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2009 J. Phys.: Condens. Matter 21 385703

(http://iopscience.iop.org/0953-8984/21/38/385703)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **21** (2009) 385703 (5pp) doi:10.1088/0953-8984/21/38/385703

Josephson supercurrent with spin-equal pairing through a half-metallic link

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Received 24 June 2009
Published 27 August 2009
Online at stacks.iop.org/JPhysCM/21/385703

Abstract
Taking into account spin-flip scattering at superconductor/half-metallic ferromagnet (S/F) interfaces in S/F/S Josephson junctions, we extend the Blonder–Tinkham–Klapwijk approach and novel Andreev reflection idea to studying the Josephson current and spatially dependent superconducting order parameters for singlet and triplet pairing states. It is found that the novel Andreev reflection at the F/S interfaces can result in electron–hole correlations in one spin subband of the F and a large supercurrent of spin-equal pairing through a long half-metallic link.

1. Introduction

It is well known that a supercurrent could exist between two superconductors (Ss) separated by a thin insulating layer (I) in the absence of a voltage drop between them, which is the so-called dc Josephson effect [1]. Its physical origin is the breakdown of time-reversal symmetry in the S/I/S structure due to the macroscopic phase difference ϕ between the two Ss, yielding supercurrent $I_s = I_c \sin\phi$ with I_c as the critical current. The Josephson effect also exists if two Ss are connected by a 'weak link' of any physical nature such as normal metal, semiconductor, and geometrical constriction. The physics of the dc Josephson effect with a weak link can be understood by the Andreev reflection [2] (AR) processes of quasiparticles with energy smaller than the superconducting energy gap [3]. In the weak link region, an electron impinging on one of the interfaces is Andreev reflected and converted into a hole moving in the opposite direction, thus generating a Cooper pair with opposite spins in one S. This hole is consequently Andreev reflected at the second interface and is converted back to an electron, leading to the destruction of the Cooper pair in the other S. As a result of this cycle, a pair of correlated electrons with opposite spins is transferred from one S to another, creating a singlet supercurrent flow across the junction [3].

If the weak link between the two Ss is a ferromagnetic metal (F) thin film, similar characteristics of the Josephson effect exist in S/F/S junctions. More interestingly, there undoubtedly appear some particular effects in them, for carriers passing through the F must feel spin-dependent potentials as a result of the ferromagnetic exchange energy. The Andreev process, recognized as the mechanism of normal to supercurrent conversion [2, 4], is modified at F/S interfaces due to the spin imbalance in the F. The AR effect is suppressed by increasing the exchange energy of the F due to occurrence of virtual AR [5–8]. Owing to the Fermi surface difference for spin-up and spin-down subbands, the AR may become an evanescent wave depending on the injection angle of the quasiparticle. An electron and the Andreev reflected hole with different momenta and in opposite spin subbands are correlated via the AR, thus providing an extension of superconducting order parameter into the F region of length of the order of ξ_F. Here ξ_F is the coherence length in the F, inversely proportional to exchange energy h_0 if h_0 is much smaller than the Fermi energy in the F [8]. It has been shown that an inhomogeneous superconducting order parameter can be induced by the proximity effect in a thin F film in contact with an S [9], and in a weak F sandwiched between two Ss [10], even though h_0 in the F is greater than the superconducting pair potential in the S. It was observed that there is a crossover from 0 to π state in S/F/S junctions and the critical current exhibits damped-oscillatory behavior with increasing F thickness, respectively, by Ryazanov *et al* [10] in Nb/Cu_xNi_{1-x}/Nb Josephson junctions and by Kontos *et al* [11] in planar Nb/Al/Al_2O_3/PdNi/Nb junctions. Such a damped-oscillatory behavior of I_c with the F thickness has been reproduced theoretically in the clean limit [12].

For a half-metallic F link with h_0 being greater than the Fermi energy of the F, the Fermi level cuts across only one spin subband, so that electronic bands exhibit metallic behavior for one spin direction and insulating behavior for the other. In this case, the singlet Cooper pair with opposite spins cannot pass through the half-metallic F region, because there is only one spin channel for electrons at the Fermi level.

Recently, Keizer *et al* [13] reported a long-range Josephson supercurrent between two s-wave superconducting NbTiN electrodes through a half-metallic CrO_2. Since singlet Cooper pairs cannot exist in the half-metallic F, it was assumed [13] that a spin-triplet supercurrent passes through the half-metallic F, and a conversion from spin-singlet to spin-triplet pairing takes place at the F/S interfaces. To realize this conversion, several theoretical works [14–20] have focused on the spin-triplet supercurrent in the presence of spin-flip scattering, most of which were based upon the quasiclassical Green's functions and Eilenberger equations [21, 22]. Recently, Niu and Xing [23] considered an F/F/S tunnel junction in the clean limit, where the two Fs have different magnetization directions. The noncollinear magnetizations provide a spin-flip effect and may give rise to a novel AR, in which the electron and the Andreev reflected hole belong in the same spin subband, so as to give a conversion from the spin-singlet pairing to a spin-triplet one. It was further shown [24] that both the spin-flip and broken time-reversal symmetry are conditions necessary for giving rise to the novel AR and spin-triplet pairing states.

In this work we extend the approach developed by Blonder, Tinkham, and Klapwijk (BTK) [4] to studying the supercurrent in S/half-metallic F/S junctions by taking into account interfacial potentials with spin-flip. This potential at the F/S interface can be regarded as an effective interfacial potential of an F/F/S structure with noncollinear magnetizations in the limit of the thickness of the middle F layer tending to vanish. It is found that not only the usual AR but also the novel AR may appear at F/S interfaces in the presence of spin-flip scattering. As a result, there could be two types of supercurrents through the F link: a short-distance singlet supercurrent composed of correlated electron pairs with opposite spins and a long-distance triplet supercurrent composed of those with the same spin. The triplet one will play a dominant role if the weak link F is half-metallic. From the four-component Nambu spinor Green's function obtained, we further calculate superconducting order parameters for singlet and triplet pairing states. Their spatial dependence in the S/half-metallic F/S junction confirms that the supercurrent through the half-metallic F link is composed of the correlated electron pairs with equal spin, which are born of the novel AR at the F/S interfaces.

2. Model and method

Consider an S/F/S Josephson junction consisting of two semi-infinite Ss and an F interlayer of thickness d. The F and Ss are separated by interfaces at $x = 0$ and d. The Ss are described by the BCS Hamiltonian of a 4×4 matrix,

$$\hat{H}_{\rm SC} = \begin{pmatrix} H_0\hat{I} & {\rm i}\Delta\hat{\sigma}_y \\ -{\rm i}\Delta\hat{\sigma}_y & -H_0\hat{I} \end{pmatrix}, \tag{1}$$

where $H_0 = -\hbar^2\nabla^2/2m + V(x) - E_{\rm F}$, $\hat{\sigma}$ is the spin Pauli matrix, and $\hat{I}$ the unit matrix. The superconducting pair potentials Δ are assumed to have the same magnitude but different phases ($\phi_{\rm L} = 0$ and $\phi_{\rm L} = \phi$), given by $\Delta(x) = \Delta(T)[\Theta(-x) + \exp({\rm i}\phi)\Theta(x-d)]$. Here $\Delta(T)$ is the temperature-dependent energy gap that follows the BCS relation $\Delta(T) = \Delta_0 \tanh[1.76(T_{\rm c}/T - 1)]$ with $T_{\rm c}$ the critical temperature of the Ss, and $\Theta(x)$ is the unit step function. The F layer is assumed to be half-metallic, i.e. the Fermi level cuts across the spin-up subband but not across the spin-down subband. Its effective single particle Hamiltonian reads

$$\hat{H}_{\rm F} = \begin{pmatrix} H_0\hat{I} + \frac{h_0}{2}\hat{\sigma}_z & 0 \\ 0 & -H_0\hat{I} - \frac{h_0}{2}\hat{\sigma}_z \end{pmatrix}, \tag{2}$$

with h_0 as the exchange energy. The interface scattering potentials at $x = 0$ and d are described by a δ-type form

$$\hat{H}_I = \begin{pmatrix} U_1\hat{I} + U_2\hat{\sigma}_y & 0 \\ 0 & -U_1\hat{I} + U_2\hat{\sigma}_y \end{pmatrix} [\delta(x) + \delta(x-d)], \tag{3}$$

where U_1 is the interfacial scattering potential in the BTK approach and U_2 is the spin-flip one, the latter being newly suggested in this work.

We adopt the BTK approach [4] to study the S/F/S junction. This approach has been widely applied to describing quasiparticle states in Ss with spatially varying pair potentials. For simplicity, the effective masses m are taken to be equal in both F and S regions. In the present F/S junction with spin-flip, the quasiparticle states must be expressed by four-spinor wavefunctions, respectively, for the electron-like quasiparticle (ELQ) and holelike quasiparticle (HLQ) with spin up and down. From $\hat{H}_{\rm SC}\hat{\psi} = E\hat{\psi}$, we have four basis wavefunctions of the left S: $\hat{e}_1 = (u, 0, 0, v)^{\rm T}$, $\hat{e}_2 = (0, u, -v, 0)^{\rm T}$, $\hat{e}_3 = (0, -v, u, 0)^{\rm T}$, and $\hat{e}_4 = (v, 0, 0, u)^{\rm T}$, in which $k^{\pm} = \sqrt{2m(E_{\rm F} \pm \Omega)/\hbar^2 - k_{\parallel}^2}$ are the perpendicular components of the wavevectors with $k_{\parallel}$ as the parallel component, $u = \sqrt{(1+\Omega/E)/2}$, $v = \sqrt{(1-\Omega/E)/2}$, and $\Omega = \sqrt{E^2 - \Delta^2}$. If the spin-flip scattering is absent, the four-component BdG equations may be decoupled into two sets of two-component equations: one for the spin-up electron-like and spin-down holelike quasiparticle wavefunctions $\hat{e}_1$ and $\hat{e}_4$, the other for $\hat{e}_3$ and $\hat{e}_2$. Similarly, the basis wavefunctions of the right S are given by $\hat{e}_5 = (u{\rm e}^{{\rm i}\phi}, 0, 0, v)^{\rm T}$, $\hat{e}_6 = (0, u{\rm e}^{{\rm i}\phi}, -v, 0)^{\rm T}$, $\hat{e}_7 = (0, -{\rm e}^{{\rm i}\phi}, u, 0)^{\rm T}$, and $\hat{e}_8 = (v{\rm e}^{{\rm i}\phi}, 0, 0, u)^{\rm T}$. In the F region, where the situation is simpler, the basis wavefunctions are $\hat{f}_1 = (1, 0, 0, 0)^{\rm T}$, $\hat{f}_2 = (0, 1, 0, 0)^{\rm T}$, $\hat{f}_3 = (0, 0, 1, 0)^{\rm T}$, and $\hat{f}_4 = (0, 0, 0, 1)^{\rm T}$.

There are eight types of quasiparticle injection processes in an S/F/S junction: an ELQ (HLQ) with spin up (down) incident on the left (right) interface from the left (right) S. We show one of them below. Suppose a beam of spin-up ELQ incident on the interface at $x = 0$ from the left S. With general solution of the Bogoliubov–de Gennes equation, the wavefunction in the left S is given by

$$\psi_1(x) = \hat{e}_1{\rm e}^{{\rm i}k_+x} + b_1\hat{e}_1{\rm e}^{-{\rm i}k_+x} + b_1'\hat{e}_2{\rm e}^{-{\rm i}k_+x} + a_1'\hat{e}_3{\rm e}^{{\rm i}k_-x} + a_1\hat{e}_4{\rm e}^{{\rm i}k_-x}, \tag{4}$$

for $x < 0$. Here coefficients b_1, b_1', a_1', and a_1 correspond to the normal reflection, the normal reflection with spin-flip, the novel AR in the spin-up subband, and the usual AR process in the spin-down subband, respectively. In the middle half-metallic F layer of $0 < x < d$, since there exist multi-reflected

ELQ and HLQ, the wavefunction is given by

$$\psi_1(x) = e\hat{f}_1 e^{ik_e x} + e'\hat{f}_2 e^{\kappa_e x} + f\hat{f}_1 e^{-ik_e x} + f'\hat{f}_2 e^{-\kappa_e x} + g\hat{f}_3 e^{ik_h x} + g'\hat{f}_4 e^{\kappa_h x} + h\hat{f}_3 e^{-ik_h x} + h'\hat{f}_4 e^{-\kappa_h x}, \quad (5)$$

where $k_{e,h} = \sqrt{2m(E_F \pm E)/\hbar^2 - k_\parallel^2}$ are the perpendicular components of the wavevectors for the electron and hole in the spin-up subband and $\kappa_{e,h} = \sqrt{2m(h_0 - E_F \mp E)/\hbar^2 + k_\parallel^2}$ are the imaginary wavevectors in the spin-down subband. In the right S region of $x > d$, we have

$$\psi_1(x) = c_1\hat{e}_5 e^{ik_+ x} + c_1'\hat{e}_6 e^{ik_+ x} + d_1'\hat{e}_7 e^{-ik_- x} + d_1\hat{e}_8 e^{-ik_- x}. \quad (6)$$

All 16 coefficients in equations (4)–(6) can be determined by matching the conditions at the left and right interfaces. For example, the matching conditions for the wavefunctions at the left interface are given by

$$\Psi_1(0^+) = \Psi_1(0^-), \quad (7)$$

$$\frac{\partial}{\partial x}\Psi_1(0^+) - \frac{\partial}{\partial x}\Psi_1(0^-) = 2k_F \begin{pmatrix} Z_1\hat{I} + Z_2\hat{\sigma}_y & 0 \\ 0 & Z_1\hat{I} - Z_2\hat{\sigma}_y \end{pmatrix} \Psi_1(0), \quad (8)$$

where $Z_1 = U_1/\hbar k_F$ and $Z_2 = U_2/\hbar k_F$ are dimensionless parameters describing the interfacial scattering with spin unchanged and with spin-flip, respectively. The wavefunctions for the other seven types of quasiparticle injection processes can be obtained in a similar way, which are ψ_2, ψ_3, and ψ_4 for the quasiparticle propagating from left to right, and ψ_5, ψ_6, ψ_7, and ψ_8 for that propagating from right to left.

Next, we wish to construct the Nambu spinor Green's function in the S/F/S structure. For the quasiparticle propagating towards the right (left), there are four wavefunctions with outgoing boundary conditions to the right (left), ψ_1, ψ_2, ψ_3, and ψ_4 (ψ_5, ψ_6, ψ_7, and ψ_8), and also four wavefunctions with incoming boundary conditions to the left (right), $\tilde{\psi}_1$, $\tilde{\psi}_2$, $\tilde{\psi}_3$, and $\tilde{\psi}_4$ ($\tilde{\psi}_5$, $\tilde{\psi}_6$, $\tilde{\psi}_7$, and $\tilde{\psi}_8$) [25]. As an example, $\tilde{\psi}_1(x) = \hat{e}_1 e^{ik_+ x}$ for $x < 0$, $\tilde{\psi}_1(x) = c_1\hat{e}_5 e^{ik_+ x} + r_1\hat{e}_5 e^{-ik_+ x} + c_1'\hat{e}_6 e^{ik_+ x} + r_1'\hat{e}_6 e^{-ik_+ x} + d_1'\hat{e}_7 e^{-ik_- x} + s_1'\hat{e}_7 e^{ik_- x} + d_1\hat{e}_8 e^{-ik_- x} + s_1\hat{e}_8 e^{ik_- x}$ for $x > d$, and $\tilde{\psi}_1(x)$ has the same form as that for $\psi_1(x)$ given by equation (5) for $0 < x < d$. With these wavefunctions, the retarded Green's functions are given by [25–27]

$$G^r(x > x'; E) = \sum_{i=1}^{4}\sum_{j=1}^{4} \alpha_{ij}\psi_i(x)\tilde{\psi}_j^\dagger(x'),$$
$$G^r(x < x'; E) = \sum_{i=5}^{8}\sum_{j=5}^{8} \beta_{ij}\psi_i(x)\tilde{\psi}_j^\dagger(x'), \quad (9)$$

which satisfy the following equation:

$$(E - \hat{H})G^r(x, x'; E) = \hat{K}\delta(x - x'),$$

with

$$\hat{K} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \quad (10)$$

The coefficients α_{ij} and β_{ij} can be determined by satisfying the following boundary conditions: $G^r(x, x + 0^+, E) = G^r(x, x - 0^+, E)$, and $dG^r(x, x', E)/dx|_{x=x'+0^+} - dG^r(x, x', E)/dx|_{x=x'-0^+} = (2m/\hbar^2)\hat{K}$. After carrying out a little tedious calculation, we can get the 4×4 retarded Green's functions. The dc Josephson current at a given temperature can be expressed by the Andreev reflection amplitudes in terms of the finite-temperature Green's function formalism as

$$I_s = \frac{e\hbar k_B T}{4im} \lim_{x'->x}\left(\frac{\partial}{\partial x'} - \frac{\partial}{\partial x}\right)\sum_{k_\parallel}\sum_{\omega_n} \mathrm{Tr}[G(x, x', k_\parallel, \omega_n)]$$
$$= \frac{k_B T e\Delta}{4\hbar}\sum_{k_\parallel}\sum_{\omega_n}\frac{k^+(\omega_n) + k^-(\omega_n)}{\Omega_n} \times \left[\frac{a_1(\omega_n,\phi) - a_2(\omega_n,\phi)}{k^+(\omega_n)} + \frac{a_3(\omega_n,\phi) - a_4(\omega_n,\phi)}{k^-(\omega_n)}\right] \quad (11)$$

where $\omega_n = (2n + 1)\pi k_B T$ are the Matsubara frequencies with $n = 0, \pm 1, \pm 2, \ldots$, and $\Omega_n = \sqrt{\omega_n^2 + \Delta^2(T)}$. $k^+(\omega_n)$, $k^-(\omega_n)$, and $a_i(i\omega_n, \phi)$ with $i = 1, 2, 3, 4$ are obtained from k^+, k^-, and a_i by analytically continuing E to $i\omega_n$. The superconducting order parameters $F_{14}(x)$ for singlet pairing and $F_{13}(x)$ for spin-equal pairing are determined by the corresponding off-diagonal component of the Green's function with $x = x'$,

$$F_{1i}(x) = \frac{1}{\pi}\sum_{k_\parallel}\int_0^\infty dE\, \mathrm{Im}[G_{1i}(x, x, k_\parallel, E)]. \quad (12)$$

3. Results and discussion

First, we wish to point out that although a_i in equation (11) is the usual AR coefficient of an electron on the left S side in the ith process, via the spin-flip at the S/F interface, it is closely related to the novel AR one of a hole on the F side. The former (usual AR) indicates the destruction of a Cooper pair with opposite spins in the left S, and the latter (novel AR) stands for the creation of a pair of correlated electrons with equal spin in the middle F. The physical picture of the Josephson supercurrent with spin-equal pairing through a half-metallic F is as follows. In the half-metallic F, a spin-up electron moving towards right is novelly Andreev reflected at the right F/S interface and converted into a hole moving towards left still in the spin-up subband; at the same time, via the interfacial spin-flip, a Cooper pair with opposite spins is generated in the right S. Then, this hole moving towards left is novelly Andreev reflected at the left S/F interface and is converted back to a spin-up electron, leading to the destruction of the Cooper pair in the left S. After this cycle, a pair of correlated electrons with equal spin is transferred from the left interface to the right one. As a result, via the interfacial spin-flip, a Cooper pair with opposite spins is destroyed in the left S and created in the right S.

In what follows we calculate the critical current I_c from equation (11), and superconducting order parameters $F_{14}(x)$ and $F_{13}(x)$ from equation (12). It is assumed that the spin-up band of the F and the energy band of the S have the same energy zero point. Parameters used in the calculation are $h_0/E_F = 2.2$, which satisfies the half-metallic condition $h_0 > E_F$, $E_F = 1000\Delta_0$, and $k_B T = 0.1\Delta_0$. The numerical

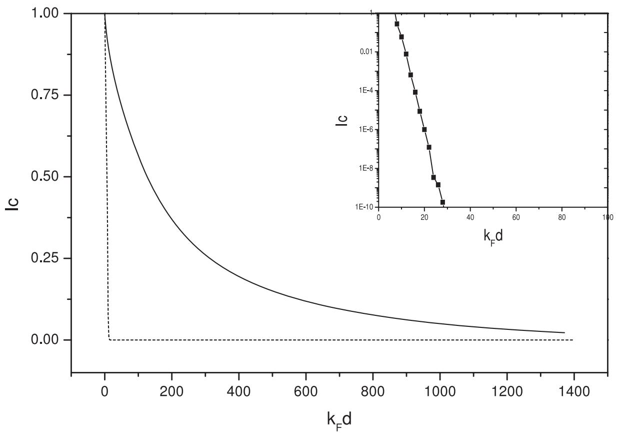

Figure 1. Critical current I_c as a function of the thickness of the middle FM layer for $Z_2 = 0.05$ (solid line) and $Z_2 = 0$ (dashed line as well as in the inset). Here $k_B T = 0.1\Delta_0$, $E_F = 1000\Delta_0$, $h_0 = 2200\Delta_0$, and $Z_1 = 0.75$ are taken.

calculation indicates that I_c is a fast-oscillated function of thickness d of the half-metallic F layer on an atomic scale. Taking its average, we plot in figure 1 the superconducting critical current I_c in an S/F/S Josephson junction as a function of d, in which I_c $(d = 0)$ is taken as the unit of current. It is found that, in the presence of interfacial spin-flip $(Z_2 \neq 0)$, I_c decreases slowly with increasing d, and has a finite value even when d is equal to several hundreds of nanometers. This indicates that the decaying length is of the same order of magnitude as the superconducting coherent length in bulk S. On the other hand, I_c decreases rapidly in the absence of spin-flip $(Z_2 = 0)$, as shown in the inset of figure 1, which stems from the fact that I_c decays exponentially with κd. From the line slope in the inset, it is estimated that the decay length $1/\kappa$ is on the order of $\hbar/\sqrt{2m(h_0 - E_F)}$ for a half-metallic F. Such a big difference between the two cases in the decay length for I_c may be understood by the following argument. In the $Z_2 \neq 0$ case, the novel AR gives rise to the correlated electron pair with equal spin, which can pass through the half-metallic F with one spin channel at E_F; while in the $Z_2 = 0$ case, there is only a singlet electron pair that cannot pass through the half-metallic F.

To confirm the argument above, in figure 2 we show calculated results for the spatial variation of superconducting order parameters for singlet and triplet pairing in the 0-state S/half-metallic F/S Josephson junction. In figure 2(a), the singlet order parameter $F_{14}(x)$ exists only in the S regions of $x < 0$ and $x > d$, and vanishes in the middle F region of $0 < x < d$ due to lack of two spin channels at E_F. In contrast, the order parameter F_{13} for the spin-equal pairing appears in the whole half-metallic region, as shown in figure 2(b). It is diminished slowly with distance from the F/S interface and exhibits a minimum at the center of the F layer. The finite $F_{13}(x)$ in the half-metallic F is a result of interference of the correlated electrons and holes in the same spin subband, and stems from the novel AR at the F/S interfaces. It then follows that the appearance of I_c and $F_{13}(x)$ in the half-metallic F is of the same origin, the coherence of electron and hole in one spin subband via the novel Andreev bound states. With increasing

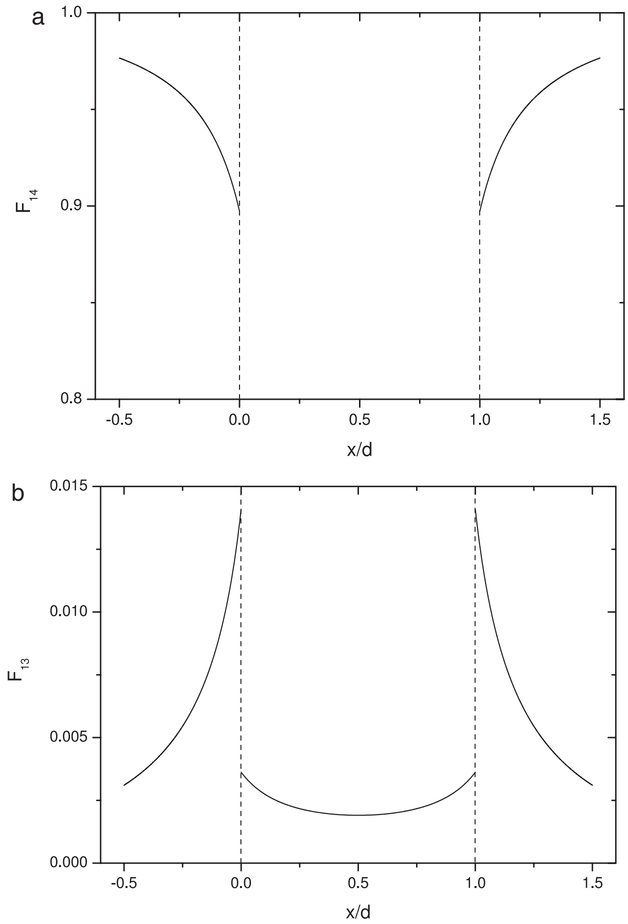

Figure 2. Spatial variation of superconducting order parameters F_{14} (a) and F_{13} (b) in the unit of F_{14} of bulk S. Here $k_F d = 500$ and other parameters are the same as in figure 1, and the interfaces are indicated by the dashed lines.

d, the coherence-broken effect is enhanced, producing a slow decrease in $F_{13}(x)$ and I_c.

In summary, the BTK theory approach has been extended to studying the Josephson supercurrent through a long half-metallic link in the S/F/S junction by taking into account an interfacial Hamiltonian of a 4×4 matrix, including spin-flip scattering. A new expression for the Josephson critical current is obtained, which is closely related to the AR coefficients, the usual AR ones in the Ss or the novel AR ones in the middle F. A clean physical picture is given of how the singlet Cooper pair with opposite spins is transferred from one S to the other via the correlated electron flow in one spin subband of the middle half-metallic F link. It is shown that the novel AR at the F/S interfaces plays a dominant role in the conversion from the spin-singlet to spin-equal pairing, giving rise to a long superconducting coherent length in the middle F. The S/half-metallic F/S Josephson junction could exhibit a large supercurrent even when the F thickness reaches the order of magnitude of the coherent length in bulk S.

Acknowledgments

This work was supported by the State Key Program for Basic Research of China under grants Nos 2006CB921803 and 2004CB619004. ZMZ was partly supported by the National Natural Science Foundation of China under grant No 10504011.

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