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Current–Phase Relation in SFS Josephson Junctions in the Presence of *s-d* Scattering

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Abstract—The analytical equations for the current–phase relation (CPR) coefficients for Josephson junctions with a ferromagnetic interlayer in the model where the scattering from *s*- to *d*-band is considered to be the main type scattering of charge carrier in a ferromagnet are obtained. It is shown that the magnitude of the coefficients oscillates and decays with an increase of the interlayer thickness. Both the oscillation period and the decay length for the first and the second harmonics differ by two times. The temperature dependence of the critical current demonstrating 0-π temperature transitions is obtained. The possibility of design a flux qubit based on such Josephson junctions is demonstrated.

Keywords: superconductivity, Josephson junctions, superconductor–ferromagnet structure, flux qubit

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INTRODUCTION. JOSEPHSON JUNCTIONS AND THE POSSIBILITY OF THEIR APPLICATION FOR DESIGN OF A QUANTUM COMPUTER

A Josephson junction consists of two superconductors (S) with a weak link. The authors of the present paper considered the contacts separated by a ferromagnetic interlayer (F) (Fig. 1). The interaction of the wave functions of the left and the right superconducting banks produce the stationary Josephson effect: a superconducting current J_S flows through the interlayer. The shape of the dependence of the current J_S on the phase difference φ of the superconducting order parameter on the banks can be obtained for the following reasons: first, the current in the absence of a phase difference has to be zero; second, a change in the phase difference sign has to yield a change in the current direction; and, third, a 2π change in the phase difference has no affect on the current [1]. The most elementary and, thus, the most widely-met relationship that satisfies these conditions is the sinusoidal relationship:

$$J_S(\varphi) = J_C \sin(\varphi),$$

where J_C is the critical current of a junction, i.e., the maximum possible superconducting current flowing through the interlayer. There are other possible cases where, in particular, the higher harmonics can be present in the expansion:

$$J_S(\varphi) = A\sin\varphi + B\sin 2\varphi + C\sin 3\varphi + \ldots. \quad (1)$$

The critical current in the junctions with a ferromagnetic interlayer can be negative, $J_C < 0$. This state is called a π-state since the phase difference in the absence of a current, i.e., in the ground state, becomes equal to π rather than to zero [2]. The cause of the occurrence of such a state is related to the influence of the magnetic field on a superconducting pair. Since the latter consists of electrons with oppositely spin directions then, due to Zeeman splitting, the contribution of the exchange field to the energies of pairing electrons is different. This leads to oscillations in the order parameter. A superconducting state of the LOFF-type (Larkin, Ovchinnikov, Fulde, Ferrell) [3, 4] appears. Then, the order parameter could be approximately written as follows:

$$\Psi_f = \Psi_{f0}\exp(-z/\xi_f) = \Psi_{f0}\exp(-z/\xi_{f1})\exp(-iz/\xi_{f2}),$$
$$\frac{1}{\xi_f} = \frac{1}{\xi_{f1}} + i\frac{1}{\xi_{f2}},$$

where Ψ_{f0} is the order parameter at the superconductor–ferromagnet interface, ξ_f is the complex coherence length, ξ_{f1} is the decay length, and $2\pi\xi_{f2}$ is the period of the order parameter oscillations. For nonsinusoidal current–phase dependence (1), the sign of odd harmonics changes when the phase difference varies by π. If the ground state is reached at the zero

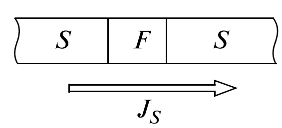

Fig. 1. Josephson junction with a ferromagnetic interlayer. S, superconductor; F—ferromagnet; J_S—superconducting current.

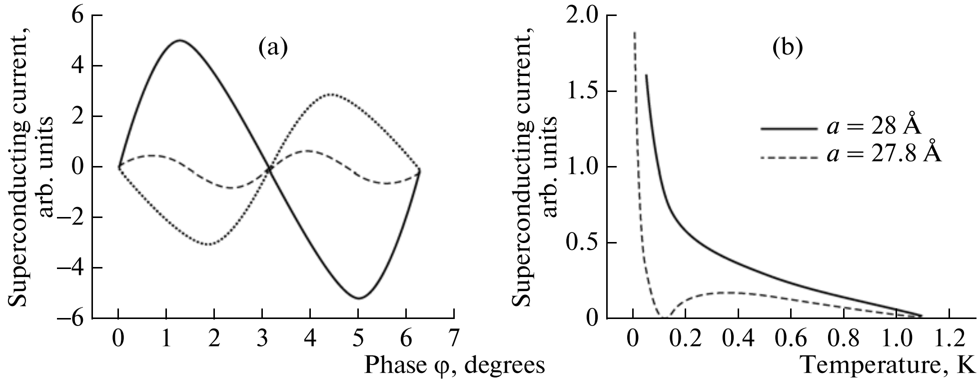

Fig. 2. (a) Current–phase dependence. The dashed line shows the π-state, the interlayer thickness is $a = 32$ Å; the solid line shows the 0 state, $a = 23$ Å; the dashed–dotted line shows the transition from the 0 to the π-state, $a = 27.8$ Å. $T = 0.5$ K, $l = 28$ Å; (b) Temperature dependence of superconducting current. The solid line shows the 0 state (interlayer thickness is $a = 28$ Å). The dashed–dotted line shows the transition from the 0 to the π-state (interlayer thickness is $a = 27.8$ Å). The temperature of the transition from the 0 to the π-state is $T = 0.12$ K, $l = 28$ Å.

phase difference, it is a 0 state and the first coefficient in expansion (1) is $A > 0$. If the ground state is reached at the phase difference equal to π, it is a π-state and $A < 0$. All π-junctions are rather significant owing to their possible application for design of a qubit.

For a qubit design, it is necessary to construct a system with a double-well potential [5]. Tunneling between the wells that removes degeneration is possible and in this case the asymmetric and symmetric superpositions of states in the left and the right minima correspond to two basic qubit states [6]. The implementation of such qubits necessitates having junctions with a nontrivial current–phase dependence [7, 8]. Let us consider a double-junction low-induction superconducting interferometer as a scheme for implementation of a so-called "flux" qubit. It consists of two Josephson junctions connected in parallel. Such a qubit is called a "flux" qubit, since a "trapped" magnetic flux serves as the value that encodes the data. Let us consider the case with identical junction parameters and identical current-phase characteristics. The conditions for the qubit are [7–9]:

$$|2(B_1 + B_2)| > |A_1 + A_2|,$$
$$\frac{(A_1 + A_2)}{2(B_1 + B_2)} \le 0. \qquad (2)$$

It follows from these conditions that it is necessary to find junctions whose current-phase dependence substantially differs from a sinusoidal one.

1.MODEL

1.1. The Density of States for s- and d-Electrons

Researchers from the Ryazanov group [10] presented experimental data that show that ξ_{f2} in a ferromagnetic exceeds the decay length of the order parameter ξ_{f1} by about three times, which comes into contradiction with the solution following from the Uzadel equation [2]. Since this fact needed explanation, it was proposed to take the following mechanisms of scattering in a ferromagnet into account: Professor Buzdin [11] proposed explaining it by scattering with a spin-flip while Vedyaev's group [12] proposed a model taking the *s-d* scattering in a ferromagnet into account. The present paper uses a model for calculation of the current-phase dependence that was developed by the Vedyaev group.

The authors of [13] demonstrated a model calculation of the state densities for nickel and a copper–nickel alloy (see Figs. 3 and 4 in [13], respectively). It was shown in [13] that the density of *d*-electrons at the Fermi level is substantially higher and, since the prob-

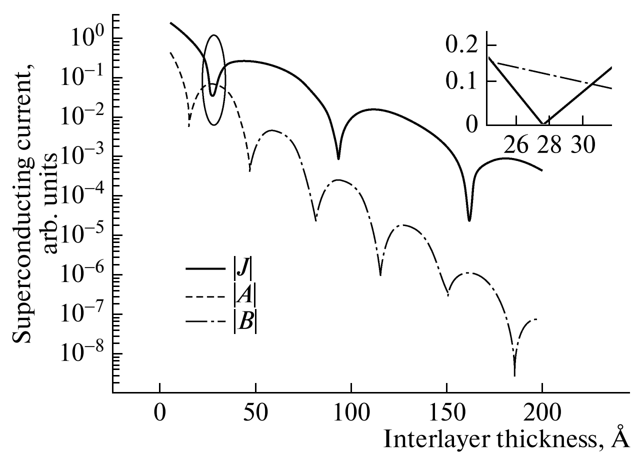

Fig. 3. Dependence of the critical current (solid line) and Harmonics *A* and *B* of current–phase relation on interlayer thickness (dashed and dashed–dotted lines, respectively). The region of the first minimum of the first harmonic (25–31 Å) is shown in the insert. The dashed line on the insert shows the doubled *B* harmonic. The region where the quibit conditions satisfy: 27.7–30.5 Å, T = 0.5 K, $l = 28$ Å.

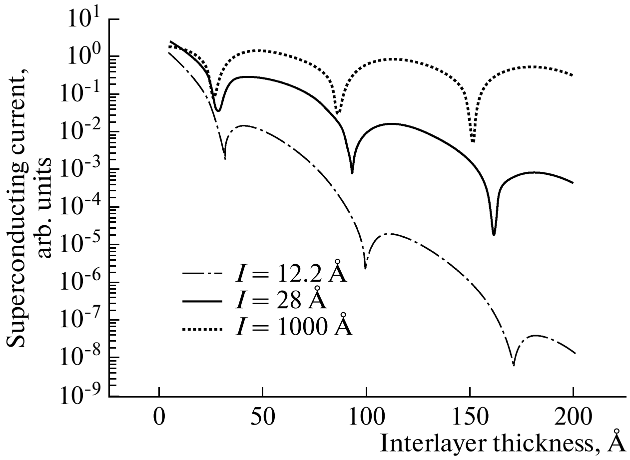

Fig. 4. Critical current as a function of interlayer thickness at different mean free paths l. The solid line (l = 28 Å), the dashed–dotted line (l = 12.2 Å), the dashed line (l = 1000 Å). The region where the quibit conditions satisfy at l = 12.2 Å: 30.55–31.1 Å, T = 0.5 K.

ability of scattering is proportional to the density of the states, the probability of scattering to the d-zone has to be larger. We considered the junctions with superconductors from aluminum, which does not have electrons in the d-zone and, thus, d-electrons are specularly reflected at the superconductor–ferromagnet interface and do not form superconducting pairs. That is why scattering in the d-zone yields decay of the pairs.

1.2. Equation for Current in a Model Taking s-d Scattering into Account

For the above-described type of scattering, the researchers from the Vedyaev group solved the Gor'kov equations and derived the following equation for the superconducting current [12]:

$$J = \frac{4e}{\pi}T\sum_{\omega}\int kdk\,\mathrm{Re}\frac{(1-R^2)\sin\varphi}{\mathrm{Den}(\varphi, a, \ldots)}, \quad (3)$$

where T is the temperature; k is the Fermi qiasimomentum; R is the coefficient of Andreev scattering: $R = \frac{c^2 - c_2c_1}{c^2 + c_1c_2}$, where c, c_1, and c_2 are the real parts of the quasiparticle momentums p, $p_\uparrow$, and $p_\downarrow$ for a superconductor and a ferromagnet, respectively; φ is the phase difference of the order parameter; a is the thickness of the ferromagnetic interlayer; $\omega = \pi T(2n + 1)$ are the Matsubara frequencies; n is an integer; and Den is an oscillating function that depends on the transition parameters. Since the phase φ is the argument of the function Den, the current–phase dependence is different from the sinusoidal one.

1.3. Equation for Harmonics of the Current–Phase Dependence

Let us consider the current–phase dependence described by Eq. (3). Let us introduce the following terms: the row bit vector is $\boldsymbol{\lambda}_1$: $\lambda_1 = (\cos(ap_\uparrow)\sin(ap_\uparrow))$, and the column bit vector is $\boldsymbol{\lambda}_2$: $\lambda_2 = \begin{pmatrix}\cos(ap_\downarrow)\\ \sin(ap_\downarrow)\end{pmatrix}$, where $p_\uparrow$, $p_\downarrow$ are the pulses of electrons in the states with a spin antiparallel and parallel the magnetization in a ferromagnet that are the solutions to the Gor'kov equations [12]. Let us introduce the matrix Q:

$$Q = \begin{pmatrix} \frac{\Delta^2+\omega^2}{\Delta^2}(1-R^2) + \frac{\omega^2}{\Delta^2}P^2(1-r^2) & 2i\omega\frac{\sqrt{\Delta^2+\omega^2}}{\Delta^2}P(1+rR) \\ -2i\omega\frac{\sqrt{\Delta^2+\omega^2}}{\Delta^2}P(1-rR) & \frac{\Delta^2+\omega^2}{\Delta^2}(1+R^2) + \frac{\omega^2}{\Delta^2}P^2(1+r^2) \end{pmatrix},$$

where Δ is the energy gap in a superconductor and r is the reflection coefficient: $r = \frac{c_1 - c_2}{c_1 + c_2}$, $P = \frac{c_1c + c_2c}{c^2 + c_1c_2}$. Using the introduced terms, the equation for current (3) can be written in a more convenient form:

$$J = \frac{4e}{\pi}T\sum_{\omega}\int \mathrm{Re}\left(\frac{(1-R^2)\sin\varphi}{(1-R^2)\cos\varphi + \lambda_1 Q\lambda_2}\right)dE.$$

Now it is possible to find coefficients of the expansion of this equation into the Fourier series over φ. Using the equations for the course-of-value function of the second-type Chebyshev polynomials $U_n(\cos\varphi)$ [14] we get:

$$z_{1,2} = -\frac{(\lambda_1 Q \lambda_2)}{(1-R^2)} \pm \sqrt{\left(\frac{(\lambda_1 Q \lambda_2)}{(1-R^2)}\right)^2 - 1}.$$

The following equations were derived for the coefficients A and B:

$$A = -2\sum_{\omega}\int z dE,$$
$$B = -2\sum_{\omega}\int z^2 dE, \quad (4)$$

where z is chosen as one of the values z_1 or z_2, which satisfies the condition $|z| < 1$.

2. INVESTIGATION OF THE CURRENT–PHASE DEPENDENCE OF SFS JUNCTIONS

2.1 The Search for Regions where the Transition from the 0-State to the π-State Takes Place

Using the obtained equations (4), the current–phase dependence for the Josephson junction with an interlayer from a ferromagnetic metal was investigated. The model parameters of the superconductor correspond to aluminum: the critical temperature is T_C = 1.196 K, and the Fermi quasimomentum is k_f = 1.75 Å^{-1} [15]. The parameters of the ferromagnetic interlayer approximately correspond to those of nickel: the Fermi quasimomentum is k_f = 1.18 Å^{-1} and H = 0.2 eV [16]. Figure 2a shows the superconducting current as a function of phase at different interlayer thicknesses. The solid line marks the dependence far from the 0-π transition: it is an ordinary 0 state with a sinusoidal dependence. The dashed line shows this dependence far from the 0-π transition as well, but for a different interlayer thickness: with respect to the previous curve it has a π-phase shift and the current direction is opposite to that in the 0 state, i.e., it is a sinusoidal π-state. The intermediate state of the transition from the 0 state to the π-state is shown with a dashed–dotted line. Its shape is different from the sinusoidal one and at least the second harmonic has to be present in the current-phase dependence. The transition from the 0 state to the π-state can be also observed when studying the temperature dependence of the critical current. Such a transition was observed in the experiment performed by the Ryazanov group [17]. Figure 2b shows the curve of the temperature transition. If the absolute value of the critical current in 0 and π-states simply decreases with temperature, there is a temperature in the intermediate state at which the critical current changes its direction and the junction gets from the 0 state over to the π-state: the current–phase dependence at this point has to be nonsinusoidal. In the given plot, the temperature is 0.12 K.

2.2. Dependence of the Critical Current and Harmonics on the Interlayer Thickness

The curves demonstrating the dependence of the coefficients on the interlayer thickness were calculated to investigate the higher-order harmonics in detail. The calculation results are shown in Fig. 3. The minima of the curves indicate a transition through zero and a change of the sign. The regions where the first harmonic is positive correspond to the 0 state of the region; the regions where it is negative correspond to the π-state. The plots for the current and the first coefficient coincide for practically all interlayer thicknesses and, thus, the current is determined mainly by the first harmonic, i.e., it is sinusoidal, $J_S(\varphi) = A\sin\varphi$. The regions where the first harmonic changes its sign correspond to the intermediate state of the 0/π-transition. The coefficient A in these regions passes through zero while the coefficient B is still nonzero and, thus, the nonsinusoidal state shown on the previous figures, $J_S(\varphi) = B\sin 2\varphi$ occurs in such regions. The oscillation periods of the first and the second coefficients differ by about two times. This yields the formation of the regions where the first coefficient A is at its minimum, while the second coefficient B is close to the maximum and the current–phase dependence is nonsinusoidal. With the thickness of the interlayer increasing, the coefficients not only oscillate but decay as well. Moreover, the second coefficient B decays twice as quickly as the first coefficient A, the decay length of the latter in this case is approximately equal to the specified length of the free path. The larger the interlayer thickness, the lower the current is in the regions with a nonsinusoidal dependence. However, even at small thicknesses the currents in these regions are negligible as compared to the current in the 0 and π-states and, thus, it is difficult to reveal a nonsinusoidal dependence in practice and it seems reasonable to consider the regions with small interlayer thicknesses where the critical current is still relatively high and the differences in the harmonics are not so substantial. The authors of [18, 19] presented the experimental evidence for the existence of the second harmonic, which allows us to perform further calculations aimed at seeking such junctions.

2.3. The Effect of the Mean Free Path on Critical Current Decay

In the applied model, the decay coefficient of the order parameter is proportional to the mean free path [12], and, thus, it seems appropriate to consider the junctions with a large mean free path. The insert in Fig. 3 shows the results of a more detailed calculation of the region shown by an oval on the basic plot. Hypothetically, the current–phase dependence in this region is nonsinusoidal and this region can be considered as one that is suitable for qubit design. A study of the conditions (2) in this region shows that they are satisfied at 27.2–30.5 Å. The calculations for the junctions with a smaller mean free path l were also performed. These results are shown in Fig. 4. It is seen that at smaller l the current decays faster, since the smaller the value of l, the larger the scattering effect. For a smaller mean free path, the region where these conditions are met is very narrow. Thus, the purer junctions are more promising for qubit design. Nevertheless, such a narrow region can be also achieved if one creates a junction with an interlayer whose thickness is close to the required value and then "catches" the sought region by varying the temperature.

To study the effect of *s-d* scattering on the current flow, the dependence of the critical current on the interlayer thickness was calculated for a very large mean free path. The results are shown in Fig. 4. The decay of the current for a "clean" junction is slower: it follows the power law rather than the exponential one [19].

CONCLUSIONS

The analytical equations for the coefficients of the current–phase relation of SFS Josephson junctions in a model where *s-d* scattering was considered as the main type of scattering in a ferromagnetic material were obtained. It was shown that the oscillation periods of the first and the second harmonics of the current–phase dependence differ by about two times and the second coefficient decays twice faster with an increase in the interlayer thickness. For the specified materials that the junctions were made from, junction parameter regions exist where the current–phase dependence is different from the sinusoidal one. The possibility of design a flux qubit based on SFS Josephson junctions is demonstrated. The transitions with a sufficiently large mean free path are the most promising.

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