Enhanced Andreev Tunneling via the Kondo Resonance in a Quantum Dot at Finite Bias

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We study the nonequilibrium transport through a quantum dot coupled to normal and superconducting leads. We use the modified second-order perturbation theory to calculate the differential conductance and the local density of states at the quantum dot. In the strong but finite Coulomb interaction regime, the differential conductance shows an anomalous peak not at a zero bias voltage but at a finite bias voltage. We also observe an additional Kondo resonance besides the nonequilibrium steady-state conditions. Furthermore, if such a QD is coupled to superconducting and normal leads (the N-QD-S system), more interesting phenomena, such as the Andreev reflection, can be observed.

In order to elucidate the interplay between the Andreev reflection and the Kondo effect, extensive experimental studies and theoretical studies of N-QD-S systems have been conducted. Although some theoretical studies have already addressed the nonequilibrium transport in N-QD-S systems focusing on the influence of the Kondo effect, there remain several important issues to be resolved. For example, there is still controversy about the zero-bias anomaly in the differential conductance: some studies have shown the absence of a zero-bias anomaly in the Kondo limit. Moreover, most theoretical studies of the nonequilibrium transport have been concerned with the limit of infinitely strong Coulomb interaction at the QD. However, since sufficiently large Coulomb interactions exclude the superconducting correlations at the QD, no interplay between the Andreev reflection and the Kondo effect may be observed under such an assumption. Thus, it is necessary to consider the intermediate interaction regime.

In order to clarify the interplay between the Andreev reflection and the Kondo effect, we investigate the nonequilibrium transport in the N-QD-S system over a broad range of Coulomb interactions. For this purpose, we extend the modified second-order perturbation theory, which gives the self-energy interpolating between the weak and strong coupling limits, to a nonequilibrium case by employing the Keldysh technique. This method enables us to study the nonequilibrium system in the intermediate interaction regime. From the results of the differential conductance and the local density of states (LDOS) at the QD, we elucidate how the Kondo effect affects the Andreev transport at a finite bias. In particular, a unique phenomenon in transport is observed in the intermediate regime: the nonequilibrium Andreev tunneling via the normal Kondo resonance causes an anomalous peak in the differential conductance not at a zero bias voltage but at a finite bias voltage. Its origin is discussed in detail from the viewpoint of the competition/cooperation between the Kondo and superconducting correlations. Note that since the anomalous peak appears only in the intermediate regime and seems to disappear in the limit of the infinitely strong Coulomb interaction, the results obtained here are consistent with most of the previous reports in this extreme limit.

We describe the N-QD-S system in terms of an Anderson impurity coupled to both the normal metal and the BCS superconductor, \( H = H_{QD} + H_N + H_S + H_{TN} + H_{TS} \), where \( H_{QD} = \epsilon_0 \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U d_{\uparrow}^\dagger d_{\downarrow}^\dagger d_{\downarrow} + d_{\downarrow}^\dagger d_{\uparrow} \) represents the Hamiltonian for the QD, \( H_N = \sum_{\sigma} (\epsilon_{k\sigma} - \mu_N)c_{N\sigma}^\dagger c_{N\sigma} \) and \( H_S = \sum\Delta_{k\sigma} (\epsilon_{k\sigma} - \mu_S)c_{S\sigma}^\dagger c_{S\sigma} + \sum\epsilon c_{S\uparrow}^\dagger c_{S\downarrow}^\dagger + H.c. \) denote the normal lead and superconducting lead, respectively (\( \Delta \)) is the superconducting gap. We assume that the bias voltage \( V \) is applied only to the normal lead: \( \mu_N = eV \) and \( \mu_S = 0 \). The tunneling Hamiltonians between the QD and the two leads are \( H_{TN} = \sum_{k\sigma} (\Delta c_{S\uparrow}^\dagger c_{N\sigma} + H.c.) \) and \( H_{TS} = \sum_{k\sigma} (\Delta c_{S\downarrow}^\dagger c_{N\sigma} + H.c.) \), where \( \Gamma_{N(S)} \) is the tunneling amplitude between the QD and the normal (superconducting) lead. We consider the wide-band limit of electrons in the leads, in which \( \Gamma_{N(S)} = \pi \Gamma_{N(S)} T_{N(S)} \) is defined at \( \Delta = 0 \) represents the resonance strength between the QD and the normal (superconducting) lead.

The time-dependent current flowing from the normal (superconducting) lead into the QD, \( \dot{I}_{N(S)}(t) \), is described by \( \dot{I}_{N(S)}(t) = (ie/\hbar) \sum_k \Gamma_{N(S)}(\omega) c_{N(S)k\sigma}^\dagger d_{\sigma}(t) + H.c. \). Since we consider the nonequilibrium steady-state transport, the expectation values of the current \( \langle \dot{I}_{N(S)} \rangle \) is time-independent. Using the standard Keldysh Green’s function formalism, \( \langle \dot{I}_{N(S)} \rangle \) can be expressed in terms of the local retarded and lesser Green’s functions at the QD, \( G^< (\omega) \) and \( G^> (\omega) \). The bold font represents a \( 2 \times 2 \) Nambu matrix. These Green’s functions include the self-energies due to the Coulomb interaction \( U \) in addition to those due to the coupling between the QD and the leads. In
order to obtain the self-energies for $U$, we use the modified second-order perturbation theory\textsuperscript{11,13} in the Keldysh Green’s function formalism which is a generalization of Cuevas’s approach\textsuperscript{11} in the equilibrium N-QD-S system to the system under nonequilibrium conditions. Following ref. 11, the modified retarded self-energy $\Sigma_{\text{ff}}^{\text{r}}(\omega)$ is given by a functional of the bare second-order self-energy $\Sigma_{\text{ff}}^{\text{r}}(\omega)$ such that $\Sigma_{\text{ff}}^{\text{r}}(\omega)$ has an appropriate form in both the atomic limit, $\Gamma_{N,S}/U \to 0$, and weak-interaction limit, $U/\Gamma_{N,S}/\Gamma_{S} \to 0$. In a similar manner, we obtain the modified lesser self-energy, $\Sigma_{\text{ff}}^{\text{l}}(\omega)$.

We can calculate the bare second-order self-energies $\Sigma_{\text{ff}}^{\text{r}}$ and $\Sigma_{\text{ff}}^{\text{l}}$ using the perturbation theory with respect to $U$ in the standard Keldysh Green’s function formalism. The only point to note in this approach is that the Hamiltonian for the QD is replaced by the following modified one when we calculate the self-energy: $H_{\text{QD}}^\text{d} = i\bar{\sigma}_{d} \sum_{\sigma} d_{d\sigma}^{\dagger} d_{d\sigma} + (\Delta d_{d\uparrow}^{\dagger} d_{d\downarrow}^{\dagger} + \text{H.c.}) + \tilde{\lambda}(\tilde{I}_{N} + \tilde{I}_{S})$, where the effective parameters $\epsilon_{d}$ and $\Delta_{d}$ are introduced to ensure that the self-energies have the correct forms in the atomic limit.\textsuperscript{11,13} In addition, we introduce the source term $\lambda$ coupled to the current operator in order to conserve the current, because the simple application of the second-order self-energy in the N-QD-S system without the source term may break the current conservation law: $\langle \tilde{I}_{N} \rangle + \langle \tilde{I}_{S} \rangle \neq 0$.\textsuperscript{15} The effective parameters $\tilde{\lambda}$ and $\Delta_{d}$ are then fixed under the following conditions, which respectively indicate the consistency of the electron number, the effective counter gap to the proximity effect at the QD, and the current conservation: $(\tilde{\lambda}) = (\tilde{\lambda})_{0}$, $\Delta_{d} = \Sigma_{d}^{\text{r}}(0)$, and $\langle \tilde{I}_{N} \rangle + \langle \tilde{I}_{S} \rangle = 0$. In the first equality, $\lambda$ and $\lambda_{0}$ are the expectation values of the electron number at the QD with the full Hamiltonian and with the modified one.

First, we discuss how the differential conductance $dI/dV$ is affected by the Coulomb interaction. Figure 1(a) shows the differential conductance as a function of the bias voltage $V$ for several values of $U$ with the symmetric coupling $\Gamma_{S}/\Gamma_{N} = 1$. We only show $dI/dV$ for a positive bias voltage since it is an even function of $V$ in this case ($\epsilon_{d} + U/2 = \mu_{S} = 0$). For $U = 0$, the zero-bias conductance takes its maximum value $4e^{2}/h$, where the Andreev tunneling between the QD and the superconducting lead is balanced by the normal electron tunneling between the QD and the normal lead. This balance is ensured by the condition of $\Gamma_{S}/\Gamma_{N} = 1$ with $U = 0$. With the enhancement of the Coulomb interaction, the differential conductance decreases gradually in the entire voltage range, because the Coulomb interaction suppresses both the Andreev tunneling and the normal electron tunneling, but in different ways: the interaction makes the former much weaker than the latter. This is evident in renormalized parameters, $\tilde{\Gamma}_{N}$ and $\tilde{\Gamma}_{S}$, which are defined for $V = 0$ and $T = 0$ as

$$\tilde{\Gamma}_{N} = z\Gamma_{N}, \quad \tilde{\Gamma}_{S} = z\Gamma_{S} + [\text{Re} \Sigma_{d}^{\text{r}}(\omega)]_{11},$$

(1)

where $z$ is the renormalization factor $z = (1 + \Gamma_{S}/\Delta - d [\text{Re} \Sigma_{d}^{\text{r}}(\omega)]_{11}/\omega_{0}^{2})^{-1}$. Figure 1(b) shows the $U$ dependence of these renormalized parameters. It is seen that $\tilde{\Gamma}_{S}$ decreases more rapidly than $\tilde{\Gamma}_{N}$ with an increase in $U$. For $\tilde{\Gamma}_{S} < \tilde{\Gamma}_{N}$, the coupling between the QD and the superconducting lead effectivley becomes weaker than the coupling between the QD and the normal lead, making the Kondo singlet dominant at the QD. As a result, the system loses the above subtle balance in tunneling processes, leading to a global reduction in conductance. Note here that the differential conductance markedly changes its voltage dependence with an increase in $U$ (Fig. 1(a)). In particular, the monotonic curve of the differential conductance for $U/\Gamma_{N} = 0$ gradually develops a double-peak structure, as seen for $U/\Gamma_{N} = 10$. As $U$ further increases, the two peaks become more prominent. The peak in the vicinity of $V = 0$ becomes sharper and gradually approaches a zero-bias voltage: e.g., it is located at $eV/\Gamma_{N} \approx 0.05$ for $U/\Gamma_{N} = 20$. The anomalous sharp peak is commonly observed when the Kondo effect is dominant at the QD ($\tilde{\Gamma}_{S}/\tilde{\Gamma}_{N} < 1$ and $U/\Gamma_{N} \gg 1$) though its height decreases with increasing $U$. On the other hand, the broad peak at $eV/\Gamma_{N} \approx 0.6$ is insensitive to the increase in $U$. The above novel characteristic feature is one of the main findings of this study, which is quite different from an ordinary zero-bias anomaly in a QD coupled to two normal leads.\textsuperscript{1} Note that with increasing $U$, the anomalous peak gets close to the zero-bias voltage but decreases in height. Eventually, the anomalous peak seems to disappear in the limit of $U \to \infty$, which is consistent with the absence of the zero-bias anomaly in refs. 4, 5, 6, and 10 where an infinitely strong Coulomb interaction is assumed. The monotonic decrease in the zero-bias conductance with increasing $U$ is also consistent with the results of equilibrium studies.\textsuperscript{11,12}

We also show the differential conductance in the cases with asymmetric couplings ($\Gamma_{S}/\Gamma_{N} \neq 1$) and a strong Coulomb interaction $U/\Gamma_{N} = 20$ in Fig. 2(a). For $\Gamma_{S}/\Gamma_{N} > 1$ (< 1), the sharp peak near the zero-bias voltage increases (decreases) in height and changes its position toward a slightly higher (lower) bias voltage. To be more specific, let us denote the position and height of the sharp peak as $V_{A}$ and $G_{A}$, respectively, which are plotted in Fig. 2(b) together with the renormalized parameters. A significant feature is that the peak position ($eV_{A}$) is approximately given by $\tilde{\Gamma}_{N}$ for small $\tilde{\Gamma}_{S}$'s, where $\tilde{\Gamma}_{N}$ corresponds roughly to the Kondo temperature. Also note that the peak height $G_{A}$ approaches zero for $\tilde{\Gamma}_{S} \to 0$ because the Andreev tunneling completely disappears in that limit. These facts indicate that the origin of this characteristic peak is related to both the Kondo effect and the proximity effect. Note that the other broad peak is also affected by the change in $\tilde{\Gamma}_{S}$. For smaller $\tilde{\Gamma}_{S}/\tilde{\Gamma}_{N}$ values, the broad peak at $eV/\Gamma_{N} \approx 0.6$ in the symmetric case ($\tilde{\Gamma}_{S}/\tilde{\Gamma}_{N} = 1$) shifts toward the gap edge,

![Figure 1](image-url)
eV/Γ_N = 1. In contrast, for larger Γ_S/Γ_N values, the broad peak shifts in the opposite direction and merges with the sharp peak near the zero-bias voltage. All the above characteristic features of the conductance will be clearly explained below in terms of the interplay between the Kondo/proximity effects under nonequilibrium conditions.

Let us now discuss how the LDOS at the QD, ρ(ω), in the strong Coulomb interaction regime changes its profile as bias voltage increases. The computed results are shown in Fig. 3. Let us first look at the LDOS in the equilibrium state (V = 0) for U/Γ_N = 20, which is compared with that in the case of U/Γ_N = 0 shown in the inset. The two resonances emerging inside the superconducting gap for U/Γ_N = 0 represent the Andreev resonant states, which are approximately described by the superposition of two Lorentzians with renormalized parameters: they are located at ω = ±Γ_S with a width Γ_N. It is seen that the Andreev resonance for U/Γ_N = 0 is strongly renormalized and merged into a single sharp Kondo resonance at the Fermi level for U/Γ_N = 20 because Γ_S decreases more rapidly than Γ_N (see Fig. 1(b)). The resulting Kondo resonance is sensitive to the change in bias voltage, so that the LDOS for U/Γ_N = 20 significantly alters its shape with an increase in V. Indeed, as bias voltage increases, the position of the Kondo resonance shifts following the Fermi level of the normal lead μ_N; e.g., for μ_N/Γ_N = eV/Γ_N = 0.2, the peak position is located at ω/Γ_N ≈ 0.2. This implies that the ordinary Kondo resonance is formed by conduction electrons in the normal lead. A noteworthy feature for eV/Γ_N = 0.2 is that another resonance develops, though small, near the counterposition of the Kondo resonance ω ≈ −μ_N. This additional Kondo resonance was previously observed by Sun et al. but has not been discussed in detail, particularly as regards its physical relevance to the transport properties. We will address this issue below and demonstrate that it indeed provides a source of the marked change in nonequilibrium transport properties. For eV/Γ_N = 0.6, the peak value of the additional Kondo resonance is slightly increased while the normal Kondo resonance is suppressed, leading to a broad two-peak structure, which is analogous to that in the U/Γ_N = 0 case. The two-peak structure therefore indicates that the superconducting pairing state, which is strongly suppressed by the large Coulomb interaction at V = 0, is revived and becomes dominant over the Kondo singlet state. With further increase in bias voltage (eV/Γ_N = 1,2), however, the Andreev resonance is suppressed again since the applied bias voltage also makes the superconducting pairing state unstable. In these cases, the weight of the LDOS is transferred to the region at ω ≈ ±U/2, corresponding to the characteristic energy of charge excitations at the QD (data not shown), which indicates that the QD is in the local-moment (free-spin) regime. Therefore, we conclude that as bias voltage increases, the LDOS first exhibits a crossover from the Kondo-dominant regime to the superconducting-dominant regime, and then to the local-moment regime.

The above discussions on the LDOS enable us to clarify the origin of the two peaks in the differential conductance in the large-U regime in Figs. 1(a) and 2(a). We first recall that the zero-bias conductance is substantially suppressed by U, as has been shown in Fig. 1(a). However, for a small bias voltage, the effective cotunneling process is enhanced owing to the nonequilibrium Andreev tunneling via the Kondo resonance, which gives rise to the anomalous increase in the differential conductance at a small but finite bias voltage. Consequently, we can say that the anomalous increase found in the conductance near zero bias is a unique nonequilibrium phenomenon induced by the interplay of the Kondo effect and superconducting proximity effect. Here, we determine why the anomalous peak is located at eV/Γ_N ≈ 1. For U = 0 in Fig. 1(a), the zero-bias conductance has a maximum value for Γ_S/Γ_N = 1. Namely, the maximum transport probability is realized when the width and position of the Andreev resonance have the same value. This specific correspondence holds for the zero-bias conductance even in the interacting case because the low-energy physics of the N-QD-S system can be described by the local Fermi liquid theory. For instance, as Γ_S becomes smaller than Γ_N with increasing U, the system loses the above specific balance, resulting in the suppression of the zero-bias conductance. Even under such conditions as Γ_S/Γ_N ≪ 1, however, the peak position of the Andreev resonance is shifted and determined by the bias voltage V instead of by Γ_S, as shown in Fig. 3. Accordingly, we can state the following by generalizing the above correspondence to the nonlinear case: In nonequilibrium cases with eV/Γ_N ≈ 1, where the position of the Andreev resonance is the same as its width,
These characteristic peak in the conductance is indeed caused by the Kondo eﬀect. Using the modified second-order perturbation theory, we have elucidated that the diﬀerential conductance develops two characteristic peaks in its bias voltage dependence as the Coulomb interaction is enhanced. In particular, the peak near the zero-bias voltage characterizes a unique phenomenon caused by a nonequilibrium Andreev tunneling via the Kondo resonance. It has indeed been conﬁrmed that the sharp peak disappears with increasing temperature, reﬂecting the suppression of the Kondo resonance. The two-peak structure found for the voltage dependence of the conductance characterizes a crossover from the Kondo-dominant regime to the superconducting-dominant regime, and then to the local-moment regime. In real experiments, different patterns in the temperature dependence of the peaks may be observed, which can give strong evidence of the interplay between the Andreev reﬂection and the Kondo eﬀect at a ﬁnite bias. We think that the transport experiments proposed here will provide an important test bed for a deeper understanding of the nonequilibrium Kondo/Andreev physics in QD systems.

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