Josephson Current in S-FIF-S Junctions: Nonmonotonic Dependence on Misorientation Angle

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Spectra and spin structures of Andreev interface states in S-FIF-S junctions are investigated with emphasis on finite transparency and misorientation angle $\varphi$ between in-plane magnetizations of ferromagnetic layers in a three-layer interface. It is demonstrated that the Josephson current in S-FIF-S quantum point contacts can exhibit a nonmonotonic dependence on the misorientation angle. The characteristic behavior takes place, if the $\pi$-state is the equilibrium state of the junction in the particular case of parallel magnetizations.

For our analysis, we examine a smooth plane interface between two superconductors which consists of two layers of the same ferromagnetic metal separated by an insulating nonmagnetic barrier. Two identical ferromagnetic layers are characterized by their thickness $t$ and internal exchange fields $|h_{1,2}| = h$, which, being parallel to the layers, make an angle $\varphi$ with each other.

The normal-state scattering $S$ matrix is represented as $S = S(1 + \tau_z)/2 + \tilde{S}(1 - \tau_z)/2$, where the Pauli-matrices $\tau_z$ are taken in particle-hole space and $S(p_y) = S^T(-p_y)$. 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 $\hat{S}_{ii} = \begin{pmatrix} r_{ii}^{\uparrow\uparrow} & r_{ii}^{\uparrow\downarrow} \\ r_{ii}^{\downarrow\uparrow} & r_{ii}^{\downarrow\downarrow} \end{pmatrix}$ contains, in general, spin-dependent interface reflection amplitudes for normal-state quasiparticles in $i$-th half-space, while $\hat{S}_{ij} = \begin{pmatrix} d_{ij}^{\uparrow\uparrow} & d_{ij}^{\uparrow\downarrow} \\ d_{ij}^{\downarrow\uparrow} & d_{ij}^{\downarrow\downarrow} \end{pmatrix}$ with $i \neq j$ incorporates spin-dependent transmission amplitudes for normal-state quasiparticles from side $j$. For the interface potentials conserving particle current, the scattering matrix has to satisfy the unitarity condition: $SS^\dagger = 1$. If the interface Hamiltonian possesses time-reversal symmetry, one obtains an additional constraint on the scattering matrix: $S(p_f, h_{1,2}) = \hat{\sigma}_y S^T(-p_f, -h_{1,2})\hat{\sigma}_y$. Assume, for simplicity, the exchange fields to be much smaller compared to the Fermi energies. For the diagonalization of the $S_{11}$-matrix we choose the $z$-axis along the magnetization in the first (left) ferromagnetic layer. Then the other $S_{ij}$-matrices are nondiagonal unless $\varphi = 0, \pi$:

\begin{align*}
\hat{S}_{21} &= d \exp \left( \frac{i\Theta}{4} (\hat{\sigma}_y \sin \varphi + \hat{\sigma}_z \cos \varphi) \right) \exp \left( \frac{i\Theta}{4} \hat{\sigma}_z \right), \\
\hat{S}_{12} &= d \exp \left( \frac{i\Theta}{4} \hat{\sigma}_z \right) \exp \left( \frac{i\Theta}{4} (\hat{\sigma}_y \sin \varphi + \hat{\sigma}_z \cos \varphi) \right), \\
\hat{S}_{11} &= r \exp \left( \frac{\Theta}{2} \hat{\sigma}_z \right),
\end{align*}

where $d$ and $r$ are the normal-state transmission amplitudes for up and down spin quasiparticles, respectively. The misorientation angle $\varphi$ can be considered, in general, as a variable parameter. Let, for instance, the magnetization axis be pinned in one ferromagnetic layer, while in the other one there is an easy in-plane magnetization layer. Then one can vary the misorientation angle (keeping other parameters fixed) by applying an external weak magnetic field to the interface. We find that the Josephson current as a function of the misorientation angle $\varphi$ manifests a characteristic nonmonotonic behavior, if, at $\varphi = 0$, the $\pi$-state is the equilibrium state of the junction.

The dc Josephson effect in junctions with ferromagnetic interfaces exposes remarkable features which have been intensively studied in recent years theoretically [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17] and experimentally [15, 16]. Apart from interfaces with a fixed magnetization, considerable attention has been drawn also to more complicated cases, when the magnetization is spatially dependent inside the interface. An important particular model for this kind of interfaces is a three-layer $FIF$-interface, where two metallic ferromagnetic layers with in-plane magnetizations, making angle $\varphi$ with each other, are separated by an insulating magnetically inactive interlayer [9, 10, 11, 14, 16]. In the present article we identify theoretically spectra and spin polarization of Andreev states bound to the three-layer $FIF$-constrictions with finite transmission, separating clean $s$-wave superconductors. Then we determine the Josephson current in the S-FIF-S quantum point contacts. This problem was not studied previously in the literature. In the dirty limit, considered in [1, 10, 13], Andreev bound states are fully destroyed. Considerations of Ref. [11] imply the absence of Andreev bound states in clean S-FIF-S junctions. This can be justified only for short superconductors, whose lengths are less than their coherence lengths. Spectra of Andreev states and the Josephson layer. Then one can vary the misorientation angle (keeping other parameters fixed) by applying an external weak magnetic field to the interface. We find that the Josephson current as a function of the misorientation angle $\varphi$ manifests a characteristic nonmonotonic behavior, if, at $\varphi = 0$, the $\pi$-state is the equilibrium state of the junction.
Here $Θ = \frac{4\hbar}{\hbar V f x}$. Quantities $r$, $r'$ and $d$ are the respective reflection and transmission amplitudes of the potential barrier $V$, satisfying the condition $rd^* = -d r^*$. We carry out calculations within the quasiclassical theory of superconductivity, based on the equations for the so-called Riccati amplitudes or coherence functions. Considering a quantum point contact with FIF-constriction, the order parameter is taken spatially constant. We include interface exchange fields in the quasiclassical boundary conditions. Since they imply, as usual, that all interface potentials are much larger than the superconducting order parameter, one should assume $|h_{1,2}| \gg Δ$. With the above normal-state $S$ matrix we get four branches of interface Andreev bound states:

$$
\varepsilon_{1,2} = |Δ| \cos \frac{Φ_{1,2}}{2}, \quad \varepsilon_{3,4} = -|Δ| \cos \frac{Φ_{1,2}}{2},$$

where the quantities $Φ_{1,2}(χ, Θ, φ)$ are defined as

$$
cos Φ_{1,2}(χ, Θ, φ) = cos Θ - 2D cos Θ sin^2 \frac{χ}{2} +$$

$$
+ 2D cos χ sin^2 \frac{Θ}{2} sin^2 \frac{φ}{2} ± 2\sqrt{D} sin \frac{χ}{2} sin Θ cos \frac{φ}{2} ×$$

$$
\times \sqrt{1 - D sin^2 \frac{χ}{2} + D cos^2 \frac{χ}{2} tan^2 \frac{Θ}{2} sin^2 \frac{φ}{2}}. \quad (3)
$$

Here, $χ$ is the phase difference of the two superconductors. The energies $ε_i$ ($i = 1, 2, 3, 4$) implicitly depend on quasiparticle momentum directions via the parameter $Θ$ and the transmission coefficient $D$.

For $φ = 0$ the spectra Eq. (3) reduce to those found in Ref. [13]. In the particular case of antiparallel orientation of the left and the right magnetization $φ = π$, the spectra of Andreev interface states [2], [3] take the form

$$
ε_1 = ε_2 = -ε_3 = -ε_4 = |Δ| \sqrt{D cos^2 \frac{χ}{2} + R cos^2 \frac{Θ}{2}}. \quad (4)
$$

Being symmetric with respect to the transformation $Θ → -Θ$, the spectrum [2] is doubly degenerated. In the limit of a nonmagnetic interface ($Θ = 0$), our result, Eqs. [2] and [3], leads to a well known spectrum of spin-degenerate interface Andreev bound states [23, 24, 25, 26]

$$
ε_B = ±|Δ| \sqrt{1 - D sin^2(χ/2)}.
$$

Quasiparticle spin is a good quantum number in the BCS theory of superconductivity, if one can disregard spin-flip effects stimulated, for instance, by magnetic impurities, spin-orbit interactions or magnetically active interfaces. In the presence of a paramagnetic spin interaction with an externally applied magnetic field or an internal exchange field, spin degeneracy of quasiparticle states is lifted and only states with parallel or antiparallel spin-to-field orientations are still eigenstates of the problem. This can lead to effects having physics common with the Larkin-Ovchinnikov-Fulde-Ferrell state [27, 28] and, in particular, associated with opposite signs of the Zeeman terms for electrons forming a Cooper pair in singlet superconductors.

A Bogoliubov quasiparticle in the superconductor has well defined spin, although its electron and hole components are described with Zeeman terms of opposite signs. Also, an electron and its Andreev reflected partner (hole) at an interface, separating singlet superconductors and leading to no spin-flip processes, have identical spin orientations and opposite signs of Zeeman terms. With opposite velocity directions and electric charges, while in identical spin states, they carry jointly the electric supercurrent across the interface, but no equilibrium spin current. Hence, definite spin polarization of interface Andreev bound states is fully compatible with the fact that Cooper pairs in singlet superconductors carry no spin current. Andreev states bound to nonmagnetic interfaces are spin degenerated. For a ferromagnetic interface with uniformly oriented magnetization Andreev interface states are spin polarized, being parallel or antiparallel to the magnetization. The ferromagnetic interface lifts spin degeneracy of the Andreev states, but still does not mix the spin-polarized channels, carrying the Josephson current. This is not the case, however, if various orientations of magnetization are present in the interface, as this takes place in the FIF-interface with $φ ≠ 0$. Quasiparticle Andreev interface states with the spectra of Eqs. [2], [3] are characterized by a nontrivial spin structure, which substantially depends (together with the spectra themselves) on $φ$, $Θ$, and $D$. In general, each of the two incoming and two outgoing parts of quasiparticle trajectories, forming an Andreev interface state, has its own specific spin polarization. This should be compatible with no spin current they carry, on the whole, across the interface. Figs. [4] and [5] demonstrate the evolution of spectra and spin polarizations of four branches of Andreev interface states as functions of $Θ$ in tunnel junctions (with transparency $D = 0.1$) and highly transparent junctions ($D = 0.95$) respectively. Two particular relative orientations of magnetization $φ = 0.1π$ (left column) and $φ = 2π/3$ (right column) are chosen. For definiteness, we consider spin polarizations of Andreev states on the incoming part of the quasiparticle trajectory in the right superconductor. The spin polarization gradually changes with the parameter $Θ$ in all cases considered. A characteristic scale of $Θ$ for the spin reconstruction diminishes with decreasing the misorientation angle $φ$. For vanishing $φ$ the scale vanishes and there are abrupt jumps from parallel to antiparallel (or vice versa) spin orientations with respect to the magnetization, taking place at those values of $Θ$, where $ε_i(Θ) = ±Δ$ [4].
The spectra of Andreev states and their spin polarizations as functions of the misorientation angle \( \varphi \) are shown in Fig. 3. The spin polarization at \( \varphi \neq 0 \) makes a finite angle with both magnetization directions and differs on different incoming and outgoing trajectories related by the bound state. As already mentioned above, for antiparallel magnetizations \( (\varphi = \pi) \) the spectra are doubly degenerated. Spin polarizations, shown in Fig. 3 for \( \varphi = \pi \), can be considered as correct eigenfunctions in zeroth order approximation in small deviations \( \varphi \approx \pi \).

The spin structure of Andreev interface states at nonzero \( \varphi \) should be taken into account in producing nonequilibrium occupation of the states. For \( \varphi = 0 \) only the interlevel transitions accompanied with spin-flip processes are possible under certain conditions [10]. On account of the complicated spin structure of the Andreev states at nonzero \( \varphi \), there are actually no strict restrictions to a change of quasiparticle spin in the transition.

The **Josephson current** is carried by the bound states [3], analogously to the situation in nonmagnetic symmetric junctions [21, 22, 23, 24]. Hence, in a quantum point contact with a FIS constriction the total Josephson current carried by four Andreev states [3] can be found as

\[
J(\chi, T) = 2e \sum_m \frac{d^2}{d \chi^2} n(\varepsilon_m) = -2e \sum_{\varepsilon_m > 0} \frac{d^2}{d \chi^2} \tanh \frac{\varepsilon_m}{2T}.
\]

It is not difficult to calculate the current in this scheme numerically. The Josephson critical current as a function of the misorientation angle \( \varphi \), normalized to its value at \( \varphi = 0 \), is shown in Fig. 4 for various \( \Theta \) and for two values of the transparency \( D = 0.01, 0.8 \) (the upper and the lower panels respectively) and the temperature \( T = 0.1T_c, 0.8T_c \) (the right and the left columns).

We define the current critical as a positive quantity, as it is usually determined experimentally. There are
two qualitatively different regimes for the behavior of the Josephson critical current as a function of \( \varphi \) in all particular cases displayed in Fig. 4. The two regimes are separated by a characteristic value \( \Theta^*(T, D) \), which depends on the temperature and the transparency. For \( \Theta < \Theta^* \) the current is a monotonous function of the misorientation angle, reaching the maximum for the antiparallel orientation of the magnetizations. For \( \Theta > \Theta^* \) the current manifests, however, a nonmonotonic dependence on the misorientation angle with well pronounced minimum at some intermediate value of \( \varphi \) and the maximum at \( \varphi = \pi \). In the case \( \Theta = \pi \) the currents at \( \varphi = 0 \) and \( \varphi = \pi \) are equal to each other. The parameter \( \Theta^* \) admits a simple physical interpretation, associated with the junction at \( \varphi = 0 \). At zero misorientation angle the junction acquires a uniformly oriented ferromagnetic interface. Then the Josephson current is equivalent to that studied in 8,12,13,14. It can be shown, that for \( \varphi = 0 \) and \( \Theta = \Theta^*(T, D) \) the 0 – \( \pi \) transition takes place in the junction just at the given temperature \( T \). Hence, for \( \Theta > \Theta^*(T, D) \) the equilibrium state of the junction with \( \varphi = 0 \) is the \( \pi \)-state, while for \( \Theta < \Theta^*(T, D) \) it is the 0-state. We omit an analytical examination of the total Josephson current in the case \( \varphi = 0 \), since the results exactly coincide with those obtained in Refs. 13,14.

Furthermore, there is no 0 – \( \pi \) transition in the junction with antiparallel magnetization, \( \varphi = \pi \), in the three-layer interface. Indeed, it is straightforward to get from Eq. (2) the Josephson current in the particular case \( \varphi = \pi \):

\[
J(\chi, T) = \frac{eD|\Delta|\sin \chi}{\sqrt{D \cos^2 \chi + R \cos^2 \frac{\Theta}{2}}} \times \tan \left( \sqrt{\frac{D \cos^2 \chi + R \cos^2 \frac{\Theta}{2}}{2T}} \right) .
\]
the eigenstates on another side (with the spin polarization rotated by the angle $\varphi$ with respect to the initial one), one confirms in the tunneling limit that the current is of the form (6).

In conclusion, we have investigated theoretically spectra and spin structures of interface Andreev states in S-FIF-S junctions. Both finite transparency and the misorientation angle between in-plane magnetizations of ferromagnetic layers were taken into account. We demonstrated that the Josephson critical current as a function of the misorientation angle always manifests a nonmonotonic behavior, if at $\varphi = 0$ the equilibrium state of the quantum point contact is the $\pi$-state.

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[1] L. N. Bulaevskii, V. V. Kuzii, and A. A. Sobyanin, JETP Lett. 25, 290 (1977)[Pis’ma Zh. Eksp. Teor. Fiz. 25, 314 (1977)].
[2] A. I. Buzdin, L. N. Bulaevsky, and S. V. Panyukov, JETP Lett. 35, 178 (1982) [Pis’ma Zh. Eksp. Teor. Fiz. 35, 147 (1982)].
[3] A. Millis, D. Rainer, and J. A. Sauls, Phys. Rev. B 38, 4504 (1988).
[4] A. I. Buzdin, B. Bujicic, and M. Yu. Kupriyanov, Sov. Phys. JETP 74, 124 (1992) [Zh. Eksp. Teor. Fiz. 101, 231 (1992)].
[5] E. A. Demler, G. B. Arnold, M. R. Beasley, Phys. Rev. B 55, 15174 (1997).
[6] S.-K. Yip, Phys. Rev. B 62, R6127 (2000).
[7] T. T. Heikkilä, F. K. Wilhelm, G. Schön, Europhys. Lett. 51, 434 (2000).
[8] M. Fogelström, Phys. Rev. B 62, 11812 (2000).
[9] E. Koshina and V. Krivoruchko, Phys. Rev. B 63, 224515 (2001); JETP Lett. 71, 123 (2000) [Pis’ma Zh. Eksp. Teor. Fiz. 71, 182 (2000)].
[10] V. Krivoruchko and E. Koshina, Phys. Rev. B 64, 172511 (2001).
[11] F. S. Bergeret, A. F. Volkov and K. B. Efetov, Phys. Rev. Lett. 86, 3140 (2001); Phys. Rev. B 64, 134506 (2001).
[12] J. C. Cuevas, M. Fogelström, Phys. Rev. B 64, 104502 (2001).
[13] N. M. Chchelkatchew, W. Belzig, Yu. V. Nazarov, and C. Bruder, JETP Lett. 74, 323 (2001) [Pis’ma Zh. Eksp. Teor. Fiz. 74, 357 (2001)].
[14] X. Waintal and P. W. Brouwer, Phys. Rev. B 65, 054407 (2002).
[15] Yu. S. Barash and I. V. Bobkova, Phys. Rev. B 65, 144502 (2002).
[16] A. A. Golubov, M. Yu. Kupriyanov, and Ya. V. Fominov, JETP Letters 75, 190 (2002) [Pis’ma Zh. Eksp. Teor. Fiz. 75, 223 (2002)].
[17] A. A. Golubov, M. Yu. Kupriyanov, and Ya. V. Fominov, [cond-mat/0204568] (unpublished).
[18] V. V. Ryazanov, V. A. Obozov, A. Yu. Rusanov, A. V. Veretennikov, A. A. Golubov, and J. Aarts, Phys. Rev. Lett. 86, 2427 (2001).
[19] T. Kontos, M. Aprili, J. Lesueur, F. Genet, B. Stephandiis, R. Boursier, [cond-mat/0201104] (unpublished).
[20] N. Schopohl and K. Maki, Phys. Rev. B 52, 490 (1995); N. Schopohl, [cond-mat/9804062] (unpublished).
[21] M. Eschrig, Phys. Rev. B 61, 9601 (2000).
[22] A. V. Zaitsev, Zh. Eksp. Teor. Fiz. 86, 1742 (1984) [Sov. Phys. JETP 59, 1015 (1984)].
[23] A. Furusaki and M. Tsukada, Physica (Amsterdam) 165B-166B, 967 (1990).
[24] A. Furusaki and M. Tsukada, Phys. Rev. B 43, 10164 (1991).
[25] C. W. J. Beenakker and H. van Houten, Phys. Rev. Lett. 66, 3056 (1991).
[26] C. W. J. Beenakker Phys. Rev. Lett. 67, 3836 (1991); 68, 1442 (1992).
[27] A. I. Larkin and Yu. N. Ovchinnikov, Sov. Phys. JETP 20, 762 (1965) [Zh. Eksp. Teor. Fiz. , (1964)].
[28] P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964).