Spin-Triplet Pairing States in Ferromagnet/Ferromagnet/*d*-Wave Superconductor Heterojunctions with Noncollinear Magnetizations

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Tunneling conductance in clean ferromagnet/ ferromagnet/d-wave superconductor (F/F/d-wave S) double tunnel junctions is studied by use of four-component Bogoliubov–de Gennes equations. The novel Andreev reflection appears due to noncollinear magnetizations, in which the incident electron and the Andreev-reflected hole come from the same spin subband, resulting in spin-triplet pairing states near the F/S interface. In the highly polarized Fs case, the conductance within the energy gap exhibits a conversion from a zero-bias dip in the parallel magnetizations to a spilt zero-bias peak in the perpendicular magnetizations.

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The proximity effect in ferromagnet/superconductor (F/S) has been of long-standing research interest and recently attracted much attention [1–4]. The proximity effect has two implications. The first one is the mutual leakage of magnetic and superconducting properties near the F/S interface, such as rapidly damped oscillations of singlet superconductivity on the F side and spin-dependent gapless superconductivity on the S side. The second one is that the competition between two types of mutually exclusive long-range orderings gives rise to a rich variety of new phenomena. An interesting result is that spin-triplet pair states may exist due to noncollinear magnetizations. In recent experiments [5] on S/F structures (with F = Co or Ni), a considerable increase of conductance in the strong F was observed below the superconducting critical temperature T_c. This behavior is difficult to be understood by the usual proximity effect, because the penetration length ξ_F of the singlet pairing is very short for a large exchange splitting of the F. In order to explain experimental phenomena, Bergeret *et al.* [6] suggested that not only the singlet, but also the triplet pairing is induced in the F due to the proximity effect in the presence of a local inhomogeneity of the magnetization near the S/F interface. For the F/S structures, such a long-range spin-triplet pairing suggested in Refs. [3,6–13] seems to have been observed in the half-metallic F [14–16]. Sefrioui *et al.* [14] and Peña *et al.* [15] reported a long-range F/S proximity effect in $La_{0.7}Ca_{0.3}MnO_3$(LCMO)/$YBa_2Cu_3O_7$(YBCO) superlattices where LCMO is a half-metallic F with a fully spin-polarized conduction band and YBCO is a high-T_c S with d-wave symmetry. The superconductivity persists even in the case of the thickness of the F layers essentially exceeding ξ_F. Since singlet Cooper pairs cannot exist in the half-metallic F with only one spin subband, it is reasonable to assume that the superconducting coupling between neighboring S layers is realized via the triplet component. [3] Very recently, Keizer *et al.* [16] reported a long-range Josephson supercurrent through the half-metallic F CrO_2, from which they inferred that it is a spin-triplet supercurrent.

In most previous theoretical works on the spin-triplet pairing in F/S structures, the S layer was assumed to be of s wave. To see the possible triplet superconducting correlations in LCMO/YBCO superlattices, it is highly desirable to study the highly polarized F/d-wave S multilayered structure with noncollinear magnetization configurations. In addition, the spin-triplet pairing states were studied mainly in the diffusive limit. It is also interesting to investigate effects of the triplet pairing component in the clean limit. In this work, we extended the Blonder-Tinkham-Klapwijk approach [17] to calculating the differential conductance of clean F/F/d-wave S double tunnel junctions with an arbitrary angle between magnetizations of the two Fs. It is found that the noncollinear magnetizations can lead to a novel Andreev reflection (AR) and spin-triplet pairing states near the F/S interface. In the novel AR, the incident electron and the Andreev-reflected hole come from the same spin subband, forming a triplet pair with parallel spins, while in the usual AR [18], they come from different spin subbands, leading to a singlet pairing with opposite spins. For the highly polarized Fs, the conductance spectrum exhibits a split zero-bias conductance peak (ZBCP), which is induced by the novel AR rather than usual AR process. In the half-metal/half-metal/d-wave S structure, there is no usual AR process, and conductance contribution of the novel AR is quite different from that of the quasiparticle tunneling. As a result, the triplet superconducting component may be distinguished by experimental measurements of conductance spectra in the present structure.

We consider a F/F/S double tunnel junction with CuO_2 (a-b) planes of the d-wave S normal to the F/S interface. The barrier potential at the interfaces is modeled by $U(r) = U_1\delta(x) + U_2\delta(x - L)$, where the x axis is chosen to be perpendicular to the interface. The magnetization in the middle F layer is assumed along the z axis, while that in the left F layer is assumed to orient along the (0, sinα, cosα) direction. Neglecting the self-consistency of spatial distribution of the pair potential in the S [19], we take the pair potential $\Delta_\pm = \Delta_0 \cos(2\theta_s \mp 2\beta)$, where θ_s is the angle between the F/S interface normal and the momentum of the quasiparticle, β is the angle between the a axis of the crystal and the interface normal, and subscripts $+$ and $-$ correspond to the pair potentials for electronlike and holelike quasiparticles, respectively.

Using the four-spinor wave function $\Psi(\mathbf{r}) = [u_\uparrow(\mathbf{r}), u_\downarrow(\mathbf{r}), v_\uparrow(\mathbf{r}), v_\downarrow(\mathbf{r})]^T$, we write the Bogoliubov–de Gennes (BdG) equation as [20]

$$\begin{pmatrix} \hat{H}_+(\mathbf{r}) & \Delta(\mathbf{r})\hat{\sigma}_1 \\ \Delta^*(\mathbf{r})\hat{\sigma}_1 & -\hat{H}_-(\mathbf{r}) \end{pmatrix} \Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{1}$$

Here E is the quasiparticle energy measured from Fermi energy E_F, and the 2×2 blocks are given by $\hat{H}_\pm(\mathbf{r}) = [-\hbar^2\nabla^2/2m + U(x) - E_F]\hat{\mathbf{1}} - \hat{\sigma}_3 h(x)\cos\alpha(x) \mp \hat{\sigma}_2 h(x) \times \sin\alpha(x)$, with $\hat{\sigma}_i$ $(i = 1, 2, 3)$ the Pauli matrices. For simplicity, we have assumed the left and middle F layers to have the same exchange energy h_0, and all the layers to have the same electron effective mass m.

Consider a beam of spin-up electrons incident on the interface at $x = 0$ from the left F at an angle θ to the interface normal. Define $\breve{e}_1 = (1,0,0,0)^T$, $\breve{e}_2 = (0,1,0,0)^T$, $\breve{e}_3 = (0,0,1,0)^T$, and $\breve{e}_4 = (0,0,0,1)^T$ as basis wave functions. With general solutions of Eq. (1), the wave function in the left F is given by

$$\Psi_{\rm LF} = (e^{iq_{xe+}x} + b_\uparrow e^{-iq_{xe+}x})\breve{e}_1 + b_\downarrow e^{-iq_{xe-}x}\breve{e}_2 + a_\uparrow e^{iq_{xh+}x}\breve{e}_3 + a_\downarrow e^{iq_{xh-}x}\breve{e}_4, \tag{2}$$

for $x \le 0$. Here coefficients $b_\uparrow$, $b_\downarrow$, $a_\uparrow$, and $a_\downarrow$ correspond to the normal reflection, the normal reflection with spin flip, the novel AR, and the usual AR process, respectively. In the middle F and right S regions, we have

$$\Psi_{\rm MF} = (f_1 e^{iq_{xe+}x} + f_2 e^{-iq_{xe+}x})\breve{e}_1 + (f_3 e^{iq_{xe-}x} + f_4 e^{-iq_{xe-}x})\breve{e}_2 + (f_5 e^{iq_{xh+}x} + f_6 e^{-iq_{xh+}x})\breve{e}_3 + (f_7 e^{iq_{xh-}x} + f_8 e^{-iq_{xh-}x})\breve{e}_4, \tag{3}$$

for $0 \le x \le L$, and

$$\Psi_{\rm S} = [c_\uparrow(u_+ e^{i\phi_+}\breve{e}_1 + v_+\breve{e}_4) + c_\downarrow(u_+ e^{i\phi_+}\breve{e}_2 + v_+\breve{e}_3)]e^{ik_{x+}x} + [d_\downarrow(v_- e^{i\phi_-}\breve{e}_1 + u_-\breve{e}_4) + d_\uparrow(v_- e^{i\phi_-}\breve{e}_2 + u_-\breve{e}_3)]e^{-ik_{x-}x}, \tag{4}$$

for $x \ge L$. Here different spin quantization axes have been taken in the left and middle F layers, which will be considered in matching conditions at $x = 0$. In Eq. (4) $u_\pm^2 = 1 - v_\pm^2 = (1 + \Omega_\pm/E)/2$ with $\Omega_\pm = \sqrt{E^2 - |\Delta_\pm|^2}$ and $e^{i\phi_\pm} = \cos(2\theta_s \mp 2\beta)/|\cos(2\theta_s \mp 2\beta)|$. The wave vectors for electrons and holes in the S are given by $k_{x\pm} = \sqrt{(2m/\hbar^2)(E_F \pm \Omega_\pm) - k_\parallel^2}$, and those in the Fs are given by $q_{xe(h)\pm} = \sqrt{(2m/\hbar^2)[E_F \pm h_0 + (-)E] - k_\parallel^2} = \sqrt{q_{e(h)\pm}^2 - k_\parallel^2}$ with $k_\parallel = \sqrt{(2m/\hbar^2)(E_F + h_0 + E)}\sin\theta$.

All the coefficients $a_{\uparrow(\downarrow)}$, $b_{\uparrow(\downarrow)}$, $c_{\uparrow(\downarrow)}$, $d_{\uparrow(\downarrow)}$, and f_i $(i = 1$–$8)$ can be determined by matching conditions at the left and right interfaces. The matching conditions for wave functions (2)–(4) are given by $\breve{T}\Psi_{\rm LF}(x=0) = \Psi_{\rm MF}(x=0)$, $\Psi_{\rm MF}(x=L) = \Psi_S(x=L)$, $\frac{d\Psi_{\rm MF}(x)}{dx}|_{x=0} - \breve{T}\frac{d\Psi_{\rm LF}(x)}{dx}|_{x=0} = 2Z_1 k_F \breve{T}\Psi_{\rm LF}(x=0)$, and $\frac{d\Psi_S(x)}{dx}|_{x=L} - \frac{d\Psi_{\rm MF}(x)}{dx}|_{x=L} = 2Z_2 k_F \Psi_{\rm MF}(x=L)$, where $\breve{T} = \cos(\frac{\alpha}{2})\hat{1}\otimes\hat{1} + i\sin(\frac{\alpha}{2})\hat{\sigma}_3\otimes\hat{\sigma}_1$ is the transformation matrix for changing the spin quantization axis, and $Z_i = U_i/\hbar v_F$ $(i = 1$ or $2)$ is a dimensionless parameter describing the magnitude of interfacial resistance with v_F the Fermi velocity. For spin-down electrons incident on the interface at $x = 0$, coefficients $a_{\uparrow(\downarrow)}$, $b_{\uparrow(\downarrow)}$, $c_{\uparrow(\downarrow)}$, $d_{\uparrow(\downarrow)}$, and f_i $(i = 1$–$8)$ can be similarly obtained by the BdG equation and boundary conditions.

The zero-temperature differential conductance of the present double tunnel junction can be obtained as $\sigma_T(E) = \frac{2e^2}{h}G(E)$ with [21,22]

$$G(E) = \frac{1}{2}\int d\theta\cos\theta[\sigma_\uparrow(\theta) + \sigma_\downarrow(\theta)], \tag{5}$$

$$\sigma_\uparrow(\theta) = \frac{1}{2}(1+P) \times \left(1 + |a_\uparrow|^2 + |a_\downarrow|^2\frac{q_{xh-}}{q_{xe+}} - |b_\uparrow|^2 - |b_\downarrow|^2\frac{q_{xe-}}{q_{xe+}}\right), \tag{6}$$

$$\sigma_\downarrow(\theta) = \frac{1}{2}(1-P) \times \left(1 + |a_\uparrow|^2\frac{q_{xh+}}{q_{xe-}} + |a_\downarrow|^2 - |b_\uparrow|^2\frac{q_{xe+}}{q_{xe-}} - |b_\downarrow|^2\right). \tag{7}$$

Here $\sigma_{\uparrow(\downarrow)}$ is the tunneling conductance for an incident electron in the majority (minority) band with $P = h_0/E_F$ for $h_0 \le E_F$ as the spin polarization in the F layers, and the integral over θ in Eq. (5) is over all the incident angles for which the parallel wave vectors can be conservative. For half-metallic Fs where the electrons are fully polarized, $P = 1$ and so $\sigma_\downarrow$ is vanishing. In this case, since the Fermi wave vector for down spin is zero ($q_{e-} = 0$ and $q_{h-} = 0$), we have $|a_\downarrow|^2 q_{xh-}/q_{xe+} = 0$ and $|b_\downarrow|^2 q_{xe-}/q_{xe+} = 0$ in Eq. (6). As a result, only those terms related to $a_\uparrow$ and $b_\uparrow$ have contribution to the spin-up tunneling conductance.

Before presenting the calculated results for the tunneling conductance, we first make a physical analysis for the formation of the spin-triplet pairing component in the F/F/S structure with noncollinear magnetizations. For the left and middle F layers in the parallel configuration ($\alpha = 0$), from Eqs. (2)–(4) and the boundary conditions we obtain $b_\downarrow = a_\uparrow = 0$ for $x \le 0$, $f_3 = f_4 = f_5 = f_6 = 0$ for $0 \le x \le L$, and $c_\downarrow = d_\uparrow = 0$ for $x \ge L$. Since there is no spin flip in the tunneling process, the four-component

BdG equations are decoupled into two sets of two-component equations: one for $\check{e}_1$ and $\check{e}_4$, the other for $\check{e}_2$ and $\check{e}_3$. In this case, the vanishing $a_\uparrow$ indicates that there is only usual AR, no spin-triplet correlations with equal spin pairs. If the magnetizations of the 2 F layers are noncollinear, e.g., perpendicular to each other ($\alpha = \pi/2$), the situation is quite different. Owing to the spin mixing induced by the noncollinear magnetizations, nonzero coefficients $a_\uparrow$ and f_5 are obtained in our calculation. Nonzero $a_\uparrow$ and f_5 at the F/F and F/S interfaces evidently indicate that there is a novel AR process in which the incident electron and the Andreev-reflected hole come from the same spin subband.

For a noncollinear F/F bilayer, a spin-up incident electron can generate a spin-down reflecting wave component at the interface to ensure the interfacial matching conditions satisfied. Similarly, for a noncollinear F/F/S structure, there exists a novel AR as discussed above. In the F/S structure, the usual AR effect leads to singlet pairing correlations in the F. Its microscopic mechanism is the quantum coherence between the electron near E_F and the corresponding Andreev-reflected hole in the F. [1] In the present noncollinear F/F/S structure, the quantum coherence in the F/F bilayer between the electron and the novel Andreev-reflected hole can result in spin-triplet pairing correlations. Such a novel AR process leads not only to appearance of the triplet pairing correlations in the F/F bilayer, but also to that of the triplet pairing component [4,6,9] in the S regime near the F/S interface. Their appearance must in turn exert an important influence on the tunneling conductance of the F/F/S double tunnel junction.

In what follows we show some numerical results, and first study the case of the parallel configuration ($\alpha = 0$). In Fig. 1 the normalized tunneling conductance σ_T with different polarizations of Fs is shown as a function of quasiparticle energy E measured from E_F. In numerical calculations we take $\Delta_0/E_F = 0.02$, $\beta = \pi/4$ (the x axis along the {110} direction, corresponding to a node in the d-wave order parameter), and $k_F L = 5$. For the N/N/d-wave S structure with N the normal metal of $h_0 = 0$, a ZBCP arises from the usual AR, in which the incident electron and the Andreev hole come from different spin subbands. With increasing polarization P, the peak at $E = 0$ decreases and gradually evolute to a zero-bias conductance dip (ZBCD). This behavior stems from the fact that the usual AR decreases with increasing P. For the half-metallic Fs, the absence of the spin-down electron makes it impossible to form the spin-singlet Cooper pairs. As a result, the usual AR is completely suppressed [22,23] and only quasiparticle tunneling makes contribution to σ_T. In this case, Eqs. (6) and (7) are reduced to $\sigma_\uparrow(\theta) = 1 - |b_\uparrow(\theta)|^2$ and $\sigma_\downarrow(\theta) = 0$. The ZBCD behavior shown in Fig. 1 is a characteristic of the d-wave S with energy gap nodes, while in the s-wave case the conductance is vanishing within the energy gap.

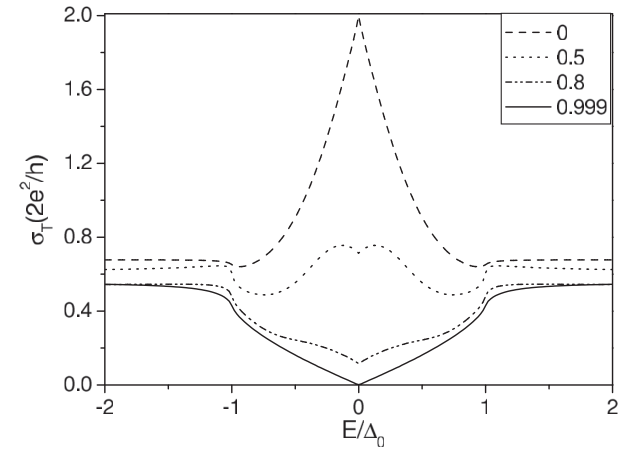

FIG. 1. Differential conductance spectra of F/F/d-wave S ($\beta = \pi/4$) junctions at zero temperature for $\alpha = 0$, $Z_1 = 0.5$, and $Z_2 = 0$ with the various polarizations indicated.

Next, we focus on the noncollinear case of $\alpha = \pi/2$. As shown in Fig. 2, the ZBCP behavior reappears in the large P case, even though there is a small splitting at $E = 0$. For the N/N/d-wave S structure of $h_0 = 0$, the curve is independent of α. With increasing P, the ZBCP splits across and the splitting increases, as shown by the dashed, dotted, dash-dotted, and solid lines in Fig. 2. For the highly polarized Fs, the appearance of ZBCP is not of the usual AR origin, but of the novel AR origin. In the novel AR process, the induction of spin-triplet superconducting correlations leads to breaking the time-reversal symmetry. The ZBCP splitting is just attributed to the broken time-reversal symmetry states.

In order to see the effect of the triplet correlations on the tunnel conductance, we divide Eq. (5) into three parts: the usual AR contribution $G_{\mathrm{AR}} = \frac{1}{2}\int d\theta \cos\theta \sigma_{\mathrm{AR}}(\theta)$, the novel AR contribution $G_{\mathrm{NAR}} = \frac{1}{2}\int d\theta \cos\theta \sigma_{\mathrm{NAR}}(\theta)$, and the quasiparticle contribution G_{Qp}. From Eqs. (6) and (7), it follows that $\sigma_{\mathrm{AR}}(\theta) = (1+P)|a_\downarrow|^2 \frac{q_{xh-}}{q_{xe+}} + (1-P)|a_\uparrow|^2 \frac{q_{xh+}}{q_{xe-}}$ and $\sigma_{\mathrm{NAR}}(\theta) = (1+P)|a_\uparrow|^2 + (1-P)|a_\downarrow|^2$. G_{NAR} are

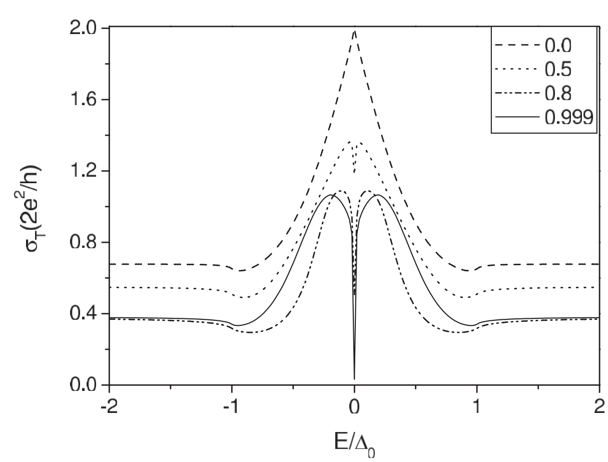

FIG. 2. The same as in Fig. 1 except that $\alpha = \pi/2$.

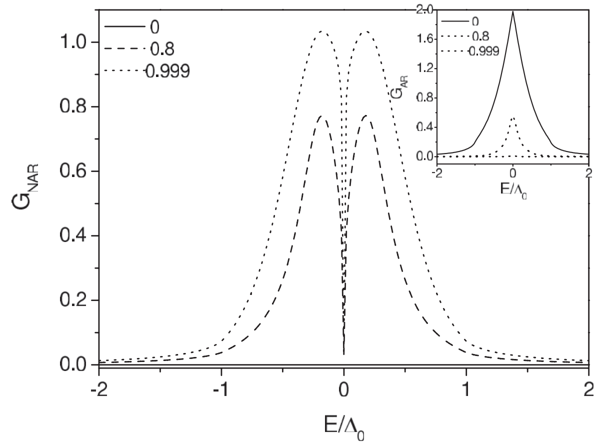

FIG. 3. G_{NAR} (G_{AR} in the inset) as a function of energy for $\alpha = \pi/2$, $Z_1 = 0.5$, and $Z_2 = 0$ with the various polarizations indicated.

closely related to the formation of the spin-rotation-induced triplet component. G_{NAR} (G_{AR}) is shown as a function of energy for $\alpha = \pi/2$ in Fig. 3 (its inset). For the N/N/d-wave S structure of $h_0 = 0$, G_{AR} is maximal and G_{NAR} vanishes. This indicates that there is no spin-triplet correlation in this systems as expected. With increasing P, G_{AR} decreases and G_{NAR} increases, the latter forming a peak with zero-bias dip. Such a splitting of the G_{NAR} peak at $E = 0$ also arises from the broken time-reversal symmetry states. As P is further increased close to 1, the usual AR is completely suppressed and the novel AR arrives at its maximum. Both the tunnel conductance and G_{NAR} have very similar behavior of the zero-bias peak for $P = 0.8$ and especially for $P = 0.999$, as shown in Figs. 2 and 3, indicating that the novel AR is the origin of the zero-bias conductance peak for the highly polarized Fs at $\alpha = \pi/2$. The experimental observation of the latter will provide direct evidence for the formation of spin-triplet pairing states.

We have extended the zero-temperature calculation to the finite temperature case and found that the conductance spectra have no qualitative difference at lower temperatures. [24] For $\alpha = 0$, the conductance spectra still exhibit ZBCD behavior in the large P case, except that the zero-bias conductance has a slight increase with temperature. For $\alpha = \pi/2$, the ZBCP behavior remains qualitatively unchanged, only its splitting becomes small with increasing temperature.

In summary we have applied the extended BTK theory to study the differential conductance of F/F/d-wave S double tunnel junctions. It is found that if magnetizations of the two Fs are noncollinear, it cannot be avoided for the novel AR and spin-triplet pairing states to appear in this structure. For the highly polarized Fs, there is no usual AR process, and the novel AR can be separated from the normal reflection. In this case, the conductance within the d-wave gap along the $\{110\}$ direction exhibits ZBCD behavior in the parallel configuration ($\alpha = 0$) due to the absence of the usual AR. With changing from $\alpha = 0$ to $\alpha = \pi/2$, the conductance exhibits a conversion from the ZBCD to ZBCP characteristic, the former coming from the quasiparticle tunneling into the d-wave S and the latter stemming from the novel AR of forming the triplet pairing states. With the spin-valve technique the angle α is easily controlled by an external magnetic field. It is expected that experimental measurements of conductance spectrum in the present structure will be able to confirm such a spin-triplet pairing effect.

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