Nonequilibrium Transport through a Quantum Dot Coupled to Normal and Superconducting Leads

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Abstract. We study the nonequilibrium transport through a quantum dot coupled to normal and superconducting leads. The mean-field phase diagram obtained for the nonequilibrium steady state demonstrates that the superconducting pair correlation suppresses, via proximity effects, electron correlations due to the Coulomb repulsion. We calculate the conductance due to the Andreev reflection at a finite voltage, and find that the maximum of conductance signals how the superconducting correlation is developed in the quantum dot.

1. Introduction
Recent remarkable developments in the nanotechnology make it possible to fabricate a quantum dot (QD) connected to the superconducting leads, providing a number of intriguing phenomena due to the interplay between the Kondo effect and superconductivity. Especially, the Andreev transport through a quantum dot coupled to normal and superconducting leads (N-QD-S) has drawn much interest and has stimulated intensive theoretical analyses \cite{1, 2, 3, 4, 5, 6, 7, 8} and experimental investigations \cite{9}. Among them, some theoretical studies have addressed the nonequilibrium steady state under a finite bias voltage with particular emphasis on the influence of the Kondo effect \cite{1, 7}. However, these studies have focused on the strong Coulomb interaction limit, so that it is desirable to study the nonequilibrium transport properties in the whole parameter region covering the weak to strong coupling limit.

In this paper, we investigate the nonequilibrium transport properties in the N-QD-S system by taking into account the effect of Coulomb interaction in the QD. By combining the mean-field and second-order perturbation theory with the Keldysh Green’s function formalism, we calculate the conductance and the superconducting pair correlation in the QD. From these results, we clarify how the interplay between the proximity effects and the local electron correlations such as the Kondo effect affects the nonequilibrium transport properties.

2. Model
The Hamiltonian for a QD coupled to normal and superconducting leads with a bias voltage \( V \) is given by

\[
H = H_{\text{QD}} + H_{\text{N}} + H_{\text{S}} + H_{\text{TN}} + H_{\text{TS}}
\] (1)

where \( H_{\text{QD}} = \epsilon_{d} \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\sigma}^{\dagger} d_{\sigma} d_{\downarrow} \) is the Hamiltonian for the QD. \( H_{\text{N}} = \sum_{k \alpha} (\epsilon_{k} - \mu_{N}) c_{k \alpha}^{\dagger} c_{k \alpha} \)

and \( H_{\text{S}} = \sum_{q \sigma} (\epsilon_{q} - \mu_{S}) a_{q \sigma}^{\dagger} a_{q \sigma} + \sum_{q} (\Delta a_{q}^{\dagger} a_{-q}^{\dagger} + \text{H.c.}) \) denote the normal and superconducting
leads (Δ is the superconducting gap), respectively. The normal and superconducting leads have different chemical potentials \( \mu_N \) and \( \mu_S \) due to the bias voltage \( V \) (\( \mu_N - \mu_S = eV \)).

\[
H_{TN} = \sum_{k_\sigma}(t_{Nk_\sigma}^\dagger d_{k_\sigma} + \text{H.c.}) \quad \text{and} \quad H_{TS} = \sum_{q_\sigma}(t_{Sq_\sigma}^\dagger d_{q_\sigma} + \text{H.c.})
\]

represent the tunneling between the QD and the two leads. We consider the wide band limit of electrons in the leads, in which \( \Gamma_{S(N)} = \pi t_{S(N)}^2 \rho_{S(N)} \) represents the resonance strength between the QD and the superconducting (normal) lead. In this study, we use the Hartree-Fock (HF) approximation for the Coulomb interaction term: \( U d_{\uparrow}^\dagger d_{\downarrow}^\dagger d_{\downarrow} d_{\uparrow} + U(\Psi^\dagger \Psi + \text{H.c.}) \), where \( n_\sigma = \langle d_{\sigma}^\dagger d_{\sigma} \rangle \) and \( \Psi = \langle d_{\uparrow}^\dagger d_{\downarrow} \rangle \) are determined self-consistently. We calculate the differential conductance \( G = dI/dV \) (\( I \) : current) and the superconducting pair correlation in the QD, \( \Psi = \langle d_{\uparrow}^\dagger d_{\downarrow} \rangle \), at zero temperature. In order to focus on the transport due to the Andreev reflection, we consider the region where the superconducting gap \( \Delta \) is larger than the other parameters.

3. Numerical Results

3.1. Mean-field phase diagram

As well known, the HF approximation of the Anderson model may give a magnetic solution in addition to a nonmagnetic one in the strong coupling regime [10]. The magnetic state obtained at the HF level, which may be relevant to the high temperature region, should be replaced by the Kondo singlet state at low temperatures. Nevertheless, the HF analysis is quite helpful for getting some insight into correlation effects due to the Coulomb interaction, as demonstrated for the Anderson model out of equilibrium [11]. Here, we make use of the HF approximation for the N-QD-S system to obtain the mean-field phase diagram.

Figure 1(a) shows the mean-field phase diagram obtained as a function of the bias voltage \( V \) and the Coulomb interaction \( U \). In this figure, the boundaries between the magnetic and nonmagnetic regions are drawn for several values of the resonance strength \( \Gamma_S \). Note that \( \Gamma_S \) represents the strength of the proximity effect which induces the pair correlation at the dot. It is seen in Fig. 1(a) that the magnetic region becomes smaller with increasing \( \Gamma_S \), which implies that the superconducting proximity effect tends to suppress the appearance of magnetic moment in the QD. Therefore, the HF approximation is applicable to the N-QD-S system for larger values of \( U \) when \( \Gamma_S \) gets larger. In the case of \( \Gamma_S/\Gamma_N = 3 \), we see that the boundary exhibits the reentrant behavior around \( U/\Gamma_N = 8 \) (see the area enclosed by a dot-dashed circle in Fig. 1(a)). We make a brief comment on this behavior. When the bias voltage is turned on, charge fluctuations in the QD are enhanced, which makes the magnetic solution unstable. At the same time, however, the pair correlation in the QD which suppresses the magnetic moment, is also weakened with
the increase of bias voltage. This can be confirmed from the results shown in Fig. 1(b), where the absolute value of the pair correlation $|\Psi|$ monotonically decreases with the increase of $V$. Therefore, nontrivial competition occurs between magnetic and superconducting correlations, leading to a remarkable phenomenon where the magnetic moment can emerge at a finite bias voltage by suppressing the pair correlation. This explains why the reentrant behavior appears for $\Gamma_S/\Gamma_N = 3$. We think that the reentrant behavior is characteristic of a nonequilibrium state in our N-QD-S system, which does not appear if two leads are assumed to be both normal [11]. Our analysis naturally suggests that the Kondo effect in the N-QD-S system, if it is properly incorporated, could be enhanced under a weak bias voltage.

### 3.2. Transport properties in the N-QD-S system

Let us now discuss the nonequilibrium transport properties in our N-QD-S system by using the results obtained in the HF approximation.

**Figure 2.** Color-scale representation of (a) differential conductance $G/G_0$ ($G_0 = 4e^2/h$) and (b) pair correlation in the QD $|\Psi|$ as a function of $eV/\Gamma_N$ and $U/\Gamma_N$. We set $\Gamma_S/\Gamma_N = 3$ and the other parameters are the same as in Fig. 1. The dot-dashed line is the phase boundary shown in Fig. 1(a).

Figure 2(a) is the color-scale representation of the differential conductance $G$ as a function of $eV/\Gamma_N$ and $U/\Gamma_N$ for $\Gamma_S/\Gamma_N = 3$. At $U = 0$, the conductance takes a maximum at a finite bias voltage, which reaches the unitary limit $G_0 = 4e^2/h$ (see the vertical axis of Fig. 2(a)). As the Coulomb interaction $U$ increases, the conductance maximum shifts to smaller values of $eV/\Gamma_N$ keeping its unitary limit value of $G_0 = 4e^2/h$. To elucidate what the conductance maximum implies, we also show the color-scale representation of the pair correlation in the QD, $|\Psi|$, in Fig. 2(b). It is seen that the pair correlation $|\Psi|$ decreases with increase of $U$ or $V$. In particular, around the region where the conductance takes the maximum in Fig. 2(a), $|\Psi|$ changes its value drastically. As already discussed in the equilibrium case ($V = 0$) [8], this drastic change signals the enhancement of the Andreev reflection in the N-QD-S system. From Figs. 2(a) and (b), we can say that the above interpretation can be extended to the nonequilibrium case; namely the conductance maximum can be a proper quantity describing how the pair correlation is developed in the QD under nonequilibrium conditions. Note that the conductance maximum discussed here is located mostly inside the nonmagnetic region where our HF analysis may be reliable. This in turn justifies our discussions on the conductance maximum in Fig. 2(a).

### 3.3. Some preliminary results on electron correlations

Finally, we present some preliminary results of the second order perturbation theory (SOPT) in $U$. We can take into account the Kondo effect to a certain extent in this treatment, although
the following results may not be directly applicable to the strong correlation regime in Fig. 1.

![Figure 3](image)

**Figure 3.** Conductance $G$ as a function of the bias voltage $V$, which is calculated by the SOPT. We set $\Gamma_S/\Gamma_N = 3$.

Figure 3 shows the conductance calculated by the SOPT as a function of $V$. As $U$ increases, the conductance peak shifts to a smaller bias voltage, which coincides with the behavior of conductance shown in Fig. 2(a). However, for $U/\Gamma_N = 2$ or 4, the conductance peak does not reach the unitary limit $G_0 = 4e^2/h$. This is due to the inelastic scattering by the Coulomb interaction at finite $V$, which is not incorporated in the HF approximation. For $U/\Gamma_N = 7$, the peak reaches unitary limit again at the zero bias limit, because the low-energy properties of the N-QD-S system in equilibrium are described by the local Fermi liquid theory [8]. We think that the result in Fig. 3 captures some essential features due to electron correlations, but is still not sufficient to clarify the nonequilibrium transport properties over the wide range covering the weak to strong correlation limit. The investigation in this direction is now in progress.

4. Summary
We have investigated the nonequilibrium transport for N-QD-S system by means of the Hartree-Fock approximation and the second-order perturbation theory. We have obtained the mean-field phase diagram of the N-QD-S system, which exhibits the interesting reentrant behavior suggesting that the magnetic correlation can overcome the pair correlation under a finite bias voltage. We have also found that the conductance maximum clearly characterizes how the pair correlation is developed in the QD under nonequilibrium conditions.

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