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Quantum dot between two superconductors

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Abstract. – Novel effects emerge from an interplay between multiple Andreev reflections and Coulomb interaction in a quantum dot coupled to superconducting leads and subject to a finite potential bias V. Combining an intuitive physical picture with a rigorous path integral formalism, we evaluate the current I through the dot and find that the interaction shifts the subharmonic pattern of the I-V curve toward higher V. For a sufficiently strong interaction the subgap current (at $eV < 2\Delta$) is virtually suppressed.

Recent progress in nanotechnology enables the fabrication and experimental investigation of superconducting contacts of atomic size with few conducting channels [1, 2]. Transport properties of such systems are essentially determined by the mechanism of multiple Andreev reflections [3] (MAR) which is responsible for Josephson current as well as for dissipative currents at subgap voltages. Theoretical analysis of MAR and current-voltage characteristics in small superconducting junctions is reported in a number of papers [4–6]. In these works, an essential ingredient is the assumption that electron-electron interaction inside the contact can be neglected. It might indeed be justified provided a metallic contact is sufficiently large and/or strongly coupled to massive superconducting leads.

However, in very small contacts (quantum dots), the Coulomb interaction is not effectively screened, hence it is expected to substantially affect transport properties of the system. For instance, it is well known both from theory [7] and experiment [8] that tunneling through a quantum dot between superconductors can virtually be suppressed due to Coulomb effects. Thus, to the fascinating physics of SNS and SIS junctions, one should add that of an SAS junction composed of superconducting leads coupled by an *interacting* quantum dot [9].

In this work, the physics of interplay between MAR and interaction effects in SAS junctions subject to a finite bias is exposed. It encodes the salient features of superconductivity, strong correlations and nonlinear response. A simple intuitive physical picture is combined with a rigorous path integral technique by which irrelevant degrees of freedom are eliminated and an effective action is constructed (in the spirit of the Feynman-Vernon influence functional [10]). Similar ideas proved to be useful elsewhere, see, *e.g.*, [11, 12]. In the present context they have been applied for the relatively simple case of an SAS junction at *zero* bias, focusing on the equilibrium Josephson current [13, 14]. Our main achievements are: a) Derivation of a tractable expression for the nonlinear tunneling current in the presence of interactions and b) prediction of novel physical effects pertaining to the I-V curve of an SAS junction at subgap bias.

Let us commence with a simple and physically transparent picture of an interplay between MAR and Coulomb effects. Consider a quasiparticle (hole) which suffers n Andreev reflections inside the superconducting junction, thereby gaining an energy neV, where V is the voltage bias. As soon as $neV = 2\Delta$ the quasiparticle leaves the junction and does not contribute anymore to the subgap current. Hence, the number of Andreev reflections n for a given voltage is $n \simeq 2\Delta/eV$.

Consider first a highly transparent junction for which the transparency parameter Γ is the largest energy scale (see definition of Γ after eq. (15)). Assume now that the Coulomb interaction inside the junction is switched on. For our qualitative discussion it suffices to account for it in terms of an effective capacitance C and its related charging energy $E_C = e^2/2C$. At $T = 0$ and for $eV \leq E_C$ a single electron tunneling (and, hence, also MAR) is blocked, so in what follows we will consider the case $eV > E_C > 0$. In order to leave the junction, the quasiparticle should gain an energy neV equal to $2\Delta + (n+1)E_C$. The last term originates from the fact that during the MAR cycle with a given n a charge $(n+1)e$ is transferred between the electrodes. Hence, an additional energy $(n+1)E_C$ should be paid. This fixes the number n at a given voltage as $n = \left[\frac{2\Delta+E_C}{eV-E_C}\right]$. Thus, in the presence of Coulomb interaction quasiparticles spend more time inside the junction and suffer more Andreev reflections. At low temperature T, the transfer of charge $(n+1)e$ is blocked by interaction at voltages $eV \leq (n+1)E_C$. One then arrives at the condition $eV \leq eV_{\rm th} = E_C\left(1+\sqrt{1+\frac{2\Delta}{E_C}}\right)$, under which the MAR current is suppressed due to Coulomb repulsion. For $E_C \ll \Delta$ the voltage threshold is $eV_{\rm th} \simeq \sqrt{2\Delta E_C} \gg E_C$, *i.e.* in this case MAR should be blocked even at voltages *much higher* than E_C/e.

Recall now that subharmonic peaks in the I-V curves occur each time the MAR cycle with a given n is blocked. In the absence of interaction, these peaks are located at voltages $V_n = 2\Delta/en$. It follows immediately from the above discussion that in the presence of Coulomb interaction the peaks should be shifted to higher voltages, $V_n = \frac{E_C}{e} + \frac{2\Delta+E_C}{en}$, *i.e.* one expects the subharmonic peaks to be shifted by $\delta V_n = (E_C/e)(1+1/n)$ towards larger V as compared to the noninteracting case.

Thus, even a naive analysis of the interplay between MAR and Coulomb effects in junctions with large Γ allows one to predict several novel effects which can be experimentally tested. In cases when the Coulomb interaction in the dot is the largest energy, and for moderate values of Γ, the estimation of the voltage threshold based on eq. (2) is not justified. The physics resembles that of an Anderson center as a weak link and discussed in ref. [7] pertaining to Josephson currents. Here we also expect that the main processes contributing to the subgap current are MAR. Yet, while the number of MAR at low voltages is rather large, the current remains small. This is due to the low effective transparency of the junction as a consequence of interaction. The high-n processes are damped by higher powers of Γ. The interaction introduces an important parameter which is proportional to the difference between spin-up and spin-down population of the dot level and obeys a self-consistent equation ((20) below). We now put these qualitative arguments on a firm basis by formulating a realistic model of an SAS junction, followed by calculations of the resulting I-V characteristics.

The model and basic formalism. – Consider, in two dimensions, a quantum dot at $\boldsymbol{r} = 0$ weakly coupled to (half planar) superconducting electrodes. The Hamiltonian of the system is decomposed as

$$\boldsymbol{H} = \boldsymbol{H}_{\mathrm{L}} + \boldsymbol{H}_{\mathrm{R}} + \boldsymbol{H}_{\mathrm{dot}} + \boldsymbol{H}_{\mathrm{t}}. \tag{1}$$

The Hamiltonians of the left ($x < 0$) and right ($x > 0$) superconducting electrodes have the standard BCS form

$$\boldsymbol{H}_j = \int \mathrm{d}\boldsymbol{r}[\Psi^\dagger_{j\sigma}(\boldsymbol{r})\xi(\boldsymbol{\nabla})\Psi_{j\sigma}(\boldsymbol{r}) - \lambda\Psi^\dagger_{j\uparrow}(\boldsymbol{r})\Psi^\dagger_{j\downarrow}(\boldsymbol{r})\Psi_{j\downarrow}(\boldsymbol{r})\Psi_{j\uparrow}(\boldsymbol{r})]. \tag{2}$$

Here $\Psi^\dagger_{j\sigma}$ ($\Psi_{j\sigma}$) are the electron creation (annihilation) operators, $\xi(\boldsymbol{\nabla}) = -\boldsymbol{\nabla}^2/2m - \mu$, and $j = \mathrm{L}, \mathrm{R}$ for left and right electrodes. The dot itself is modeled as an Anderson impurity center with Hamiltonian

$$\boldsymbol{H}_{\mathrm{dot}} = \epsilon_0 \sum_\sigma C^\dagger_\sigma C_\sigma + U C^\dagger_\uparrow C_\uparrow C^\dagger_\downarrow C_\downarrow\,, \tag{3}$$

where $C^\dagger_\sigma$ and C_σ are dot electron operators. The impurity site energy ϵ_0 (counted from the Fermi energy μ) is assumed to be far below the Fermi level $\epsilon_0 < 0$. The presence of a strong Coulomb repulsion $U > -\epsilon_0$ between electrons in the same orbital guarantees that the dot is at most singly occupied.

Electron tunneling through the dot is described by the term

$$\boldsymbol{H}_{\mathrm{t}} = \mathcal{T} \sum_{j=\mathrm{L,R}} \sum_\sigma \Psi^\dagger_{j\sigma}(0) C_\sigma + \mathrm{h.c.}, \tag{4}$$

where $\mathcal{T}$ is an effective transfer amplitude.

Using the single-level Anderson model in our problem is justified if the dot level spacing δ is large, in our case $\delta > 2\Delta > eV$. This requirement can be easily met in experiments. *E.g.*, in a recent experiment on tunable Kondo effect in GaAs/AlGaAs quantum dots [15], the estimate is $\delta \approx 0.15$ meV. Thus, for $\Delta \approx 1$ K the above inequality is satisfied. With smaller dots [8] δ can be pushed higher.

The dynamics of the system is completely contained within the evolution operator on the Keldysh contour K, which consists of forward- and backward-oriented time paths. Its kernel J is given by a path integral,

$$J = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi\mathcal{D}\bar{C}\mathcal{D}C \exp[iS], \tag{5}$$

over Grassman fields corresponding to the fermion operators, with $\bar{\Psi} = (\Psi^\dagger_{\mathrm{L}\uparrow}, \Psi^\dagger_{\mathrm{L}\downarrow}, \Psi^\dagger_{\mathrm{R}\uparrow}, \Psi^\dagger_{\mathrm{R}\downarrow})$ and similar definitions for Ψ, $\bar{C}$ and C. The action $S = \int_K L\mathrm{d}t$, where L is the Lagrangian pertaining to the Hamiltonian (1).

In order to avoid dealing with fields defined on both branches of the Keldysh contour, one performs a rotation $C \to c$ and $\Psi \to \psi$ in Keldysh space:

$$\bar{c} = \bar{C}\sigma_z\hat{Q}^{-1}, \qquad c = \hat{Q}C; \qquad \hat{Q} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \tag{6}$$

and similarly for $\bar{\psi}$ and ψ. Here σ_z is the third Pauli matrix operating in Keldysh space. The new Grassman variables $\bar{c}$, c, $\bar{\psi}$, ψ are now defined solely on the forward time branch. Averages of the corresponding products of these fields determine the standard 2×2 Green-Keldysh matrix composed of retarded ($\hat{G}^{\mathrm{R}}$), advanced ($\hat{G}^{\mathrm{A}}$) and Keldysh ($\hat{G}^{\mathrm{K}}$) Green functions which, in turn, are 2×2 matrices in spin (Nambu) space.

The path integral (5) is expressed in terms of the new Grassman variables in the same way, and the action S is now defined as $S = S_{\rm dot} + S_0[\bar\psi, \psi]$, where

$$S_{\rm dot} = \int {\rm d}t \left[\bar c \left(i\frac{\partial}{\partial t} - \tilde\epsilon \tau_z \right) c + \frac{U}{2}(\bar c c)^2 \right], \tag{7}$$

$$S_0 = \int {\rm d}t \sum_{j={\rm L,R}} \left[\int_j {\rm d}\boldsymbol{r} \bar\psi_j(\boldsymbol{r},t) \hat G_j^{-1} \psi_j(\boldsymbol{r},t) + (\mathcal{T} \bar\psi_j(0,t)\tau_z c(t) + {\rm c.c.}) \right], \tag{8}$$

where $\tilde\epsilon = \epsilon_0 + U/2$ and the Pauli matrices $\tau_{x,y,z}$ act in Nambu space. The operator $\hat G^{-1}_{\rm L,R}$ has the standard form

$$\hat G^{-1}_{\rm L,R}(\xi) = i\frac{\partial}{\partial t} - \tau_z \xi(\boldsymbol{\nabla}) + \tau_+ \Delta_{\rm L,R} + \tau_- \Delta^*_{\rm L,R}, \tag{9}$$

where $\tau_\pm = (\tau_x \pm i\tau_y)/2$ and $\Delta_{\rm L,R}$ are the (spatially constant) BCS order parameters of the electrodes.

Effective action and transport current. – The basic algorithm of our approach is to integrate out the electron variables in the superconducting electrodes which play the role of an effective environment for the dot. This procedure yields the influence functional $F[\bar c, c]$ for the c-fields in the dot:

$$F \equiv \exp[iS_{\rm env}[\bar c, c]] = \int \mathcal{D}\bar\psi \mathcal{D}\psi \exp[iS_0[\bar\psi, \psi]], \tag{10}$$

which is evaluated exactly. Gaussian integration in (10) is carried out separately for L- and R-electrodes.

Consider, say, the left superconductor and omit the subscript $j = L$ for the moment. The first step is to integrate out the fermion fields *inside* the superconductor thereby arriving at an intermediate effective action in terms of the fermion fields defined on the surface $x = 0$. It is useful at this point to Fourier transform the fields $\psi(x, y)$ along the (translationally invariant) y direction. The problem then reduces to a one-dimensional one with fermion fields $\psi_k(x)$ where k is the quasiparticle momentum in the direction normal to x. In order to evaluate the Gaussian integral, we will look for a saddle point field $\tilde\psi_k(x)$ defined by $\hat G^{-1}(\xi_x)\tilde\psi_k(x) = 0$, where $\xi_x = -(1/2m)(\partial^2/\partial x^2) - \mu_k$ and $\mu_k = \mu - k^2/2m$.

Decomposing $\tilde\psi$ into bulk and surface fields $\tilde\psi_k(x) = \psi^b_k(x) + \psi_k(0)$ and integrating out $\psi^b_k(x)$ we arrive at the intermediate effective action $\tilde S$ of a superconductor lead expressed only via the ψ-fields at the surface,

$$\tilde S = i \int {\rm d}t \int {\rm d}t' \sum_k \frac{v_x}{2} \bar\psi_k(0,t)\tau_z \hat g(t,t')\psi_k(0,t'). \tag{11}$$

Here $v_x = \sqrt{2\mu_k/m}$ and

$$\hat g(t,t') = \exp\left[\frac{i\varphi(t)\tau_z}{2}\right] \int \hat g(\epsilon) e^{-i\epsilon(t-t')} \frac{{\rm d}\epsilon}{2\pi} \exp\left[-\frac{i\varphi(t')\tau_z}{2}\right], \qquad \hat g = \begin{pmatrix} \hat g^{\rm R} & \hat g^{\rm K} \\ \hat 0 & \hat g^{\rm A} \end{pmatrix}, \tag{12}$$

where $\varphi(t) = \varphi_0 + 2e\int^t V(t_1){\rm d}t_1$ is the time-dependent phase of the superconducting order parameter and $V(t)$ is the electric potential of the electrode. The Fourier-transformed retarded and advanced Eilenberger functions have the standard form

$$\hat g^{\rm R/A}(\epsilon) = \frac{(\epsilon \pm i0)\tau_z + i|\Delta|\tau_y}{\sqrt{(\epsilon \pm i0)^2 - |\Delta|^2}}, \tag{13}$$

and $\hat{g}^{\mathrm{K}} = (\hat{g}^{\mathrm{R}} - \hat{g}^{\mathrm{A}})\tanh(\epsilon/2T)$ is the Keldysh function.

The second step in our derivation amounts to integrating out the ψ-fields on the surface. The integral

$$\int \mathcal{D}\bar{\psi}(0)\mathcal{D}\psi(0)\exp\left[i\tilde{S} + i\int \mathrm{d}t(\mathcal{T}\bar{\psi}_k(0)\tau_z c + \text{c.c.})\right] \tag{14}$$

can be easily evaluated. Carrying out exactly the same procedure for the right electrode, making use of the identity $\hat{g}^2_{\mathrm{L,R}} = 1$ and adding up the results we obtain

$$S_{\mathrm{env}} = i\Gamma \int \mathrm{d}t \int \mathrm{d}t' \bar{c}(t)\tau_z \hat{g}_+(t,t')c(t'). \tag{15}$$

Here and below we define $\Gamma = 4\sum_k \mathcal{T}^2/v_x$ and $\hat{g}_\pm = (\hat{g}_{\mathrm{L}} \pm \hat{g}_{\mathrm{R}})/2$. Equation (15) is one of our central results. It enables the expression of the kernel J (5) solely in terms of the fields $\bar{c}$ and c:

$$J = \int \mathcal{D}\bar{c}\,\mathcal{D}c \exp[iS_{\mathrm{dot}} + iS_{\mathrm{env}}], \tag{16}$$

where $S_{\mathrm{dot}} + S_{\mathrm{env}} \equiv S_{\mathrm{eff}}[\bar{c}, c]$ represents the effective action for a quantum dot between two superconductors.

In order to complete our derivation, let us express the current through the dot in terms of the correlation function for the variables $\bar{c}$ and c. Starting from the general expression for the current and representing the correlator for the ψ-fields in terms of that for the c-fields, we find

$$I = \frac{e\Gamma}{4}\mathrm{Tr}[\hat{g}_- \langle \bar{c}c\rangle|_K + \text{h.c.}]\,. \tag{17}$$

Thus, the problem of calculating the current through an interacting quantum dot is reduced to that of finding the correlator $\langle \bar{c}c\rangle$ in the model defined by the effective action $S_{\mathrm{eff}} = S_{\mathrm{dot}} + S_{\mathrm{env}}$ (7), (15). It should be emphasized that our approach is appropriate for studying both equilibrium and nonequilibrium electron transport. In the noninteracting limit $U \to 0$ the results of previous studies can be easily recovered within our formalism.

Mean-field approximation. – Consider now the case $U \neq 0$ and decouple the interacting term in (7) by means of the Hubbard-Stratonovich transformation [13, 14] introducing new scalar fields $\gamma_\pm$. The kernel J now reads

$$J = \int \mathcal{D}\bar{c}\mathcal{D}c\mathcal{D}\gamma_+\mathcal{D}\gamma_- \exp[iS[\gamma] + iS_{\mathrm{eff}}|_{U=0}], \tag{18}$$

$$S[\gamma] = \int \mathrm{d}t\left(\bar{c}\gamma_+\sigma_x c + \bar{c}\gamma_- c - \frac{2}{U}\gamma_+\gamma_-\right). \tag{19}$$

Here we will assume that the effective Kondo temperature [7] $T_{\mathrm{K}} = \sqrt{U\Gamma}\exp[-\pi|\epsilon_0|/2\Gamma]$ is smaller than the superconducting gap Δ. In this case interactions can be accounted for within the mean-field approximation. The fields $\gamma_\pm$ in (19) are considered as time-independent parameters determined self-consistently from the saddle point conditions $\delta J/\delta\gamma_\pm = 0$:

$$\gamma_+ = \frac{U}{2}\int \mathrm{d}t\langle \bar{c}c\rangle, \qquad \gamma_- = \frac{U}{2}\int \mathrm{d}t\langle \bar{c}\sigma_x c\rangle. \tag{20}$$

As it turned out from our numerical analysis, the effect of the parameter γ_+ is merely the renormalization of the tunneling rate Γ. Absorbing γ_+-terms in Γ we arrive at the final effective action of our model

$$S_{\mathrm{eff}}[\gamma] = \int \frac{\mathrm{d}\epsilon}{2\pi}\int \mathrm{d}\epsilon' \bar{c}\hat{M}(\epsilon,\epsilon')c, \qquad \hat{M}(\epsilon,\epsilon') = \delta(\epsilon-\epsilon')(\epsilon + \gamma_- - \tau_z\tilde{\epsilon}) + i\tau_z\Gamma\hat{g}_+(\epsilon,\epsilon'). \tag{21}$$

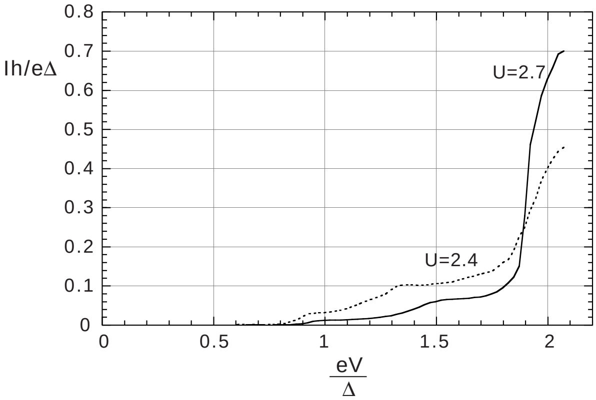

Fig. 1 – The *I*-*V* curves for an SAS junction at subgap voltages. The parameters are $\epsilon_0 = -1.5$, $\Gamma = 0.6$, $U = 2.4$ (dotted line) and 2.7 (solid line).

The physical justification for using the mean-field approximation is the suppression of the Kondo resonance by superconducting order parameter. Such a suppression occurs due to strong decreasing of the density of states at the Fermi energy in the region of order Δ. Thus, the number of low-energy electrons which are able to screen the local impurity spin is small [16, 17]. Therefore, we can expect that the damping of the screening enlarges the parameter space (ϵ_0, U) for which the single occupancy (dublet states) becomes the ground state of the system. Indeed, the complete solution includes competition between singlet state responsible for Kondo physics that cannot be obtained by the mean-field approximation (MF) and doublet states which can be reached by MF. These doublet states whose characteristics depend on the applied voltage were obtained by solving eq. (20) as a function of bias. In s-superconductors both the spin-up and spin-down electrons of the Cooper pair interact with the local spin and the new important parameter which distinguishes which doublet or singlet states are relevant is the ratio Δ/T_K. Thus, roughly, one may say: if $\Delta > T_\mathrm{K}$ then the doublet states is preferable and the MF can be used; if $\Delta \le T_\mathrm{K}$ then the Kondo singlet is stabilized and the other methods like noncrossing approximation or variational wave function approach are more suitable. Such reasoning was used for example in recent works on the subject (see refs. [13, 17]). In our case even for largest value of $U = 2.7$, for all Γ and for $\epsilon/\Delta = 1.5$ which we used, the criterion $\Delta > 2T_\mathrm{K}$ (it was obtained in the above-mentioned works) is fulfilled.

Subgap current in SAS junctions. – In order to find the correlator $\langle \bar{c}c \rangle = i\hat{M}^{-1}$ and the current (17), we numerically inverted the matrix (21) and simultaneously solved the self-consistency equation for γ_- (20). The resulting *I*-*V* characteristics for an SAS junction in the presence of Coulomb interaction are displayed in fig. 1. One observes all the main features which characterize an interplay between MAR and Coulomb interaction: i) at relatively low voltages the current is essentially suppressed due to interaction, ii) for higher voltages (but still $eV < 2\Delta$) MAR is possible and results in a nonzero subgap current which increases with V and iii) the subharmonic peaks in the differential conductance occur and are shifted to higher voltages as compared to the noninteracting case. An increase of U results in a stronger current suppression and a more pronounced shift of the subharmonic peaks. Close to the gap edge $eV = 2\Delta$ the current shoots up sharply.

The parameters used in our numerical analysis are chosen in a way to observe all the key features i), ii) and iii). The transparency of the junction is chosen to be $\Gamma = 0.6$ and the current is evaluated for $U = 2.4$, and $U = 2.7$. Here we notice that the MAR were considered for interacting quantum dot also in ref. [18]. In this work $\Gamma \ll 1$ and the factorized form for the effective tunneling rate was suggested . In our case all higher-order virtual processes take place and must be included into calculations of the current. Thus the expressions for the current are much more complicated and cannot be represented in a factorized form. The same is correct for the saddle point dynamical mean field equations that defined the position and the width of doublet states. The case $U_{-} > \infty$ was considered in [19] in the limit $T_{\mathrm{K}} \ll T_{\mathrm{c}}$.

In summary, we presented a detailed analysis of an SAS junction at finite bias and derived its effective action using Keldysh path-integral techniques. Our approach applies for both equilibrium and nonequilibrium current transport in the presence of interactions. The repulsive Coulomb interaction leads to novel effects in the pattern of the subgap current. In particular, it shifts the peaks of the differential conductance toward larger bias. When the interaction is sufficiently strong the subgap current is highly suppressed. Our predictions can be directly tested in experiments with superconducting quantum dots.

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