Coexistence of ferromagnetism and superconductivity in normal mental/superconductor/ferromagnet structures*

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We extend the Blonder, Tinkham and Klapwijk theory to the study of the inverse proximity effects in the normal mental/superconductor/ferromagnet structures. In the superconducting film, there are the gapless superconductivity and the spin-dependent density of states both within and without the energy gap. It indicates an appearance of the inverse-proximity-effect-induced ferromagnetism and a coexistence of ferromagnetism and superconductivity near the interface. The influence of exchange energy in the ferromagnet and barrier strength at the superconductor/ferromagnet interface on the inverse proximity effects is discussed.

Keywords: coexistence of ferromagnetism and superconductivity, inverse proximity effects, normal mental/superconductor/ferromagnet structures

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1. Introduction

As a ferromagnet (F) is deposited on top of a superconductor (S), S and F provide leakage sources of the Cooper pairs and spin-polarized electrons, respectively. On the one hand, Cooper pairs can diffuse or leak from S to F, leading to the proximity effect[1] with the occurrence of superconducting-like properties on the F side. On the other hand, the inverse proximity effect occurs on the S side near the interface,[2] in which the leakage of spin-polarized electrons from F to S results in an induced spin-dependent density of states (DOS) on the S side. The special reflection process known as Andreev reflection (AR)[3] plays an important role in the proximity effect and the inverse proximity effect. In the process an electron with an energy lower than the superconducting gap is reflected back as a hole along the time-reversed path at the interface. The inducements of superconductivity in F and its suppression in S are attributed to a coherent coupling of electrons and holes in F and a pair-breaking effect in S, both produced by the AR process.

Proximity effects in F/S structures have recently attracted much attention in experimental and theoretical investigations. When the Cooper pairs are injected from S into F, they are not broken instantaneously and can survive for a time corresponding to a traveled length on the order of $\xi_{\rm F}$, where $\xi_{\rm F} = \hbar v_{\rm F}/2h_0$ is the coherence length in F, $2h_0$ is the exchange energy corresponding to the difference in energy between spin up and spin down bands in F, and $v_{\rm F}$ is the Fermi velocity. As a result, there appears a proximity-effect-induced DOS on the F side. An alternative argument is that the electron (hole) and the AR hole (electron) in F have opposite spins and different Fermi momenta, the interference between their wave functions causes the induced DOS to have a damped oscillation from "0" state to "π" state.[4−13] Another interesting topic in the F/S structure is inverse proximity effects, i.e., the induction of a magnetic moment in the S in contact with F. Similar to the penetration of superconductivity into the F, the spin-polarized electrons in F may penetrate the S over some distances, leading not only to pair-breaking effects but also to magnetic leakage spin-splitting effects near the F/S interface on the S side. Near the interface the Bose condensate of Cooper pairs does not contain all the pairs, and some of them have smaller or vanishing binding ener-

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gies, leading to the decrease of superconducting order parameter $F(x)$ and energy gap Δ. Theoretical calculations based on the Blonder, Tinkham and Klapwijk (BdG) approach[14,15] and on the quasi-classical theory[16−18] have shown that the DOSs for spin-up and spin-down electrons are different in the S over the length on the order of ξ_S, where ξ_S is the superconducting coherent length. Bergeret *et al.*[18] have calculated the magnetic moment induced by inverse proximity effects in the S/F junctions from the ballistic to the diffusive limit. However, it has not been studied how the magnitude of the exchange energy h_0 and the interfacial barrier strength affect the inverse proximity effects, which is addressed in the present work. And the DOS of S/F structures can be measured with planar tunneling spectroscopy of the N/S/F structures or low-temperature scanning tunnel microscopy (STM).[19] It is highly desired to investigate the inverse proximity effects in the N/S/F structures, which is another motivation for this work. And we expect our results to be observed in the future experiments.

Very recently, the possibility of the coexistence of the ferromagnetism and the s-wave superconductivity near the F/S interface has been suggested. The electrons in the F tend to be parallel aligned due to the exchange energy h_0 while the Cooper pair in an s-wave S must be composed of a spin-up electron and a spin-down one. The requirements for the alignments of the electron spins in the F and the S are so different that the coexistence of the ferromagnetism and the s-wave superconductivity is quite difficult to realize. It was shown that their coexistence condition was given by $h_0/\Delta_0 < 0.707$ for zero centre-of-momentum Cooper pairs[20] and $0.707 < h_0/\Delta_0 < 0.754$ for the FFLO states[21,22] with the Cooper pair having a finite centre-of-mass momentum $Q = 2h_0/\hbar v_F$, where Δ_0 is the superconducting energy gap. The exchange energy h_0 in the F is typically at least 2 orders of magnitude larger than the superconducting gap Δ_0 in the S in bulk materials and consequently the coexistence is difficult to observe. Until recently, whether or not the itinerant ferromagnetism can coexist with s-wave superconductivity is still in dispute.[23,24] However, this condition for the coexistence may be largely relaxed near the F/S interface where the Cooper pairs are injected from the S into the F by the proximity effect and the spin-polarized electrons from the F into the S by the inverse proximity effect. As a result, it is highly desirable to study probable coexistence of ferromagnetism and superconductivity near the F/S interface, which is one of motivations in this work.

2. Model and theory

Consider an N/I_1/S/I_2/F double-barrier junction as shown in Fig. 1.

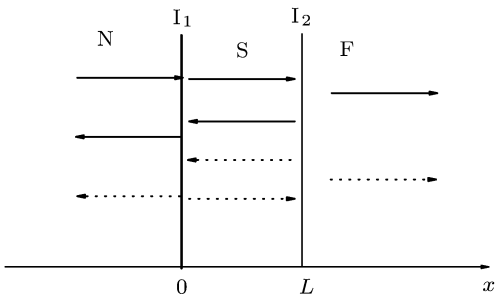


Fig. 1. Schematic illustration of an N/I_1/S/I_2/F junction and reflection and transmission of quasi-particles in the junction. The solid-line arrow represents the electron in N, and F or ELQ in S, while the dot-line arrow refers to the hole in N and F or HLQ in S.

The materials on the left and the right sides are N and F respectively, and they are separated from the central S by two thin insulating interfaces. The two interfaces at $x = 0$ and $x = L$ are described by two δ-type barrier potentials $V(x) = U_1\delta(x) + U_2\delta(x-L)$, where L is the thickness of S interlayer and $U_{1(2)}$ depends on the product of barrier height and width. We use an effective single-particle Hamiltonian to describe the electrons (holes) in N and F, and the S is assumed to be s-wave pairing and described by a BCS-like Hamiltonian. In the one-dimensional Blonder, Tinkham and Klapwijk (BTK) model[25] the quasi-particle wave functions satisfy the following Bogoliubov-de Gennes (BdG) equation:[26]

$$\begin{bmatrix} H_0(x) - \eta_\sigma h(x) & \Delta(x) \\ \Delta^*(x) & -H_0(x) - \eta_\sigma h(x) \end{bmatrix} \begin{bmatrix} u_\sigma \\ v_{\bar\sigma} \end{bmatrix} = E \begin{bmatrix} u_\sigma \\ v_{\bar\sigma} \end{bmatrix}. \tag{1}$$

Here $H_0(x) = -(\hbar^2/2m)(\mathrm{d}^2/\mathrm{d}x^2) + V(x) - E_F$, E is the quasi-particle energy relative to the Fermi energy E_F, $h(x) = h_0\Theta(x-L)$ is the exchange energy in F, $\eta_\sigma = 1$ for $\sigma = \uparrow$ and $\eta_\sigma = -1$ for $\sigma = \downarrow$, $\bar\sigma$ represents the spin opposite to σ. In general, equation (1) should be a four-component BdG equation for u_σ and v_σ with

$\sigma =\uparrow$ and $\downarrow$, where u_σ and v_σ denote the spin-σ electron-like quasi-particle (ELQ) and hole-like quasi-particle (HLQ), respectively. After the spin-flip process has been neglected near the interface, the four-component BdG equation may be decoupled into two sets of two-component equations: $(u_\sigma, v_{\bar\sigma})$ describing the spin-σ ELQ and spin-$\bar\sigma$ HLQ.

Consider a spin-σ electron incident on the interface at $x = 0$ from the left N as shown in Fig. 1. There are four possible trajectories: normal reflection (b_σ), Andreev reflection ($a_{\bar\sigma}$), transimission as ELQ (c_σ) and transimission as HLQ ($d_{\bar\sigma}$). With general solutions of BdG equation (1), the wave functions in three regions have the following forms:

$$\psi_\sigma(x) = \begin{pmatrix}1\\0\end{pmatrix}\mathrm{e}^{\mathrm{i}\,k_\mathrm{e}x} + a_{\bar\sigma}\begin{pmatrix}0\\1\end{pmatrix}\mathrm{e}^{\mathrm{i}\,k_\mathrm{h}x} + b_\sigma\begin{pmatrix}1\\0\end{pmatrix}\mathrm{e}^{-\mathrm{i}\,k_\mathrm{e}x} \tag{2}$$

in the left region ($x \le 0$),

$$\psi_\sigma(x) = c_\sigma\begin{pmatrix}1\\0\end{pmatrix}\mathrm{e}^{\mathrm{i}\,k_\mathrm{e}^\sigma x} + d_{\bar\sigma}\begin{pmatrix}0\\1\end{pmatrix}\mathrm{e}^{-\mathrm{i}\,k_\mathrm{h}^{\bar\sigma}x} \tag{3}$$

in the right region ($x \ge L$), and

$$\psi_\sigma(x) = e\begin{pmatrix}u\\v\end{pmatrix}\mathrm{e}^{\mathrm{i}\,q_\mathrm{e}x} + f\begin{pmatrix}u\\v\end{pmatrix}\mathrm{e}^{-\mathrm{i}\,q_\mathrm{e}x} + g\begin{pmatrix}v\\u\end{pmatrix}\mathrm{e}^{\mathrm{i}\,q_\mathrm{h}x} + h\begin{pmatrix}v\\u\end{pmatrix}\mathrm{e}^{-\mathrm{i}\,q_\mathrm{h}x} \tag{4}$$

in the middle region ($0 \le x \le L$). Here $k_{\mathrm{e(h)}} = k_\mathrm{F} \pm mE/(\hbar^2 k_\mathrm{F})$, $k^\sigma_{\mathrm{e(h)}} = k^\sigma_\mathrm{F} \pm mE/(\hbar^2 k^\sigma_\mathrm{F})$ with $k^\sigma_\mathrm{F} = k_\mathrm{F}\sqrt{1+\eta_\sigma h_0/E_\mathrm{F}}$ and $k_\mathrm{F} = \sqrt{2mE_\mathrm{F}}/\hbar$; $q_{\mathrm{e(h)}} = k_\mathrm{F} \pm m\Omega/(\hbar^2 k_\mathrm{F})$ with $u = \sqrt{(1+\Omega/E)/2}$, $v = \sqrt{(1-\Omega/E)/2}$ and $\Omega = \sqrt{E^2 - \Delta_0^2}$. Coefficients $a_{\bar\sigma}$, b_σ, c_σ and $d_{\bar\sigma}$ correspond to the probability amplitudes for AR, normal reflection, transmissions within the same branch and between different branches, respectively. The wave functions must satisfy the boundary conditions at $x = 0$ and $x = L$ as follows:

$$\begin{cases} \psi_\sigma(0_-) = \psi_\sigma(0_+), \quad \dfrac{\mathrm{d}\psi_\sigma(x)}{\mathrm{d}x}\Big|_{x=0_+} = \dfrac{\mathrm{d}\psi_\sigma(x)}{\mathrm{d}x}\Big|_{x=0_-} + 2k_\mathrm{F}Z_1\psi_\sigma(0), \\ \psi_\sigma(L_-) = \psi_\sigma(L_+), \quad \dfrac{\mathrm{d}\psi_\sigma(x)}{\mathrm{d}x}\Big|_{x=L_+} = \dfrac{\mathrm{d}\psi_\sigma(x)}{\mathrm{d}x}\Big|_{x=L_-} + 2k_\mathrm{F}Z_2\psi_\sigma(L), \end{cases} \tag{5}$$

where $Z_1 = mU_1/(\hbar^2 k_\mathrm{F})$ and $Z_2 = mU_2/(\hbar^2 k_\mathrm{F})$ are the dimensionless barrier strengths. From Eqs. (2)–(5) we obtain

$$a_{\bar\sigma} = -k_\mathrm{e}uv\{4q_\mathrm{e}q_\mathrm{h}K_1(u^2-v^2) + [2q_\mathrm{e}q_\mathrm{h}K_1e_{1+} - 2q_\mathrm{e}p_{2+}(u^2-v^2)e_{1-}]\}/D, \tag{6}$$

$$\begin{aligned} b_\sigma = {} & -k_\mathrm{e}\{(u^2-v^2)^2[(R_3p_{2-} + q_\mathrm{e}q_\mathrm{h}R_1)e_{2+} + q_\mathrm{e}(p_{2-} + R_3R_1)e_{2-}] \\ & - [p_{2+}R_3(u^2-v^2)^2 + q_\mathrm{e}q_\mathrm{h}K_1]e_{1+} + (u^2-v^2)q_\mathrm{e}[p_{2+} + K_1R_3]e_{1-} + D/k_\mathrm{e}\}/D, \end{aligned} \tag{7}$$

where

$$\begin{aligned} D = {} & -4q_\mathrm{e}q_\mathrm{h}K_1K_2u^2v^2 + [p_{1+}p_3(u^2-v^2)^2 + q_\mathrm{e}q_\mathrm{h}K_1K_2]e_{1+} - q_\mathrm{e}(u^2-v^2)(K_1p_{1+} + K_2p_{2+})e_{1-} \\ & - (u^2-v^2)^2[(p_{1-}p_{2-} + q_\mathrm{e}q_\mathrm{h}R_1R_2)e_{2+} + q_\mathrm{e}(p_{1-}R_1 + p_{2-}R_2)e_{2-}], \end{aligned} \tag{8}$$

$$p_{1\pm} = (k_\mathrm{e} + 2\,\mathrm{i}\,k_\mathrm{F}Z_1)(k_\mathrm{h} - 2\,\mathrm{i}\,k_\mathrm{F}Z_1) \pm q_\mathrm{e}q_\mathrm{h}, \quad p_{2\pm} = (k_\mathrm{e}^\sigma + 2\,\mathrm{i}\,k_\mathrm{F}Z_2)(k_\mathrm{h}^{\bar\sigma} - 2\,\mathrm{i}\,k_\mathrm{F}Z_2) \pm q_\mathrm{e}q_\mathrm{h}, \tag{9}$$

$$\begin{aligned} R_1 &= k_\mathrm{e}^\sigma - k_\mathrm{h}^{\bar\sigma} + 4\,\mathrm{i}\,k_\mathrm{F}Z_2, \quad R_2 = k_\mathrm{e} - k_\mathrm{h} + 4\,\mathrm{i}\,k_\mathrm{F}Z_2, \\ R_3 &= k_\mathrm{h} - 2\,\mathrm{i}\,k_\mathrm{F}Z_1, \quad K_1 = k_\mathrm{e}^\sigma + k_\mathrm{h}^{\bar\sigma}, \quad K_2 = k_\mathrm{e} + k_\mathrm{h}, \end{aligned} \tag{10}$$

$$e_{1\pm} = \mathrm{e}^{\mathrm{i}(q_\mathrm{e}-q_\mathrm{h})L} \pm \mathrm{e}^{-\mathrm{i}(q_\mathrm{e}-q_\mathrm{h})L}, \; e_{2\pm} = \mathrm{e}^{\mathrm{i}(q_\mathrm{e}+q_\mathrm{h})L} \pm \mathrm{e}^{-\mathrm{i}(q_\mathrm{e}+q_\mathrm{h})L}. \tag{11}$$

From Eqs. (6) and (7) we obtain the probabilities $A_{\bar\sigma} = |a_{\bar\sigma}|^2\,\mathrm{Re}(q_\mathrm{h}/q_\mathrm{e})$, and $B_\sigma = |b_\sigma|^2$, respectively, corresponding to the AR and the normal reflection coefficients. Finally, the tunnelling conductance is given by[25]

$$G = \sum_{\sigma=\uparrow,\downarrow} G_\sigma = \sum_{\sigma=\uparrow,\downarrow} \frac{2e^2}{h}(1 - B_\sigma + A_{\bar\sigma}). \tag{12}$$

3. Results and discussion

We first calculate the tunneling conductance in the N/I_1/S/F double junctions to study the inverse proximity effects, in which I_1 is assumed to be a delta-type barrier and the S/F interface is the ohmic contact. The parameters used in the calculations are taken as follows: the dimensionless potential strength of barrier I_1 is $Z_1 = 4.0$, $Z_2 = 0$ for the S/F ohmic contact, the Fermi energy $E_F = 1.4$ eV, and the superconducting energy gap $\Delta_0 = 1.4$ meV. Figure 2 shows the energy dependences of conductance for different values of thickness L. The conductance is normalized by its value at $E = 5\Delta_0$ beyond which the conductance is almost constant. It is shown that the conductance are strikingly different from zero for $E < \Delta_0$, indicating gapless superconductivity, which stems from the pairing breaking and time-reversal symmetry breaking due to the injection of spin-polarized electrons from F into S. Near the interface the Bose condensate of Cooper pairs does not contain all the pairs, and some of them have smaller and vanishing binding energies. At $L = 0.5\xi_S$ the conductance has the biggest departure from its bulk behaviour as shown by the solid line, where $\xi_S = \hbar v_F/2\Delta_0$ is the coherent length in S. With the value of L increasing, the conductance within the energy gap gradually decreases. When $L = 5.0\xi_S$, the conductance within the energy gap almost vanishes and the peak occurs on the edge of energy $E = \Delta_0$, which is very close to that in bulk S.

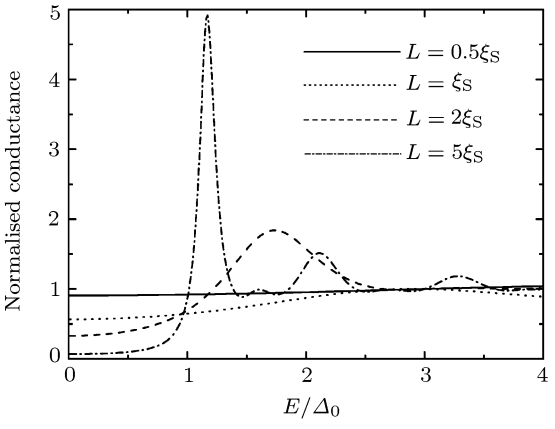


Fig. 2. Energy dependences of the normalized conductance for different values of thicknesses of S film.

Next, we discuss the effects of barrier strength at the S/F interface on conductance in S. As shown in Fig. 3, we plot the barrier strength dependences of normalized conductance for $L = 0.5\xi_F$, ξ_F, $1.5\xi_F$, $2.0\xi_F$, separately, with $h_0/E_F = 0.01$ and $E = 0$. It is found that the conductance decreases monotonically with the increase of Z_2 and/or the thickness L. When $Z = 0$ and $L = 0.5\xi_F$, the conductance has the biggest deviation from its bulk behaviour (zero), which is shown by the dash-dot line. With the barrier strength Z_2 or the thickness L increasing , the conductance within the energy gap gradually decreases. This effect of barrier strength is closely associated with the change of AR at the interface. Our calculation indicates that at $Z_2 = 0$ the AR coefficient is the largest and it decreases with Z_2 increasing.

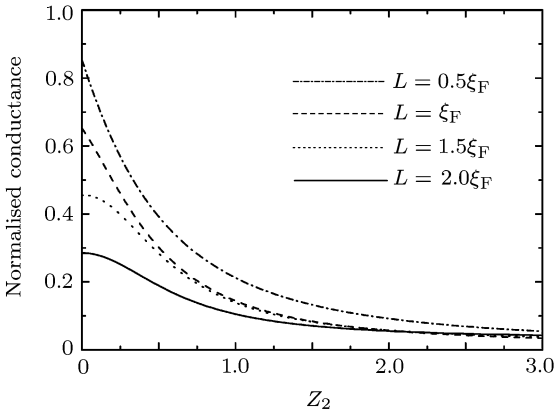


Fig. 3. Normalized conductances as a function of barrier strength Z_2 for different thicknesses of S film.

Finally, we discuss the probable coexistence of ferromagnetism and superconductivity in the S film near the interface. Figures 4(a)–4(d) show the energy dependences of the spin-dependent conductance for $L = 0.5\xi_F$, ξ_F, $2.0\xi_F$, $3.0\xi_F$, respectively, with $Z_2 = 0$ and $h_0/E_F = 0.05$. In Fig. 4(a), where $L = 0.5\xi_F$, the normalized conductances for spin-up and spin-down electrons are obviously different both within and without energy gaps as shown by the solid and dotted lines, indicating an inverse-proximity-effect-induced ferromagnetism in the S film. With the increase of

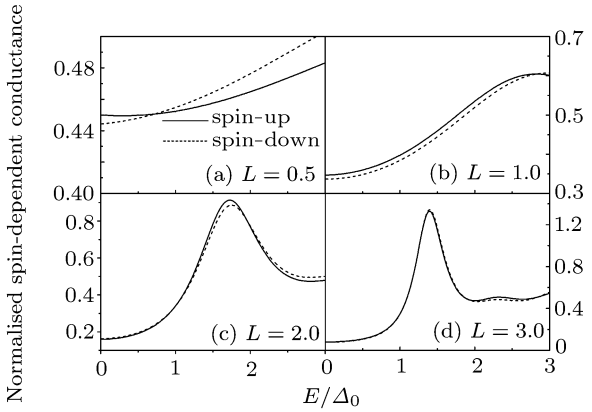


Fig. 4. Energy dependences of normalized spin-dependent conductance for different thicknesses of S film.

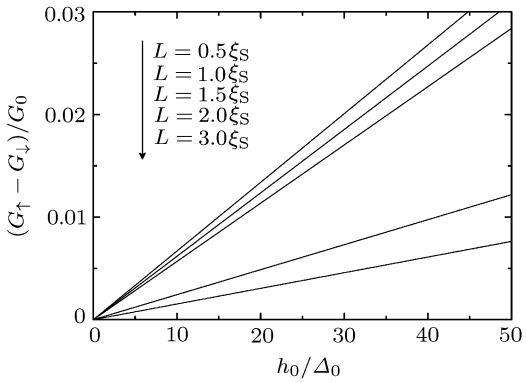


Fig. 5. Difference between spin-up and spin-down conductances at $E = 0$ as a function of the exchange energy h_0 for different thicknesses of the S film.

the distance away from the interface, the difference between spin-up and spin-down conductance gradually decreases and almost vanishes at $L = 3.0\xi_S$ as shown in Fig. 4(d). It suggests the possible coexistence of the ferromagnetism and the s-wave superconductivity in the S film near the S/F interface. The difference in conductance between spin-up and spin-down electrons is sensitive to the magnitude of exchange energy h_0, which is depicted in Fig. 5 for different values of thickness L, where $E = 0$. An increase of exchange energy h_0 will increase the difference in conductance between spin-up and spin-down electrons, while an increase of thickness L will decrease it. From the figure we also see clearly that the difference equals zero for $h_0 = 0$ in despite of L, which indicates that the spin-dependent conductance in the S film is entirely induced by the injection of spin-polarized electrons from F side through inverse proximity effects.

4. Conclusion

The BTK theory is extended to the calculation of the tunnelling conductance for the $N/I_1/S/I_2/F$ double junctions. Inverse proximity effect in the S film induces the spin-dependent conductance within the energy gap, indicating an appearance of gapless superconductivity and a coexistence of ferromagnetism and superconductivity in a small regime near the interface. The inverse proximity effect is weakened by increasing the barrier strength at the interface, and the induced ferromagnetism in S near the interface is enhanced by increasing the exchange energy in F.

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