Long-range supercurrents induced by the interference effect of opposite-spin triplet state in clean superconductor-ferromagnet structures

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Abstract
By now it is known that in an s-wave superconductor-ferromagnet-superconductor (SFS) structure the supercurrent induced by spin singlet pairs can only transmit a short distance of the order of magnetic coherence length. The long-range supercurrent, taking place on the length scale of the normal metal coherence length, will be maintained by equal-spin triplet pairs, which can be generated by magnetic inhomogeneities in the system. In this paper, we have shown an unusual long-range supercurrent, which can take place in clean $SF_1F_2S$ junction with non-parallel orientation of magnetic moments. The mechanism behind the enhancement of Josephson current is provided by the interference of the opposite-spin triplet states deriving from $S/F_i$ and $F_j/S$ interfaces when both ferromagnetic layers have the same values of the length and exchange field. This discovery can offer a natural explanation for recent experiments (Robinson et al 2010 Phys. Rev. Lett. 104 207001; Baek et al 2014 Nat. Commun. 5 3888).

1. Introduction
The interplay between superconductivity and ferromagnetism in hybrid structures has currently attracted considerable attention because of the rich unusual physical phenomena [1–7] and potential practical applications [8–11]. Much effort has been devoted to obtaining a better understanding of the exotic phenomena appeared in heterostructures involving superconductor ($S$) and ferromagnet ($F$). To mention a few of these, it is natural to highlight the experimental and theoretical study of the transport properties in $SF$ heterostructures.

When a conventional s-wave $S$ is adjacent to a homogeneous $F$, the superconducting proximity effect in this $F$ is rather short ranged due to the differential action of the ferromagnetic exchange field acting on the spin-up and spin-down electrons that form a Cooper pair. In this case, the spin-split of the electronic energy bands in the ferromagnetic region will make the opposite-spin Cooper pair acquire a finite center-of-mass momentum

$$Q = 2\hbar v/\hbar v_F$$

where $\hbar$ and $v_F$ are the exchange field strength and the Fermi velocity, respectively. As a result, the Cooper pair $|\uparrow \downarrow\rangle e^{iQ R} - |\downarrow \uparrow\rangle e^{-iQ R}$ can be rewritten as a mixture of spin singlet component

$$\langle |\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle \cos(Q \cdot R)$$

and spin triplet component with zero spin projection along the magnetization axis

$$\langle |\uparrow \downarrow\rangle + |\downarrow \uparrow\rangle \sin(Q \cdot R)$$

where $R$ is the distance from the $S/F$ interface. For simplicity, we will hereafter refer to the wave function of this triplet component as opposite-spin triplet state. Accordingly, the above singlet and triplet components are short range and decays at a distance $\xi_f$ from the superconductor [6, 7]. Here $\xi_f$ is the superconducting coherence length in the $F$ layer, which is much smaller than the correlation length $\xi_s$ in normal metal ($N$). Another peculiarity in such systems is the spatial oscillations of these two components inside the $F$
region [18]. Owing to this oscillatory nature, the critical current of SFS junctions becomes an oscillating function of the $F$ layer thickness [12–16]. This oscillating behavior of the supercurrent corresponds to the transition between so-called ’0 state’ and ‘π state’ [5, 6].

In contrast, it is useful to seek ways to enhance the proximity effect. Several options have recently been proposed in literatures. First, the presence of the inhomogeneous magnetization may strongly modify the SF proximity effect [8, 17, 18]. In the presence of domain wall at the $S/F$ interface, the magnetization direction rotates in a spiral fashion in a region near the interface [19, 20]. The spin quantization follows the rotating magnetization, and the resulting triplet mixing and the spin–flip scattering will produce equal-spin triplet pairing ($|↑↑⟩$ or $|↓↓⟩$) with a long-range penetration into the ferromagnetic material [8, 18]. The primary reason is that since two triplet-paired electrons at the Fermi surface have no momentum difference and propagate with the same phase, they are not affected by the exchange field and decay at a distance $\xi_n$. This long-range proximity effect, giving rise to induced superconducting correlations in ferromagnets and half-metals, is prime examples of the potential that lies within this field of research. It has been observed in Co [21–23] and Ho [24–27], as well as in the half-metal CrO$_2$ [28, 29] and LaCaMnO [30–35]. Its origin is related with the presence of the spin–flip scattering at the $S/F$ interface, which is induced by the non-collinear magnetic domain or magnetic impurity.

Recently, the second way to enhance the supercurrent has been proposed in SFS junction containing a noncollinear thin magnetic domain in the center of ferromagnetic region [36, 37]. The magnetic domain will induce a spin–flip scattering process, which reverses the spin orientations of the singlet Cooper pair and simultaneously changes the sign of the corresponding electronic momentum. Under these conditions the singlet Cooper pair will create an exact phase-cancellation effect and gets an additional $\pi$ phase shift as it passes through the entire ferromagnetic region, so that the supercurrent can not be suppressed.

The third approach requires the magnetizations of the bilayer ferromagnetic Josephson junction to be arranged antiparallel. This situation was originally described by Bergeret et al [38] for an $SF_1IF_zS$ tunnel junction ($I$ stands for an insulating layer) then later by Blanter et al [39] for an $SF_1F_2S$ junction. However, the physical origin of this enhanced proximity effect is more subtle. With the simplest picture of this situation, Blanter et al argue that the pair wave function describing Cooper pairs from the left-hand $S$ accumulates a phase $\delta_\varphi_{1} = Q \cdot R_1$ while traversing $F_1$, where $R_1$ is the thickness of $F_1$. Because the magnetization of $F_2$ is antiparallel to that of $F_1$, the role of majority and minority bands is reversed, and the pair wave function will accumulate an additional phase $\delta_\varphi_{2} = -Q \cdot R_2$ traversing $F_2$. If the two $F$ layers have the same thickness, then the net change in the pair wave function is zero. The ferromagnetic bilayer behaves as a piece of normal metal and the proximity effect will be fully restored. However, this explanation does not specify which pairing form $|↑↑⟩ - |↓↓⟩$ or $|↑↓⟩ + |↓↑⟩$ provides the main contribution to the long-range Josephson current. Soon afterwards, the same conclusion for clean junction was proposed theoretically by Pajović et al [40] via solving the Bogoliubov–de Gennes (BdG) equation, but they just took into account a single transverse channel case for simplicity, which is generally inconsistent with the realistic situation. Moreover, experimental studies of the Josephson junctions with double magnetic barriers of collinear magnetizations were carried out by Bell et al [41] and later by Robinson et al [42] and Baek et al [43]. In these studies, enhanced maximum supercurrents were observed for the antiparallel states compared with the parallel states.

In addition, Mel’nikov et al [44] pointed out that in clean $SF_1F_2S$ junction the interference of particle- and hole-like wave functions could provide the possibility of the canceling the particle–hole phase difference ($Q \cdot R$), which is gained by the electron- and hole-like parts of the pair wave function in the ferromagnetic regions. However, several key issues still need to be resolved and further studied: (i) What kind of interference, either the singlet or triplet components, can provide a long-range contribution to the Josephson current through a ferromagnetic system? (ii) How interference of the particle- and hole-like wave functions in the ferromagnetic regions could enhance the Josephson current? (iii) What roles should the exchange fields of two ferromagnetic layers play in the interference effect?

In order to improve the above theories, in this paper we study the interference effect in clean $SF_1F_2S$ junction with non-parallel magnetizations by considering an oblique injection process. Note that in contrast to the model of reference [40] we consider the multiple transverse channel that is more agree with the realistic case of the planar junctions. We investigate the dependence of the critical Josephson current on the thicknesses of both $F$ layers. It is shown a slowly decaying characteristic for non-parallel orientation of magnetizations in the $F$ layers. Furthermore, by changing the relative magnetization direction of two ferromagnetic layers from parallel to antiparallel, the critical current is varied from a small to a large value. In this process, the amplitude of wave function of spin singlet state changes slightly but the opposite-spin triplet state could switch from a finite value to be canceled out in central region of the entire $F$ layer. So we attribute the enhancement of critical current to the interference effect of opposite-spin triplet wave functions in the $F$ region. This effect can weaken the role of the center-of-mass momentum acquired by the Cooper pair, and the situation is similar to the transition of the Cooper pair in normal metal, in which case only the singlet state exists but the opposite-spin triplet state disappears. Moreover, it is found that the critical current is inversely proportional to the exchange field of both $F$
layers. When the two $F$ layers are converted into half-metals, the Josephson current will be prohibited completely. That is because the singlet and triplet states will all be suppressed by the exchange splitting of two $F$ layers, and the interference effect could disappear entirely in the $F$ region. On the other hand, if the both $F$ layers have different features, the critical current will oscillator decay with the difference of lengths or exchange fields, which can be attribute to the variation of the interference between the two opposite-spin triplet states deriving from $S/F_1$ and $F_2/S$ interfaces.

2. Model and formula

The $SF_1F_2S$ junction we consider is shown schematically in figure 1. We denote the ferromagnetic layer thicknesses by $L_1$ and $L_2$, respectively. The $y$-axis is chosen to be perpendicular to the layer interfaces with the origin at the $S/F_1$ interface, and the whole system satisfies translational invariance in the $x$–$z$ plane. The exchange field in the $F_1$ layer is directed along the $z$-axis while within the $F_2$ layer, it is oriented at an angle $\theta$ in the $x$–$z$ plane.

The BCS mean-field effective Hamiltonian \[6, 45\] is

$$H_{\text{eff}} = \int d\vec{r} \left\{ \sum_\alpha \psi^\dagger_\alpha(\vec{r}) H_\alpha \psi^\dagger_\alpha(\vec{r}) + \frac{1}{2} \sum_{\alpha,\beta} (i\vec{\sigma})_{\alpha\beta} \Delta(\vec{r}) \times \psi^\dagger_\alpha(\vec{r}) \psi^\dagger_\beta(\vec{r}) + \text{h.c.} \right\} - \sum_{\alpha} \psi^\dagger_\alpha(\vec{r}) (\vec{h} \cdot \vec{\sigma}) \psi^\dagger_\alpha(\vec{r}),$$

(1)

where $H_\alpha = -\hbar^2 \nabla^2 / 2m - E_F$, $\psi^\dagger_\alpha(\vec{r})$ and $\psi^\dagger_\alpha(\vec{r})$ represent creation and annihilation operators with spin $\alpha$, and the vector $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is composed of Pauli spin matrices. $m$ is the effective mass of the quasiparticles in both $S$s and $F$s, and $E_F$ is the Fermi energy. $\Delta(\vec{r}) = \Delta(T)|e^{i\phi_L} \Theta(-y) + e^{i\phi_R} \Theta(y - L_2)|$ describes the superconducting pair potential with $L_F = L_1 + L_2$. Here $\Delta(T)$ accounts for the temperature-dependent energy gap. It satisfies the BCS relation $\Delta(T) = \Delta_0 \tanh(1.74\sqrt{T_c/T - 1})$, where $\Delta_0$ is the energy gap at zero temperature and $T_c$ is the superconducting critical temperature. $\phi_{L(R)}$ is the phase of the left (right) $S$, and $\Theta(y)$ is the unit step function. The exchange field $\vec{h}$ due to the ferromagnetic magnetizations in the $F$ region can be written as

$$\vec{h} = \begin{cases} \hat{h}_1 \hat{z}, & 0 < y < L_1 \\ \hat{h}_2(\sin \theta \hat{x} + \cos \theta \hat{z}), & L_1 < y < L_F. \end{cases}$$

(2)

To diagonalize the effective Hamiltonian, we make use of the Bogoliubov transformation

$$\psi^\dagger_\alpha(\vec{r}) = \sum_\mu\mu \alpha \gamma^\dagger_\alpha(\vec{r}) + \gamma^\dagger_\alpha(\vec{r}) \gamma^\dagger_\alpha(\vec{r})$$

and take into account the anticommutation relations of the quasiparticle annihilation operator $\gamma^\dagger$ and creation operator $\gamma$. The resulting BdG equation can be expressed as \[6, 45\]

$$\begin{pmatrix} H_0 - \Delta(y) & -h_0(y) & 0 & \Delta(y) \\ -h_0(y) & H_0 + h_0(y) & -\Delta(y) & 0 \\ 0 & -\Delta^*(y) & -H_0 + h_0(y) & h_0(y) \\ \Delta^*(y) & 0 & h_0(y) & -H_0 - h_0(y) \end{pmatrix} \begin{pmatrix} \psi^\dagger_1(\vec{r}) \\ \psi^\dagger_1(\vec{r}) \\ \psi^\dagger(\vec{r}) \\ \psi^\dagger(\vec{r}) \end{pmatrix} = E \begin{pmatrix} \psi_1(\vec{r}) \\ \psi_1(\vec{r}) \\ \psi(\vec{r}) \\ \psi(\vec{r}) \end{pmatrix}.$$

(3)
2.1. Blonder–Tinkham–Klapwijk (BTK) approach

In what follows, we adopt the BTK approach to calculate the Josephson current. The BdG equation (3) can be solved for each superconducting electrode and each ferromagnetic layer, respectively. We have four different incoming quasiparticles, electronlike quasiparticles (ELQs) and holelike quasiparticles (HLQs) with spin-up and spin-down. For an incident spin-up electron in the left superconducting electrode, the wave function is

$$\Psi^S_L(y) = \hat{M}_e e^{i k_y y} + a_1 \hat{M}_f e^{i k_y y} + b_1 \hat{M}_e e^{-i k_y y} + a'_1 \hat{M}_f e^{i k_y y} + b'_1 \hat{M}_e e^{-i k_y y}. \quad (4)$$

In this particular process, the coefficients $b_1, b'_1, a'_1$, and $a_1$ correspond to the normal reflection, the normal reflection with spin-flip, the novel Andreev reflection, and the usual Andreev reflection, respectively. Moreover, $\hat{M}_e = [u e^{i \phi/2}, 0, 0, v e^{-i \phi/2}], \hat{M}_f = [v e^{i \phi/2}, 0, 0, u e^{-i \phi/2}], \hat{M}_1 = [0, -v e^{i \phi/2}, u e^{-i \phi/2}, 0]^T$, and $\hat{M}_4 = [0, u e^{i \phi/2}, -v e^{-i \phi/2}, 0]^T$ are the four basis wave functions of the left $S$, in which the quasiparticle amplitudes are defined as $u = \sqrt{(1 + \Omega/E)/2}, v = \sqrt{(1 - \Omega/E)/2}$ and $\Omega = \sqrt{E^2 - \Delta^2}$. $k_{eh}(\phi) = \sqrt{2m [E_f + (-)\Omega]/\hbar^2 - k_f^2}$ are the perpendicular components of the ELQs (HLQs) wave vector with $k_f$ as the parallel component.

The corresponding wave function in the right superconducting electrode is

$$\Psi^S_R(y) = c_1 \hat{N}_e e^{i k_y y} + d_1 \hat{N}_f e^{i k_y y} + c'_1 \hat{N}_e e^{i k_y y} + d'_1 \hat{N}_f e^{-i k_y y}, \quad (5)$$

where the transmission coefficients $c_1, d_1, c'_1$, and $d'_1$ correspond to the reflection processes described above. The basis wavefunctions $\hat{N}_p (p = 1 \sim 4)$ in the right $S$ can be obtained from $\hat{M}_p$ by performing the substitution $\phi_e \rightarrow \phi_R$.

By contrast, the magnetism in the $F$ layers can be described by transformation matrix [46]. When the local magnetization orientation is along the $+z$-axis, the Hamiltonian of the $F$ layer reads

$$H = \text{diag}[H_c - h_z, H_c + h_z, -H_c + h_z, -H_c - h_z]. \quad (6)$$

As above, $H_c$ and $h_z$ are electron Hamiltonian and effective exchange field, respectively. However, if the random magnetization orientation $\theta$ in the $x$-$z$ plane is defined relative to the $+z$-axis, the Hamiltonian can be rearranged as

$$\hat{H} = \begin{pmatrix}
H_c - h_z \cos \theta & -h_z \sin \theta & 0 & 0 \\
-h_z \sin \theta & H_c + h_z \cos \theta & 0 & 0 \\
0 & 0 & -H_c + h_z \cos \theta & h_z \sin \theta \\
h_z \sin \theta & -h_z \cos \theta & 0 & -H_c - h_z \cos \theta
\end{pmatrix}. \quad (7)$$

In this situation, the transformation matrix $\hat{T}$ satisfies the constraint $\hat{H} = \hat{T} \hat{H} \hat{T}^{-1}$. With the equations (6), (7) and making use of the unitary property of $\hat{T}$, we can obtain

$$\hat{T} = \begin{pmatrix}
\cos \frac{\theta}{2} & -\sin \frac{\theta}{2} & 0 & 0 \\
\sin \frac{\theta}{2} & \cos \frac{\theta}{2} & 0 & 0 \\
0 & 0 & \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\
0 & 0 & \sin \frac{\theta}{2} & \cos \frac{\theta}{2}
\end{pmatrix}. \quad (8)$$

As a result, the expression for the wave function in the $F_z$ layer is given by

$$\Psi^S_{F_z}(y) = \hat{T} \{ [e \cdot \exp(ik_{F_z}^e y) + f \cdot \exp(-ik_{F_z}^f y)] \hat{e}_1 \\
+ [e' \cdot \exp(ik_{F_z}^e y) + f' \cdot \exp(-ik_{F_z}^f y)] \hat{e}_2 \\
+ [g \cdot \exp(-ik_{F_z}^h y) + h \cdot \exp(i k_{F_z}^h y)] \hat{e}_3 \\
+ [g' \cdot \exp(-ik_{F_z}^h y) + h' \cdot \exp(i k_{F_z}^h y)] \hat{e}_4 \}.$$

Here $\hat{e}_1 = [1, 0, 0, 0]^T$, $\hat{e}_2 = [0, 1, 0, 0]^T$, $\hat{e}_3 = [0, 0, 1, 0]^T$, $\hat{e}_4 = [0, 0, 0, 1]^T$ are basis wave functions in the ferromagnetic region, and $k_{F_z}^{eh}(\psi) = \sqrt{2m [E_f + (-)\Omega + \rho \hbar^2]/\hbar^2 - k_f^2}$ with $\rho(\psi) = 1(-1)$ are the perpendicular components of wave vectors for ELQs and HLQs. It is worthy to note that the parallel component $k_f$ is conserved in transport processes of the quasiparticles. From the conversion $\theta \rightarrow 0$ and $h_z \rightarrow h$, we can obtain the wave function $\Psi^S_{F_z}(y)$ in the $F_z$ layer.

All scattering coefficients can be obtained by continuity of the wave functions and their derivatives at the interfaces:
\[
\Psi_{\phi}^{F}(y_{\phi}) = \Psi_{\phi}^{F}(y_{\phi}), \partial_{y_{\phi}}[\psi_{\phi}^{F} - \psi_{\phi}^{E}]\|_{y_{\phi}} = 2k_{F}Z_{F}\psi_{\phi}^{F}(y_{\phi});
\]
\[
\Psi_{\phi}^{F}(y_{\phi}) = \Psi_{\phi}^{F}(y_{\phi}), \partial_{y_{\phi}}[\psi_{\phi}^{F} - \psi_{\phi}^{E}]\|_{y_{\phi}} = 2k_{F}Z_{F}\psi_{\phi}^{F}(y_{\phi});
\]
\[
\Psi_{\phi}^{F}(y_{\phi}) = \Psi_{\phi}^{F}(y_{\phi}), \partial_{y_{\phi}}[\psi_{\phi}^{F} - \psi_{\phi}^{E}]\|_{y_{\phi}} = 2k_{F}Z_{F}\psi_{\phi}^{F}(y_{\phi}).
\]

Here, \(Z_{F} \sim Z_{F}\) are dimensionless parameters describing the magnitude of the interfacial resistances. \(y_{\phi} = 0\), \(L_{S1}, L_{S2}\) are local coordinate values at the layer interfaces, and \(k_{F} = \sqrt{2mE_{F}}\) is the Fermi wave vector. The wave functions for the other types of quasiparticle injection processes can be obtained in a similar way. From the boundary conditions, we obtain a system of linear equations that yield the scattering coefficients. With all the scattering coefficients at hand, we can use the finite-temperature Green’s function formalism [47–49] to calculate the Josephson current

\[
I_{c}(\phi) = \frac{k_{B}T}{4\hbar} \sum_{k_{n}} \frac{k_{e}(\omega_{n}) + k_{h}(\omega_{n})}{\Omega_{n}} \left[ \frac{a_{1}(\omega_{n}, \phi) - a_{2}(\omega_{n}, \phi)}{k_{e}} + \frac{a_{3}(\omega_{n}, \phi) - a_{4}(\omega_{n}, \phi)}{k_{h}} \right],
\]

where \(\omega_{n} = \pi k_{B}T(2n + 1)\) are the Matsubara frequencies with \(n = 0, 1, 2, \ldots\) and \(\Omega_{n} = \sqrt{\omega_{n}^{2} + \Delta^{2}(T)}\). \(k_{e}(\omega_{n}), k_{h}(\omega_{n}), a_{j}(\omega_{n}, \phi)\) with \(j = 1, 2, 3, 4\) are obtained from \(k_{e}, k_{h}, a_{j}\) by analytic continuation \(E \rightarrow i\omega_{n}\). In this case the critical current is defined by \(I_{c} = \max_{\phi}|I_{c}(\phi)|\).

### 2.2. Bogoliubov’s self-consistent field method

In principle, to acquire the time dependent triplet amplitude functions and the local density of the states (LDOS), we need to solve the BdG equation (3) by Bogoliubov’s self-consistent field method [45, 50–52]. The \(S_{1}, F_{1}, S_{2}\) junction is placed in a one-dimensional square potential well with infinitely high walls, then the eigenvalues and eigenvectors of the equation (3) have the following substitutions: \(E \rightarrow E_{n}\) and \([u_{1}(\vec{r}), u_{2}(\vec{r}), v_{1}(\vec{r}), v_{2}(\vec{r})]^{T} \rightarrow [u_{n}(\vec{r}), u_{n}(\vec{r}), v_{1}(\vec{r}), v_{2}(\vec{r})]^{T}\). Accordingly, the corresponding quasiparticle amplitudes can be expanded in terms of a set of basis vectors of the stationary states \([51, 53]\), \(u_{n0}(\vec{r}) = \sum_{q} u_{n0}^{q} \zeta_{q}(y)\) and \(v_{n0}(\vec{r}) = \sum_{q} v_{n0}^{q} \zeta_{q}(y)\) with \(\zeta_{q}(y) = \sqrt{2/L} \sin(qy/L)\). Here, \(q\) is a positive integer and \(L = L_{S1} + L_{F} + L_{S2}\). \(L_{S1}\) and \(L_{S2}\) are the thicknesses of the left and right superconducting electrodes, respectively. The pair potential in the BdG equation (3) satisfies the self-consistency condition [45]

\[
\Delta(y) = \frac{g(y)}{2} \sum_{n, q'\neq 0}^{\infty} (u_{nq}^{q}v_{nq}^{q} - u_{nq}^{q}v_{nq}^{q}) \zeta_{q}(y)\zeta_{q'}(y) \tanh \left( \frac{E_{n}}{2k_{B}T} \right),
\]

where the primed sum of \(E_{n}\) is over eigenstates corresponding to positive energies smaller than or equal to the Debye cutoff energy \(\omega_{D}\), and the superconducting coupling parameter \(g(y)\) is a constant in the superconducting regions and zero elsewhere. The matrix elements of equation (3) are then written as

\[
H_{c}(q, q') = \int_{0}^{L} \zeta_{q}(y) \left[ -\frac{1}{2m} \frac{\partial^{2}}{\partial y^{2}} + \varepsilon_{\perp} - E_{F} \right] \zeta_{q'}(y) dy,
\]

\[
h_{x}(q, q') = h_{x} \sin \theta \int_{L_{S1} + L_{F} + L_{S2}}^{L_{S1} + L_{F} + L_{S2}} \zeta_{q}(y)\zeta_{q'}(y) dy,
\]

\[
h_{z}(q, q') = h_{z} \int_{0}^{L_{S1} + L_{F} + L_{S2}} \zeta_{q}(y)\zeta_{q'}(y) dy + h_{z} \cos \theta \int_{L_{S1} + L_{F} + L_{S2}}^{L_{S1} + L_{F} + L_{S2}} \zeta_{q}(y)\zeta_{q'}(y) dy,
\]

\[
\Delta(q, q') = \int_{0}^{L} \zeta_{q}(y) \Delta(y) \zeta_{q'}(y) dy,
\]

where \(\varepsilon_{\perp}\) in equation (13) is the continuous energy in the transverse direction. The BdG equation (3) is solved by an iterative schedule. One first starts from the stepwise approximation for the pair potential and iterations are performed until the change in value obtained for \(\Delta(y)\) does not exceed a small threshold value.

The amplitude functions of the spin triplet state with zero and net spin projection are defined, respectively, as follows [51]:

\[
f_{0}(y, t) = \frac{1}{2} \sum_{n, q'\neq 0}^{\infty} (u_{nq}^{q}v_{nq}^{q} + u_{nq}^{q}v_{nq}^{q}) \zeta_{q}(y)\zeta_{q'}(y) \eta_{n}(t),
\]

\[
f_{y}(y, t) = \frac{1}{2} \sum_{n, q'\neq 0}^{\infty} (u_{nq}^{q}v_{nq}^{q} - u_{nq}^{q}v_{nq}^{q}) \zeta_{q}(y)\zeta_{q'}(y) \eta_{n}(t),
\]

where \(\eta_{n}(t) = \cos(E_{n}t) - i\sin(E_{n}t)\tan(EN/2k_{B}T)\), and the sum of \(E_{n}\) is in general performed over all positive energies. Additionally, the amplitude function of the spin singlet state can be written as \(f_{S} = \Delta(y)/g(y)\). In this paper the singlet and triplet amplitude functions are all normalized to the value of the
singlet pairing amplitude in a bulk superconducting material. The LDOS is given by [51]

\[
N(y, \epsilon) = -\sum_{q} \sum_{q' \neq q} (u_{qq'}^{+}\sigma_{q'}^{+} + u_{qq'}^{+}\sigma_{q}^{+}) f'(\epsilon - E_{a})
+ (v_{qq'}^{+}\sigma_{q'}^{+} + v_{qq'}^{+}\sigma_{q}^{+}) f'(\epsilon + E_{a}) \zeta_{q}(y) \zeta_{q'}(y),
\]

where \(f'(\epsilon) = \partial f / \partial \epsilon\) is the derivative of the Fermi function. The LDOS is normalized by its value at \(\epsilon = 3\Delta_{0}\) beyond which LDOS is almost constant.

3. Results and discussions

Unless otherwise stated, in BTK approach we use the superconducting gap \(\Delta_{0}\) as the unit of energy. The Fermi energy is defined as \(E_{F} = 1000 \Delta_{0}\), and the temperature is taken to be \(T / T_{c} = 0.1\). We assume all interfaces between the layers are transparent for electrons \(Z_{1,3} = 0\). All lengths and the exchange field strengths are measured in units of the inverse of the Fermi wave vector \(k_{F}\) and the Fermi energy \(E_{F}\), respectively. In Bogoliubov’s self-consistent field method, we consider the low-temperature limit and set \(k_{F} L_{S1} = k_{F} L_{S2} = 400\) and \(\omega_{D}/E_{F} = 0.1\), the other parameters are the same as the ones described above.

The detailed dependence of the critical current on the thickness \(k_{F} L_{1} (= k_{F} L_{2})\) is shown in figure 2(a) for different misorientation angles \(\theta\). We can find a significant change in the magnitude of critical current depending on the relative orientation of the two magnetizations. Considering first the parallel orientation \((\theta = 0)\), the well known \(0-\pi\) oscillations are reproduced, where the current change sign for certain values of thickness. It should however be noted that we have taken absolute value for the critical current.

By comparison, the dependence of critical current \(I_{c}\) on the exchange field \(h_{J}/E_{F} (= h_{J}/E_{F})\) is plotted in figure 2(b). It can be clearly seen that for various \(\theta\) the current \(I_{c}\) decreases monotonically with increasing \(h_{J}/E_{F}\) and it is reduced to zero at \(h_{J}/E_{F} = 1\), which implies a vanishing of the Josephson current. This phenomenon shows that the strong exchange splitting of the energy bands inside the \(F\) layers could effectively damp the tunneling of pairing electrons. For \(\theta = 0\), the critical current becomes an oscillating function of the \(h_{J}/E_{F}\), and it is accompanied by an exponential decay. This oscillating effect will diminish with the enhancement of \(\theta\) and also disappearing at some larger \(\theta\). We confirm the obvious fact that the critical current is increased with \(\theta\) for any fixed \(h_{J}/E_{F}\). Inset of figure 2(b) shows this characteristic of the critical current for \(h_{J}/E_{F} = 0.1\). It displays a nonmonotonic dependence of the critical current on \(\theta\), where a low dip corresponds to \(\theta = 0.12\pi\) and the maximum is located at \(\theta = \pi\). The main reason is because the junction starts out in the \(\pi\) state for the parallel orientation and turns into 0 state for the antiparallel one. From the above current
and the LDOS in the center of the layers. The LDOS is calculated at $k_F T = 0.0008$. Parameters used in all panels are $k_F l_1 = k_F l_2 = 100$ and $h_i/E_0 = h_r/E_0 = 0.1$.

![Figure 3. The current–phase relation $I_L(\phi)$ (a) and the LDOS in the center of F layer ($k_F T = 100$) (b) for several values of the misorientation angle $\theta$. The LDOS is calculated at $k_F T = 0.0008$. Parameters used in all panels are $k_F l_1 = k_F l_2 = 100$ and $h_i/E_0 = h_r/E_0 = 0.1$.](image)

characteristics, we could draw a conclusion that the phase state of the Josephson junction can be toggled between $\pi$ and 0 by changing the relative orientation of the two magnetizations when selecting the appropriate lengths of the two layers. Such peculiar behavior has been demonstrated by recent experiment [54]. In contrast, if the 0 state is the equilibrium state of the junction for $\theta = 0$, one can acquire a monotonic variation of the critical current when $\theta$ varies from 0 to $\pi$. These behaviors agree with the statement made in references [2, 55].

In order to clearly illustrate above features of the critical current, we plot the current–phase relation $I_L(\phi)$ and the LDOS in figures 3(a) and (b), respectively, for several misorientation angles $\theta$. If the two ferromagnetic layers have the same directions of the magnetic moments the wave-vector mismatches for spin-up and spin-down particles at both sides of the interface will result in an interface scattering. Additionally, for the antiparallel orientation of magnetic moments the wave-function could maintain continuously in above transmission process. However, the center-of-mass momentum $Q$ will be transformed into $-Q$ when the Cooper pair penetrates into the $F_2$ layer. As a result, the right-going wave function of the Cooper pair arising from the $S/F_1$ interface can be written as

$$\psi = \psi_{S/F_1}(\theta) = \psi_{S/F_1}^{Q,R_i} e^{iQ R_i} + \psi_{S/F_1}^{Q,R_i'} e^{-iQ R_i'},$$

where $R_i$ and $R_i'$ represent the distance from the $S/F_1$ and $F_1/F_2$ interfaces, respectively. This wave function can be decomposed into the singlet and triplet components. Accordingly, the right-going singlet component is given
by

\[ f_s = \begin{cases} 
(\uparrow\uparrow) - (\downarrow\downarrow) \cos (QR), & \text{in } F_1 \text{ layer,} \\
(\uparrow\downarrow) - (\downarrow\uparrow) \cos [Q(L_1 - R'_1)], & \text{in } F_2 \text{ layer}
\end{cases} \]

and the associated right-going triplet component reads as

\[ f_0 = \begin{cases} 
i(\uparrow\downarrow) + (\downarrow\uparrow) \sin (QR), & \text{in } F_1 \text{ layer,} \\
i(\uparrow\uparrow) + (\downarrow\downarrow) \sin [Q(L_1 - R'_1)], & \text{in } F_2 \text{ layer.}
\end{cases} \]

From above descriptions, we can demonstrate that \( f_s \) and \( f_0 \) are all symmetrical about the \( F_1/F_2 \) interface.

On the other hand, the left-going wave function \( \chi^- \) has the same transmission characteristic, but the only difference is that it generates at the \( F_2/S \) interface, in which case its original center-of-mass momentum becomes \( -Q \). Consequently, this wave function can be expressed as

\[ \chi^- = \begin{cases} 
(\uparrow\uparrow) e^{iQ(R_1 - L_1)} - (\downarrow\downarrow) e^{-iQ(R_1 - L_1)}, & \text{in } F_1 \text{ layer,} \\
(\uparrow\downarrow) e^{-iQ R'_1} - (\downarrow\uparrow) e^{iQ R'}, & \text{in } F_2 \text{ layer,
\end{cases} \]

where \( R_1 \) and \( R'_1 \) are the distance from the \( F_1/F_2 \) and \( F_2/S \) interfaces, respectively. Hence we can get the left-going singlet component

\[ f_s = \begin{cases} 
(\uparrow\downarrow) - (\downarrow\uparrow) \cos \{Q(R_1 - L_2)\}, & \text{in } F_1 \text{ layer,} \\
(\uparrow\uparrow) - (\downarrow\downarrow) \cos (QR'), & \text{in } F_2 \text{ layer,
\end{cases} \]

and the left-going triplet component

\[ f_0 = \begin{cases} 
i(\uparrow\downarrow) + (\downarrow\uparrow) \sin \{Q(R_1 - L_2)\}, & \text{in } F_1 \text{ layer,} \\
-i(\uparrow\uparrow) + (\downarrow\downarrow) \sin (QR'), & \text{in } F_2 \text{ layer.
\end{cases} \]

From above equations, we can find that because the factor \( \cos (QR') \) of the singlet component \( f_0^- \) is an even function of center-of-mass momentum \( Q \), \( f_0^- \) will not change its sign when passing from the \( F_2 \) layer into the \( F_1 \) layer, then it will overlap with \( f_1^- \). In contrast, the triplet component \( f_0^- \) will be added a negative sign because the factor \( \sin (QR') \) of this component is an odd function of \( Q \). Thus the sign of \( f_0^- \) is opposite to \( f_0^- \), and these two components could be canceled out each other. In addition, it is known that in normal metal the singlet component decays more slowly and the triplet component does not exist, then the supercurrent could transmit a long distance in the SNS junction. Compared with this situation, the long-range Josephson current also could be induced in the \( SF_s/F_1 \) junction with antiparallel magnetizations by the interference effect. This is because the

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**Figure 4.** The singlet components (top row) and the imaginary parts of opposite-spin triplet components (bottom row) plotted as a function of the coordinate \( k_F y \) for three values of lengths \( k_F L_1 = k_F L_2 = 70 \) (left column), \( 87 \) (middle column) and \( 100 \) (right column) in the antiparallel magnetization configuration \( (\theta = \pi) \). Here \( f_{1s0} \) and \( f_{2s0} \) correspond to \( S/F/F \) and \( F/F/S \) configurations, respectively. Parameters used in all panels are \( h/\hbar = h/\hbar = 0.1, \omega_{2l} = 4 \), and \( \phi = 0. \)
interference effect can revise the configurations of the singlet and triplet components, and also can make the characteristics of the two components closer to what they show in the normal metal. In figure 4, we show the numerical results about the singlet and triplet components through solving the BdG equation (3), which further demonstrate our above discussions. It is found that the total $f_1$ will be enhanced by the coherent superposition of $f_{1}^{+}$ and $f_{1}^{-}$, but $f_0$ will be canceled out in the central $F$ region due to the opposite signs of $f_{0}^{-}$ and $f_{0}^{+}$.

In the following, we want to know which components can make a crucial contribution to the enhancement of the Josephson current. So we turn to discuss the spatial dependence of the singlet and triplet components on the direction of magnetizations. As shown in figure 5, we plot the singlet component $f_1$ as a function of the coordinate $k_{xy}$ for several values of $\theta$. It is found that the amplitude of $f_1$ increases slightly as $\theta$ increases from 0 up to $\pi$. The main reason is because the singlet component is an even function of $Q$ and as a result $f_{1}^{+}$ and $f_{1}^{-}$ are nearly symmetrical to each other for different orientations of magnetic moments. From above features we can exclude the contribution of the singlet component to the long-range proximity effect when the magnetization direction switches from parallel to antiparallel.

Now let us analyze the dependence of the triplet components on the misorientation angle $\theta$. As illustrated in figure 6, for parallel orientation ($\theta = 0$) $f_0$ is symmetrical about the center of the $F$ layer. At this time, the equal-spin triplet component $f_1$ does not exist in the entire ferromagnetic region because of the homogeneous magnetization. When the magnetization direction of the $F_2$ layer rotates from the $z$-axis to $x$-axis, $f_0$ in the $F_2$ region decreases gradually, but $f_1$ increases and reaches maximum at $\theta = 0.5\pi$. This is because the magnetization oriented along the $x$-direction will induce the opposite-spin triplet component with respect to the $x$-axis ($|\uparrow\rangle = |\downarrow\rangle$). If one views with respect to the $z$-axis, such state is equivalent to the equal-spin triplet component $-|\uparrow \downarrow\rangle$ [8, 18]. It is interesting to note that for the perpendicular magnetizations the spatial oscillations of $f_0$ in the $F_1$ region will instead exhibit a monotonic spatial variation with jumping into the $F_2$ region. Meanwhile, $f_1$ has the same characteristics as it passes from the $F_2$ layer into the $F_1$ layer. Here we should point out that there are two important effects to enhance the supercurrent: (i) the emergence of long-range $f_1$, and (ii) the interference of the $f_0$ and $f_1$. It is well known that $f_1$ could induce a long-range supercurrent. If two $F$ layers are highly asymmetric, $f_1$ becomes much larger than $f_0$, then the interference between of them will be reduced accordingly. In this case, the long-range proximity effect manifests itself as a large second harmonic ($I_2 \gg I_1$) in the spectral decomposition of the Josephson current–phase relation

$$I(\phi) = I_1 \sin(\phi) + I_2 \sin(2\phi) + \cdots.$$  

This phenomenon has been proposed in references [57–59]. In contrast, the first harmonic could preval as the interference of $f_0$ and $f_1$ was restored again in symmetric junction with equal ferromagnetic layers. The comparison of these two cases is shown in figure 7. As can be seen from the picture, the amplitude of critical current in the symmetric configuration is larger than that in the asymmetric one. Additionally, since $\theta$ turns from $0.5\pi$ to $\pi$, $f_1$ gradually decreases but $f_0$ in the $F_2$ region will increase instead, which leads to the enhancement of the interference effect. In the antiparallel configuration $f_1$ completely vanishes, but the interference effect becomes most apparent, which is displayed by the cancellation of $f_0$ in the middle region of the $F$ layer. As a result, in the above process the critical current will continue to increase and reach maximum in antiparallel case. This physical picture can clearly explain recent experimental phenomena [42, 43]. It is emphasized that the Josephson current in the antiparallel configuration is obviously smaller than that in SNS junctions for the same length between two superconducting electrodes, which has been described in the introduction. This is because the interference effect does not make the triplet component $f_0$ cancel out completely in the entire $F$ region, and also could not let the singlet component $f_1$ grow big enough.
As mentioned above, in antiparallel configuration the critical current $I_c$ decreases monotonically from a finite value to zero with the increasing exchange field. This behavior can be attributed to the fact that the singlet and triplet components are all suppressed by the exchange splitting of two $F$ layers. In figure 8, we show the distribution of these two components for three exchange fields $h_1/E_F = 0.1, 0.5, \text{ and } 1.0$. With increasing $h_1/E_F$, the magnitude of $f_3$ and $f_0$ in the entire $F$ region are all reduced, and both of them will drop to zero at $h_1/E_F = 1$. The reason can be summarized as follows: for weak exchange field $h_1/E_F = 0.1$, the Andreev reflections could occur at $S/F_1$ and $F_2/S$ interfaces, in which case the singlet and triplet components are all present in the two $F$ layers. Meanwhile, the interference effect of the triplet components will take place, which can create an enhanced supercurrent flowing across the junction. When the exchange fields are increased, the Andreev reflections can be suppressed by the exchange splitting, and as a result the singlet and triplet components will decrease correspondingly. In particular, for a fully spin-polarized half-metal ($h_1/E_F = 1$) the Andreev reflections could be totally inhibited, then above two components just exist near the $S/F_1$ and $F_2/S$ interfaces but are unable to form in two $F$ regions. Hence the Josephson current would be suppressed completely. From the inset of figure 8, we can find that two distinguishable peaks in the LDOS become weak with increasing $h_1/E_F$, and they even disappear for $h_1/E_F = 1$. These actions further demonstrate the fact that two components are no available in the $F$ regions and the interference effect of the triplet components would vanish accordingly.

To understand further the interference effect of the opposite-spin triplet state, we investigate the intriguing influence of the length and exchange field on the Josephson current when both ferromagnetic layers have
different physical features, as seen in figures 9(a) and (b). Take the first one for example, the variation of $I_c$ with the thickness $k_L$ looks like a Fraunhofer pattern. This phenomenon appears more and more obvious as the misorientation angle $\theta$ increases from 0 to $\pi$. In parallel orientation ($q_p = 0$), the critical current shows the 0–$\pi$ conversion on the condition of the nonexistence of interference effect, in which case the amplitude of critical current is weak enough. It is important to note that for perpendicular orientation ($q_p = 0.5$) the long range second harmonic current will be induced in highly asymmetric junction, which corresponds to the circular regions denoted in figure 9, then the interference effect can be almost negligible. By contrast, $I_c$ dependence exhibits a remarkable oscillating behavior in the thickness range $< k_L < 130$, which marks the enhancement of the interference effect. Moreover, $I_c$ reaches its maximum value for $k_L = 100$ and above or below this thickness its amplitude will decrease.

If the two $F$ layers are arranged antiparallel to each other ($\theta = \pi$), the interference effect would appear most likely to occur, meanwhile, their contribution to the Josephson current reaches maximum. In this configuration, we consider in figure 10 the current–phase relations $I_c(\phi)$ and the corresponding LDOSs in particular points A, B, C and D of figure 9(a). If the $F_1$ and $F_2$ layers have identical thickness, as shown in point A, the Josephson current is positive and the LDOS displays a valley at $\phi = 0$ and two distinguishable peaks at $\phi = \pm 0.5\Delta$. Besides, when the thickness $k_L$ decreases to 91, corresponding to point B, the Josephson junction is located at the 0–$\pi$
transition point. The first harmonic current vanishes, and the second harmonic will be fully revealed. Subsequently, the sign of $I_c$ turns to negative at $kF_2 = \frac{83}{32}$ (point C), and the LDOS at $\epsilon = 0$ will be converted from valley to peak. This indicates that the ground state of junction converts into $\pi$ state. At last, the junction will return to the critical point of $0-\pi$ transition at $kF_2 = \frac{66}{32}$ (point D). From figure 9 (a), we can clearly see that the critical current oscillating with $kF_2$ displays an unequal period. The detailed explanation will be described in the following paragraph. In addition, if the both $F$ layers have the same lengths but different exchange fields, the critical current $I_c$ shows the similar characteristics (see figure 9 (b)). This feature illustrates that the interference effect is simultaneously related to the difference of the center-of-mass momenta which are acquired by the spin-opposite triplet pair from the $F_1$ and $F_2$ layers.

As previously mentioned, the interference of $f_0^+$ and $f_0^-$ provides the main contribution to the Josephson current. To gain further insight into the interference effect in the asymmetric junctions, we choose the antiparallel configuration as an example for discussion. In figure 10, we present results for the dependence of the triplet components $f_0$ on the thickness $kF_2$ when the $F_1$ layer has a fixed thickness $kF_1 = 100$ (point D). From figure 9 (a), we can clearly see that the critical current oscillating with $kF_2$ displays an unequal period. The detailed explanation will be described in the following paragraph. In addition, if the both $F$ layers have the same lengths but different exchange fields, the critical current $I_c$ shows the similar characteristics (see figure 9 (b)). This feature illustrates that the interference effect is simultaneously related to the difference of the center-of-mass momenta which are acquired by the spin-opposite triplet pair from the $F_1$ and $F_2$ layers.

As previously mentioned, the interference of $f_0^+$ and $f_0^-$ provides the main contribution to the Josephson current. To gain further insight into the interference effect in the asymmetric junctions, we choose the antiparallel configurations as an example for discussion. In figure 11, we present results for the dependence of the triplet components $f_0$ on the thickness $kF_2$ when the $F_1$ layer has a fixed thickness $kF_1 = 100$. It is known that the strength of interference effect is relate to the phase difference and amplitude of two wave functions emanating from different directions. We first talk about the contributions of the phase difference between $f_0^+$ and $f_0^-$ to the oscillation of the critical current. Here we fix the thickness of $F_1$ layer and shorten that of $F_2$ layer, which is similar to set constant $f_0^+$ and shift $f_0^-$ from left to right. When both $F$ layers have the same length, the phase difference of two triplet components $f_0^+$ and $f_0^-$ is $\pi$ at every position of the $F$ region. In this case, the interference effect manifests obviously and could induce an enhancement of the Josephson current. As the thickness $kF_2$ is reduced to 91, $f_0^-$ moves 1/4 period, then the $F_2$ interface shifts from the red vertical dashed–dotted line to the green one. Correspondingly, the junction is situated at the critical point of $0-\pi$ phase transition. For $kF_2 = 83$, $f_0^+$ moves to the right 1/2 period, accordingly, the junction converts to $\pi$ state.
Decreasing the $F_2$ layer thickness down to $k_L F_2 = 66$ means that $f_0$ shifts $3/4$ period, the junction returns to the critical point of phase transition. As mentioned before, the critical current has unequal oscillation period with varying $k_L F_2$, which is determined by the inhomogeneous spatial oscillation of $f_0$. On the other hand, as the length $k_L F_2$ turns from 100 to 0, the mutual cancellation between $f_0$ and $\bar{f}_0$ will decrease. Consequently, the magnitude of $f_0$ could be enhanced by the superposition of $f_0$ and $\bar{f}_0$. This indicates the weakening of interference effect that can make the Josephson current diminish.

**4. Conclusion**

In this paper, we have investigated the relationship between the long-range Josephson current and the pairing correlations in clean $SF_1/F_2/S$ junctions with the misorientation magnetizations through solving the BdG equations. The interference effect of the opposite-spin triplet component was pointed out to be a source of this current. The main reason is because the Josephson critical current will enhance when the magnetizations rotate from the parallel to the antiparallel orientation. In this process, the amplitude of the singlet component changes slightly but the interference effect of the triplet components $f_0$ and $\bar{f}_0$ will increase correspondingly, and in the antiparallel configuration the interference of both components cloud nearly cancel each other in central ferromagnetic region. This behavior can be attribute to two facts: (i) The triplet components $f_0$ and $\bar{f}_0$ derive, respectively, from the $S/F_1$ and $F_2/S$ interfaces and transmit to opposite directions. They experience a scattering occurred at the $F_1/F_2$ interface and take this interface as an emission source to continually spread into another ferromagnetic layer. (ii) The antiparallel magnetizations will provide opposite center-of-mass momentum to the Cooper pair, then two singlet components $f_3$ and $\bar{f}_3$ almost maintains invariant, but the triplet components $f_0$ and $\bar{f}_0$ have opposite sign and could cancel each other out in the $F$ region. Furthermore, if the feature of the $F_1$ layer remains unchanged, the interference effect will make the critical current oscillate with the length and exchange field of the $F_2$ layer. Therefore, this finding provides new insight into the physical mechanism to the
long-range proximity effect in the Josephson junctions with non-parallel magnetizations and can be important for the implementation of interference effect in superconducting spin electronic devices.

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