all the coupled equations for these Green's 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 nonequilibrium process one should work with the Keldysh formalism of nonequilibrium complex-time Green's functions [23,24].

In the study of the nonequibrium complex-time Green's functions by means of the perturbation theory with respect to the Coulomb interaction one usually retains some chain of ladder diagrams and assumes also the noncrossing approximation (NCA). The systems of equations for the Green's functions were solved by means of different numerical methods, for example the Quantum Monte Carlo technique [13] and the numerical renormalization group method [10, 12, 14, 17]. The electron two-point Green's functions were shown to have resonance related to the Kondo effect. Beside of Kondo resonance,

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the Fano quasi-bound state in the energy spectrum of the electron system of the QD and the leads might also give some resonant contribution.

In this work, the exact analytical expressions of the Kondo and the Fano resonance terms are derived with the help of the computer algebra systems Mathematica and Maple by explicitly solving the matrix equations for the underlying Green's functions. From these analytical expressions, we obtain the whole set of resonances and the conditions for their existence. In particular, we shall demonstrate the distinction between the Kondo and the Fano resonances, if they do exist.

II. SYSTEM OF DYSON EQUATIONS

Consider the nanosystem consisting of a single-level QD connected to two leads through the potential barriers with the total Hamiltonian

$$\begin{aligned} H &= E\sum_{\sigma} c_{\sigma}^{+}c_{\sigma} + UN_{\uparrow}N_{\downarrow} \\ &+ \sum_{\boldsymbol{k}}\sum_{\sigma}\left\{E_a(\boldsymbol{k})a_{\sigma}^{+}(\boldsymbol{k})a_{\sigma}(\boldsymbol{k}) + E_b(\boldsymbol{k})b_{\sigma}^{+}(\boldsymbol{k})b_{\sigma}(\boldsymbol{k})\right\} \\ &+ \sum_{\boldsymbol{k}}\sum_{\sigma}\left\{V_a(\boldsymbol{k})a_{\sigma}^{+}(\boldsymbol{k})c_{\sigma} + V_a^{*}(\boldsymbol{k})c_{\sigma}^{+}a_{\sigma}(\boldsymbol{k})\right. \\ &\left. + V_b(\boldsymbol{k})b_{\sigma}^{+}(\boldsymbol{k})c_{\sigma} + V_b^{*}(\boldsymbol{k})c_{\sigma}^{+}b_{\sigma}(\boldsymbol{k})\right\}, \end{aligned} \tag{1}$$

where $a_{\sigma}(\boldsymbol{k})$, $b_{\sigma}(\boldsymbol{k})$ and $a_{\sigma}^{+}(\boldsymbol{k})$, $b_{\sigma}^{+}(\boldsymbol{k})$ are the annihilation and creation operators of the electrons with momenta $\boldsymbol{k}$ in the two leads,

$$N_{\sigma} = c_{\sigma}^{+}c_{\sigma},$$

and $G_{\sigma\sigma'}(t-t')_C$ denotes the complex time single-electron Green's function and is given by

$$\begin{aligned} G_{\sigma\sigma'}(t-t')_C &= \delta_{\sigma\sigma'}G(t-t')_C \\ &= -i\left\langle T_C\left[c_{\sigma}(t)c_{\sigma'}^{+}(t')\right]\right\rangle, \end{aligned} \tag{2}$$

which is a set of four functions

$$G_{\sigma\sigma'}(t-t')_{\alpha\beta} = \delta_{\sigma\sigma'}G(t-t')_{\alpha\beta}, \qquad \alpha,\,\beta = 1,\,2 \tag{3}$$

with the Fourier transforms

$$\widetilde{G}_{\sigma\sigma'}(\omega)_{\alpha\beta} = \delta_{\sigma\sigma'}\widetilde{G}(\omega)_{\alpha\beta}.$$

Due to the presence of the Coulomb interaction term in the Hamiltonian in Eq. (1), the differential equation for the Green's function in Eq. (2) contains a new Green's function $H(t-t')_C$ defined as

$$\begin{aligned} H_{\sigma\sigma'}(t-t')_C &= \delta_{\sigma\sigma'}H(t-t')_C \\ &= -i\left\langle T_C\left[N_{-\sigma}c_{\sigma}(t)c_{\sigma'}^{+}(t')\right]\right\rangle. \end{aligned} \tag{4}$$

From the Heisenberg equations of motion for the operators $c_{\sigma}(t)$, $a_{\sigma}(\boldsymbol{k},t)$ and $b_{\sigma}(\boldsymbol{k},t)$, we can derive the differential equations for the Green's functions. Applying the mean field approximation to the products of the four operators and neglecting the terms of fourth and higher orders with respect to the tunneling coupling constants $V_a(\boldsymbol{k})$ and $V_b(\boldsymbol{k})$, we obtain the system of Dyson equations containing three self-energy parts, $\Sigma^{(i)}(t-t')_{\alpha\beta}$, $i = 1,\,2,\,3$, a vertex $\rho(t-t')_{\alpha\beta}$ and the constant

$$n = \langle c_{\alpha}^{+}c_{\alpha}\rangle = -iG(-0)_{11}.$$

In the derivation of the equations the contributions of all crossing terms have been taken into account: there was no necessity to use the NCA. Moreover, in all previous works on the Green's functions of quantum dots in the Keldysh formalism, the system of equations was solved by using numerical methods. In the present work, we use the analytical expressions for the exact solution of the system of Dyson equations.

In terms of the 2×2 matrices $\hat{G}(\omega)$, $\hat{H}(\omega)$, $\hat{\Sigma}^{(i)}(\omega)$ and $\hat{\rho}(\omega)$ with the matrix elements being the Fourier transforms of the functions $G(t-t')_{\alpha\beta}$, $H(t-t')_{\alpha\beta}$, $\Sigma^{(i)}(t-t')_{\alpha\beta}$ and $\rho(t-t')_{\alpha\beta}$, the system of Dyson equations becomes that of two matrix equations. From these two matrix equations, we derive two similar systems of algebraic equations, each of which consists of four equations for $G(\omega)_{\alpha 1}$ and $H(\omega)_{\alpha 1}$ or $G(\omega)_{\alpha 2}$ and $H(\omega)_{\alpha 2}$, $\alpha = 1,\,2$. For the investigation of the electron transport through the QD, it is necessary to study the function $G(\omega)_{11}$. By solving the system of equations for the functions $G(\omega)_{\alpha 1}$ and $H(\omega)_{\alpha 1}$, we have derived the expression of this function in the form

$$G(\omega)_{11} = \frac{Z(\omega)}{Y(\omega)}. \tag{5}$$

The explicit forms of the rather cumbersome numerator $Z(\omega)$ and denominator $Y(\omega)$ in Eq. (5) were found from the system of two matrix equations for $\hat{G}(\omega)$ and $\hat{H}(\omega)$ by solving exactly. This was done by using the computer algebra methods implemented in Maple and Mathematica. We used both computer algebra systems to verify the expressions obtained and to analyze the possible applicability of each of these software systems in view of much more tedious computations related to the extension of the study in the present paper.

III. KONDO AND FANO RESONANCES

Now we consider the resonances of the Green's function in Eq. (5). It contains the dispersion integrals with the spectral functions

$$\begin{aligned} \Gamma_{a,b}^{(p)}(\omega) &= \pi\sum_{\boldsymbol{k}}\left[\frac{e^{-\beta E_{a,b}(\boldsymbol{k})}}{1+e^{-\beta E_{a,b}(\boldsymbol{k})}}\right]^{p} \\ &\times |V_{a,b}(\boldsymbol{k})|^{2}\,\delta[\omega - E_{a,b}(\boldsymbol{k})], \\ &p = 0,\,1,\,2, \end{aligned} \tag{6}$$

$$\lambda_{a,b} = \pi \sum_{\boldsymbol{k}} \ell_a(\boldsymbol{k}) \left|V_{a,b}(\boldsymbol{k})\right|^2 \delta[\omega - E_{a,b}(\boldsymbol{k})], \tag{7}$$

$$\ell_a(\boldsymbol{k}) = \frac{1}{Z}\left\{\frac{e^{-\beta E} - [1+e^{-\beta E}]n_a(\boldsymbol{k})}{E - E_a(\boldsymbol{k})} + \frac{e^{-\beta(E+U)} - [1+e^{-\beta(E+U)}]n_a(\boldsymbol{k})}{E+U-E_a(\boldsymbol{k})}e^{-\beta E}\right\}, \tag{8}$$

$$n_a(\boldsymbol{k}) = \left\langle a_\sigma^+(\boldsymbol{k}) a_\sigma(\boldsymbol{k})\right\rangle = \frac{e^{-\beta E_a(\boldsymbol{k})}}{1+e^{-\beta E_a(\boldsymbol{k})}}, \tag{9}$$

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

Denote μ_a, μ_b and Ω_a, Ω_b as the chemical potentials and the tops of the energy bands of the systems of conducting electrons in the leads "a" and "b", respectively. Because

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

where $E_{a,b}^{(0)}(\boldsymbol{k})$ are the kinetic energies of the conducting electrons in the leads, $0 \le E_{a,b}^{(0)}(\boldsymbol{k}) \le \Omega_{a,b}$, the spectral functions $\Gamma_{a,b}^{(p)}(\omega)$ and $\lambda_{a,b}(\omega)$ vanish for $\omega < -\mu_{a,b}$ and $\omega > \Omega_{a,b} - \mu_{a,b}$. For the study of the divergence of $\Sigma^{(i)}(\omega)_{\alpha\beta}$ and $\rho(\omega)_{\alpha\beta}$, we set $\mu_a = \mu_b$, $\Omega_a = \Omega_b$, $\Gamma_a^{(0)}(\omega) = \Gamma_b^{(0)}(\omega)$ and $\lambda_a(\omega) = \lambda_b(\omega)$ and we approximately replace the values of the latter two functions in the interval $-\mu < \omega < \Omega - \mu$ by some constants Γ and λ, respectively. Then, we have following behaviors of the Green's function in Eq. (5) in the neighborhoods of the divergence points of the functions $\Sigma^{(i)}(\omega)_{\alpha\beta}$, neglecting the finite very small terms of the second order with respect to the tunneling coupling constants:

a) As $\omega \to -\mu$ and at low temperature $T \approx 0$, the Green's function in Eq. (5) has an asymptotic form

$$G(\omega)_{11} \approx -\frac{\left[1 - n + \frac{1}{2}(E+\mu)\frac{\lambda}{\Gamma}\right]U}{E+2U+\mu} \times \frac{1}{\frac{1}{2}(E+\mu) + \frac{2\Gamma}{\pi}\ln\left|\frac{\omega+\mu}{\Omega}\right| + 2i\Gamma} - \frac{E+\mu+\left[1+n-(E+U+\mu)\frac{\lambda}{\Gamma}\right]U}{E+2U+\mu} \times \frac{1}{(E+U+\mu) + \frac{2\Gamma}{\pi}\ln\left|\frac{\omega+\mu}{\Omega}\right| + 2i\Gamma}. \tag{10}$$

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

$$\omega_1^{(\pm)} = -\mu \pm \Omega \exp\left\{-\frac{\pi}{4\Gamma}(E+\mu)\right\}, \tag{11}$$

and two more resonances at two more points,

$$\omega_2^{(\pm)} = -\mu \pm \Omega \exp\left\{-\frac{\pi}{2\Gamma}(E+U+\mu)\right\}. \tag{12}$$

Between these four resonances, there are dips. If $E+\mu < 0$ but $E+U+\mu > 0$, $G(\omega)_{11}$ 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's function $G(\omega)_{11}$ 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 Fano resonances.

b) As $\omega \to 0$ and at $T = 0$ the Green's function $G(\omega)_{11}$ has the asymptotic form

$$G(\omega)_{11} \approx -\frac{E + (1-n)U}{E(E+U) + \frac{2\Gamma U}{\pi}\ln\left|\frac{\mu}{\omega}\right| + 2i(3E+2U)\Gamma}. \tag{13}$$

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

$$\omega_3^{(\pm)} = \pm\mu \exp\left\{-\frac{\pi}{2\Gamma}\left|\frac{E(E+U)}{U}\right|\right\}, \tag{14}$$

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

$$T_K = \frac{1}{k}\mu \exp\left\{-\frac{\pi}{2}\frac{|E(E+U)|}{\Gamma U}\right\}, \tag{15}$$

where k is the Boltzmann constant, instead of the formula in Eq. (13), we have

$$G(\omega)_{11} \approx \frac{\pi}{2}\frac{E+(1-n)U}{\Gamma U} \times \frac{1}{\ln|T/T_K| - i\pi(3E+2U)\Gamma}. \tag{16}$$

The resonances in the neighborhood of the point $\omega = 0$ have the same physical origin as the Kondo effect in 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's function $G(\omega)_{11}$ has the asymptotic form

$$G(\omega)_{11} \approx \frac{E+nU}{E(E+U) - \frac{2\Gamma U}{\pi}\ln\left|\frac{\mu}{\omega-2E-U}\right| - 2iE\Gamma}. \tag{17}$$

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

$$\omega_4^{(\pm)} = 2E + U \pm \mu \exp\left\{-\frac{\pi}{2\Gamma}\frac{E(E+U)}{U}\right\}, \tag{18}$$

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

$$T'_K = \frac{1}{k}\mu \exp\left\{-\frac{\pi}{2}\frac{E(E+U)}{\Gamma U}\right\}; \quad (19)$$

instead of the formula in Eq. (17), we have

$$G(\omega)_{11} \approx \frac{\pi}{2}\frac{E+nU}{\Gamma U}\frac{1}{\ln|T/T'_K| - 2iE\Gamma}. \quad (20)$$

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's function $G(\omega)_{11}$ has the asymptotic form

$$G(\omega)_{11} \approx \frac{1-n+(E+U+\mu)\frac{\lambda}{\Gamma}}{(E+U+\mu)+\frac{2\Gamma}{\pi}\ln\left|\frac{\omega-2E-U-\mu}{\Omega}\right| - 2i\Gamma} \times \frac{U}{E+\mu}. \quad (21)$$

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

$$\omega_5^{(\pm)} = 2E + U + \mu \pm \Omega e^{-\frac{\pi}{2}\frac{E+U+\mu}{\Gamma}}, \quad (22)$$

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

IV. CONCLUSION

By means of the equation of motion method, the system of Dyson equations for the complex-time nonequilibrium electron Green's functions of a system consisting of a single-level QD connected with two conducting leads was derived in the mean field approximation with respect to the products of four creation and destruction operators of the electron and to second order with respect to the effective tunneling coupling constants. All the crossing terms are included in the equations. The exact solution of the system of Dyson equations obtained by solving them with the help of the computer algebra systems Mathematica and Maple may have resonances of four types, dependending 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's function $G(\omega)_{11}$ at these resonances were derived. The results of the present study complement and agree with the numerical calculations in previous works [6-19] on the electron Green's functions in a QD.

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