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Electron Transport Through Josephson Junction Containing a Dimeric Structure

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Abstract The dc Josephson effect in a superconductor/dimeric molecule/superconductor junction has been investigated by means of the nonequilibrium Green's function method and the Keldysh diagram technique. The application of the atomic representation has allowed to simplify considerably the computation of the supercurrent and occupation numbers and receive the general expressions which take into account all processes of the Andreev reflection in the loopless approach. It is significant that the expressions for the current and occupation numbers are valid for different multilevel structures in the Josephson junction. The sf-exchange interaction between the electron spin and the spins of the dimer leads to the suppression of the critical current due to a new set of Andreev bound states.

Keywords Josephson junction · Andreev reflection · Spin-flip processes · Spin dimer

1 Introduction

Josephson structures attract attention of researchers due to the opportunity to use them as bits of information in future quantum computers and in traditional electronics devices [1,2]. Quantum transport between superconductors (SCs) is coherent because of the proximity effect, it allows to explore the fundamental characteristics of mesoscopic samples [3]. In addition, the substantial properties of SC contacts can be

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investigated in such structures [4,5]. A large number of studies in this area have been devoted to the interaction of the Andreev reflection (AR) mechanism [6] with Coulomb blockade and Kondo correlations [7]. In particular, it is shown that in the SC/quantum dot (QD)/SC system in the magnetic case, and a large Coulomb interaction the main contribution to the supercurrent is provided by the tunnel processes in which the spin ordering of Cooper pairs is reversed. As a result, the critical current becomes negative, $I = I_c \sin(\Theta + \pi) = -I_c \sin\Theta$ ($\Theta = \Theta_L - \Theta_R$—the phase difference between SCs), and a π-junction is realized [8–10]. On the other hand, the Kondo effect may prevent Cooper pairing at low temperatures, $T < T_K$ (T_K—the Kondo temperature) and $\Delta < T_K$ (Δ—the superconducting order parameter), and a 0-junction is restored [8,11]. In this study, we have investigated the effect of the spin-flip processes on the dc Josephson current in the junction containing dimeric molecule when $\Delta > T_K$. Thus, to solve this problem, we have neglected the Coulomb correlations both on an outer molecular orbital and between the electrons on the orbital and Cooper pairs in the SCs. For example, the last type of correlations can give rise to the Mahan–Nozieres–De Dominicis effect [12,13] in normal tunnel junctions which was first discussed by Matveev and Larkin [14].

2 Model

The system under consideration is a Josephson junction with a dimeric structure in the central part (see Fig. 1). It can model a molecule with two localized magnetic ions coupled by antiferromagnetic exchange interaction and the outer electron orbital in the experiment [15]. The Hamiltonian of the system consists of several components, $\hat{H} = \hat{H}_L + \hat{H}_R + \hat{H}_D + \hat{H}_T$. The terms $\hat{H}_L$ and $\hat{H}_R$ describe left and right uncoupled SCs and represented by a BCS Hamiltonian

$$\hat{H}_{L(R)} = \sum_{k(p)\sigma} \xi_{k(p)} c^+_{k(p)\sigma} c_{k(p)\sigma} + \sum_{k(p)} \left(\Delta e^{i\Theta_L} c^+_{k(p)\uparrow} c^+_{-k(p)\downarrow} + h.c. \right), \qquad (1)$$

where $c^+_{k(p)\sigma}$ creates an electron with wave vector k (p) and spin σ at the single-particle energy level $\xi_{k(p)}$ referred to the chemical potential, i.e., $\xi_{k(p)} = \varepsilon_{k(p)} - \mu$ ($\mu = 0$). The Hamiltonian of the dimeric molecule has form

$$\hat{H}_D = \sum_\sigma \varepsilon_d a^+_\sigma a_\sigma + I\,(\mathbf{S}_1\mathbf{S}_2) + A\,[(\sigma\mathbf{S}_1) + (\sigma\mathbf{S}_2)]\,. \qquad (2)$$

The first term in (2) characterizes the single-electron energy ε_d on the outer orbital which can be changed applying a gate voltage. It is assumed that the dimer's spin

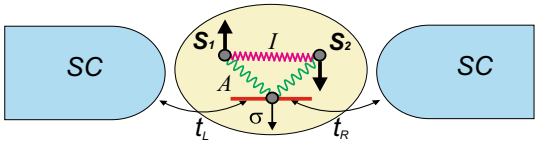

Fig. 1 The Josephson junction with dimeric molecule. (Color figure online)

moments, $\mathbf{S}_1$ and $\mathbf{S}_2$, are antiferromagnetically coupled with the intensity $I > 0$ ($\mathbf{S}_1 = \mathbf{S}_2 = 1/2$). Consequently, the singlet state is a ground one and triplet levels are higher at I in case of the absence of electrons at the molecule or the doubly occupied orbital. If the outer orbital has one electron, eight spin states are possible due to the sf-type exchange interaction defined by the parameter A.

The last term in $\hat{\mathrm{H}}$ is a tunnel Hamiltonian,

$$\hat{H}_{\mathrm{T}} = t_{\mathrm{L}} \sum_{k\sigma} c_{k\sigma}^{+} a_{\sigma} + t_{\mathrm{R}} \sum_{p\sigma} c_{p\sigma}^{+} a_{\sigma} + h.c., \tag{3}$$

where $t_{\mathrm{L}}, t_{\mathrm{R}}$ - the coupling coefficient of the molecule to left and right SCs respectively.

3 Josephson Current in Atomic Representation

The application of the atomic representation for the Hamiltonian (2) is convenient for the consideration of the electron transport through a multilevel structure as it was shown in the works [16,17]. The introduction of the Hubbard operators, X^{α} (where $\alpha = \alpha(n, m), n\, m$—the indices of the initial and final states of the transition $\alpha(n, m)$), allows to simplify essentially the application of Wick's theorem in the construction of the perturbation series in the tunnel parameters. The Hamiltonian (2) is diagonal in the atomic representation, $\hat{H}_{\mathrm{D}} = \sum_{n=1}^{16} E_n X^{nn}$. The second-quantization operators are described in terms of the Hubbard operators with the use of the representation parameters, $\gamma_{\sigma}(\alpha)$, $a_{\sigma} = \sum_{\alpha} \gamma_{\sigma}(\alpha) X^{\alpha}$. The sixteen states of the isolated dimeric molecule are distributed among the three sectors of the Hilbert space with the different number of electrons in the outer orbital.

It is useful to employ the Nambu representation with the two-component operators, $\Psi_{k(p)} = \left[c_{k(p)\uparrow} \quad c_{-k(p)\downarrow}^{+}\right]^{T}$, $\Psi_{\alpha} = \left[X^{\alpha} \quad X^{-\alpha}\right]^{T}$, to describe the transport properties of the Josephson junctions [3]. To simplify the current calculation, we also take an unitary transformation $\hat{U} = \exp\left\{\frac{i}{2}\left[\sum_{k\sigma} \Theta_{\mathrm{L}} c_{k\sigma}^{+} c_{k\sigma} + \sum_{p\sigma} \Theta_{\mathrm{R}} c_{p\sigma}^{+} c_{p\sigma}\right]\right\}$ [18] which carries the phases $\Theta_{\mathrm{L(R)}}$ in the tunnel Hamiltonian,

$$\begin{aligned} \hat{H}_{\mathrm{T}} &= \sum_{k\alpha} \Psi_{k}^{+} \hat{t}_{\mathrm{L}\alpha} \Psi_{\alpha} + \sum_{p\sigma} \Psi_{p}^{+} \hat{t}_{\mathrm{R}\alpha} \Psi_{\alpha} + h.c., \\ \hat{t}_{\mathrm{L(R)}\alpha} &= \hat{t}_{\mathrm{L(R)}} \hat{\gamma}_{\alpha} = t_{\mathrm{L(R)}} diag\left(e^{i\Theta_{\mathrm{L(R)}}/2} \gamma_{\uparrow}(\alpha), -e^{-i\Theta_{\mathrm{L(R)}}/2} \gamma_{\downarrow}(\alpha)\right). \end{aligned} \tag{4}$$

To calculate the Josephson current, we introduce the matrix Green's functions with the time arguments defined at the Keldysh contour, $\hat{G}_{ij}^{ab}(\tau - \tau') = -i_C \left\langle \Psi_i(\tau) \Psi_j^{+}(\tau') \right\rangle$ [19]. The indices $a,\ b$ take values $+$ or $-$ depending on whether the lower or upper branch of the Keldysh contour the times τ, τ' belong. Considering the operator (4) as a perturbation and writing a diagram series for the mixed Green's function $\hat{G}_{k(p)\alpha}^{+-}(\tau, \tau)$ [19,20], the Josephson current is expressed as

$$I = -e\left\langle \frac{dN_{\mathrm{L}}}{dt} \right\rangle = \int\limits_{-\infty}^{+\infty} \mathrm{d}\omega f\left(\omega\right) j\left(\omega\right) = I_{\mathrm{d}} + I_{\mathrm{cont}},$$

$$I_{\mathrm{d}} = \frac{e\Gamma^2}{\pi} \sin\Theta \int\limits_{-\Delta}^{+\Delta} \mathrm{d}\omega f\left(\omega\right) \times$$

$$\times Im\left\{ \frac{L_1 L_2 \beta_0^2}{1 + \Gamma\left(L_1 + L_2\right)\beta + \Gamma^2 L_1 L_2 \left(\beta^2 - \beta_0^2 \cos^2\frac{\Theta}{2}\right)} \right\}, |\omega| < \Delta,$$

$$I_{\mathrm{cont}} = \frac{e\Gamma^3}{\pi} \sin\Theta \left(\int\limits_{-\infty}^{-\Delta} + \int\limits_{+\Delta}^{+\infty} \right) \mathrm{d}\omega f\left(\omega\right) \times$$

$$\times Re\left\{ \frac{i\beta\beta_0^2 L_1 L_2 \left(L_1 + L_2\right)}{\left[1 + \Gamma^2 L_1 L_2 \left(\beta^2 - \beta_0^2 \cos^2\frac{\Theta}{2}\right)\right]^2 - \Gamma^2\beta^2\left(L_1 + L_2\right)^2} \right\}, \ |\omega| > \Delta, \tag{5}$$

where $f\left(\omega\right) = 1/\left\{1 + \exp\left[\omega/kT\right]\right\}$—the Fermi equilibrium distribution function; $\beta = \frac{\omega}{\sqrt{\Delta^2 - \omega^2}}$ when $|\omega| < \Delta$ and $\beta = \frac{i|\omega|}{\sqrt{\omega^2 - \Delta^2}}$ when $|\omega| > \Delta$; $\beta_0 = \beta\frac{\Delta}{\omega}$. All the information on the energy spectrum and the system's occupation numbers is stored in the functions L_1 and L_2,

$$L_1 = \sum_{\alpha} \frac{b_\alpha \gamma_\uparrow^2\left(\alpha\right)}{\omega + E_\alpha + i\delta}, L_2 = \sum_{\alpha} \frac{b_\alpha \gamma_\downarrow^2\left(\alpha\right)}{\omega - E_\alpha + i\delta}, \tag{6}$$

where $b_\alpha = N_n + N_m$—the sum of the occupation numbers of the transition $\alpha(n, m)$. To derive (5) it was assumed that the junction is symmetrical, i.e., the broadening of the levels due to the coupling with contacts are the same, $\Gamma_{\mathrm{L}} = \pi\nu_0 t_{\mathrm{L}}^2 = \Gamma_{\mathrm{R}} = \Gamma/2$ (ν_0—the DOS of the contacts in the normal phase). We also expressed the lesser Green's functions with the advanced and retarded ones as $\hat{G}_{ij}^{+-}\left(\omega\right) = f\left(\omega\right)\left[\hat{G}_{ij}^{a}\left(\omega\right) - \hat{G}_{ij}^{r}\left(\omega\right)\right]$ using the fluctuation-dissipation theorem valid in equilibrium. The Josephson current has two components: I_{cont}—a contribution from the continuous spectrum $|\omega| > \Delta$ and I_{d}—a current carried by Andreev bound states (ABSs) when $|\omega| < \Delta$. The energies of the ABSs are the zeros of the integrand of I_{d}. It is significant to emphasize that in the single-level QD limit ($A = 0$) such an equation is similar to the corresponding formulae in the articles [21,22]. The expression (5) takes into account all possible processes of the multiple AR on the spin dimer in the loopless approach. It should be noted that the formula (5) obtained for the Josephson current can be applied to different multilevel systems in the junction and cannot be reduced to the one for the case of direct tunneling between SCs [23].

4 Analysis of Numerical Results

In the calculations below, all the energy quantities are scaled by the energy gap Δ and the system is considered to be at zero temperature. The dependence I_c on the phase Θ in the tunnel regime ($\Gamma << \Delta$) can be neglected as follows from formula (5). Hence, the critical current in this case is defined as $I_c = I$ ($\Theta = \pi/2$). The occupation numbers in L_1 and L_2 were found from the self-consistent calculation of the quantum kinetic equations $N_m = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} \left[\hat{G}^{+-}_{\alpha\alpha}(\omega)\right]_{11}$ using the condition $\sum_m N_m = 1$.

The dependence of the critical current on the gate voltage $I_c(\varepsilon_d)$ for different intensities of the sf-interaction is depicted in Fig. 2. When $A = 0$, a Cooper pair tunnels in a single-level QD (see red curve). The corresponding current density j_d has a maximum associated with the transmission through the ABS (dashed curve close to the point $\omega = -0.1\Delta$ in Fig. 3). This ABS is attributed to the transition from the ground state to a one electron excited state of the system. Despite having opposite sign the contribution of the states with $\omega < -\Delta$, I_{cont}, to the supercurrent is significantly less than I_d and does not affect the resulting critical current (see the inset of Fig. 3). The critical current is maximum in the presence of the electron-hole symmetry $\varepsilon_d = 0$. When $A > I$ and $|\varepsilon_d| < A - I$, the spin-flip processes lead to the fact that the ground state of the system becomes a spin doublet with one electron in the molecule with the energy $E_d = \varepsilon_d + I/4 - A$. Consequently, there are two classes of possible excitations of the system: either the zero-electron states or the two-electron states. Each transition results in the creation of a corresponding Andreev bound state. Transport via these states causes the appearance of two closely spaced peaks in the current density (solid curve in Fig. 3) instead of the one for $A = 0$. As a result, these resonances give contributions of opposite signs and, therefore, the current I_d is significantly decreased. Furthermore, $|I_{cont}|$ becomes comparable with I_d. This factor gives an additional contribution to the resulting suppression of the critical current (see curves when $A \neq 0$ in Fig. 2). Our data tend to qualitatively support the results of the experimental work [15] that the Josephson current and the proximity effect are very sensitive to the magnetic state of the dimeric structure. In the regions $|\varepsilon_d| > A - I$,

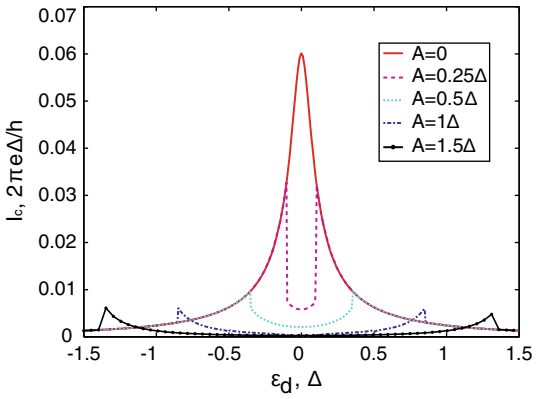

Fig. 2 The critical current as a function of the gate voltage for different A. Parameters: $I = 0.15\ \Delta$, $\Gamma = 0.1\ \Delta$. (Color figure online)

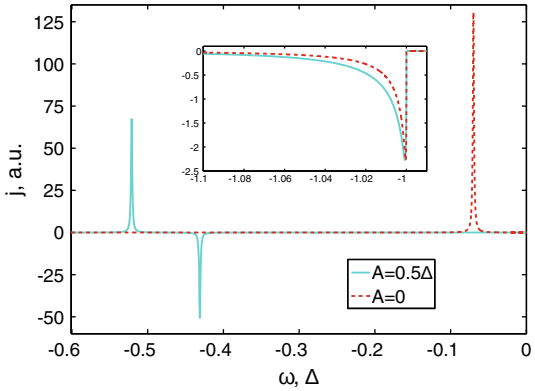

Fig. 3 The current density distribution for $\varepsilon_d = -0.03\ \Delta$. The other parameters are the same as in Fig. 2. *Inset* the current density in the region $\omega < -\Delta$. (Color figure online)

the ground state of the molecule is the dimer in the spin singlet and one electron at the outer orbital. Consequently, the spin degrees of freedom of the electron and dimer do not interact even though $A \neq 0$. And the transport problem is reduced again to the transmission through the single-level QD. If the sf exchange is ferromagnetic ($A < 0$) that the suppression of the critical current is realized under the conditions $A < -2I$ and $|\varepsilon_d| < |A/2 + I|$, when the molecule's ground state is one-electron spin quartet with the energy $E_q = \varepsilon_d + I/4 + A/2$. Thus, the switching of the junction between the states with low and high supercurrent by varying the gate voltage is shown.

5 Conclusions

We have studied the quantum transport in a Josephson junction containing a multilevel structure. The explored structure is a dimeric molecule which consists of a spin dimer in the singlet ground state and the outer electron orbital. A general expression describing the dc Josephson current in the system with a nonequidistant energy spectrum is received using the Keldysh diagram technique and the atomic representation. It is shown that the sf-type exchange interaction between the electron spin of the Cooper pair and the spins of the dimer causes to a significant decrease of the critical current due to the change of the ground state of the dimeric molecule and the emergence of the new set of ABSs. This effect is implemented under the conditions: $A > I$ and $|\varepsilon_d| < A - I$ or $A < -2I$ and $|\varepsilon_d| < |A/2 + I|$.

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