Distribution of pairing functions in superconducting spin-valve switching modes

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Abstract. We investigated the critical temperature T_c of SF1F2 trilayers (S is a singlet superconductor, F1 and F2 are ferromagnetic metals), where the long-range triplet superconducting pairing is generated at canted magnetizations of the F layers. We examined the spin-singlet and spin-triplet pairing distributions and their amplitudes as a function of the layers thicknesses under different values of the angle α in the SF1F2 structure to clarify which one of the pairing distributions and how may affect the superconducting T_c.

1. Introduction

We investigated the critical temperature T_c of SF1F2 trilayers (S is a singlet superconductor, F1 and F2 are ferromagnetic metals), where the long-range triplet superconducting pairing is generated at noncollinear magnetizations of the F layers [1]. An asymptotically exact numerical method [2] is employed to calculate T_c as a function of the trilayer parameters, such as mutual orientation of magnetizations, interfaces transparencies, and the layers thicknesses. Earlier we demonstrated that T_c in the semi-infinite SF1F2 structures can be a non-monotonic function of the angle α between magnetizations of the two F layers [3], contrary to the monotonic $T_c(α)$ behavior calculated for the F1SF2 superconducting spin-valve design [4]. The existence of the anomalous dependence of the spin-triplet correlations on the angle α in FFS structures in limit of thin F films was shown recently [5]. We examined the spin-singlet and spin-triplet pairing distributions and amplitudes as a function of the layers thicknesses at different values of the angle α in the SF1F2 structure to clarify which one of the pairing distributions and how may impact on the superconducting T_c.

2. The model and numerical method

At first we found a nonmonotonic dependence of T_c in a SF1F2 trilayer as a function of the angle α between the exchange fields of the two F layers (figure 1).

The S layer is of the thickness d_S $(-d_S < x < 0)$, the middle F1 layer is of the thickness d_{F1} $(0 < x < d_{F1})$, the outer F2 layer is of the thickness d_{F2} $(d_{F1} < x < d_{F1}+d_{F2})$, the x axis is normal to the plane of the layers. The exchange field in the middle F1 layer is along the z direction, $\mathbf{h} = (0, 0, h)$, while the exchange field in the outer F2 layer is in the yz plane: $\mathbf{h} = (0, h\sin\alpha, h\cos\alpha)$. The angle α varies between 0 (parallel configuration, P) and π (antiparallel configuration, AP).
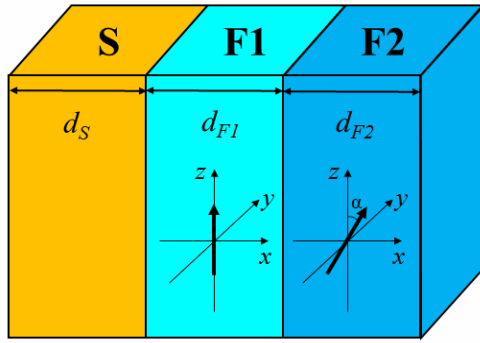
Figure 1. SF1F2 trilayer. The S/F1 interface corresponds to $x = 0$. The thick arrows in the F layers denote direction of the exchange fields $\mathbf{h}$ lying in the (y, z) plane. The angle between the in-plane exchange fields is α.

We consider SF1F2 structure in the dirty limit, which is described by the Usadel equations. Near T_c, the Usadel equations are linearized and contain only the anomalous Green function $\hat{f}$ [1]:

$$\frac{D}{2}\nabla^2 \hat{f} - |\omega|\hat{f} - \frac{i\,\mathrm{sgn}\,\omega}{2}\left\{\hat{\tau}_0(\mathbf{h}\hat{\boldsymbol{\sigma}}), \hat{f}\right\} + \Delta\hat{\tau}_1\hat{\sigma}_0 = 0. \tag{1}$$

Here, D is the diffusion constant, $\hat{f}$ is 4×4 matrix, $\omega = \pi T_c(2n + 1)$ where the integer n is the Matsubara frequency, $\hat{\tau}_i$ and $\hat{\sigma}_i$ are the Pauli matrices in the Nambu-Gor'kov and spin spaces, respectively. $\hat{\tau}_k\hat{\sigma}_l$ is direct product of these matrices. The order parameter Δ is real-valued in the superconducting layer, while in the ferromagnetic layers it is zero. In general, the diffusion constant D acquires a proper subscript, S or F, when equation (1) is applied to the superconducting or ferromagnetic layers, respectively.

The Green function has the following components:

$$\hat{f} = \hat{\tau}_1\left(f_0\hat{\sigma}_0 + f_3\hat{\sigma}_3 + f_2\hat{\sigma}_2\right). \tag{2}$$

Here, f_0 is the singlet component, f_3 is the triplet with zero projection on the z axis, and f_2 is the triplet with ±1 projections on z (the latter is present only at $\alpha \neq 0, \pi$).

There are the following symmetries:

$$\begin{aligned}
f_0(-\omega) &= f_0(\omega), \qquad & f_0 \text{ is purely real} \\
f_3(-\omega) &= -f_3(\omega), \qquad & f_3 \text{ is purely imaginary} \\
f_2(-\omega) &= -f_2(\omega), \qquad & f_2 \text{ is purely imaginary,}
\end{aligned} \tag{3}$$

which makes it sufficient to consider only positive Matsubara frequencies, $\omega > 0$.

Problem of calculating T_c can be reduced to an effective set of equations for the singlet component in the S layer: the set includes the self-consistency equation and the Usadel equation,

$$\Delta\ln\frac{T_{cS}}{T_c} = 2\pi T_c\sum_{\omega > 0}\left(\frac{\Delta}{\omega} - f_0\right), \tag{4}$$

$$\frac{D}{2}\frac{d^2 f_0}{dx^2} - \omega f_0 + \Delta = 0, \tag{5}$$

with the boundary conditions:

$$\left.\frac{df_0}{dx} = 0\right|_{x=-d_S}, \qquad \left.-\xi_S\frac{df_0}{dx} = Wf_0\right|_{x=0}. \tag{6}$$

Here, T_{cS} and $x_S = \sqrt{D_S / 2pT_{cS}}$ are the superconducting transition temperature and coherence length for an isolated S layer, respectively. This is exactly the problem for which the multimode method (as well as the method of fundamental solution) was developed in [2] and then applied to F1SF2 [4] and semi-infinite SF1F2 [3] spin valves. We only need to determine the explicit expression for W in equation (6), solving the boundary problem for the SF1F2 structure.

The Usadel equation (1) generates the following characteristic wave vectors:

$$k_\omega = \sqrt{\frac{2\omega}{D}}, \quad k_h = \sqrt{\frac{h}{D}}, \quad \tilde{k}_h = \sqrt{k_\omega^2 + 2ik_h^2}. \tag{7}$$

In the S layer the solution of equation (1) is (A and B are purely imaginary):

$$\begin{pmatrix} f_0 \\ f_3 \\ f_2 \end{pmatrix} = \begin{pmatrix} f_0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ A \\ B \end{pmatrix} \cdot \frac{\cosh\left(k_\omega\left(x + d_S\right)\right)}{\cosh\left(k_\omega d_S\right)}. \tag{8}$$

Note that here we keep $f_0(x)$ as is, because we cannot solve the equation for this component since it contains $\Delta(x)$. In the middle F1 layer the solution of equation (1) has the following form (C_1 and S_1 are purely imaginary, $C_3 = -C_2^*$, $S_3 = -S_2^*$):

$$\begin{pmatrix} f_0 \\ f_3 \\ f_2 \end{pmatrix} = C_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \cosh\left(k_\omega x\right) + C_2 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \cosh\left(\tilde{k}_h x\right) + C_3 \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \cosh\left(\tilde{k}_h^* x\right)$$

$$+ S_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \sinh\left(k_\omega x\right) + S_2 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \sinh\left(\tilde{k}_h x\right) + S_3 \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \sinh\left(\tilde{k}_h^* x\right). \tag{9}$$

In the outer F2 layer (E_1 is purely imaginary, $E_3 = -E_2^*$):

$$\begin{pmatrix} f_0 \\ f_3 \\ f_2 \end{pmatrix} = E_1 \begin{pmatrix} 0 \\ -\sin\alpha \\ \cos\alpha \end{pmatrix} \cosh\left(k_\omega x\right) + E_2 \begin{pmatrix} 1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix} \cosh\left(\tilde{k}_h x\right) + E_3 \begin{pmatrix} -1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix} \cosh\left(\tilde{k}_h^* x\right)$$

$$+ H_1 \begin{pmatrix} 0 \\ -\sin\alpha \\ \cos\alpha \end{pmatrix} \sinh\left(k_\omega x\right) + H_2 \begin{pmatrix} 1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix} \sinh\left(\tilde{k}_h x\right) + H_3 \begin{pmatrix} -1 \\ \cos\alpha \\ \sin\alpha \end{pmatrix} \sinh\left(\tilde{k}_h^* x\right). \tag{10}$$

The boundary conditions at the free interface F2 of the structure take the form:

$$\left.\frac{df_i}{dx} = 0\right|_{x = d_{F1} + d_{F2}}. \tag{11}$$

The boundary conditions at the SF1 and F1F2 interfaces have the form [6]:

$$\left.\left(f_i + \gamma_B \xi \frac{df_i}{dx}\right)\right|_{\text{left}} = f_i\big|_{\text{right}}, \quad \left.\left(\gamma\xi \frac{df_i}{dx}\right)\right|_{\text{left}} = \left.\left(\xi \frac{df_i}{dx}\right)\right|_{\text{right}}, \tag{12}$$

where g_B and g are the spin-independent suppression parameters:

$$\gamma_{BSF1} = R_{BSF1} A_B / \rho_S \xi_S, \quad \gamma_{SF1} = \rho_{F1} \xi_{F1} / \rho_S \xi_S,$$
$$\gamma_{BF1F2} = R_{BF1F2} A_B / \rho_{F1} \xi_{F1}, \quad \gamma_{F1F2} = \rho_{F2} \xi_{F2} / \rho_{F1} \xi_{F1}. \tag{13}$$

R_{BF1S}, R_{BF2F1} and A_B are the resistance and the area of the SF1 and F1F2 interfaces, r_S, r_{F1} and r_{F2} are the resistivities of the S, F1 and F2 layers, respectively.

We choose the simplest formulation: all the interfaces are transparent ($g_B = 0$), the diffusion constants and the conductivities are the same ($g = 1$), the absolute values of the exchange fields in

the two F layers coincide, f_0 is a constant within the S layer. Our strategy now is to obtain the effective boundary conditions (6) for $f_0(x)$ by eliminating all other components in the three layers.

The boundary conditions (11) and (12) give 14 equations. We are mainly interested in one of them, determining the derivative of the singlet component on the S side of the SF1 interface ($x = 0$):

$$\left.\frac{df_0}{dx}\right|_{x=0} = \tilde{k}_h S_2 - \tilde{k}_h^* S_3. \tag{14}$$

The remaining 13 boundary conditions form a system of 13 linear equations for 13 coefficients in equations (8)-(10). The solution of this system is nonzero due to $f_0(x)$ in equation (8). Then, we substitute the S_2 coefficient into equation (14) and thus explicitly find W in equation (6). All the information about the two F-layers is contained in the single real-valued function $W(\alpha)$.

3. Results and discussions

The results of numerical calculations of T_c as a function of the angle α, and pairing distributions under different values of the layers thicknesses in SF1F2 trilayer are given in figures 2 - 4.

Figure 2 (a) demonstrates the *direct* spin-valve effect ($T_c^{AP}(\alpha = 180°) > T_c^{P}(\alpha = 0°)$). The basic physical reason of the difference $\Delta T_c = T_c^{AP} - T_c^{P}$ is partial compensation of the pair-breaking ferromagnetic exchange field, when the magnetizations of the F1 and F2 layers are aligned antiparallel. As far as the F-layers are thin compared with the coherent lengths, the compensation is pretty good providing large ΔT_c. The both triplet pairing components f_2 and f_3 tend to have a maximum mostly at the outer surface of the F2 layer.
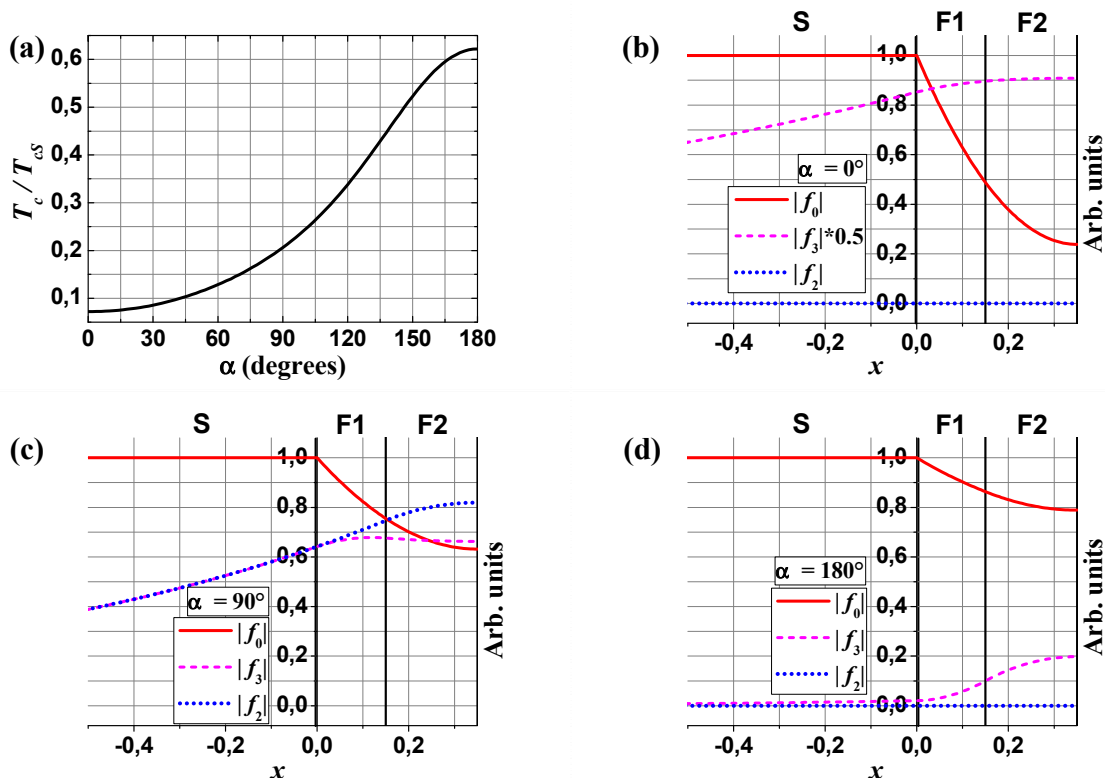
Figure 2. Critical temperature T_c vs. misalignment angle α (a). Spin-singlet and spin-triplet pairing distributions at $\alpha = 0°$ (b), 90° (c) and 180° (d) for $n = 2$; $d_{F1}/\xi_{F1} = 0.15$, $d_{F2}/\xi_{F2} = 0.2$, and table 1; the functions moduli have been drawn here and hereafter.

Figure 3(a) demonstrates the *triplet* spin-valve effect (T_c(non-collinear) $< T_c(\alpha = 180°)$, $T_c(\alpha = 0°)$). In this mode, the oscillating behavior of the singlet superconducting pairing in the F layers is observed. The minimal critical temperature T_c corresponds to the long-range triplet pairing f_2 changing sign in the outer F2 layer, and double crossing zero by the singlet pairing component f_0 in the F layers (figure 3(c)), which does not present at the maximum temperatures (figures 3(b) and 3(d)). The zero spin-projection triplet component f_3 is located close to the S/F1 interface.
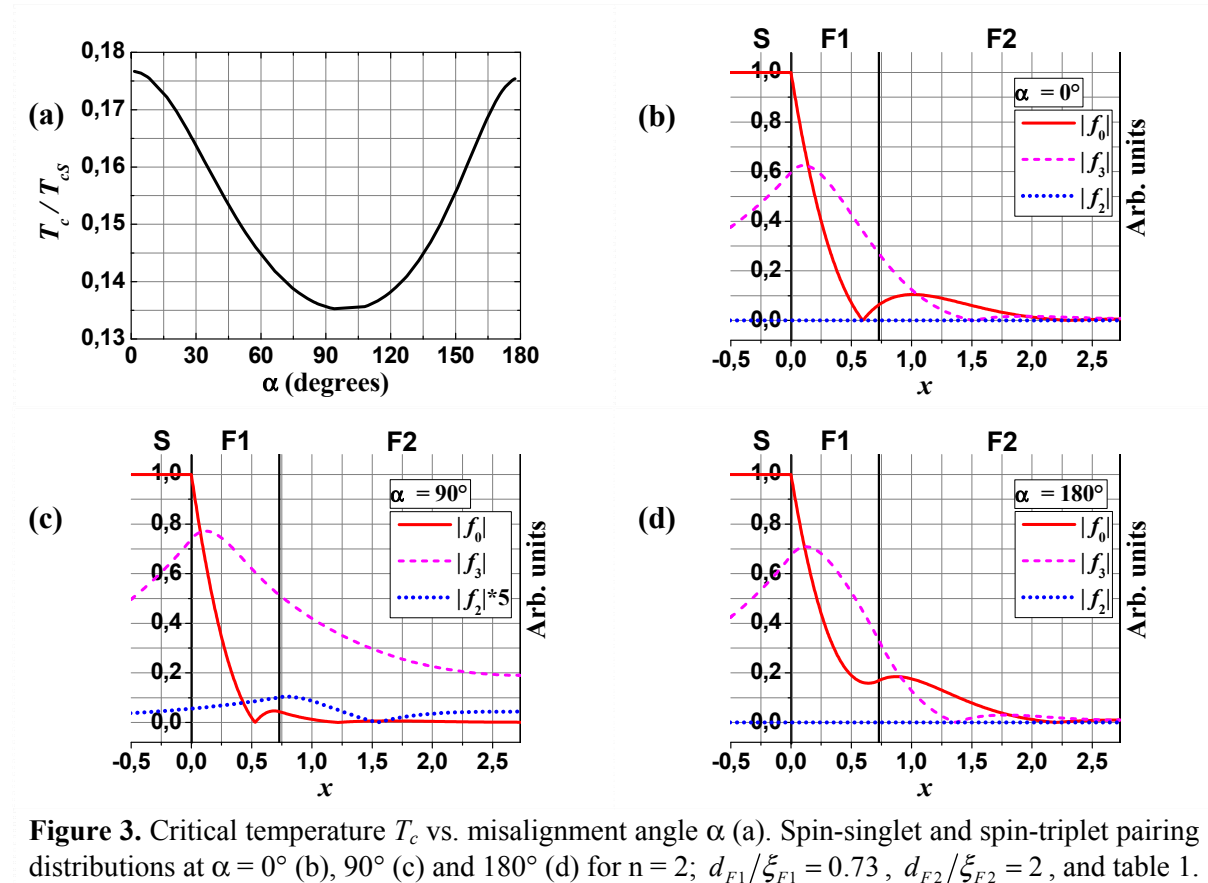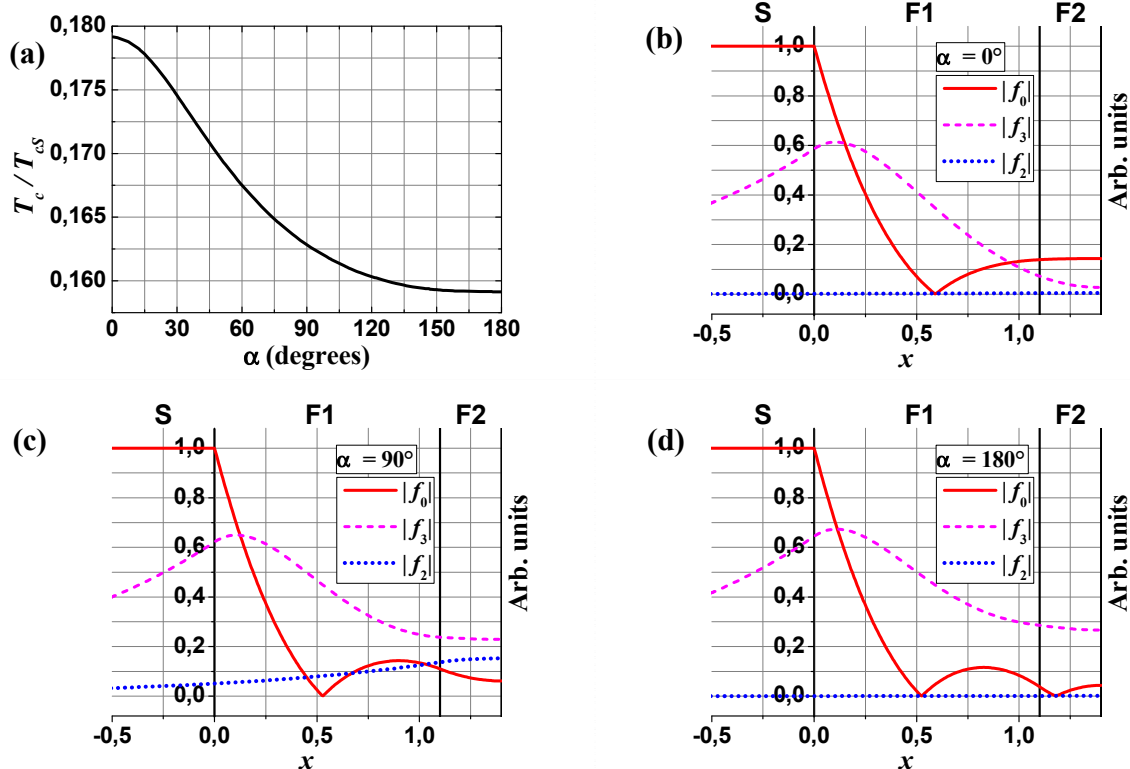

Figure 3. Critical temperature T_c vs. misalignment angle α (a). Spin-singlet and spin-triplet pairing distributions at $\alpha = 0°$ (b), 90° (c) and 180° (d) for n = 2; $d_{F1}/\xi_{F1} = 0.73$, $d_{F2}/\xi_{F2} = 2$, and table 1.

Figure 4(a) demonstrates the *inverse* spin-valve effect ($T_c(\alpha = 0°) > T_c(\alpha = 180°)$). In this mode the long-range triplet pairing component f_2 has a maximum at the outer surface of the F2 layers, while the zero spin-projection triplet component f_3 is always located close to the S/F1 interface. The minimum critical temperature T_c corresponds to the peculiar behavior – double crossing of zero by the singlet superconducting component f_0 in the F layers (figure 4(d)) which is not the case at $\alpha = 0°$ (figure 4(b)).

Table 1. Common parameters of the SF1F2 trilayer.

Parameter	value
d_S/ξ_S	2.75
γ	1
γ_B	0
ξ_F/ξ_S	1

Figure 4. Critical temperature T_c vs. misalignment angle α (a). Spin-singlet and spin-triplet pairing distributions at $\alpha = 0°$ (b), 90° (c) and 180° (d) for $n = 2$; $d_{F1}/\xi_{F1} = 1.1$, $d_{F2}/\xi_{F2} = 0.3$, and table 1.

4. Conclusion

We have considered a finite-thickness SF1F2 spin valve. We visualized distributions of spin-singlet and spin-triplet superconducting pairing components and attributed their peculiarities to different spin-valve switching modes of the SF1F2 trilayer heterostructure. This may be important to plan experimental detecting of the triplet pairings and the inverse proximity effect in SF hybrids by, for example, polarized neutron reflection [7, 8].

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