

# $\pi - 0$ transition in superconductor-ferromagnetic-superconductor junctions

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Superconductor-ferromagnetic-superconductor (SFS) Josephson junctions are known to exhibit a transition between  $\pi$  and 0 states. In this note we find the  $\pi - 0$  phase diagram of an SFS junction depending on the transparency of an intermediate insulating layer (I). We show that in general, the Josephson critical current is nonzero at the  $\pi - 0$  transition temperature. Contributions to the current from the two spin channels nearly compensate each other and the first harmonic of the Josephson current as a function of phase difference is suppressed. However, higher harmonics give a nonzero contribution to the supercurrent.

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In the last years, many interesting phenomena were investigated in Superconductor (S) – Ferromagnetic (F) – Superconductor (SFS) Josephson contacts. One of the most striking effects is the so called  $\pi$ -state of SFS junctions [1–4] in which the equilibrium ground state is characterized by an intrinsic phase difference of  $\pi$  between the two superconductors. Investigations of  $\pi$  junctions have not only academic interest, e.g., in [5, 6] a solid-state implementation of a quantum bit was proposed based on a superconducting loop with 0 and  $\pi$  Josephson junctions.

The existence of the  $\pi$ -state in an SFS junction was recently experimentally demonstrated by the group of Ryazanov [4]. In this experiment, the temperature dependence of the critical current was measured. At a certain temperature the critical current was found to drop almost to zero, this has been interpreted as the transition from the 0 to the  $\pi$  state. The transition temperature  $T_{\pi 0}$  was shown to exhibit a strong dependence on the concentration of ferromagnetic impurities, i.e., on the exchange field  $E_{ex}$  in the ferromagnetic film.

In this note, we present a theory of the  $\pi - 0$  transition in short SFS junctions. Our goal is to understand which parameters (exchange field, temperature, ...) stabilize a  $\pi$ -state and how the phase diagram looks like. We investigate the current-phase relation and the critical current near the transition to the  $\pi$ -state. Most importantly, we find that in general, the critical current is not

zero at  $T_{\pi 0}$ , and it may not even reach a local minimum. The identification of the critical current drop and the  $\pi - 0$  transition is only possible if the current is given by the standard Josephson expression  $I(\varphi) \propto \sin(\varphi)$ , which is valid for the limiting case of tunnel barriers only. Even if the main contribution to the current is of this form, the higher harmonics contribution  $I(\varphi) \propto \sin(2\varphi)$  would not vanish at  $T_{\pi 0}$ . Consequently,  $I_c \neq 0$  at the transition point.

We consider SFS junctions in the “short” limit defined by  $\hbar/\tau \gg \Delta(T = 0)$ ; here,  $\tau$  is the characteristic time needed for an electron to propagate between the superconductors. In this case, we can employ a powerful scattering formalism [7] which allows one to express the energies of Andreev states in the junction in terms of the transmission amplitudes of the junction in the normal state. These Andreev states give the main contribution to the phase-dependent energy of the junction, therefore  $I(\varphi)$  can be calculated. Any junction is characterized by a set of “transport channels” labelled by  $n = 0, 1, \dots, N$ , each channel is characterized by the transmission coefficient  $D_n$ . If one disregards ferromagnetism, the Andreev levels are degenerate with respect to the spin index  $\sigma$ . Their energies are given by  $E_{n\sigma} = \pm\Delta(1 - D_n \sin^2(\varphi/2))^{1/2}$ .

We generalize the scattering approach to cover SFS junctions. In this case, the phase of the transmission amplitudes also becomes important. To see this, we introduce the parameter  $\gamma$ :  $\cos(\gamma(\varphi)) \equiv 1 - 2D_n \sin^2(\varphi/2)$ . If we assume that ferromagnetism does not change the

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transport channels, the energies of the Andreev states become

$$E_{n\sigma}(\varphi) = \Delta \left| \cos \left( \frac{\gamma(\varphi) + (\Phi_{n,\sigma} - \Phi_{n,-\sigma})}{2} \right) \right|, \quad (1)$$

where  $\Phi_{n,\sigma}$  is the phase of the transmission amplitude for an electron with spin  $\sigma$  in the channel  $n$ . Thus we observe that the different phase shifts for different spin directions result in a spin-dependent energy shift of the Andreev states. To specify the model further, we consider the layout shown in Fig.1. It consists of

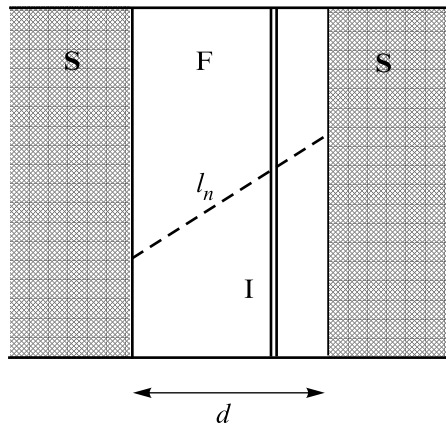


Fig.1. Junction configuration. The current flows from one superconductor (S) to the other through the ferromagnetic (F) layer (width  $d$ ) which a scattering region denoted by I. The exchange field is supposed to be parallel to the SF boundaries

two bulk superconductors, a ferromagnetic layer with exchange energy  $E_{ex} \ll E_F$ , and a scattering region denoted by I. We assume that the F-layer is ballistic and that the order parameter  $\Delta$  is constant in the superconductors:  $\Delta(x) = \Delta e^{\pm i\varphi/2}$ , and  $\Delta(x) = 0$  in F.

We believe that the model considered is quite a general one. It is applicable to quasiballistic SFS multilayers (recently a quasiballistic SF junction was prepared by Kontos et al. [8]) with either specular or disordered interfaces [9]; also to Josephson junctions where electrons tunnel through small ferromagnetic nanoparticles [10, 11]. We shall restrict ourselves to the case, when the width of the scattering region is much smaller than the width  $d$  of the junction. The transport channels can be associated with different incident angles. Then  $\Phi_{n,\sigma} - \Phi_{n,-\sigma} = \sigma\pi(2E_{ex}d/\pi\hbar v_F)l_n = \sigma\pi\Theta l_n$ , where  $l_n > 1$  is the length of a quasiparticle path between the superconductors divided by  $d$ , see Fig.1. Eq. (1) reproduces the energy spectrum obtained in the limiting case  $D = 1$  in [12].

The contribution to the free energy of the junction which depends on  $\varphi$  is given by

$$\Omega(\varphi) = -T \sum_{n,\sigma} \ln \left[ \cosh \left( \frac{E_{n\sigma}(\varphi)}{2T} \right) \right]. \quad (2)$$

The continuous spectrum is neglected in (2); one can easily check that it gives a  $\varphi$ -independent contribution to the free energy. The summation over the channels  $n$  can be evaluated by converting the sum to an integral:  $\sum_n \dots = \int dl \rho(l)$ , where  $\rho(l) = \sum_n \delta(l - l_n)$  and  $\int \rho(l) dl = N$ , the number of channels. If there is only one channel in the junction, the weight function  $\rho$  defined above reduces to  $\delta(l - 1)$ . If, on the other hand, the number of channels  $N$  is much bigger than unity,  $\rho(l) = 2N/l^3 \theta(l - 1)$ . (We assumed  $D$  to be independent on  $n$ .) A similar distribution of  $l$  can be found for SFS junctions with disordered boundaries, see [9]. At some points of these notes, we shall use the distribution  $\rho(l) = N\delta(l - 1)$ , since it allows us proceed analytically, and the results obtained with it are qualitatively the same as with the other distributions. We shall refer to this distribution as the  $\delta$ -distribution. (When  $\rho(l) = N\delta(l - 1)$ , our parameter  $\Theta$  is closely related to spin-mixing angle introduced in [11].)

Which exchange field in F is sufficient to ensure that the SFS junction can be put into a  $\pi$ -phase by changing the temperature? The  $\pi$ -state is the result of the ferromagnetic exchange field in the F-layer. If it is too small, then the junction will remain in the 0-phase at all temperatures. We show below which values of exchange field and temperature guarantee that the junction will be in the  $\pi$ -phase.

In an equilibrium situation with zero current, the temperature  $T_{\pi 0}$  separating the  $\pi$  and 0 phases is determined from the condition that the free energy  $\Omega$  reaches its minimum at  $\varphi = 2\pi n$  and at  $\varphi = \pi + 2\pi n$ ,  $n = 0, \pm 1, \dots$  (the free energy of an ordinary junction has a global minimum at  $\varphi = 2\pi n$ ). The numerical solution of this equation for  $T_{\pi 0}(D)$  is shown in Fig.2. Here and below, we use the approximation  $\Delta(T)/\Delta(0) = \tanh(1.74\sqrt{T_c/T - 1})$  in doing numerical calculations. If  $D = 1$ , the  $\pi$ -phase can exist only in the domain  $2n + 1/2 < \Theta < 3/2 + 2n$ ,  $n = 0, \pm 1, \dots$ . At finite  $D$ , there are regions of  $\Theta$  in which either the  $\pi$ -phase or the 0-phase is stable for all temperatures,  $I_c(T)$  has no cusps in these regions. For  $\Theta \rightarrow 1/2 + n$ ,  $T_{\pi 0} \rightarrow T_c$  for arbitrary transparency.

There are regions in the phase diagram where  $\Omega$  has two minima,  $\varphi = 2\pi n$  and  $\varphi = \pi(2n + 1)$ ,  $n = 0, \pm 1, \dots$ . We shall consider these regions below.

The  $(T, \Theta)$  phase diagram of the junction is depicted in the inset of the Fig.2. The diagram is periodic in

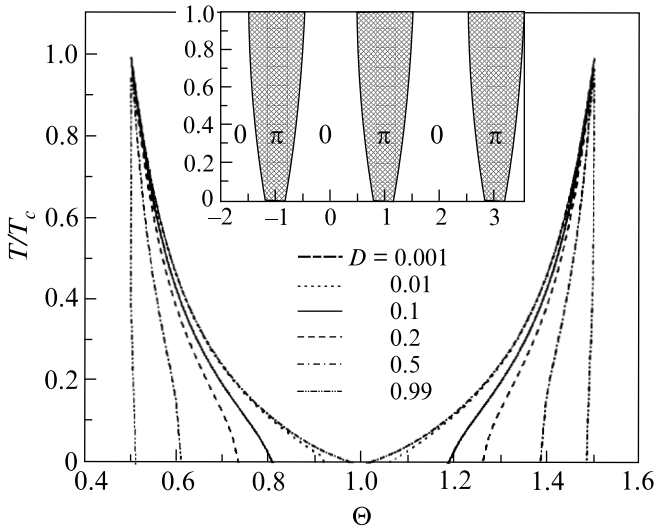


Fig.2. The temperature of the  $\pi - 0$  transition at zero current versus the dimensionless exchange field  $\Theta = 2E_{ex}d/\pi\hbar v_F$  at different values of junction transparencies  $D$ . Only trajectories with  $l = 1$  are taken into account which is justified if either one channel or many channels are present. Inset: phase diagram of the junction at  $D = 0.1$ . The gray regions correspond to the  $\pi$ -phase, the white regions to the 0-phase

$\Theta$  with period  $2\pi$ . It follows from the graph that large value of the exchange field  $\Theta = 2E_{ex}d/\pi\hbar v_F$  do not guarantee that the SFS junction is a  $\pi$ -junction.

Evidence of the existence of a  $\pi$  phase in SFS junctions was experimentally demonstrated by the group of Ryazanov [4]. The experimental curves  $I_c(T)$  showed cusps at a certain temperature (which we shall denote by  $T_{\pi 0}$ ); the critical current at the cusp was close to zero. There are qualitative arguments in [4] that the cusp corresponds to transition of the junction to the  $\pi$ -state and  $I_c \equiv 0$  at the cusp. We agree with the first statement, but disagree with the second. In our opinion, there is no qualitative argument for the critical current to be zero at the temperature of the cusp. Our model gives qualitatively similar curves  $I_c(T)$  to those presented by Ryazanov et al., but  $I_c \neq 0$  at the cusp, where the junction undergoes transition between 0 and  $\pi$ -states. This will be discussed below in more detail.

The Josephson current  $I$  carried by the Andreev levels (1) can be found from the free energy (2) using the relation  $I(\varphi) = \frac{e}{\hbar} \partial_\varphi \Omega(\varphi)$ . Using  $\partial_\varphi \gamma = D \sin(\varphi) / \sin(\gamma)$ , we obtain

$$I(\varphi) = \sum_{\sigma} \sum_n \frac{e D \sin(\varphi)}{\hbar \sin(\gamma)} \Delta \sin\left(\frac{\gamma + \sigma\pi\Theta l_n}{2}\right) \times \times \tanh\left(\frac{\Delta}{2T} \cos\left(\frac{\gamma + \sigma\pi\Theta l_n}{2}\right)\right). \quad (3)$$

If  $\Theta = 0$  and  $D = 1$ , Eq.(3) reduces to the usual formula for the Josephson current in a short ballistic SNS junction, leading to the critical current  $I_c = Ne\Delta/\hbar$  at  $T = 0$  [7, 13].

If  $D \ll 1$ , we can proceed analytically in the calculation of  $I_c(T)$ . Then  $\gamma \approx 2\sqrt{D} |\sin(\varphi/2)| \ll 1$  and we can expand the Josephson current (3) in  $\gamma$ . This leads to

$$I(\varphi) = \frac{e\Delta D}{2\hbar} \sin(\varphi) g(\Theta, T), \quad (4)$$

where

$$g(\Theta, T) = \int dl \rho(l) \left\{ \cos(\pi\Theta l/2) \times \times \tanh\left(\frac{\cos(\pi\Theta l/2) \Delta}{2T}\right) - \frac{\Delta \sin^2(\pi\Theta l/2)}{2T \cosh^2(\cos(\pi\Theta l/2) \Delta/2T)} \right\}. \quad (5)$$

If  $g > 0$  in (5), the junction is in the ordinary state. In the opposite case, the junction is in the  $\pi$ -state.

Solving  $g(\Theta, T) = 0$  gives us the transition temperature  $T_{\pi 0}$ . For  $\rho(l) \propto \delta(l - 1)$ ,  $g(\Theta, T) = 0$  can be solved only in the domain  $2n + 3/2 \leq \Theta \leq 1/2 + 2n$ ,  $n = 0, \pm 1, \dots$ . As a consequence, the  $\pi$ -phase exists only in these domains. If  $\Theta \rightarrow 1/2 + n$  then  $T \rightarrow T_c$ ;  $\Theta \rightarrow 1 + 2n$  leads to  $T \rightarrow 0$ .

In the region  $|T - T_{\pi 0}| \sim DT_c$ , the current is no longer given by Eq.(4). Higher harmonics in  $\varphi$  have to be taken into account. Since the  $n$ -th harmonic is proportional to  $D^n \sin(n\varphi)$  (follows from (3)) and  $D \ll 1$ , the second harmonic gives the main contribution to the Josephson current:  $I(\varphi) \propto D^2 \sin(2\varphi)$ . That means the critical current is not zero at the temperature of  $\pi - 0$  transition,  $I_c \propto D^2$ . Near  $T_{\pi 0}$  the currents of the spin channels  $\sigma = \pm 1$  flow in opposite directions and nearly compensate each other; therefore  $I_c$  is suppressed.

Near the critical temperature  $T_c$ , we also can proceed analytically. Then we obtain from (3) for the Josephson current:

$$I(\varphi) = \frac{e\Delta^2}{2T\hbar} \sin(\varphi) \int dl \rho(l) D \sin(\pi\Theta l). \quad (6)$$

Using the  $\delta$ -distribution of the trajectory lengths, we find that the junction is in the  $\pi$ -state when  $1 + 2n < < \Theta < 2 + 2n$ ,  $n = 0, \pm 1, \dots$

Fig.3 shows the typical dependence of the critical current on temperature. The critical current in the figure is normalized to the critical current  $I_{c0} = = N(e\Delta/\hbar)(1 - \sqrt{1 - D})$  at zero temperature and zero

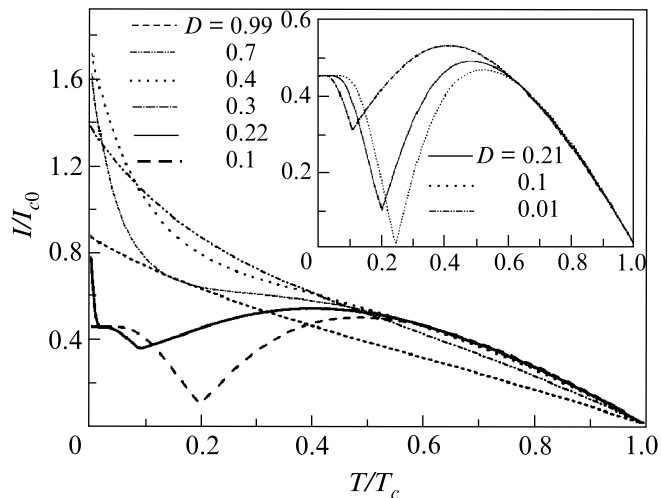


Fig.3. Dependence of the critical current on temperature for  $\Theta = 0.7$  at different transparencies  $D$ . Cusps in the  $I_c(T)$  curves indicate the  $\pi - 0$  transition.  $I_c$  is always nonzero at the cusp, see the inset. The plot of the critical current for  $D = 0.22$  has two cusps. At low temperature and  $I \lesssim I_c$ , the junction with  $D = 0.22$  is in the  $\pi$ -state, at intermediate temperatures (between two cusps) – in the 0-state, and for temperatures near  $T_c$  – again in  $\pi$ -state

exchange field. The plot corresponding to  $D = 0.22$  exhibits two cusps. When the temperature is low the junction is in the  $\pi$ -state; for intermediate temperatures (between the two cusps) the junction will be in the 0-state, for  $T \lesssim T_c$  – again in the  $\pi$ -state. (There is a schematic plot in [1] where  $I_c(T)$  of a SFS junction has many cusps with nonzero critical current in the cusps. However, Ref. [1] does not provide an explanation of this fact.) The critical current for  $D = 0.3, 0.4, 0.7$  in Fig.3 is greater than the critical current  $I_{c0}$  corresponding to zero temperature and zero  $\Theta$ . The exchange field enhances the Josephson current in the SFS junction [14].

Below we shall investigate the  $\pi - 0$  transition when a *d.c.* current  $I < I_c$  is injected into the junction. We shall pay attention to the regime when  $I$  is smaller than  $I_c$  at the cusp. Suppose that the temperature is changed at fixed  $I$ . Then at the  $\pi - 0$  transition temperature, the phase across the junction will jump approximately by  $\pi$ .

There are several solutions  $\varphi(T)$  of the equation  $I = I(\varphi)$ , where  $I(\varphi)$  is given by (3). We will assume that the damping is large, such that the phase is stabilized at one of the minima of the Gibbs energy  $\Xi(I, T, \varphi) = \Omega(T, \varphi) - \varphi I \hbar / e$  [15]. The phase values corresponding to the minima of the Gibbs energy are depicted by solid lines in Fig.4b. If the temperature is increased from  $T = 0$ , the phase will continuously change with  $T$  until  $T$  reaches the dark gray region in

Fig.4a where  $\Xi$  has two minima of  $\varphi$  in  $[-\pi, \pi]$ . Here the phase will choose one of the minima depending on the dynamics of the junction, which depends on the properties of the external circuit. Outside of this region at higher temperatures, the phase will also follow continuously adiabatic changes of  $T$ .

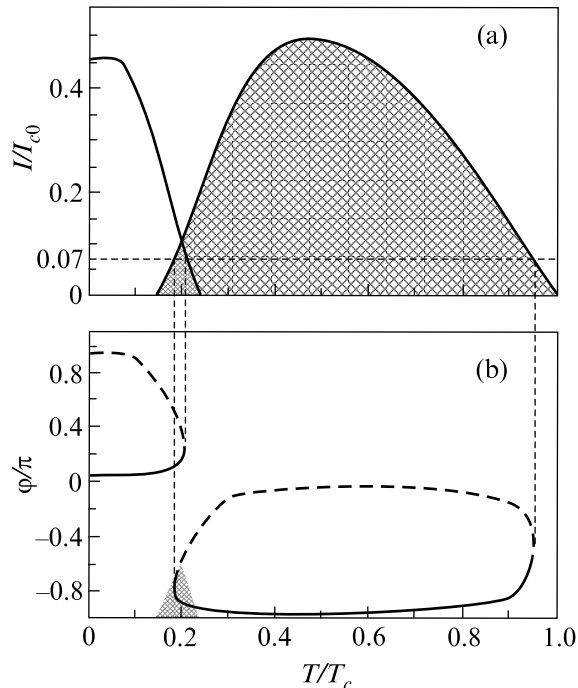


Fig.4. (a) The phase diagram of the junction for  $D = 0.1$ ,  $\Theta = 0.7$ . The light gray region corresponds to the  $\pi$ -phase, the white to the 0-phase. The Gibbs potential has two minima of  $\varphi$  in  $[-\pi, \pi]$  in the dark gray region. The critical current (solid thick line) is the upper boundary of the phase diagram. (b) Temperature dependence of the phases corresponding to the *d.c.* current  $I = 0.07I_{c0}$  (dashed line parallel to the temperature axes in (a)). The thick solid line represents the stable solution of the equation  $I = I(\varphi)$  (minimum of the Gibbs energy), the dashed curve exhibits the unstable solution (maximum of the Gibbs energy). The equilibrium transition temperature ( $I = 0$ ) corresponds to  $T/T_c = 0.2$

In conclusion, we investigated the phase transition between the  $\pi$  and 0 phases in a ballistic SFS junction with a scatterer in the F layer. We calculated the  $(T, \Theta)$  and  $(I, T)$  phase diagrams of the junction. It was shown that there is no reason for the critical current to be zero at the transition temperature  $T_{\pi 0}$ . The currents of the two spin channels nearly compensate each other at  $T_{\pi 0}$ , and the current scales as  $D^2 \sin(2\varphi)$ ,  $D \ll 1$  instead of  $D \sin(\varphi)$ , as it does far from the transition.

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