Interplay of spin-discriminated Andreev bound states forming the 0-\(\pi\) transition in Superconductor-Ferromagnet-Superconductor Junctions

Yu. S. Barash\(^1\), I. V. Bobkova\(^2\)

\(^1\)Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany
\(^2\)Lebedev Physical Institute, Leninsky Prospect 53, Moscow 119991, Russia

The Josephson current in \(S-F-S\) junctions is described by taking into account different reflection (transmission) amplitudes for quasiparticles with spin up and down. We show that the 0-\(\pi\) transition in the junctions can take place at some temperature only for sufficiently strong spin-activity of the interface. In particular, Andreev interface bound state energies in one spin channel have to be all negative, while in the other one positive. Only one spin channel contributes then to the zero-temperature Josephson current. At the temperature of the 0-\(\pi\) transition two spin channels substantially compensate each other and can result in a pronounced minimum in the critical current in tunnel junctions. The minimal critical current is quadratic in small transparency and contains first and second harmonics of one and the same order.

Growing interest at the time being to spin-dependent transport in superconductor-ferromagnet systems concerns, in particular, the dc Josephson effect. The possibility for forming the \(\pi\)-junction owing to interfaces containing magnetic impurities, was indicated for the first time in \(^3\). Since then the supercurrent across magnetically active interfaces has been studied theoretically both in \(S-FM-S\) junctions with a ferromagnetic metal separating superconductors \(^4\), and in \(S-FI-S\) junctions with interfaces made of a ferromagnetic insulator or semiconductor \(^5\). The 0-\(\pi\) transition in \(S-F-S\) junctions was predicted under certain conditions in both cases \(^6\). Recently the effect has been observed experimentally in \(S-FM-S\) junctions \(^7\).

0-\(\pi\) transition in \(S-FM-S\) highly transparent junctions is mostly discussed with respect to the proximity effect in a ferromagnetic metal \(^8\). An exchange field in a ferromagnetic metal between two superconductors induces specific oscillations in the exponentially decaying Cooper pair density. For this reason an exchange field dependent oscillations in the critical current can arise in \(S-FM-S\) sandwiches. In \(S-FI-S\) junctions the proximity effect in a ferromagnetic insulator or semiconductor usually is much weaker, as compared with the case of a ferromagnetic metal, and can be disregarded. It has been found experimentally that a ferromagnetic semiconductor represents a ferromagnetic barrier in tunnel junctions, providing different transmission probabilities for up and down spins \(^9\). In \(S-FM-S\) tunnel junctions the proximity in a ferromagnetic metal does not manifest itself in the critical current in the dominating, linear in small transparency term. In all these cases spin-discrimination by the interface is especially important, as it results in proximity effects induced by a ferromagnetic layer in adjacent superconducting regions. If the interface thickness is less than the superconducting coherence length, the interface effects on the junction properties are conveniently described by the \(S\)-matrix approach. As this was demonstrated in \(^3\), a quasiparticle scattering on magnetically active interfaces can themselves lead to a formation of a \(\pi\)-junction, even in the absence of any proximity-induced processes inside interfaces. The physics for this is associated with interface Andreev bound states caused by the spin-discriminating processes (for instance, by the effects of an exchange field in a ferromagnet). In the present paper we report the spectra of Andreev interface states, which arise on magnetically-active interfaces with arbitrary spin-dependent reflection and transmission amplitudes, and analyze their interplay in forming the Josephson current.

Since interface bound states depend explicitly on the phase difference, they are directly associated with the Josephson current through the junction. This is in accordance with the general relation between the Josephson current and the spectra of Andreev interface bound states \(^4\). We develop on this basis comparatively simple analytical description of the dc Josephson current in \(S-F-S\) junctions, when the proximity in ferromagnets is not important. We find exact conditions for the presence of the 0-\(\pi\) transition and demonstrate that interface bound states from different spin channels have to be strongly discriminated in this case. In particular, both interface bound state energies in one spin channel have to be negative, while positive in the other channel.

Our approach is based on the quasiclassical formulation of the superconductivity \(^8\). The quasiclassical equations, as is known, have to be completed with respective boundary conditions. For smooth flat surfaces or interfaces not distinguishing quasiparticle spin directions, the boundary conditions for the quasiclassical Green’s function were derived for the first time in \(^11\). Later on they were generalized to incorporate spin-active potentials \(^8\). This permitted to solve some particular problems for systems with impenetrable spin-active boundaries \(^12\) and for junctions in the tunneling limit \(^8\). The possibility for studying various magnetically active interfaces with finite transmission has appeared only recently, when the particular formulation of the quasiclassical theory with its basic quantities, equations, the corresponding boundary and asymptotic con-
tronics, was substantially modified and simplified. The achievements are associated with making clear a general structure of the quasiclassical matrix Green’s function, reducing the calculation of the Green’s function to finding its ingredients, the so-called Riccati amplitudes or coherence functions \[ R_{\pm} \]. For magnetically active interfaces this formulation was developed in [3]. Using this approach, we present analytical results, explicitly describing how magnetically-active interfaces with spin-dependent transmission amplitudes influence the Josephson current.

Consider a smooth plane interface between two superconductors or normal metals. Interface is characterized by the normal-state scattering \( S \) matrix, which can be described as follows. Exploiting Pauli-matrices \( \hat{r}_i \) in particle-hole space, a scattering matrix is represented as \( S = S(1 + \hat{r}_z)/2 + \hat{S}(1 - \hat{r}_z)/2 \), where \( \hat{S}(p) = S^T(\mp p) \). Each component \( \hat{S}_{ij} \) in matrix \( S = \| \hat{S}_{ij} \| (i,j = 1,2) \) is in its turn a matrix in spin space. Matrix \( \hat{S}_{ii} \) contains, in general, spin-dependent reflection amplitudes of normal-state quasiparticles from the interface in \( i \)-th half-space, while \( \hat{S}_{ij} \) with \( i \neq j \) incorporates spin-dependent transmission amplitudes of normal-state quasiparticles from side \( i \). For the interface potentials conserving particle current, the scattering matrix has to satisfy the unitarity condition: \( SS^\dagger = I \). If the interface Hamiltonian possesses the time-reversal symmetry, one gets an additional constraint on the scattering matrix: \( S(p_f, \mu) = \hat{\sigma}_y S^T(-p_f, -\mu) \hat{\sigma}_y \). Assuming the scattering matrix diagonal in spin space and obeying \( S(p) = S(-p) \), one obtains from here \( \hat{S}_{12}(p_f) = \hat{S}_{21}(p_f) = \hat{d}(p_f) \). For a barrier potential of the form \( \hat{V}(x) = V(x)\hat{1} + \mu(x)\hat{\sigma}_i \), it is convenient to take the \( z \)-axis along the only characteristic ‘magnetization’ vector \( \mu \). Then \( \hat{S}_{ij} \)-matrices are diagonal. Diagonal components of \( \hat{S}_{1} \) and \( \hat{S}_{2} \) are \( r_{1,\uparrow}(\downarrow) \) and \( r_{2,\uparrow}(\downarrow) \) respectively, and the diagonal components of \( \hat{S}_{12} = \hat{S}_{21} \) are \( d_{\downarrow}(\uparrow) \). On account of the above relations one also obtains \( S(p_f) = S^T(p_f) \).

It follows from the unitarity of the scattering matrix \( r_{2,\uparrow}(\downarrow) d_{\uparrow}(\downarrow) + d_{\downarrow}(\uparrow) r_{1,\uparrow}(\downarrow) = 0, |r_{1,\uparrow}(\downarrow)|^2 + |d_{\downarrow}(\uparrow)|^2 = |r_{2,\uparrow}(\downarrow)|^2 + |d_{\uparrow}(\downarrow)|^2 \). Remembering this and introducing \( \Theta_{\uparrow,\downarrow}(\Theta_{\uparrow,\downarrow}) = \Theta_{\uparrow,\downarrow}(\Theta_{\uparrow,\downarrow}) \), we get \( d_{\downarrow} \rightarrow \alpha |d_{\downarrow}| \exp \left( \frac{i}{\hbar}(\Theta_{\uparrow,\downarrow} + \Theta_{\downarrow,\uparrow} + \Theta_{\uparrow,\uparrow} + \Theta_{\downarrow,\downarrow}) \right) \). Here \( \alpha = \pm 1 \). One can then show that \( \alpha = -1 \) for a nonmagnetic barrier, while \( \alpha = 1 \) for a purely magnetic \( V = 0 \) and sufficiently high barrier. For a rectangular potential \( \alpha = -\text{sgn}[(V - (p^2_{f-x}/2 + h)/(V - (p^2_{f-x}/2 - h))], \) where \( h = n_{z} \). Hence, \( \alpha = 1 \), if the wave function in one spin channel exponentially decays in the barrier region, while in the other channel it oscillates. In general, \( \alpha \) can depend on quasiparticle momentum direction.

We have calculated spectra of interface bound states on magnetically active interfaces with the scattering \( S \)-matrix described above. Our main results are as follows.

For a symmetric barrier potential \( \hat{V}(-x) = \hat{V}(x) \), when \( \Theta_{\uparrow,\downarrow} = \Theta_{\downarrow,\uparrow} \), two branches of energies of the Andreev interface bound states in \( S-F-S \) symmetric junctions, corresponding to one spin channel (spin up for electron-like quasiparticles), take the form

\[
\varepsilon_{\pm} = |\Delta| \text{ sgn} \left( \sin \left( \frac{\Phi_{\uparrow}}{2} \right) \right) \cos \left( \Phi_{\uparrow}/2 \right),
\]

where

\[
\Phi_{\pm}(\alpha, \chi) = \Theta \pm \text{arccos} \left[ \sqrt{R_{\uparrow} R_{\downarrow}} - \alpha \sqrt{D_{\uparrow} D_{\downarrow}} \cos \chi \right],
\]

\( R_{\uparrow}(\downarrow) = |r_{\uparrow}(\downarrow)|^2, D_{\uparrow}(\downarrow) = |d_{\uparrow}(\downarrow)|^2 \) and \( \Theta = \Theta_{\uparrow} - \Theta_{\downarrow} \). The solution for the other spin channel is obtained from Eq.(3) by the substitution \( \Theta \rightarrow -\Theta \). Energies \( \varepsilon_{\pm} \) implicitly depend on quasiparticle momentum directions via the parameter \( \Theta \), reflection and transmission coefficients, and, possibly, \( \alpha \).

Eq.(4) describes, in particular, how spin-filtering effects suppress the Josephson current, when the transmission coefficient for quasiparticles with one spin orientation is sufficiently small as compared to the other one. As it is seen, spin-dependent transmission (and reflection) coefficients enter the spectra of interface Andreev bound states (as well as the Josephson current) as an effective transparency \( \sqrt{D_{\uparrow} D_{\downarrow}} \) (and a reflectivity \( \sqrt{R_{\uparrow} R_{\downarrow}} \)). There is, however, no general prescriptions for replacing spin-independent coefficients by spin-dependent ones without particular calculations, since the relations \( R_{\uparrow}(\downarrow) = 1 - D_{\uparrow}(\downarrow) \) make it ambiguous. According to Eqs.(1), (3), the difference between spin-dependent phases of reflection amplitudes \( \Theta = \Theta_{\uparrow} - \Theta_{\downarrow} \) plays a crucial role, lifting spin-degeneracy of the Andreev bound states. In the particular case \( D_{\uparrow} = D_{\downarrow}, \alpha = -1 \) the whole bound state spectra of two spin channels reduce to those found in [10]. For an impenetrable spin-active surface the spectrum Eq.(4) transforms to \( \varepsilon_{B,\pm} = |\Delta| \text{ sgn} (\sin (\chi/2)) \). Then the whole spectra of two spin channels \( \varepsilon_{B,\pm} = \pm |\Delta| \text{ sgn} (\sin (\chi/2)) \) coincide with obtained in [3]. For a nonmagnetic interface (\( D_{\uparrow} = D_{\downarrow} = D, \Theta = 0, \alpha = -1 \)) our result Eq.(4) leads to well known one positive and one negative spin-degenerate interface Andreev bound states [20,27,28].

\( \varepsilon_{B,\pm} = \pm |\Delta| \sqrt{1 - D \sin^2 (\chi/2)} \). With increasing parameter \( \Theta \) bound states in Eq.(4) can change their signs both continuously or abruptly, due to a factor \( \text{sgn}(\sin (\Phi_{\pm}/2)) \) in the latter case. For this reason, under certain conditions, both levels in one spin channel can be positive (or negative) at the same time. Energy spectrum formed jointly by two spin channels is symmetric with respect to the sign change.

Generic form of the spectrum given by Eq.(4) always arise, if order parameters for the incoming and the outgoing quasiparticle momenta in a reflection (or transmis-
Effects of the self-consistency on the results are not crucial. For instance, in the low-energy range (e.g. for \( \Phi \) close to \( \pi \)) the spectrum Eq. (1) remains to be valid for spatially dependent \( |\Delta(x)| \) as well, if one substitutes \( |\Delta| \) for effective surface order parameter \( |\tilde{\Delta}(0)| \), defined in [29].

Consider now the Josephson current in a symmetric \( S - F - S \) junction. The Josephson current is flowing via the bound states (\( \Pi \)), analogously to what takes place in nonmagnetic symmetric junctions [20,21,22,23,24]. Hence, in a quantum point contact with spin-active constriction the total Josephson current carrying by two spin channels can be found as \( J(\chi, T) = 2e \sum_{m} \frac{d\varepsilon_m}{d\chi} n(\varepsilon_m) \equiv -2e \sum_{\varepsilon_m > 0} \frac{d\varepsilon_m}{d\chi} \tanh \frac{\varepsilon_m}{2T} \). With Eqs. (1),(2) we find

\[
J(\chi, T) = A(\chi) \left[ \sin \left( \frac{\Phi_+}{2} \right) \tanh \left( \frac{|\Delta| \cos \frac{\Phi_+}{2}}{2T} \right) - \sin \left( \frac{\Phi_-}{2} \right) \tanh \left( \frac{|\Delta| \cos \frac{\Phi_-}{2}}{2T} \right) \right],
\]

where \( A(\chi) = -ae|\Delta|\sqrt{D_T D_\perp} \sin \chi \left[ 1 - \left( \sqrt{R_T R_\perp} - \alpha \sqrt{D_T D_\perp} \cos \chi \right)^2 \right]^{-1/2} \).

In the absence of a spin-activity \( \mu(x) = 0 \) and, hence, \( \Theta = 0, \alpha = -1, D_\perp = D_T \). Then Eq.(1) reduces to well-known contributions from two spin-degenerated channels to the Josephson current of quantum point contact with finite transparency. Spin-discrimination by the interface lifts the degeneracy. The current flowing in the spin-up channel takes the form \( J_1(\chi, T) = -A(\chi) \left[ \sin \left( \frac{\Phi_+}{2} \right) \right] n_f \left( \frac{\xi_+}{T} \right) - \sin \left( \frac{\Phi_-}{2} \right) \right] n_f \left( \frac{\xi_-}{T} \right) \).

\( J_1(\chi, T) \) is obtained from here by the interchange \( \Theta \rightarrow -\Theta \).

Andreev bound states in different spin channels can carry current in opposite directions, so that one direction prevails in the total current at low temperatures, while the other one near \( T_c \). We find that in the case \( \sqrt{R_T R_\perp} - \alpha \sqrt{D_T D_\perp} \cos \chi > 0 \) the current Eq. (3) changes its sign with varying the temperature at a given phase difference \( \chi \), if \( \pi/2 < |\Theta| < \pi - \arccos \left( \sqrt{R_T R_\perp} - \alpha \sqrt{D_T D_\perp} \cos \chi \right) \). Analogously, for \( \sqrt{R_T R_\perp} - \alpha \sqrt{D_T D_\perp} \cos \chi < 0 \) the sign change is \( \pi - \arccos \left( \sqrt{R_T R_\perp} - \alpha \sqrt{D_T D_\perp} \cos \chi \right) < |\Theta| < \pi/2 \). The above conditions imply, in particular, that both interface Andreev states in one spin channel have positive energies while the energies in the other channel are negative.

In tunnel junctions, where the former condition holds, the interplay of two spin channels, in a certain rage of \( \Theta \), results in a pronounced minimum of the Josephson critical current. This is shown in Fig. 1. The appearance of the minimum can be explained as follows. Since at zero temperature only quasiparticle states with negative energies are occupied, only the respective spin channel contribute the zero-temperature Josephson current. The contribution from the second channel rises with increasing temperature and becomes important at temperatures of the order of positive bound state energies. The corresponding current in the second channel turns out to be aligned in the opposite direction as compared to the zero-temperature current. Competing contributions of different spin channels result in the 0–\( \pi \) transition in the junction. Near the transition currents from two channels substantially compensate each other. The interplay of two spin channels forming the Josephson current is shown at various temperatures in Fig. 1. 0–\( \pi \) transition takes plays at the temperature, where maximal currents in “\( \uparrow \)” and “\( \pi \)” spin channels become equal to each other.

![FIG. 1. Critical current \( J_c(T) \), normalized to its value at zero temperature \( J_c(0) \) and taken for various values of \( \Theta \); \( \Theta = 0.4\pi \) (1), \( \Theta = 0.7\pi \) (2), \( \Theta = 0.8\pi \) (3), \( \Theta = 0.9\pi \) (4). Transparencies are \( D_T = D_\perp = 0.1 \) and \( \alpha = -1 \).](image)
FIG. 2. Current-phase relations at various temperatures for the total Josephson current (solid line) and separate contributions of spin-up (dashed line) and spin-down (dotted line) channels. The parameters are chosen to be \( D_{\uparrow} = D_{\downarrow} = 0.05 \), \( \Theta = 2\pi/3 \). The current is normalized to the zero-temperature critical current in the nonmagnetic case \( \Theta = 0 \).

As this was indicated in [9], the 0-π transition takes place abruptly. It is instructive to analyze this problem in the case \( D_{\uparrow} \ll 1 \). In accordance with Eq.(3), the anomalous temperature behavior of the Josephson critical current in \( S - F - S \) junctions with small transparencies takes the form

\[
J_c(T) = -\alpha e|\Delta|\sqrt{D_{\uparrow}D_{\downarrow}} \left[ \frac{\varepsilon_{B,0}(\Theta)}{|\Delta|} \tanh \left( \frac{\varepsilon_{B,0}(\Theta)}{2T} \right) - \frac{|\Delta|}{2T} \left( 1 - \frac{\varepsilon_{B,0}^2(\Theta)}{2T} \right) \cosh^2 \left( \frac{\varepsilon_{B,0}(\Theta)}{2T} \right) \right],
\]

where \( \varepsilon_{B,0}(\Theta) = |\Delta \cos \Theta/2| \) is the positive bound state energy on an impenetrable spin-active surface.

In accordance with Eq.(1), a part of the critical current, which is linear in effective transmission coefficient \( \sqrt{D_{\uparrow}D_{\downarrow}} \), changes its sign going through zero at some temperature. The tunnelling contributions from two spin channels cancel each other there. Quadratic in transparency terms, however, survive and determines the current-phase relation and the critical current itself in the vicinity of the transition temperature. One can get from Eq.(3) and see from Fig. 2, that quadratic in transmission first and second harmonics have one and the same order of value. At the temperature, where the linear in transmission term vanishes (near the transition temperature) the critical current \( \propto D_{\uparrow}D_{\downarrow} (\sin \chi + \frac{1}{2} \sin 2\chi) \). Thus, on account of quadratic in transmission terms, the total critical current does not vanish when the transition from 0 to π junction takes place. The minimal value of the critical current \( \propto D_{\uparrow}D_{\downarrow} \) if the transparencies are small.

The second harmonic in the Josephson current Eq.(3) is also important for junctions with sufficiently high transparency. For fully transparent junctions with \( \Theta = \pi/2 \) the current-phase relation has a period \( \pi \), which leads, in particular, to a half-periodicity of the dependence of the critical current on an applied magnetic field.

For \( \Theta = \pi - \delta(|\delta| \ll 1) \) we find from Eq.(3), that the current \( \propto 1/T \) under the condition \( |\Delta||\delta|/4 \ll T \ll |\Delta|/4 \sqrt{D_{\uparrow} + D_{\downarrow} + 2\alpha \sqrt{D_{\uparrow}D_{\downarrow}} \cos \chi} \). This anomalous temperature behavior is associated with the presence of zero-energy (or low-energy) surface bound states in both banks of the junction with vanishing transparency (see also [8]). It quickly disappears with increasing transparency, when only one energy of two different bound states in the spin channel can be close or even equal to zero, while the other is roughly the order of \( \Delta \) (see Eqs.(2), (1)).

In the case of classical junctions one should carry out the integration over the Fermi surface in the presence of momentum dependent bound state energies. This does not modify strongly our main results, obtained above for quantum point contacts. Although, \( 1/T \) behavior can be substantially distorted or even smeared out in this case. For instance, if only a maximum (or a minimum) of dispersive bound states is equal to zero in S-F-S tunnel
junctions with two-dimensional s-wave superconductors, the current in a classical junction would be \( I \propto 1/\sqrt{T} \).

In conclusion, we have studied the interplay of spin-discriminated channels on the spectrum of Andreev bound states and the Josephson current through a ferromagnetic interface. The conditions for the 0-π transition in the junction are found. They imply strong discrimination of Andreev interface states in two spin channels. In particular, only one spin channel contribute to the zero-temperature Josephson current in this case. Linear in transparency Josephson current vanishes near the 0-π transition. The critical current in its minimum is quadratic in small transparency and contains two first harmonics \( \sin \chi \) and \( \sin 2\chi \) which are of the same order there.

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