Magnetization-orientation dependence of the superconducting transition temperature calculated for F/S/F trilayer structures

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(Received 18 April 2003; revised manuscript received 29 September 2003; published 9 July 2004)

We theoretically investigate the superconducting critical temperature T_c dependence on the relative orientation of the magnetizations in $F/S/F$ trilayer structures, where F is a ferromagnet and S is a superconductor. The values of T_c are obtained from the linearized Usadel equations. We discuss the usual approximations employed to solve those equations and show that they are invalid in the parameter range of interest. We also compare approximate results of several authors. Adapting the numeric method used previously for F/S bilayers to the case of $F/S/F$ trilayers, we find critical temperatures for parallel and antiparallel magnetic configurations with no approximations involved. Our results qualitatively explain experimental data and provide guidelines for optimizing the experimental systems.

DOI: 10.1103/PhysRevB.70.014505 PACS number(s): 74.62. - c, 74.50. + r, 85.70. - w, 73.43.Qt

I. INTRODUCTION

The observation of a nonmonotonic dependence of the superconducting (S) critical temperature T_c on the ferromagnetic (F) layer thickness in F/S systems¹ has generated much work on ferromagnet–superconductor proximity effects. This and other novel phenomena were predicted and observed, most notably a π -phase state in S/F/S structures.^{2–5} The experimental situation is usually such that the mean free path in the F and S layers is small and superconductivity can be described by the Usadel equations. Their solution and the choice of appropriate boundary conditions at the S/F interfaces are the subject of much theoretical development.^{$6-9$}

Theoretical models also predict that in $F/S/F$ trilayers T_c depends on the angle θ between the magnetizations M_1 and \mathbf{M}_2 of the F layers.^{10–15} This type of effect for a structure with insulating ferromagnets was predicted and observed earlier, $16,17$ but no systematic studies followed. In the case of all-metallic systems, the first experimental observation of an orientation dependent T_c was reported for $Cu_xNi_{1-x}/Nb/Cu_xNi_{1-x}.$ ¹⁸ The alloy Cu_xNi_{1-x} for $x \le 0.6$ is a weak ferromagnet that does not destroy superconductivity in layers with thickness $d_S \sim \xi_S$, where ξ_S is the coherence length of the superconducting layer.

In metallic $F/S/F$ trilayers the overall T_c is reduced by the usual proximity effect with the adjacent ferromagnetic layers,¹⁹ but the amount of reduction depends on the relative magnetization orientation in the F layers. This magnetization orientation dependence occurs when the Cooper pair size ξ_s is comparable with or smaller than the thickness of the superconducting layer, so that the pairs are influenced by both F layers simultaneously.

The usual Cooper pairs are spin-singlets that are isotropic in spin space. Their interaction with a ferromagnetic layer does not depend on the direction of the magnetization that sets the Zeeman field in the layer. A purely singlet pairing cannot explain the effect of the relative magnetization orientation on T_c ; the best one could expect is a stronger suppression of T_c in the $F/S/F$ trilayer compared to the F/S bilayer due to the additional hostile interface. However in the presence of even one magnetic layer the nature of the Cooper pairs in the S layer changes. The usual spin-singlet pairs are modified and acquire an admixture of spin-triplet nature. In the spin-triplet state the Cooper pairs have total spin equal to one and thus a direction in the spin space is selected. The interaction of a spin-triplet pair with the F-layer Zeeman field then does depend on the angle between the spin of the pair and the magnetization of the F layer. Thus the effect discussed in this paper is made possible.

Mathematically superconductivity with an arbitrary spin state of the pairs is described by a 2×2 matrix anomalous Green's function

$$
F_{\alpha\beta}(x,\omega_n) = \begin{vmatrix} f_{\uparrow\uparrow} & f_{\uparrow\downarrow} \\ f_{\downarrow\uparrow} & f_{\downarrow\downarrow} \end{vmatrix}.
$$

In the purely spin-singlet state this matrix is antisymmetric $\hat{F} \sim i\hat{\sigma}_y$. In the generic case \hat{F} can be decomposed as

$$
\hat{F} = s(i\hat{\sigma}_y) + t_{(1)}\frac{\hat{E} + \hat{\sigma}_z}{2} + t_{(0)}\hat{\sigma}_x + t_{(-1)}\frac{\hat{E} - \hat{\sigma}_z}{2},
$$

where $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ are the Pauli matrices and \hat{E} is an identity matrix. The spin-singlet component and three spin-triplet components are given by complex coefficients *s* and $t_{(-1,0,1)}$, respectively. The indices of the spin-triplet component denote the projection of the Cooper pair spin on the *z* axis. In the dirty limit superconductivity can only exist in the form of an *s* wave in the momentum space. To respect the overall symmetry of \hat{F} , the spin-triplet components of $\hat{F}(x,\omega_n)$ have to be odd functions of the Matsubara frequency ω_n . Such odd-in-omega pairing correlations were first discussed in Ref. 20.

In the absence of ferromagnets all spin-triplet components are equal to zero. For the F/S bilayers the $t_{(0)}$ component is generated near the boundary due to the interplay between the spin-singlet pairing interaction in the S layer and band splitting of the F layer. The same is true for the $F/S/F$ trilayers for the case of collinear magnetic configuration. As argued above, the presence of the $t_{(0)}$ component is responsible for the difference of T_c in parallel and antiparallel configurations.

In a noncollinear magnetic configuration the $t_{(\pm 1)}$ components are generated as well. According to recent theoretical work^{21,22} their decay length in a ferromagnet is much longer than for the spin-singlet and the $t_{(0)}$ spin-triplet component and their presence leads to very interesting phenomena of long range proximity. In the problem of T_c dependence on magnetic configuration the presence of $t_{(\pm 1)}$ is not required (but has to be taken into account if these components are indeed present).

It was shown^{10–15} that the critical temperature $T_c(\theta)$ is lowest in the parallel (P) state $T_c(\theta=0) \equiv T_{c[P]}$ and highest in the antiparallel (AP) state $T_c(\theta=\pi)\equiv T_{c[AP]}$. This can be qualitatively justified as follows. Since the triplet component is induced by *M*, it is natural that its value averaged over the superconductor is larger for the P than for the AP configuration. Then the relationship $T_{c[P]} < T_{c[A]P]}$ follows from the fact that the presence of a triplet component is detrimental to the superconductivity.

In the temperature range $T_{c[P]} < T < T_{c[AP]}$ the S layer can retain its superconductivity in the AP configuration of the F layers, but will revert to the normal state in the parallel configuration. Therefore the system not only exhibits physically interesting phenomena, but can be also used as a switching device for low-temperature applications.²³ If the coercivity of the F layers is sufficiently small, as is usually the case, the switching field of the S layer can be much smaller than the critical field of the superconductor.

The predictions of a significant difference $T_{c[AP]} - T_{c[P]}$ in previous work¹¹⁻¹³ are in sharp contrast with recent experiments which measured much smaller ΔT_c (the sign of $T_{c[AP]} - T_{c[P]}$ does correspond to the theoretical predictions). ¹⁸ One must remember, however, that the calculations 11–13 were performed using approximations—either a thin S layer approximation or a "single-mode" approximation—to solve the Usadel equations in closed form. The experimental parameters can often be out of the validity range of those approximations. This, in particular, is true for the structures used in Ref. 18. In order to perform a more meaningful comparison of the theory and experiment, it is necessary to solve the problem exactly. To achieve that we adapted the numerical method developed for the F/S bilayers^{24,25} to the case of $F/S/F$ trilayers. Numeric solution is valid in any range of parameters and thus can provide valuable guidance for experiments. We investigate the T_c dependence of various parameters, such as the F- and S-layer thickness.

The paper is organized as follows: Sec. II explains the adaptation of the method of Ref. 25 for trilayer structures. Section III discusses the regions of validity of common ap-

FIG. 1. F/S/F trilayer structure.

proximations and shows that numeric calculations are required to describe the structures studied in Ref. 18. Section IV presents our results for the difference between T_c in parallel and antiparallel configurations for various parameters. Finally we compare our calculation with experiments, and discuss the insights gained.

II. SOLUTION METHOD FOR THE TRILAYER STRUCTURES

We adapt the method, developed in Refs. 24 and 25 in the context of F/S bilayers, for the collinear F/S/F case. It is assumed that all quantities depend only on the coordinate *x* perpendicular to the layers. We also specifically consider symmetric structures with identical ferromagnets and F/S boundaries (see Fig. 1).

A. Equations and boundary conditions

In general the system of Usadel equations involves properly averaged Matsubara Green's functions $G(x, \omega_n)$, $F(x, \omega_n)$, $\omega_n(T)=2\pi T(n+1/2)$, and the self-consistent order parameter $\Delta(x)$. However to find the critical temperature it is sufficient to linearize these equations with respect to small *F* and use G of the normal metal state.¹² Then, starting from the matrix Usadel equation on $F_{\alpha\beta}(x,\omega_n)$,²¹ it is possible to prove that in the collinear case this matrix has the form

$$
F_{\alpha\beta}(x,\omega_n) = \begin{vmatrix} 0 & F(x,\omega_n) \\ -F^*(x,\omega_n) & 0 \end{vmatrix}.
$$

This means that the singlet component is $s = \text{Re } F$ and the triplet component is $t_{(0)}=i$ Im *F*. Now the matrix equation can be reduced to an equation on a scalar complex function $F(x, \omega_n)$ (we follow the notation of Ref. 25):

$$
\xi^{2}(x)\pi T_{cs}F''(x,\omega_{n}) - (|\omega_{n}| + iE_{ex}(x)\text{sgn}(\omega_{n}))F(x,\omega_{n}) + \Delta(x)
$$

= 0. (1)

The order parameter $\Delta(x)$ obeys the self-consistency condition²⁵

$$
\Delta(x) \log \left(\frac{T_{cs}}{T} \right) = \pi T \sum_{\omega_n} \frac{\Delta(x)}{|\omega_n|} - F(x, \omega_n)
$$

$$
= 2\pi T \sum_{\omega_n > 0} \frac{\Delta(x)}{|\omega_n|} - \text{Re}\{F(x, \omega_n)\}.
$$
 (2)

Here T is the temperature of the system, T_{cs} is the critical temperature of a stand-alone S layer (in our approximation it is equal to the transition temperature of a bulk superconductor), and parameters $\xi(x)$ and $E_{ex}(x)$ have constant, but different, values in the F and S layers. Coherence lengths $\xi_F = \sqrt{D_f/(2\pi T_{cs})}$ and $\xi_S = \sqrt{D_s/(2\pi T_{cs})}$ are expressed through corresponding diffusion coefficients. The band splitting parameter $E_{ex}(x) = E_i$ in the F_i layer (*i*=1 for the left F layer and $i=2$ for the right F layer) and zero in the S layer. For the parallel configuration $E_1 = E_2 = E_{ex}$ while for the antiparallel configuration $E_1=E_{ex}$, $E_2=-E_{ex}$. The order parameter $\Delta(x)$ is zero in the F layer and has to be determined in the S layer. This is a consequence of the physical assumption of the absence of pairing interaction in the F layers. We also used the symmetry property $F(-\omega_n) = F^*(\omega_n)$ to obtain the last line.

The anomalous function $F(x, \omega_n)$ experiences jumps and derivative discontinuities at the boundaries between the layers and at the outer boundaries. We will denote the values of *F* on the F and S sides of the boundary as F_F and F_S , respectively. For a symmetric structure the boundary conditions²⁶ are:

$$
\frac{dF_F}{dx} = 0
$$

on the outer boundaries of the F layers, and on the F_i/S boundaries are:

$$
\gamma \xi_F \left(\frac{dF_F}{dx} \right)_i = \xi_S \left(\frac{dF_S}{dx} \right)_i
$$

$$
(-1)^{i+1} \gamma_b \xi_F \left(\frac{dF_F}{dx} \right)_i = F_{Si} - F_{Fi}.
$$
 (3)

The parameters γ and γ_b characterize the band-structure mismatch and transparency of the boundary, respectively, and can be expressed through resistivities ρ_S and ρ_F and boundary resistivity ρ_b (in terms of boundary surface area and total boundary resistance $\rho_b = R_b A$): $\gamma = \rho_S \xi_S / (\rho_F \xi_F)$, γ_b $=p_b/(\rho_F \xi_F)$. Equations (1) and (2) with boundary conditions (3) have nonzero solutions only for $T < T_c$. We determine the T_c as the temperature at which the first $F \neq 0$ solution appears.

B. Equations reduction

The main difficulty in finding F and Δ is posed by the integral self-consistency equation (2). However, in the F layers $\Delta=0$ and one can solve the equations analytically. When this is done, it turns out that, just like in Refs. 24 and 25, knowing $F_F(x, \omega_n)$ it is possible to express the boundary conditions through F_S only. As a result we obtain a simpler system for F_S and Δ on the interval $[-d_S/2, d_S/2]$

$$
\xi_S^2 \pi T_{cs} \frac{d^2 F_S(x, \omega_n)}{dx^2} - |\omega_n| F_S(x, \omega_n) + \Delta(x) = 0,
$$

$$
\Delta(x) \ln\left(\frac{T_{cs}}{T}\right) = \pi T \sum_{\omega_n(T)} \left(\frac{\Delta}{|\omega_n|} - \text{Re}\{F_S(x, \omega_n)\}\right), \qquad (4)
$$

and boundary conditions

$$
\xi_{S}F'_{Si}=L_{i}F_{Si},\tag{5}
$$

where complex constants L_i ($i=1,2$) are defined as

$$
L_i = (-1)^{i+1} \frac{\gamma}{\gamma_b + B_i},
$$

\n
$$
B_i = \frac{1}{\xi_F k_F(i, \omega_n) \tan h(d_F k_F(i, \omega_n))},
$$

\n
$$
k_F(i, \omega_n) = \frac{1}{\xi_F} \sqrt{\frac{|\omega_n| + iE_i \text{sgn}(\omega_n)}{\pi T_{cs}}}. \tag{6}
$$

The parallel case is characterized by $L_1 = -L_2 = L$, while for the antiparallel case $L_1 = -L_2^* = L$.

The order parameter $\Delta(x)$ can be chosen to be real; this is a consequence of the requirement of the absence of a current. Then equations for the $F_{+} = 2\text{Re}\{F_{S}\}\$ and $F_{-} = 2\text{Im}\{F_{S}\}\$ parts of the anomalous function separate into

$$
\xi_S^2 \pi T_{cs} \frac{d^2 F_-}{dx^2} - |\omega_n| F_- = 0, \tag{7}
$$

and

$$
\xi_S^2 \pi T_{cs} \frac{d^2 F_+}{dx^2} - |\omega_n| F_+ + 2\Delta(x) = 0, \tag{8}
$$

with

$$
\Delta(x)\ln\left(\frac{T_{cs}}{T}\right) = \pi T \sum_{\omega_n(T)} \left(\frac{2\Delta}{|\omega_n|} - F_+(x, \omega_n)\right),\tag{9}
$$

but the boundary conditions still connect F_+ and F_- :

$$
\xi_{S}\left(\frac{F'_{+}}{F'_{-}}\right)_{i} = \begin{vmatrix} \text{Re}(L_{i}) & -\text{Im}(L_{i}) \\ \text{Im}(L_{i}) & \text{Re}(L_{i}) \end{vmatrix} \begin{pmatrix} F_{+} \\ F_{-} \end{pmatrix}_{i}
$$

The general solution of Eq. (7) is

$$
F_{-}(x) = A \cosh(k_{S}x) + B \sinh(k_{S}x),
$$

$$
k_{S}(n) = \frac{1}{\xi_{S}} \sqrt{\frac{|\omega_{n}|}{\pi T_{cs}}}.
$$
(10)

.

When the structure has identical properties of the F layers and F/S boundaries, one has a handy simplification following from the symmetry of the problem, i.e., $B=0$ in the P case and $A=0$ in the AP case. As a consequence one can separate the bulk equation and the boundary conditions on F_{+} in the form

$$
\xi_{S}F'_{+i} = (-1)^{i+1}W_{[P/AP]}(\omega_n)F_{+i},\tag{11}
$$

where the subscripts $\lfloor P \rfloor$ and $\lfloor AP \rfloor$ specify the magnetic configuration. Our calculations yield

$$
W_{[P/AP]} = \text{Re } L + \frac{\text{Im } L^2}{A_{[P/AP]} + \text{Re } L}
$$

= $\gamma \frac{A_{[P/AP]}(\gamma_b + \text{Re}[B]) + \gamma}{A_{[P/AP]}|\gamma_b + B|^2 + \gamma(\gamma_b + \text{Re}[B])},$ (12)

where

$$
A_{[P]} = k_S \xi_S \tanh(k_S d_S / 2),
$$

$$
A_{[AP]} = k_S \xi_S \coth(k_S d_S / 2).
$$
 (13)

Either of B_i or L_i from Eq. (6) can be used in this formula, since *W* does not depend on the sign of the imaginary part of *B*.

C. Mapping on the F/S problem

With symmetric boundary conditions (11) the solutions of Eqs. (8) and (9) are symmetric functions $F₊(x)$ and $\Delta(x)$. Therefore, the problem is mapped back onto the F/S problem with the superconducting layer occupying the $[-d_S/2, 0]$ interval and a boundary condition $F'_{+}(0) = 0$, i.e. on the problem treated in Ref. 25 with effective value d_{Self} $=d_S/2$. This conclusion is obvious for the P case, and indeed $W_{[P]}$ is identical to the one found for the F/S bilayer. For the AP case the only change occurs in $A_{[AP]}$. Any of the solution methods discussed in Ref. 25 can now be utilized. In Sec. IV we will present numeric results obtained with the method of fundamental solution introduced in Sec. IV of Ref. 25. But before doing that, we discuss the validity of the approximations commonly made to solve Eqs. (8) and (9), and justify the necessity of a numeric approach.

III. ANALYSIS OF COMMON APPROXIMATIONS

A. Single-mode approximation

We start with the "single-mode" approximation. As explained in Sec. III A of Ref. 25 this approximation is valid when parameters W_n are approximately independent of n . Since the sum Eq. (2) is converging, it is enough to demand *n* independence only up to a certain number n_{\ast} such that $\omega_{n*} \gg \pi T_c$ and the remainder of the sum can be neglected.

In a strong ferromagnet with $E_{ex} \gg \omega_{n*}$ the wave vector k_F , given by Eq. (6), can be considered constant for ω_n of fixed sign:

$$
k_F \approx \frac{1}{\xi_F} \sqrt{\frac{iE_{ex} \text{sgn}(\omega_n)}{\pi T_{cs}}}.
$$
 (14)

After that, the only *n* dependence of W_n comes from $A(\omega_n)$.

In the P case, *A* is never constant. It starts to grow linearly $A_{[P]} \sim \omega_n$ for small values of the argument and then has an asymptote $A_{[P]} \approx \sqrt{\omega_n / (\pi T_0)}$. In the AP case, *A* can be approximated by a constant $A_{[AP]} \approx 2\xi_S / d_S$ if $k_S(\omega_n) / d_S \le 1$, i.e., in the limit of a thin superconductor:

$$
\sqrt{\frac{\omega_{n^*}}{\pi T_{cs}}}\frac{d_S}{\xi_S} \ll 1.
$$
\n(15)

For larger values of ω_n , function $A_{[AP]}$ joins the same asymptote as $A_{[P]}$.

Now from Eq. (12) we see that the single-mode approximation is justified when either $A(\omega_n) \approx$ const, or when the second term in

$$
\operatorname{Re} L + \frac{\operatorname{Im} L^2}{A + \operatorname{Re} L} \tag{16}
$$

is negligible compared to Re *L*. The first case is realized for a thin superconductor in the AP (but not the P) configuration. The limit of a thin superconductor will be discussed in the next section for both P and AP configurations. For now, let us concentrate on the single-mode solution in the $\xi_s \le d_s$ (not too thin superconductor) case. To keep $W_{[P/AP]}(\omega_n)$ constant in this regime, one has to be able to either neglect *A* in the denominator of the second term of Eq. (16), or neglect the second term altogether. The first possibility requires $A(\omega_{n*})$ \ll Re *L*. For the not too thin superconductor $k_S(\omega_n*)d_S\geq 1$, and so $A_{\lceil P \rceil}(\omega_{n^*}) \approx A_{\lceil AP \rceil}(\omega_{n^*}) \approx \sqrt{\omega_{n^*}/(\pi T_{cs})}$. The same condition $\sqrt{\omega_{n*}/(\pi T_{cs})}$ Re *L* makes the single-mode approximation possible in both cases.

However, when the single mode approximation is valid, one also gets $W_{[P]} \approx W_{[AP]}$ and the difference of critical temperatures cannot be studied this way. The same thing happens when the second term of Eq. (16) can be neglected altogether. We conclude that the single-mode approximation does not allow the study of the dependence of the critical temperature on the configuration in the $\xi_s \le d_s$ regime.

In pioneering work¹³ the $F/S/F$ problem was studied on the basis of a single-mode approximation and, contrary to our statements, a finite *Tc*^f*AP*g−*Tc*^f*P*^g difference was predicted even in the case of a thick superconductor. The details of the calculation are not given in Ref. 13 and we cannot fully reconcile the conclusions. On one hand, Ref. 13 gives an explicit expression for T_c in the limit $d_S \ll \xi_S$, d_F/ξ_F $\ll \sqrt{\pi T_{cs}/E_{ex}}$, and even in the P case, where the single mode approximation should not be accurate according to the discussion above, it corresponds to our Eq. (18). On the other hand, it cites Ref. 27 for the single-mode approach, and we believe that a problem can be found in the ansatz proposed there. Namely the complex anomalous function inside the superconductor is assumed to have the form

$$
F_S(x, \omega_n) = \frac{\Delta(x)}{|\omega_n| + z},\tag{17}
$$

with *z* being a complex number to be determined. Then Eq. (8) gives an equation for $\Delta(x)$ that is independent of *n*:

$$
\xi_S^2 \pi T_{cs} \Delta''(x) + z \Delta(x) = 0.
$$

But Usadel equation (1) with real $\Delta(x)$ implies $F(-\omega_n)$ $=F^*(\omega_n)$ and ansatz (17) does not satisfy this condition. At best it could be rewritten as:

$$
F_S(x, \omega_n) = \frac{\Delta(x)}{|\omega_n| + z} \quad \omega_n > 0,
$$

$$
F_S(x, \omega_n) = \frac{\Delta(x)}{|\omega_n| + z^*} \quad \omega_n < 0,
$$

which in turn would lead to a requirement for Δ to satisfy

$$
\xi_S^2 \pi T_{cs} \Delta''(x) + z^* \Delta(x) = 0.
$$

Consequently, ansatz (17) works only when *z* is a real number. However, with real *z* one cannot satisfy conditions (5) on the boundary with a ferromagnet.

Note, that in the approach of Ref. 25, which we use in the present paper, only the real part of *F* has the form Eq. (17) with real *z*. The imaginary part is then determined from Usadel's equations. This is why the difficulty discussed above does not arise. However, the conditions of the validity of the single mode approximation turn out to be more stringent than those given in Ref. 27.

B. Limit of a thin superconductor

Finally we compare the thin superconductor $d_S \le \xi_S$ results of Refs. 25 and 28. A more quantitative definition of this limit is given by the requirement $k_S(\omega_n*)d_S \leq 1$, or Eq. (15).

For the P case one compares Eqs. (18) and (19) of Ref. 28 with Eq. (A2) of Ref. 25. Taking into account different definitions of coherence lengths ξ_F , ξ_S and boundary parameters γ , γ_b , and using Eq. (A2) at $d_{\text{Seff}} = d_S / 2$, one sees that these formulas are identical. In terms of parameters introduced in Eq. (6) they read

$$
\ln \frac{T_{cs}}{T_{c[P]}} = \text{Re}\left[\psi \left(\frac{1}{2} + \frac{T_{cs}}{T_{c[P]}} \frac{\xi_S}{d_S} L\right)\right] - \psi \left(\frac{1}{2}\right). \tag{18}
$$

The AP case is not treated in Ref. 25, so we have to use our extension of the method, Eqs. $(11)–(13)$. As discussed in the previous section, in the thin superconductor limit the AP case can be treated in the single-mode approximation. Parameter *W* is

$$
W = \text{Re } L + \frac{\text{Im } L^2}{2\xi_S/d_S + \text{Re } L} \approx \text{Re } L
$$

and according to Sec. III A of Ref. 25 the single-mode critical temperature is determined from a system

$$
\ln \frac{T_{cs}}{T_c} = \text{Re}\left[\psi \left(\frac{1}{2} + \frac{T_{cs}}{T_c} \frac{\Omega^2}{2}\right)\right] - \psi \left(\frac{1}{2}\right),\,
$$

$$
\Omega \tan \left(\Omega \frac{d_{\text{Self}}}{\xi_S}\right) = \text{Re } L.
$$

In the second equation the argument of the tangent is small, so

FIG. 2. Typical normalized superconducting critical temperature dependence on the thickness of the ferromagnetic layers in a F/S/F trilayer structure for parallel and antiparallel magnetic configurations of the two ferromagnetic layers. Note, that a slight violation of the property $T_c \rightarrow T_{cs}$ as $d_F \rightarrow 0$ of Eqs. (4) and (11) is due to the decrease of the accuracy of numeric procedure for small d_F . It was checked that the discrepancy vanishes as the spatial resolution of the calculation is increased. Parameters values are $\gamma=0.15$, γ_b $=0.3$, and $d_S/\xi_S=2.47$.

$$
\Omega^2 = \frac{\xi_S}{d_{\text{Seff}}} \text{Re } L,
$$

which yields

$$
\ln \frac{T_{cs}}{T_{c[AP]}} = \psi \left(\frac{1}{2} + \frac{T_{cs}}{T_{c[AP]}} \frac{\xi_S}{d_S} \text{Re } L \right) - \psi \left(\frac{1}{2} \right). \tag{19}
$$

This is exactly the same result as given by Eqs. (18) and (20) of Ref. 28.

The actual experiments of Ref. 18 were performed on a structure with $d_S > \xi_S$. Thus neither of the approximations is suitable for their description. This is even more true if one recalls that the F layers were deliberately fabricated from weak ferromagnet; so the criterion that $E_{ex} \gg \omega_{n*}$ may not be valid either. To study the behavior of the experimental samples we performed numeric calculations as explained in Sec. II C.

IV. NUMERIC RESULTS

In this section, we show results for various material parameters and layer thicknesses. Material parameters are taken from published data for Nb (ρ_s =7.5 $\mu\Omega$ cm, ξ_s =8.9 nm) and Cu_xNi_{1−*x*} with *x*=0.43 (ρ_F =60 $\mu\Omega$ cm, ξ_F =7.6 nm).^{25,29} We plot typical behavior of T_c of the trilayer system as a function of d_F for d_S =22 nm, γ_b =0.3 and E_{ex}/k_B ~ 130 K for the P and AP cases in Fig. 2. Here the parameters are chosen so that we can compare with the bilayer result of Ref. 25 with $d_{\text{Seff}} = 11$ nm. Indeed, we find the same T_c in the P configuration.

FIG. 3. The $\Delta T_c = T_{c[AP]} - T_{c[P]}$ dependence on the thickness of the ferromagnetic layers in a F/S/F trilayer structure plotted for $\gamma = 0.15$, $\gamma_b = 0.3$, and $d_S / \xi_s = 2.47$.

As shown in Fig. 2, T_c of the trilayer depends on the relative magnetization orientation of the two F layers. The difference of the T_c values between the P and AP configurations, $\Delta T_c = T_{c[AP]} - T_{c[P]}$ is shown in Fig. 3 for the same materials parameters. As d_F increases, ΔT_c goes through a maximum and finally reaches a limiting value as $d_F \rightarrow \infty$.

We now examine the spatial variation of the anomalous Green function *F*, which is proportional to the density of Cooper pairs. The superconducting order parameter is given by the anomalous Green's function taken at zero imaginary time τ :

$$
F(x, \tau = 0) = T \sum_{\omega_n} F(x, \omega_n) = T \sum_{\omega_n > 0} F_+(x, \omega_n).
$$
 (20)

In Figs. $4(a)$ and $4(b)$, *F* is plotted for the P and AP configurations. We also plotted the sum

$$
F_{-}(x) = T \sum_{\omega_n > 0} F_{-}(x, \omega_n)
$$
 (21)

to characterize the imaginary part of *F*. As discussed above, $F₋(x)$ is an even function of *x* in the P configuration and an odd function in the AP configuration.

Now, we explore the ΔT_c dependence on various parameters. First we plot a family of $T_{c[P]}(d_F)$, $T_{c[AP]}(d_F)$, and $\Delta T_c(d_F)$ curves for various values of d_S . They are shown in Figs. 5(a) and 5(b) (other parameters are the same as stated above). The critical temperatures obey $T_{c[AP]} > T_{c[P]}$, as shown in Fig. 5(a). The decrease of T_c compared to T_{cs} (proximity effect) and the value of ΔT_c are large for thin d_S in agreement with Ref. 11. However in that case T_c is often too small to measure experimentally without a dilution refrigerator. The behavior is also very sensitive to d_F . In the inset of Fig. $5(b)$, we plot the thin d_S case again to show more detail. From Fig. 5(b), we find that the region of large ΔT_c is very narrow within the thin d_F range. The d_F value

FIG. 4. (a) $F(x, \tau=0)$ Eq. (20) and (b) $F_-(x)$ Eq. (21) for parallel and antiparallel configurations. Here $\gamma = 0.15$, $\gamma_b = 0.3$, $d_S / \xi_s = 2.47$, and $d_F/\xi_F = 1.0$.

where the ΔT_c has a maximum is slightly smaller than the d_F value where T_c has its minimum. For larger d_S the proximity effect becomes smaller, so it can be easily measured, but in this regime ΔT_c is small as well.

In Figs. 6(a) and 6(b), we plot normalized values of $T_{c[P]}$, $T_{c[AP]}$ and ΔT_c as a function of *d_S* for d_F/ξ_F =0.7. This plot is analogous to Fig. 2 of Buzdin *et al.*, 11,12 except that in the previous papers,^{11,12} $T_{c[P]}$ and $T_{c[AP]}$ were plotted as a function of $1/d_S$ which might make them less easy to use. We plot $T_{c[P]}$ and $T_{c[AP]}$ as a function of the normalized thickness of the S layer. As shown in Fig. 6(a), the region where the AP configuration is superconducting while the P configuration is normal is very narrow. In that region $T_{c[AP]}$ is also small. In Fig. 6(b) there is a maximum ΔT_c , however, the maximum usually corresponds to a minimum in T_c . We plot curves for only one value of d_F , because the functional behavior of $T_{c[P/AP]}$ and ΔT_c is very similar for various d_F values.

The proximity effect depends on many parameters, and some of them (diffusion coefficients, conductivities, and γ) are readily obtained from the literature or supplemental mea-

FIG. 5. (a) Normalized $T_{c[P]}$ and $T_{c[AP]}$. (b) ΔT_c dependence on d_F for various d_S/ξ_S values as noted. Inset of (b) shows the full range of ΔT_c values. Calculated for $\gamma = 0.15$ and $\gamma_b = 0.3$.

surements. However, it is not easy to find the value of E_{ex} and γ_b from other experiments. Physically E_{ex} is related to the Curie temperature of the F layer, but it is not a straightforward dependence. It can be extracted from the measurements by matching the position of the $T_c(d_F)$ minimum. The parameter γ_b is defined as $(R_bA)/(\rho_F\xi_F)$ and depends on both bulk properties, such as the band mismatch between the two materials, 6.9 and microstructural parameters, such as the S/F interfacial roughness. We present normalized ΔT_c values as a function of d_F for various E_{ex} and γ_b in Figs. 7 and 8. As shown in Fig. 7, for large E_{ex} (strong ferromagnet) the maximum ΔT_c is large, but in that case the T_c is small and the maximum of ΔT_c happens for a very thin (\sim 1 nm) F layer. It is not even clear whether an F layer of such thickness will order ferromagnetically, $30,31$ so such conditions are not favorable experimentally. For a weak ferromagnet (small E_{ex}), the proximity effect becomes smaller, and ΔT_c is also reduced.

Next, consider the effect of the transparency parameter γ_b at the interface. When $\gamma_b \rightarrow 0$, the interface becomes transparent, and the proximity effect is enhanced. For large γ_h , the

FIG. 6. (a) $T_{c[P]}$ and $T_{c[AP]}$ and (b) ΔT_c dependence on d_S for $d_F/\xi_F = 0.7$. Surface parameters are taken to be $\gamma = 0.15$ and γ_b $=0.3$.

proximity effect becomes small causing ΔT_c to decrease. In Fig. 8, we plot ΔT_c on a logarithmic scale for various values of γ_b . Although the magnitude of ΔT_c changes dramatically with γ_b , the overall behavior is similar for all γ_b values. Note again, that γ_b is affected by not only intrinsic materials parameters but also by the interface quality which depends on the sample preparation conditions.

The overall behavior of the ΔT_c dependence on various parameters can be summarized as follows: when T_c is small, $\Delta T_c / T_c$ is large. This is natural, because ΔT_c exists due to the interference of the proximity effects, and thus strong proximity effect implies a strong magnetization direction dependence. However, from an experimental viewpoint, too strong a proximity effect can make it difficult to measure T_c .

Finally we try to fit the experimental data for the F/S/F structure studied in Ref. 18. The best theoretical fit is shown in Fig. 9. Here $d_s = 19$ nm (i.e., $d_s > \xi_s$) and the values of the other parameters are taken as $\gamma=0.135$, $\gamma_b=0.3$, and E_{ex}/k_B =110 K. The behavior of T_c shows agreement between experiment and theoretical calculations. Theoretical results also show correct qualitative trends of the experimental data.

FIG. 7. ΔT_c dependence on d_F for various E_{ex}/k_B as noted. Calculated for parameters values $\gamma = 0.15$, $\gamma_b = 0.3$, and d_S / ξ_S $=$ 2.47

However, there is a large discrepancy in the magnitude of ΔT_c . Varying two unknown parameters γ_b and E_{ex} we were not able to fit both T_c and ΔT_c . We would like to contrast this result with the case of a thin superconductor $(d_S \ll \xi_S)$, in which it is always possible to fit given data T_c and ΔT_c ³² but which is not a good approximation for the $d_S > \xi_S$ experimental situation of Ref. 18.

Possible reasons for the disagreement between theory and experiment need to be considered. First, the real sample structure is not a simple trilayer. Extra ferromagnetic pinning layers were used to stabilize the AP configuration.¹⁸ When the thickness of the CuNi layer is small, the effect of the permalloy pinning layer must be included into the calculation. Therefore, the shift of the thickness dependence in ΔT_c

FIG. 8. ΔT_c dependence on d_F for various γ_b as noted. Calculated for $\gamma = 0.15$ and $d_S / \xi_S = 2.47$.

FIG. 9. T_c and ΔT_c (inset) for the trilayers taken from Ref. 18. Experimental data are shown as symbols and theoretical fit is shown as a dashed curve (dotted curve on the inset). Theoretical curves are calculated using parameters values $\gamma=0.135$, $\gamma_b=0.3$, $d_s=19$ nm, ξ_S =8.9 nm, ξ_F =7.6 nm, and E_{ex}/k_B =110 K.

might be ascribed to an extra permalloy layer. Second, asymmetry plays a role. In the experiments, the bottom CuNi (fcc with lattice constant \sim 3.55 Å) layer was grown on permalloy whose structure is fcc with lattice constant 3.569 Å. However, the top CuNi layer was grown on Nb whose crystal structure is bcc with lattice constant 3.3 Å. Therefore the interface quality and magnetic properties at the interface between Nb and the top CuNi are different from the interface between Nb and the bottom CuNi layer. Since the portion of the proximity effect from the interface dominates, the asymmetry at the interface can cause large effects. Since ΔT_c exists due to the interference of proximity effects, if there is asymmetry between the two F layers, it might decrease ΔT_c dramatically. Therefore removing asymmetry should be one way to increase ΔT_c . Furthermore, in our calculation we ignored the spin-orbit scattering, which was considered by Demler *et al.*³³ and Oh *et al.*³⁴ Since the spin-orbit scattering suppresses the oscillation of the proximity effect, that might play an important role in the magnetization orientation dependent effect.

V. CONCLUSIONS

We show that the single-mode approximation cannot be used to study the magnetization orientation dependence of T_c in F/S/F structures with $\xi_S \le d_S$. To find $T_{c[P/AP]}$ in this case we extend the numeric method developed for F/S bilayers²⁵ to the symmetric F/S/F trilayer case and we explore the ΔT_c dependence on various parameters. Our results are valid for arbitrary material parameters as long as the dirty limit condition is satisfied.

The difference ΔT_c generally reaches its maximum value when T_c is near its minimum. The parameters that give maximum values of ΔT_c are found for various materials and thicknesses of the ferromagnetic and superconducting layers. Comparing our results with experimental data we find that by fitting two unknown parameters, E_{ex} and γ_b , a quantitative agreement with T_c can be reached. It is however impossible to obtain quantitative agreement for ΔT_c at the same time. Thus, the $\xi_S \leq d_S$ case differs from the $d_S \leq \xi_S$ case. Possible reasons for this discrepancy between theory and experiment are discussed.

Note added in proof. Recently, the work of Fominov *et* al^{35} that also treats the critical temperature of $F/S/F$ trilayers appeared in print. This paper considers a symmetric system with an arbitrary angle between the magnetization of F layers. For parallel and antiparallel collinear configurations both the present paper and Ref. 35 obtain the same equations (8) , (9) , and $(11)–(13)$ to be solved numerically.

ACKNOWLEDGMENTS

We benefited from illuminating discussions with Ya. V. Fominov, A. A. Golubov, A. I. Buzdin, L. R. Tagirov, R. R. Ramazashvili, and M. R. Norman. We thank V. V. Ryazanov for providing experimental data prior to publication. C.-Y. You was supported by INHA University Research Grant No. INHA-30348. Work at Argonne National Laboratory was supported by the U.S. Department of Energy, Division of Basic Energy Science–Material Science under Contract No. W-31-109-ENG-38.

- ¹H. K. Wong, B. Y. Jin, H. Q. Yang, J. B. Ketterson, and J. E. Hillard, J. Low Temp. Phys. **63**, 307 (1986).
- 2Z. Radović, M. Ledvij, L. Dobrosavljević-Grujić, A. I. Buzdin, and J. R. Clem, Phys. Rev. B **44**, 759 (1991), and references therein.
- 3A. I. Buzdin and M. Yu. Kupriyanov, JETP Lett. **25**, 290 (1991); A. J. Buzdin, B. Bujicic, and M. Yu. Kupriyanov, Sov. Phys. JETP **74**, 124 (1992).
- 4C. L. Chien and D. H. Reich, J. Magn. Magn. Mater. **200**, 83 (1999) and references therein.
- 5V. V. Ryazanov, V. A. Oboznov, A. Yu. Rusanov, A. V. Veretennikov, A. A. Golubov, and J. Aarts, Phys. Rev. Lett. **86**, 2427 (2001).
- ⁶ J. Aarts, J. M. E. Geers, E. Brück, A. A. Golubov, and R. Coehoorn, Phys. Rev. B **56**, 2779 (1997).
- 7M. G. Khusainov and Yu. N. Proshin, Phys. Rev. B **56**, R14283 (1997).
- 8L. R. Tagirov, Physica C **307**, 145 (1998).
- 9L. Lazar, K. Westerholt, H. Zabel, L. R. Tagirov, Yu. V. Goryunov, N. N. Garif'yanov, and I. A. Garifullin, Phys. Rev. B **61**, 3711 (2000).
- 10S. Oh, D. Youm, and M. R. Beasley, Appl. Phys. Lett. **71**, 2376 (1997).
- ¹¹ A. I. Buzdin, A. V. Vedyayev, and N. V. Ryzhanova, Europhys. Lett. **48**, 686 (1999).
- ¹² I. Baladié, A. I. Buzdin, N. V. Ryzhanova, and A. V. Vedyayev, Phys. Rev. B **63**, 054518 (2001).
- 13L. R. Tagirov, Phys. Rev. Lett. **83**, 2058 (1999).
- 14A. Bagrets, C. Lacroix, and A. Vedyayev, cond-mat/0112934 (unpublished).
- 15V. Apinyan and R. Melin, cond-mat/0107038 (unpublished).
- 16P. G. de Gennes, Phys. Lett. **23**, 10 (1966).
- 17G. Deutscher and F. Meunier, Phys. Rev. Lett. **22**, 395 (1969).
- ¹⁸ J. Y. Gu, C.-Y. You, J. S. Jiang, J. Pearson, Ya. B. Bazaliy, and S. D. Bader, Phys. Rev. Lett. **89**, 267001 (2002).
- 19K. Maki, in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969).
- 20V. L. Berezinskii, Sov. Phys. JETP **20**, 287 (1974).
- 21A. F. Volkov, F. S. Bergeret, and K. B. Efetov, Phys. Rev. Lett. **90**, 117006 (2003).
- 22F. S. Bergeret, A. F. Volkov, and K. B. Efetov, Phys. Rev. B **68**, 064513 (2003).
- 23T. W. Clinton and M. Johnson, Appl. Phys. Lett. **70**, 1170 (1997).
- 24 Ya. V. Fominov, N. M. Chtchelkatchev, and A. A. Golubov, JETP Lett. **74**, 101 (2001).
- ²⁵ Ya. V. Fominov, N. M. Chtchelkatchev, and A. A. Golubov, Phys. Rev. B **66**, 014507 (2002).
- 26M. Yu. Kupriyanov and V. F. Lukichev, Zh. Eksp. Teor. Fiz. **94**, 139 (1988) [Sov. Phys. JETP **67**, 1163 (1988)].
- 27Z. Radović, L. Dobrosavljević-Grujić, A. I. Buzdin, and J. R. Clem, Phys. Rev. B **38**, 2388 (1988).
- ²⁸ I. Baladié and A. Buzdin, Phys. Rev. B **67**, 014523 (2003).
- 29V. V. Ryazanov *et al.* (unpublished).
- ³⁰ J. S. Jiang, D. Davidović, D. H. Reich, and C. L. Chien, Phys. Rev. Lett. **74**, 314 (1995).
- 31Th. Mühge, N. N. Garif'yanov, Yu. V. Goryunov, G. G. Khaliullin, L. R. Tagirov, K. Westerholt, I. A. Garifullin, and H. Zabel, Phys. Rev. Lett. **77**, 1857 (1996).
- 32A. I. Buzdin (private communication).
- 33E. A. Demler, G. B. Arnold, and M. R. Beasley, Phys. Rev. B **55**, 15174 (1997).
- 34S. Oh, Y.-H. Kim, D. Youm, and M. R. Beasley, Phys. Rev. B **63**, 052501 (2000).
- 35Ya. V. Fominov, A. A. Golubov, and M. Yu. Kupriyanov, JETP Lett. **77**, 510 (2003).