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Theory of Proximity Effect in Ferromagnet/Superconductor Heterostructures in the Presence of Spin Dependent Interfacial Phase Shift

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We study the proximity effect and charge transport in ferromagnet (F)/superconductor (S) and S/F/I/F/S junctions (where I is insulator) by taking into account simultaneously exchange field in F and spin-dependent interfacial phase shifts (SDIPS) at the F/S interface. We solve the Usadel equations using extended Kupriyanov–Lukichev boundary conditions which include SDIPS, where spin-independent part of tunneling conductance G_T and spin-dependent one G_ϕ coexist. The resulting local density of states (LDOS) in a ferromagnet depends both on the exchange energy E_{ex} and G_ϕ/G_T. We show that the magnitude of zero-temperature gap and the height of zero-energy LDOS have a non-monotonic dependence on G_ϕ/G_T. We also calculate Josephson current in S/F/I/F/S junctions and show that crossover from 0-state to π.

1. Introduction

Physical phenomena in ferromagnet/superconductor (F/S) hybrids have recently attracted much interest due to peculiar nature of proximity effect in these structures.[1–3] The main manifestation of the proximity effect in F/S contacts is the damped oscillatory behavior of superconducting correlations induced in a ferromagnet. As a result, a number of striking phenomena can be realized in F/S bilayers and S/F/S Josephson junctions. The most spectacular one is the realization of the so-called π-state in S/F/S junctions corresponding to a spontaneous π-shift of the Josephson phase difference in the ground state of a junction.[4–22] Another striking phenomenon is the possibility of generation of odd-frequency spin-triplet s-wave pairs in F/S junctions by spin-mixing due to inhomogeneous magnetization or spin-dependent potential, predicted theoretically in refs. 23–36 and recently observed experimentally in various types of junctions.[37–41]

However, most of previous theoretical studies on F/S bilayers and S/F/S junctions were performed using standard spin-independent boundary conditions, either in the framework of Kupriyanov–Lukichev model,[42] or its extension by Nazarov within the circuit theory.[43,44] Recently general treatment of the boundary conditions at the F/S interface has been proposed,[45–50] which includes the co-called spin-dependent interfacial phase shifts (SDIPS). A number of new phenomena were predicted within this model, in particular the possibility of generation of an odd-frequency state even in the absence of an exchange field, in an N/S junction, provided SDIPS have sufficiently large magnitude.[51,52] Such SDIPS were not included into the standard treatment of the boundary conditions.[42–44] At the same time, it is natural to assume that superconductor/ferromagnet interfaces should be, in general, spin-active. Such scenario was suggested to interpret experimental data on long-ange Josephson coupling in Nb–CrO_2–Nb Josephson junctions[37,39] in terms of generation of odd-frequency long-range triplet order parameter at spin active F/S interfaces where F is half-metallic ferromagnet.[28,33,34] The importance of SDIPS has been also demonstrated theoretically at interfaces between superconductors and ferromagnetic insulators.[52] Further, several theoretical studies showed the importance of SDIPS for fitting experimental data in F/S structures involving Ni-alloys.[47,49]

Despite the general formalism which allows to include SDIPS into the boundary conditions for quasiclassical Green functions is now well developed, quantitative treatment of the boundary conditions including SDIPS in F/S junctions was performed earlier only in a number of examples considered numerically in refs. 47, 49. Therefore, no general picture emerged so far regarding interplay of two effects: exchange field in a ferromagnet and SDIPS. The purpose of this work is to study the interplay of exchange field and SDIPS in F/S junctions in a systematic way. This study allows us to identify several new physical effects arising from simultaneous presence of these two phenomena and to make predictions which can be tested experimentally.

The organization of the present paper is as follows. In §2, we introduce the quasiclassical Green's function formalism which is needed for the calculation of the local density of states and the Josephson current. In §3, the results for the local density of states in F/S junctions are discussed. As an application of the model, in §4 we present the results of calculation of the Josephson current in S/F/I/F/S junctions which consist of two S/F bilayers separated by a tunnel barrier "I". Underdamped π-junctions with tunnel barriers are desired for many applications in superconducting classical and quantum logic circuits and were recently studied experimentally in refs. 17–20 and theoretically in refs. 21, 22. In §4, the existence of temperature-induced 0–π crossover in S/F/I/F/S junctions with the variation of G_ϕ/G_T ratio is demonstrated. In §5, the conclusions and outlook are presented.

2. Model and Formulation

Here, we formulate the model for an F/S bilayer in the general case when exchange field in the F-layer and SDIPS at the F/S interface are simultaneously present. This model will be applied to the study of the density of states in F layer and Josephson effect in S/F/I/F/S junction. We assume that both S- and F-layers are in the diffusive limit. Let us choose x-direction along the normal to the F/S interface, the F-layer has finite thickness d and occupies the region $0 < x < d$

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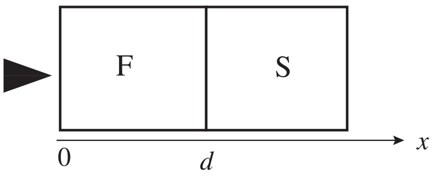

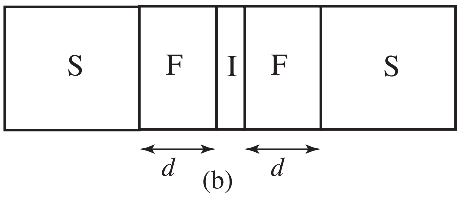

Fig. 1. (a) F/S bilayer consisting from the F-layer occupying the region $0 < x < d$ and bulk S-layer occupying the region $x > d$; (b) S/F/I/F/S Josephson junction discussed in §4 consisting from two S/F bilayers separated by a tunnel barrier "I".

while S-layer is bulk and occupies the region $x > d$ (see Fig. 1). In the Matsubara representation the Usadel equation in the F-layer has the form[1–3,53)]

$$D_{\mathrm{F}} \frac{\partial}{\partial x}\left(\hat{G}_{\mathrm{F}\sigma} \frac{\partial}{\partial x} \hat{G}_{\mathrm{F}\sigma}\right) = [\tau_3(\omega_n - i\sigma E_{\mathrm{ex}}), \hat{G}_{\mathrm{F}\sigma}], \tag{1}$$

where D_{F} is the diffusion coefficient in the ferromagnet, $\omega_n = 2\pi T(n + 1/2)$ are the Matsubara frequencies, E_{ex} is the exchange field in the ferromagnet, $\sigma = \pm 1$ for different spin subbands and τ_3 is the Pauli matrix (we set $\hbar = k_{\mathrm{B}} = 1$).

The Usadel equation in the S layer can be written as[53)]

$$D_{\mathrm{s}} \frac{\partial}{\partial x}\left(\hat{G}_{\mathrm{s}\sigma} \frac{\partial}{\partial x} \hat{G}_{\mathrm{s}\sigma}\right) = [\tau_3\omega_n + \hat{\Delta}(x), \hat{G}_{\mathrm{s}\sigma}], \tag{2}$$

where D_{s} is the diffusion coefficient in the superconductor. In eqs. (1) and (2) we use following matrix notations (we omit "F", "s", and "σ" subscripts)

$$\hat{G}(x,\omega) = \begin{pmatrix} G & F \\ F^* & -G \end{pmatrix}, \quad \hat{\Delta}(x) = \begin{pmatrix} 0 & \Delta(x) \\ \Delta^*(x) & 0 \end{pmatrix}, \tag{3}$$

where G and F are normal and anomalous Green's functions, respectively, and $\Delta(x)$ is the superconducting pair potential determined by the self-consistency equation

$$\Delta(x) \ln \frac{T_{\mathrm{c}}}{T} = \pi T \sum_{\omega>0,\sigma} \left[\frac{\Delta(x)}{\omega} - F_{\mathrm{s}\sigma}\right]. \tag{4}$$

The boundary conditions at the F/S interface have the form[45,46,48–50)]

$$2\xi_{\mathrm{S}}\left(\hat{G}_{\mathrm{S}} \frac{\partial}{\partial x} \hat{G}_{\mathrm{S}}\right) = \gamma[G_{\mathrm{T}}\hat{G}_{\mathrm{F}} + iG_{\phi}\sigma\tau_3, \hat{G}_{\mathrm{S}}], \tag{5a}$$

$$2\xi_{\mathrm{F}}\left(\hat{G}_{\mathrm{F}} \frac{\partial}{\partial x} \hat{G}_{\mathrm{F}}\right) = [G_{\mathrm{T}}\hat{G}_{\mathrm{S}} + iG_{\phi}\sigma\tau_3, \hat{G}_{\mathrm{F}}], \tag{5b}$$

which are the generalization of Kupriyanov–Lukichev boundary conditions,[42)] including additional G_{ϕ} term describing SDIPS. Here $G_{\mathrm{T}} = \rho_{\mathrm{F}}\xi_{\mathrm{F}}/R_{\mathrm{B}}$ describes the *normalized* tunneling conductance of the interface (according to Kupriyanov–Lukichev), where R_{B} is the specific boundary resistance. The parameter $\gamma = \rho_{\mathrm{S}}\xi_{\mathrm{S}}/\rho_{\mathrm{F}}\xi_{\mathrm{F}}$ describes the inverse proximity effect, i.e., the influence of the F-layer on suppression of superconductivity in the S-layer,[42)] where $\rho_{\mathrm{F,S}}$ and $\xi_{\mathrm{F,S}} = \sqrt{D_{\mathrm{F,S}}/2\pi T_{\mathrm{c}}}$ are, respectively, the normal state resistivities and coherence lengths in a ferromagnet and a superconductor and T_{c} is the critical temperature of a superconductor. Here we have assumed that $G_{\phi}^{\mathrm{S}} = G_{\phi}^{\mathrm{F}} \equiv G_{\phi}$ in both boundary conditions, while these parameters can in general be different. This assumption does not influence our main results, since we concentrate on the proximity effect in the F-layer which is controlled by G_{ϕ}^{F} while the parameter G_{ϕ}^{S} only influences on the inverse proximity effect, which can be neglected if $\gamma = \rho_{\mathrm{S}}\xi_{\mathrm{S}}/\rho_{\mathrm{F}}\xi_{\mathrm{F}}$ is small. In the following, we will use the θ parametrization $G = \cos\theta$ and $F = \sin\theta$. In normalized units, the equation in the F-layer can be rewritten as

$$\theta_{\mathrm{F}}'' - [|\omega_n| - i\sigma E_{\mathrm{ex}} \cdot \mathrm{sgn}(\omega_n)] \sin\theta_{\mathrm{F}} = 0. \tag{6}$$

In the S-layer

$$\theta_{\mathrm{S}}'' - |\omega_n| \sin\theta_{\mathrm{S}} + \Delta\cos\theta_{\mathrm{S}} = 0. \tag{7}$$

Here ω_n, E_{ex} and pair potential Δ are normalized to πT_{c}, length scale is normalized to ξ_{F} in the F layer and to $\xi_{\mathrm{S}} = \sqrt{D_{\mathrm{S}}/2\pi T_{\mathrm{c}}}$ in the S layer. The boundary conditions at $x = d$ have the form:

$$\theta_{\mathrm{F}}' = -G_{\mathrm{T}} \sin(\theta_{\mathrm{F}} - \theta_{\mathrm{S}}) - iG_{\phi}\sigma \cdot \mathrm{sgn}(\omega_n) \sin\theta_{\mathrm{F}}, \tag{8}$$

$$\theta_{\mathrm{S}}' = -\gamma G_{\mathrm{T}} \sin(\theta_{\mathrm{F}} - \theta_{\mathrm{S}}) - i\gamma G_{\phi}\sigma \cdot \mathrm{sgn}(\omega_n) \sin\theta_{\mathrm{S}}. \tag{9}$$

In the following, we will discuss the situation when SDIPS and exchange field are simultaneously present. We will first consider the proximity effect in an F/S bilayer and discuss the anomalous features of the local density of states (LDOS) in the F-layer. Based on these results, we will discuss the Josephson effect in S/F/I/F/S junctions, where two F/S bilayers are weakly coupled across the spin-independent tunnel barrier (I) and will demonstrate how the behavior of LDOS manifests itself in the Josephson current. Particularly interesting is the possibility to induce 0–π transition by increasing the magnitude of SDIPS in such junctions.

Simple analytical result can be obtained in the limit of thin F-layer $l \ll d \ll \xi_{\mathrm{F}}$, where l is the electronic mean free path, and under assumption of rigid boundary conditions, $\gamma = 0$, when the pair potential Δ in S near the F/S interface equals to its bulk value Δ_0. In this case the solution of the Usadel equation in the F-layer is greatly simplified while the diffusion approximation is still valid. The solution of the Usadel equation in F-layer has the form

$$\theta_{\mathrm{F}} = A + Bx + Cx^2. \tag{10}$$

Substituting it into the Usadel equation, we obtain

$$C = \frac{1}{2}[|\omega_n| - i\sigma E_{\mathrm{ex}} \cdot \mathrm{sgn}(\omega_n)] \sin A.$$

The boundary conditions are:

$$\theta_{\mathrm{F}}'(x = d) = -G_{\mathrm{T}} \sin(\theta_{\mathrm{F}} - \theta_{\mathrm{S}}) - iG_{\phi}\sigma \cdot \mathrm{sgn}(\omega_n) \sin\theta_{\mathrm{F}}, \tag{11}$$

$$\theta_{\mathrm{F}}'(x = 0) = 0. \tag{12}$$

Below we present the results for the case $\omega_n > 0$ only, while the case $\omega_n < 0$ can be added using general symmetry relation $F(-\omega_n, E_{ex}, \gamma_\phi) = F(\omega_n, -E_{ex}, -\gamma_\phi)$ which follows from the Usadel equation and the boundary conditions. From $\theta'_F(x=0) = 0$ we get $B = 0$, then from the first boundary condition we obtain:

$$(\omega_n - i\sigma E_{ex})d \sin A = -G_T \sin(A - \theta_S) - iG_\phi \sigma \sin A \tag{13}$$

$$\tan\theta_F = \tan A = \frac{\sin\theta_S}{[\omega_n d + i\sigma(-E_{ex}d + G_\phi)]/G_T + \cos\theta_S}, \tag{14}$$

where $\cos\theta_S = \omega_n/\sqrt{\omega_n^2 + \Delta_0^2}$ and $\sin\theta_S = \Delta_0/\sqrt{\omega_n^2 + \Delta_0^2}$. This expression is the generalization of the result of ref. 54 obtained for the case when only the exchange field is present while $G_\phi = 0$, and the generalization of the result of ref. 51 obtained for $E_{ex} = 0$. One can see that the exchange field and the G_ϕ term enter the result as a linear combination $E_{ex}d - G_\phi$. That means that in a thin ferromagnetic layer the effective exchange field is given by $E_{ex} - G_\phi/d$, i.e., in addition to an "intrinsic" term E_{ex} it includes the contribution G_ϕ/d from the spin-active interface. It is important to note that, according to ref. 52, the sign of G_ϕ term can be not determined in the present phenomenological approach (the absolute value of G_ϕ/G_T was considered as a parameter in ref. 52). To determine the sign of G_ϕ, microscopic calculation of the scattering matrix is required. Correspondingly, in our model, both combinations $E_{ex} - G_\phi/d$ and $E_{ex} + G_\phi/d$ are possible, i.e., E_{ex} and G_ϕ/d can either add or compensate each other. As will be illustrated below by calculating LDOS and Josephson current, the interplay of E_{ex} and G_ϕ/d may result in nontrivial behavior of these physical quantities as a function of G_ϕ/G_T.

3. LDOS in the Diffusive Ferromagnet Attached to Superconductor

In this section, we study proximity effect in F/S junctions. We will focus on the LDOS at the edge of ferromagnet ($x = 0$) in an F/S junction. At the same time, we also discuss the behavior of the pair amplitude as a function of energy. Since we consider the case of diffusive ferromagnet, only purely s-wave symmetry of the order parameter is possible. In the presence of E_{ex} and G_ϕ/G_T, odd-frequency spin-triplet component can mix with even-frequency spin-singlet component. Before discussing the case with simultaneous existence of both E_{ex} and G_ϕ/G_T, we start with the discussion of each effect separately.

The normalized LDOS can be obtained by making an analytical continuation $\omega_n \to -i\varepsilon$ in a solution for θ_F

$$\frac{N(E)}{N_0} = \sum_\sigma \mathrm{Re}[\cos\theta_F(\varepsilon, \sigma)], \tag{15}$$

where ε is the quasiparticle energy normalized to πT_c and N_0 is the density of states in the normal state. Below we will refer to the approximation of small F-layer thickness in order to clarify key results of this work. For arbitrary F-layer thickness and arbitrary values of the interface parameters the LDOS is calculated by selfconsistent numerical solution of the Usadel equations with the generalized boundary conditions introduced above, using the method described in ref. 54.

Superconducting pair amplitude $f = \sin\theta$ can be decomposed into even-frequency part

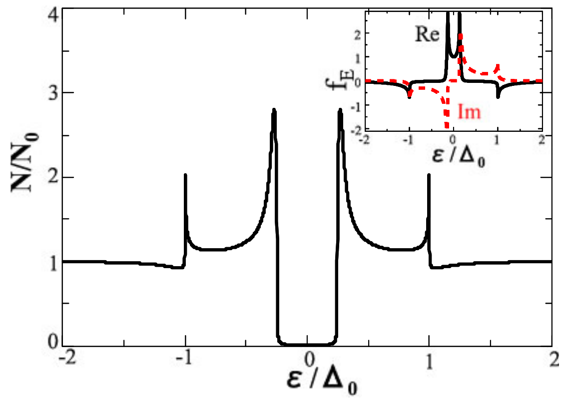

Fig. 2. (Color online) LDOS at the edge $x = 0$ of F/S junction with $E_{ex} = 0$ for $d = 0.5$ and $G_\phi = 0$. Inset: Even-frequency pair amplitude f_E at $x = 0$. Real and imaginary part of f_E is plotted as a solid and dashed line.

$$f_E = \frac{\sin\theta(E) + \sin\theta(-E)}{2}$$

and odd-frequency part

$$f_O = \frac{\sin\theta(E) - \sin\theta(-E)}{2}.$$

In the following calculations we shall fix the dimensionless tunneling conductance $G_T = 0.1$.

First, we shall discuss the case with $E_{ex} = 0$ and $G_\phi = 0$, where F/S junction can be regarded as a normal metal/superconductor junction without SDIPS. As shown in Fig. 2, the resulting LDOS has a gap structure near zero energy. It is known that in an N/S contact the magnitude of the energy gap is the order of Thouless energy[55–58] if the latter is much smaller than the superconducting gap Δ_0. In the opposite limit of large Thouless energy or, equivalently, in the limit of small thickness $d \ll \xi_N$, the energy gap in N is determined by interface transparency.[59,60] In the low-transparency regime, the gap Δ_g is given by simple analytical expression $d \ll \xi_N$, $\Delta_g = G_T \pi T_c$, in agreement with the result shown in Fig. 2. The corresponding pair amplitude is also plotted in the inset. It is known that the symmetry of pair amplitude is purely even-frequency spin-singlet s-wave.[2] In agreement with previous results,[61] the real part of the pair amplitude is an even function of ε while imaginary part is an odd function of ε.

Next, we discuss the effect of G_ϕ. In Fig. 3, we plot corresponding LDOS for $E_{ex} = 0$ for different values of G_ϕ/G_T. For $G_\phi/G_T = 0.5$, LDOS still has a energy gap structure around zero energy similar to the case with $G_\phi = 0$. For $G_\phi/G_T = 1$, LDOS has a sharp zero energy peak (ZEP), in agreement with the result of ref. 51. The sharp ZEP splits into two for $G_\phi/G_T > 1$ as shown in dotted

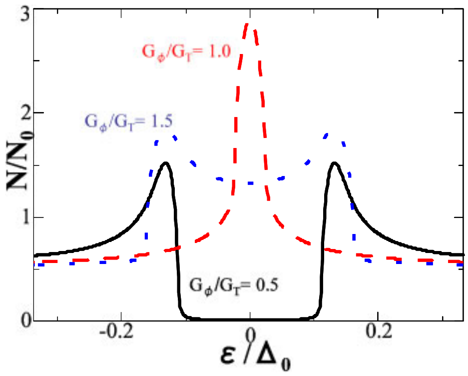

Fig. 3. (Color online) LDOS at the edge $x = 0$ of F/S junction with $E_{\rm ex} = 0$, $d = 0.5$, and $G_\phi/G_{\rm T} = 0.5$ (solid line), $G_\phi/G_{\rm T} = 1$ (dashed line), and $G_\phi/G_{\rm T} = 1.5$ (dotted line).

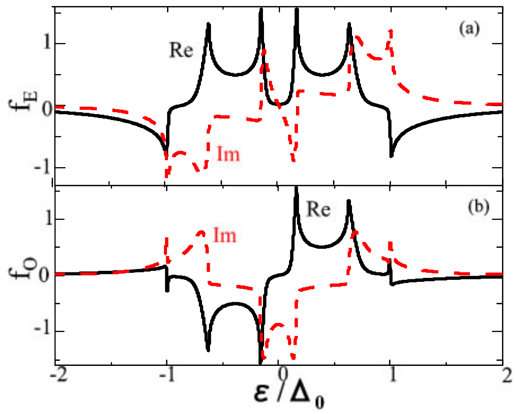

Fig. 4. (Color online) Pair amplitude at the edge $x = 0$ of F/S junction with $G_\phi/G_{\rm T} = 1.5$, $E_{\rm ex} = 0$ and $d = 0.5$. (a) Real (solid line) and imaginary (dashed line) part of even-frequency spin-singlet pair amplitude $f_{\rm E}$. (b) Real (solid line) and imaginary (dashed line) part of odd-frequency spin-triplet pair amplitude $f_{\rm O}$.

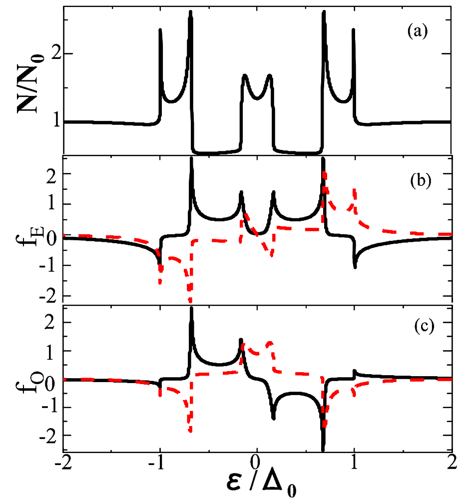

Fig. 5. (Color online) LDOS and pair amplitude at the edge $x = 0$ of F/S junction is plotted as a function of ε. $G_\phi/G_{\rm T} = 0$, with $E_{\rm ex} = 0.3$ and $d = 0.5$. (a) LDOS, (b) Real (solid line) and imaginary (dashed line) part of even-frequency spin-singlet pair amplitude $f_{\rm E}$, (c) Real (solid line) and imaginary (dashed line) part of odd-frequency spin-triplet pair amplitude $f_{\rm O}$.

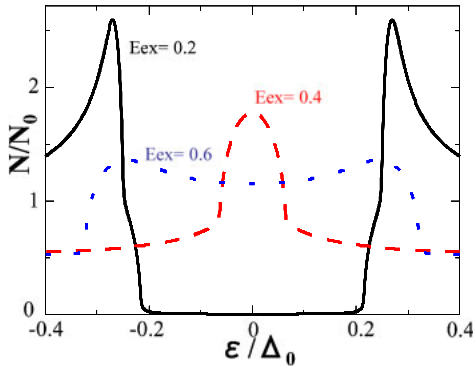

Fig. 6. (Color online) LDOS at the Ferromagnet edge $x = 0$ is plotted for $E_{\rm ex} = 0.2$ (solid line), $E_{\rm ex} = 0.4$ (dashed line), and $E_{\rm ex} = 0.6$ (dotted line). We have set $d = 0.5$ and $G_\phi/G_{\rm T} = 1$.

line with $G_\phi/G_{\rm T} = 1.5$. In order to understand the relevance of G_ϕ and the pair amplitude, we plot pair amplitude in Fig. 4. Note that not only even-frequency spin-singlet pair amplitude $f_{\rm E}$ but also odd-frequency spin-triplet pair amplitude $f_{\rm O}$ can be generated for nonzero G_ϕ.

As seen from Fig. 4, the real part of $f_{\rm O}$ is an odd-function of ε while its imaginary part is an even-function of ε by contrast to $f_{\rm E}$. For $\varepsilon = 0$, only the imaginary part of $f_{\rm O}$ is nonzero. It is consistent with the result obtained previously in ref. 51. If the relation $G_\phi > G_{\rm T}$ is satisfied, then the resulting $f_{\rm E}$ is always zero at $\varepsilon = 0$.

In order to compare the effect of G_ϕ with that of the exchange field $E_{\rm ex}$, in Fig. 5 we present the results for the case when only $E_{\rm ex}$ is nonzero. The resulting LDOS has a nonzero value at $\varepsilon = 0$.[62–68] At this energy, both real and imaginary parts of $f_{\rm E}$ vanish and only imaginary component of $f_{\rm O}$ is nonzero.[69,70] This feature is similar to that shown in Fig. 4. Therefore, decomposition of the pair amplitude into even- and odd-frequency components helps to understand the correspondence between zero-energy peak in LDOS and existence of non-zero value of imaginary part of $f_{\rm O}$ at low energies, both in the presence of exchange field and SDIPS.

In Fig. 6, LDOS at the edge of the F-layer (at $x = 0$) is plotted for various $E_{\rm ex}$ in the presence of $G_\phi/G_{\rm T}$ for fixed value of $G_{\rm T} = 0.1$. One can see that zero energy peak shown in Fig. 3 splits into two peaks, then it recovers at $E_{\rm ex} = 0.4$ and further splits at $E_{\rm ex} = 0.6$.

In order to understand the above non-trivial dependence of LDOS N for $E_{\rm ex}$, it is instructive to analyze the solutions for LDOS in the case of thin F-layer. The Usadel equation in the F-layer and the boundary conditions in the real energy representation are given by eq. (6) and eqs. (11) and (12), respectively, by making analytical continuation $\omega_n \to -i\varepsilon$ and with $\cos\theta_{\rm S} = \varepsilon/\sqrt{\varepsilon^2 - \Delta_0^2}$ and $\sin\theta_{\rm S} = \Delta_0/\sqrt{\Delta_0^2 - \varepsilon^2}$. Using the expansion (10) for $\theta_{\rm F}$, we obtain

$$\cos^2\theta_{\rm F} = -\frac{\tilde{\varepsilon}_\sigma^2}{\Delta_0^2 - \tilde{\varepsilon}_\sigma^2}, \qquad (16)$$

with

$$\tilde{\varepsilon}_\sigma = \sqrt{\Delta_0^2 - \varepsilon^2}\left[\frac{(\varepsilon + \sigma E_{\rm ex})d}{G_{\rm T}} - \frac{\sigma G_\phi}{G_{\rm T}}\right] + \varepsilon.$$

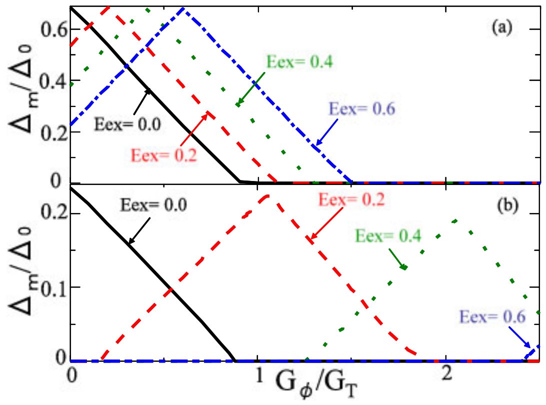

Fig. 7. (Color online) The magnitude of the energy gap Δ_m of LDOS at $x = 0$ is plotted as a function of G_ϕ/G_T for $E_{ex} = 0$ (solid line), $E_{ex} = 0.2$ (dashed line), $E_{ex} = 0.4$ (dotted line), and $E_{ex} = 0.6$ (dot-dashed line). We have set $d =$ (a) 0.1 and (b) 0.5.

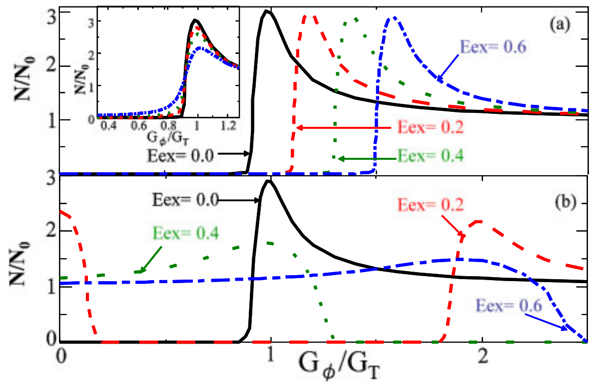

Fig. 8. (Color online) The magnitude of the LDOS at $x = 0$ with zero energy $\varepsilon = 0$ is plotted as a function of G_ϕ/G_T for $E_{ex} = 0$ (solid line), $E_{ex} = 0.2$ (dashed line), $E_{ex} = 0.4$ (dotted line), and $E_{ex} = 0.6$ (dot-dashed line). We have set (a) $d = 0.1$ and (b) $d = 0.5$. In the inset, LDOS is plotted for $E_{ex} = 0$ as a function of G_ϕ/G_T by changing $d = 0.1$ (solid line), $d = 1$ (dashed line), $d = 2$ (dotted line), and $d = 5$ (dot-dashed line).

At $E = 0$, the resulting spin averaged normalized LDOS is given by

$$\frac{N}{N_0} = \mathrm{Re}\left[\frac{|E_{ex}d/G_T - G_\phi/G_T|}{\sqrt{(E_{ex}d/G_T - G_\phi/G_T)^2 - 1}}\right].$$

As seen from this equation, the condition of the formation of ZEP of LDOS is given by

$$\left|\frac{E_{ex}d}{G_T} - \frac{G_\phi}{G_T}\right| = 1.$$

In the calculations shown in Fig. 6, the ratio $d/G_T = 5$. Since the magnitude of G_ϕ/G_T is chosen to be 1, the resulting condition can be given by $|5E_{ex} - 1| = 1$, which is satisfied by $E_{ex} = 0$ and 0.4.

As is shown by solid line on Fig. 6, the LDOS is zero in a certain energy range $-\Delta_m < \varepsilon < \Delta_m$ where Δ_m is an effective energy gap. In order to understand the conditions for the formation of an energy gap in LDOS more clearly, let us concentrate on the magnitude Δ_m of the energy gap of LDOS shown in Fig. 7. For $E_{ex} = 0$, Δ_m is reduced with the increase of G_ϕ/G_T. On the other hand, for nonzero E_{ex}, the resulting Δ_m once increases and then decreases again. The condition for a maximum Δ_m corresponds to

$$\frac{E_{ex}d}{G_T} = \frac{G_\phi}{G_T},$$

which can be reduced to

$$E_{ex} = \frac{G_\phi}{G_T}$$

for the case (a) when $d/G_T = 1$ and

$$E_{ex} = 0.2\frac{G_\phi}{G_T}$$

for the case (b) when $d/G_T = 5$.

The corresponding value of G_ϕ/G_T becomes 0, 0.2, 0.4, and 0.6 for $E_{ex} = 0$, 0.2, 0.4, and 0.6, respectively in case (a). On the other hand, the corresponding value of G_ϕ/G_T becomes 0, 1, 2, and 3 for $E_{ex} = 0$, 0.2, 0.4, and 0.6, respectively in case (b). These features are consistent with Fig. 7.

In Fig. 8, the zero energy LDOS is plotted at the edge of ferromagnet $x = 0$. As seen from Fig. 8(a), the position of the G_ϕ/G_T, where LDOS has a peak, is changing as a function of E_{ex}. As seen from above analytic calculation, the condition is satisfied for

$$\left|\frac{E_{ex}d}{G_T} - \frac{G_\phi}{G_T}\right| = 1. \tag{17}$$

For $d = 0.1$, the relation $d/G_T = 1$ is satisfied. Since G_ϕ/G_T is a positive quantity, the resulting G_ϕ/G_T can be chosen as $G_\phi/G_T = 1$, 1.2, 1.4, and 1.6, for $E_{ex} = 0$, 0.2, 0.4, and 0.6, respectively. The peak positions are consistent with the results shown in Fig. 8(a). On the other hand, for $d = 0.5$, $d/G_T = 5$ is satisfied. Since G_ϕ/G_T is a positive quantity, the resulting G_ϕ/G_T can be chosen as $G_\phi/G_T = 1$, $G_\phi/G_T = 0$ or 2, $G_\phi/G_T = 1$ or 3, and $G_\phi/G_T = 2$ or 4, for $E_{ex} = 0$, 0.2, 0.4, and 0.6, respectively. These positions are roughly consistent with Fig. 8(b). However, as compared to Fig. 8(a), the peak of LDOS is rather broad. In the inset, LDOS is plotted as a function of G_ϕ/G_T for $E_{ex} = 0$. Contrary to the case of nonzero E_{ex}, the position of peak is almost insensitive with the change of d. This result is important for experimental verification of our predictions: though our analytical results [as well as Fig. 8(a)] describe LDOS in the limit of very thin F-layer $l \ll d \ll \xi_F$ which is difficult to realize experimentally, the inset demonstrates the robustness of the LDOS peak for large F-layer thicknesses up to $5\xi_F$.

4. Josephson Current in S/F/I/F/S Junctions

In this section, we will focus on the Josephson current in S/F/I/F/S junctions. We will concentrate on the regime when both ferromagnets are thin and the tunnel barrier "I" (non-magnetically-active) is placed between two S/F bilayers. In this regime the Josephson current is given by the expression[54]

$$I = \frac{\pi T}{eR}\sum_{\omega_n}\mathrm{Im}[F_1^*(-E_{ex1}, -G_{\phi_1})F_2(E_{ex2}, G_{\phi_2})], \tag{18}$$

where R is the junction resistance and Green functions $F_{1,2}$ characterize left and right ferromagnet, respectively. This expression is valid under condition of low transparency of the tunnel barrier "I" and provides lowest (sinusoidal) harmonic of the current-phase relation.

For functions $F_{1,2}$ we have

$$F_{1,2} = \frac{\sin(\theta_S) \cdot e^{\pm i\varphi/2}}{\sqrt{1 + 2\alpha_{1,2}\cos\theta_S + \alpha_{1,2}^2}} \tag{19}$$

$$\alpha_{1,2} = \left[\omega_n + i\sigma\left(-E_{ex1,2} + \frac{G_{\phi_{1,2}}}{d_{1,2}}\right)\right]\frac{d_{1,2}}{G_{T_{1,2}}}, \tag{20}$$

where in general different values $E_{ex1,2}$, $d_{1,2}$, and $G_{\phi_{1,2}}$ are allowed in the S/F bilayers. Here ω_n and $E_{ex1,2}$ are normalized to πT_c and $d_{1,2}$ are normalized to $\xi_{F1,2}$. The above expression is a generalization of eq. (12) from ref. 54, with E_{ex} replaced by $E_{ex} + G_\phi/d$. Substituting the solutions for $F_{1,2}$ into the expression for current and summing over spin directions ($\sigma = \pm 1$), we arrive

$$I = \frac{2\pi T}{eR}\sum_{\omega_n>0}\mathrm{Re}\left[\frac{\sin^2\theta_S}{\sqrt{1 + 2\alpha_1\cos\theta_S + \alpha_1^2}\sqrt{1 + 2\alpha_2\cos\theta_S + \alpha_2^2}}\right]\sin\varphi,$$

$$\sin\theta_S = \frac{\Delta_0}{\sqrt{\omega_n^2 + \Delta_0^2}}, \quad \cos\theta_S = \frac{\omega_n}{\sqrt{\omega_n^2 + \Delta_0^2}}.$$

Hereafter, we consider the case $G_{\phi_1} = G_{\phi_2} = G_\phi$, $d_1 = d_2 = d$, and $G_{T_1} = G_{T_2} = G_T$. In the considered case the current-phase relation is sinusoidal, and below we shall discuss the Josephson critical current I_c as a function of temperature and interface parameters G_ϕ and G_T. First, we focus on the case with $E_{ex1} = E_{ex2} = E_{ex}$. In Fig. 9 the results are plotted for the case of $E_{ex} = 0$ and various G_ϕ/G_T ratios. For $G_\phi/G_T = 0$, 0.5, and 1.0, the resulting critical current is positive. That means, the junction is in the so-called 0-state corresponding to zero phase difference in the ground state. However, with increasing $G_\phi/G_T \geq 1.0$, I_c becomes negative, i.e., the junction is in the π-state when the phase difference π is realized in the ground state. Note that the 0–π transition is triggered by changing only the parameter G_ϕ/G_T.

Similar plots are shown for $E_{ex} = 0.5$ in Fig. 10, where the crossover from 0- to π-state is demonstrated with the increase of G_ϕ/G_T. As seen from the case with $G_\phi/G_T = 1.6$, I_c has a non-monotonic temperature dependence with a sharp sign change. In the considered case, since the length of both ferromagnetic films is small compared to the coherence length, it is possible to discuss the results on the basis of the analytic solution obtained above. In symmetric junction, π-state is realized when $|(E_{ex}d - G_\phi)/G_T| > 1$. For the present parameter choice, this condition is satisfied since G_ϕ/G_T has a positive nonzero value. In accordance to this statement, as seen from Fig. 10, sharp transition from 0-state (positive I_c) to π-state (negative I_c) is realized at low temperature with variation of G_ϕ/G_T.

In order to understand the origin of 0–π transition in a more detail, we concentrate on the phase of the pair amplitude at the left superconductor in detail. Note that in the presence of E_{ex} and G_ϕ/G_T, the quantity α_1^* becomes a complex number. Here we define argument of F_1 as

$$\phi = \arctan\left(\frac{\mathrm{Im}\,F_1}{\mathrm{Re}\,F_1}\right). \tag{21}$$

It is important to note that the phase shift ϕ is due to generation of odd-frequency pairing correlations, which are described by odd-frequency component of the Green function F_1. Formally, it is evident form the fact that odd-frequency component at low energies is purely imaginary quantity, therefore the term Imag F_1 in the above expression

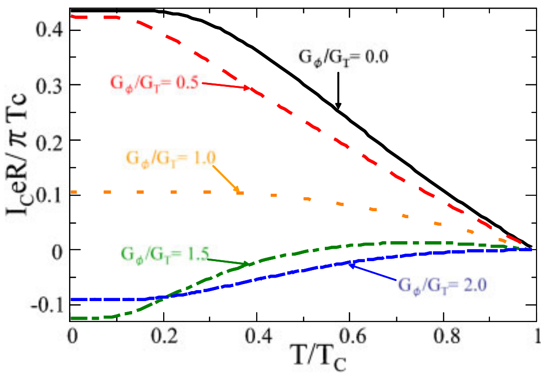

Fig. 9. (Color online) Temperature dependence of the Josephson critical current of S/F/I/F/S junction for various G_ϕ/G_T. Here $E_{ex} = 0$ both in F and F′, $G_\phi/G_T = 0$ (solid line), $G_\phi/G_T = 0.1$ (dashed line), $G_\phi/G_T = 0.5$ (dotted line), $G_\phi/G_T = 1.0$ (dot-dashed line), and $G_\phi/G_T = 1.5$ (dashed line).

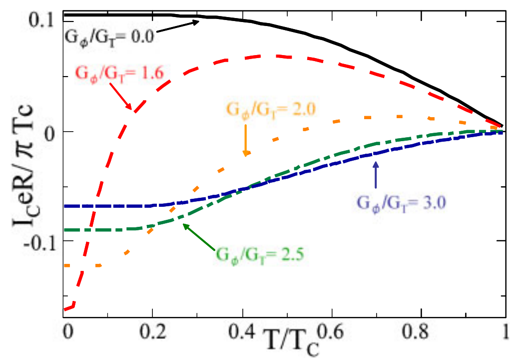

Fig. 10. (Color online) Temperature dependence of the Josephson critical current of S/F/I/F′/S junction for various G_ϕ/G_T. Here, we choose $E_{ex}d/G_T = 0.5$ both in F and F′, $G_\phi/G_T = 0$ (solid line), $G_\phi/G_T = 1.6$ (dashed line), $G_\phi/G_T = 2.0$ (dotted line), $G_\phi/G_T = 2.5$ (dot-dashed line), and $G_\phi/G_T = 3.0$ (dashed line).

is responsible for the generation of of the phase shift at the S/F interface. Here, we focus on how the phase difference ϕ changes with variation of exchange energy E_{ex}. Let us fix the magnitude of $G_\phi/G_T = 0.5$. As seen from Fig. 11, ϕ changes drastically from 0 to $\pi/2$ at $E_{ex}d/G_T = 1$–1.5, in

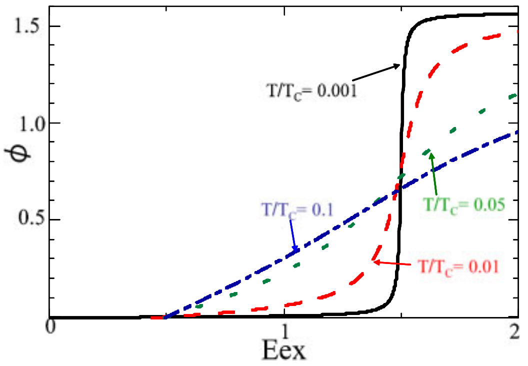

Fig. 11. (Color online) The magnitude of phase shift ϕ of pair amplitude is plotted as a function of E_{ex} for $G_\phi/G_T = 0.5$ at various temperatures: $T/T_C = 0.001$ (solid line), $T/T_C = 0.01$ (dashed line), $T/T_C = 0.05$ (dotted line), and $T/T_C = 0.1$ (dot-dashed line).

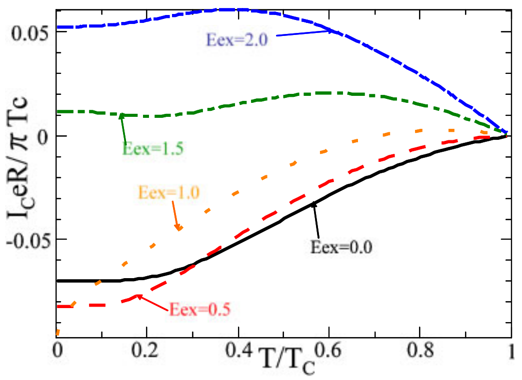

Fig. 12. (Color online) Temperature dependence of the Josephson current of S/F/I/F$'$/S junction for various E_{ex} in the first F-film and fixed exchange energy $E_{ex2} = -1$ in the second F-film and $G_\phi/G_T = 2$: $E_{ex} = 0$ (solid line), $E_{ex} = 0.5$ (dashed line), $E_{ex} = 1.0$ (dotted line), $E_{ex} = 1.5$ (dot-dashed line), and $E_{ex} = 2.0$ (dashed line).

accordance with the general criteria $|(E_{ex}d - G_\phi)/G_T| = 1$. As a result, $\pi/2$ phase shifts at both S/F interfaces add to each other and the crossover from 0 to π state occurs. Such mechanism of 0–π crossover was discussed in ref. 54 in the absence of SDIPS. In the present case, the crossover can be triggered solely by SDIPS, even in the absence of exchange field. In accordance with the above discussion, this crossover to π state is related to the generation of odd-frequency pairing component Im F_1 as a result of simultaneous action of exchange field and SDIPS. As seen from Fig. 11, the crossover becomes more gradual at higher temperatures. This fact has natural explanation in terms of odd-frequency pairing: according to eq. (18), at high temperatures the low-energy odd-frequency components of Green functions $F_{1,2}$ do not contribute to the Josephson current.

It is also interesting to consider the case when the directions of the exchange fields on the left side (F_1) and the right side (F_2) are opposite. We change $E_{ex1} = E_{ex}$ for fixed exchange energy $E_{ex2} = -1$. In Fig. 12, we show the temperature dependence of critical Josephson current in this case. It is known that 0–π transition does not appear in the antiparallel configuration in the absence of G_ϕ term.[54,71–73] However, in the presence of SDIPS, the behavior of junction becomes more complex. For $G_\phi/G_T = 2$ with $E_{ex} = 0$, the junction goes into π-state. On the other hand, with the increase of the magnitude of E_{ex}, it changes from π-state to 0-state. Based on these calculations, one can conclude that the role of G_ϕ is important to understand the actual temperature dependence of the Josephson current.

5. Conclusions

We have studied proximity effect in F/S and S/F/I/F/S junctions taking into account exchange field in F and spin dependent interfacial phase shift (SDIPS) at the same time. We have solved the Usadel equations using extended Kupriyanov–Lukichev's boundary conditions which include the term with spin-independent tunneling conductance G_T and additional term G_ϕ depending on spin. We have shown that in particularly interesting case of a thin ferromagnetic layer the effects of the exchange field and the SDIPS are additive, namely, in a thin ferromagnetic film the effective exchange field includes the contribution from the spin-active interface, in addition to an "intrinsic" term E_{ex}. The resulting local density of states in a ferromagnet depends both on the exchange energy E_{ex} in ferromagnet and G_ϕ/G_T. The energy gap in the quasiparticle spectrum and the magnitude of zero-energy LDOS exhibit a non-monotonic behavior as a function of G_ϕ/G_T. We have also calculated Josephson current in S/F/I/F/S junctions and have demonstrated the crossover from 0- to π-state with variation of the SDIPS strength G_ϕ/G_T.

In the present paper, we have considered the case of spin-singlet s-wave superconductor. It is interesting to extend these results to the case of spin-singlet d-wave and spin-triplet p-wave pairing state, where midgap Andreev bound state strongly influences the electronic transport across the interface.[74–80] Another interesting open problem is to take into account G_ϕ term in the boundary conditions in the case of unconventional pairing.[81–86] It is known that anomalous proximity effect originating from odd-frequency pairing is prominent in spin-triplet superconductor junctions. Important problem is to reveal the influence of G_ϕ on the spin-triplet superconductor proximity systems where odd-frequnecy pairing plays important roles.[87–91] Recently, the study of S/F junctions of topological insulators became a hot topic in condensed matter physics. Since anomalous helical metallic state is a background of this system, study of SDIPS in such a system is an important subject.[92–94]

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