The superconducting critical temperature and singlet and triplet pair functions of superconductor/normal-metal/ferromagnet trilayers

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We calculate the superconducting critical temperature $T_c$, the singlet pair function $\Psi^+(x)$, and triplet pair function $\Psi^-(x)$ of superconductor/normal metal/ferromagnet (S/N/F) trilayers using the linearized Usadel equation near $T_c$. The Green’s function method developed by Fominov et al. for the S/F bilayers is extended to the S/N/F trilayer systems. The S of the trilayers is taken to be an s-wave singlet pairing superconductor, and the S/N and N/F interfaces are modeled in terms of the interface resistances parameterized, respectively, by $\gamma^{SN}_6$ and $\gamma^{NF}_6$. We present the $T_c$, $\Psi^+(x)$, and $\Psi^-(x)$ for typical $\gamma^{SN}_6$, $\gamma^{NF}_6$, and the exchange energy $E_{ex}$: (a) For a small (large) $\gamma^{NF}_6$, $T_c$ of S/N/F trilayers, as $d_N$ is increased, increases (decreases) on the length scale of N coherence length $\xi_N$ with a discontinuity at $d_N = 0$ due to a boundary condition mismatch. (b) $T_c(d_F)$ shows a non-monotonic behavior like S/F bilayers with a weakened shallow dip. (c) The odd frequency triplet component $\Psi^-(x)$, induced by $E_{ex}$ and proximity effects, has a maximum near the N/F interface and decreases on the length scale $\xi_N$ in F. It also penetrates into N and S regions on the length scale $\xi_N$ and $\xi_S$, respectively. Based on these results we make comments on the experimental observation of the odd triplet components and the recent $T_c$ measurements in Nb/Au/CoFe trilayer systems.

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I. INTRODUCTION AND MOTIVATION

When different states of matter are in contact, one affects the other over the coherence length $\xi$, which is referred to as the proximity effects. For instance, when a superconductor (S) and a normal metal (N) are in contact as in an S/N bilayer, the singlet pair function $\Psi^+(x) \sim \langle \phi^+(x) | \phi(x) \rangle$, where $\phi(x)$ is the field operator of spin $\sigma$ electron at the position $x$ and $\langle \rangle$ means the thermodynamic average, penetrates into the N region and decays exponentially on the length scale of N coherence length $\xi_N$. For diffusive metals, $\xi_N = \sqrt{D_N/2\pi T}$ where $D_N$ is the diffusion constant of the normal metal and $T$ is the temperature. Note that, however, the gap energy given by $\Delta(x) = V \Psi^+(x)$ vanishes in N because the pairing interaction $V = 0$ in the N region. The superconducting temperature $T_c$ of an S/N bilayer as a function of N thickness $d_N$ also decreases exponentially on the length scale of $\xi_N$. Here, $T_c$ is defined with the current parallel to the interfaces. Therefore, $T_c$ of an S/N bilayer is determined by the highest temperature at which the singlet pair function $\Psi^+(x)$ does not vanish at least at one point within the bilayer.

The proximity effects in S/F bilayers have also been studied intensively. Like the S/N case, $\Psi^+(x)$ of an S/F bilayer decreases exponentially in the F region, and $T_c$ decreases as the F thickness $d_F$ is increased. Many of the interesting S/F proximity effects occur at the nanoscale range of layer thickness. The observation of these effects was made possible by the progress of fabrication technique of high quality hybrid S/F layers. The S/F proximity effects have the following differences compared with S/N: (a) The decay length scale in F, $\xi_{ex}$, given by $\xi_{ex} = \sqrt{D_F/E_{ex}}$, is much smaller than $\xi_N$ because the exchange energy $E_{ex}$ is much larger than $T_c$. (b) The pair function oscillates as well as decreases in the F region because the net momentum of a Cooper pair is non-zero in F. By the same reason, $T_c(d_F)$ does not monotonically decrease like S/N as $d_F$ is increased but shows a shallow dip. The oscillation has been confirmed by the observation of the “$\pi$-state” in S/F/S Josephson junction, where two superconductors separated by a ferromagnet of appropriate thickness can have a phase difference of $\pi$. (c) Triplet pairing component (TPC) is induced in addition to the dominant singlet pairing component (SPC).
The triplet pairing is realized in $^3$He and Sr$_2$RuO$_4$, for instance, in the form of $p$-wave pairing. The induced TPC in S/F systems in the diffusive limit, however, is even ($s$-wave) in momentum but odd in frequency, referred to as odd frequency triplet pairing component (OFTPC). The OFTP was first suggested by Berezinskii in the context of $^3$He superfluidity but it turned out that it is the $p$-wave triplet pairing that is realized in $^3$He. The OFTP is induced from $s$-wave SPC because time reversal symmetry is broken by the exchange field in S/F bilayers. Just like non-$s$-wave pairing components are induced from $s$-wave one when the translational symmetry is broken, OFTPC is induced in S/F bilayers from the singlet component because the time reversal symmetry is broken by the exchange field in F region. This can be seen directly from Fig. 4 where the induced TPC vanishes as $E_{xx} \to 0$.

While it is natural to expect that the characteristic length scale in F region is very short given by $\xi_{ex}$, it was realized that there exist long range proximity effects in S/F systems set by the long length scale of $\xi_F = \sqrt{D_F/2\pi T}$. For instance, the long range triplet pairing was suggested to understand the unexpected conductance increase of S/F structures below $T_c$. The condition for the occurrence of the long length TPC is that the magnetization is not unidirectional. When the magnetization in F is unidirectional, the induced triplet pairing component has the short coherence length $\xi_{ex}$ like the singlet one and can be represented as $S_z = 0$ component along the magnetization direction in F. More explicitly, it is given by $\langle \phi_\uparrow(x, \tau)\phi_\downarrow(x) + \phi_\downarrow(x, \tau)\phi_\uparrow(x) \rangle$, where $\tau$ is the imaginary time. When the magnetization is not unidirectional, on the other hand, other triplet components with $S_z = \pm 1$ given by $\langle \phi_\uparrow(x, \tau)\phi_\uparrow(x) \rangle$ and $\langle \phi_\downarrow(x, \tau)\phi_\downarrow(x) \rangle$ are also induced because $S_z = 0$ along a spin quantization axis is not pure $S_z = 0$ but a mixture of $S_z = 0$, $+1$, and $-1$ along a different axis. The $S_z = \pm 1$ TPC has the long coherence length $\xi_F$ in F because the exchange field is not pair breaking for them.

We here note the following distinctive features of the TPC which appears in S/F systems. See below for more detailed discussion. (a) The S in an S/F bilayer is a conventional s-wave singlet superconductor. The exotic state of OFTPC is induced not because the S of the S/F is exotic. It is induced because of the proximity effects and the broken time reversal symmetry. (b) TPC is induced in addition to the dominant SPC, and may have short coherence length $\xi_{ex}$ or long coherence length $\xi_F$. (c) TPC is even in momentum but odd in frequency. (d) The $T_c$ of an S/F bilayer is determined by the SPC (See Eq. (11) below), and TPC can change $T_c$ indirectly only by changing SPC through the boundary conditions. See Sec. II in the following for detailed discussions. The OFTP is an exotic state of matter, but it has not been directly observed yet. A lot of experimental and theoretical work has focused on finding fingerprints of the OFTP correlations. The basic idea is that one convert the short range triplet component into the long range one by controlling or inducing nonuniformity of the F magnetization direction, and observe the long length scale triplet component with appropriate experiments. Even when the exchange field is uniform in the F, the long range components are induced when the interface is spin active which causes spin flip or spin rotation. The present formulation can be straightforwardly applied in this case too with a modified version of the boundary conditions (BC) given by Eq. (13). Recently, there was a report which strongly hints the existence of long length OFTPC in S/F/S.

The superconductor-ferromagnet systems, as described above, exhibit very interesting and exotic behavior, and it will be important to understand them in a systematic way. To do that, we have theoretically studied the S/N/F trilayer systems. By varying the intervening N thickness $d_N$ and the interface resistances between S and N and N and F, represented in terms of $\gamma^{SN}_b$ and $\gamma^{NF}_b$, respectively, we can control the proximity effects in a systematic way. In this paper, the proximity effects in S/N/F trilayers are studied for $T_c$, SPC, and TPC. This paper is organized as follows: After this section, we present in Sec. II the generalization to S/N/F trilayers of the numerically exact Green’s function method developed by Fominov et al. for S/F bilayers. The resulting Usadel equations subject to appropriate boundary conditions are then solved self-consistently by numerical iterations for $T_c$, SPC, and TPC. The results will be presented in Sec. III for typical values of $\gamma^{SN}_b$, $\gamma^{NF}_b$, and $E_{xx}$. Based on these results, we will make some comments on the experimental observation of the odd frequency triplet components and the recent $T_c$ measurements in Nb/Au/CoFe bilayer systems. We then conclude with the summary and concluding remarks in Sec. IV. In Appendix, we collect some technical details for calculating the singlet and triplet pairing components.

II. USADEL FORMULATION

A. Usadel equation for S/N/F trilayers

We wish to understand the proximity effects in the S/N/F trilayer systems, which is schematically shown in Fig. 1. The S is a conventional s-wave singlet pairing superconductor like Nb, N is Au, Cu, or Al (above Al’s $T_c$), and F is CoFe or Ni. Each of S, N, F is characterized by the coherence length $\xi$ and resistivity $\rho$. In addition, S layer is described by superconducting critical temperature $T_{c0}$, and F by the exchange energy $E_{ex}$. The layers of thin films are in the dirty limit and we employ the dirty limit quasi-classical theory, the Usadel equation, to describe them. Moreover, since we are interested in calculating the superconducting transition temperature $T_c$ and the pair functions near $T \approx T_c$ of S/N/F, we will use the linearized Usadel equation. Near $T_c$, the normal Green function is $G = \text{sgn}(\omega)\delta_{\sigma\sigma'}$, where $\sigma$ and $\sigma'$ are the spins of two electrons forming a Cooper pair, and the anomalous function is $F \to 0$. The Usadel equation is
therefore linearized with respect to $F$. In a general case where all four components of $F$ are kept, $F$ may be represented as a $2 \times 2$ matrix or a 4 component vector. In the present problem where the exchange field is uniform over the $F$ region, only two components, SPC and short range TPC, appear in the equation and the anomalous function $F$ may be represented as a two component vector or scalar complex function. Because we will consider long range TPC in a subsequent study where a vector representation is convenient we will formulate the present problem in terms of two component vector

$$F_i(x, i\omega_n) = \left( \frac{F_i^+(x, i\omega_n)}{F_i^+(x, i\omega_n)} \right),$$

where $i = S, N, F$, and $x$ is the coordinate perpendicular to the interface and the translational symmetry is assumed parallel to the interface. The superscript $\pm$ refers to the even and odd functions of the frequency.

$$F^\pm(x, i\omega_n) \equiv \frac{F(x, i\omega_n) \pm F(x, -i\omega_n)}{2},$$

where the anomalous function $F$ is defined by

$$F(x, i\omega_n) = - \int_0^\beta d\tau e^{i\omega_n \tau} T\phi_\tau(x, \tau) \phi_\tau(x, 0),$$

where $T\phi$ is the $\tau$ ordering operator. Then, $F(x, -i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} T\phi_\tau(x, \tau) \phi_\tau(x, 0)$, and the even function $F^+$ represents the SPC and the odd function $F^-$ the TPC of the anomalous function. We will also use the SPC (TPC) to stand for $\Psi^+(x)$ ($\Psi^-(x)$) which is just the summation over Matsubara frequencies of $F^+(x, i\omega_n)$ ($F^-(x, i\omega_n)$) as given in Eq. (8).

$$\xi_{S}^{2} \pi T_{c} \frac{\partial^{2}}{\partial x^{2}} F_{S}(x, i\omega_n) = |\omega_n| F_{S}(x, i\omega_n) - \Delta(x), \hspace{1cm} (0 < x < d_{S}),$$

$$\xi_{N}^{2} \pi T_{c} \frac{\partial^{2}}{\partial x^{2}} F_{N}(x, i\omega_n) = |\omega_n| F_{N}(x, i\omega_n),$$

$$(-d_{N} < x < 0),$$

$$\xi_{F}^{2} \pi T_{c} \frac{\partial^{2}}{\partial x^{2}} F_{F}(x, i\omega_n) = |\omega_n| F_{F}(x, i\omega_n) + i \text{sgn}(\omega_n) E_{0} \sigma_{i} F_{F}(x, i\omega_n),$$

$$(-d_{F} - d_{N} < x < -d_{N}).$$

where $\omega_n = 2\pi T (n + \frac{1}{2})$ is the Matsubara frequency and $\sigma_{1}$ is the Pauli spin matrix. $\Delta(x) = \begin{pmatrix} \Delta(x) \\ 0 \end{pmatrix}$. Eq. (9) explicitly shows that the exchange field $E_{ex}$ couples the SPC $F^+_S$ and TPC $F^-_F$ and induces TPC from SPC. The coherence length is $\xi = \sqrt{\frac{\pi T_{c}}{2}}$ in the dirty limit where $D$ is the diffusion constant. Then,

$$\xi_{S} = \sqrt{\frac{D_{S}}{2\pi T_{c}}}, \quad \xi_{N} = \sqrt{\frac{D_{N}}{2\pi T_{c}}}, \quad \xi_{F} = \sqrt{\frac{D_{F}}{2\pi T_{c}}} \tag{7}$$

in each S, N, and F layer, as discussed in Introduction. The singlet component $F^+_S$ determines the gap function $\Delta(x)$

$$\Delta(x) = V g(\epsilon_F) \pi T_{c} \sum_{\omega_n > 0} F^+_S(x, i\omega_n),$$

where $V$ and $g(\epsilon_F)$ are, respectively, the pairing interaction and the density of states per spin at the Fermi level. It satisfies the self-consistency relation

$$\Delta(x) \ln \left( \frac{T_{c}0}{T_{c}} \right) = \pi T_{c} \sum_{\omega_n} \left[ \frac{\Delta(x)}{|\omega_n|} - F^+_S(x, i\omega_n) \right], \tag{9}$$

where $T_{c}$ is the superconducting critical temperature of the S/N/F trilayer and $T_{c0}$ is that of the S layer alone without the N and F layers. Eq. (9) explicitly shows that $T_{c}$ is determined by the singlet component alone. The triplet components may affect $T_{c}$ only by changing the singlet component through the boundary conditions discussed below.

Being a differential equation, the Usadel equation must be supplemented by boundary conditions. The appropriate BC for the Usadel equation are well established and given as follows,$^{25}$

$$\frac{d}{dx} F_{F}(-d_{F} - d_{N}) = 0, \tag{10}$$

$$\xi_{N} \frac{d}{dx} F_{N}(-d_{N}) - \gamma_{NF} \xi_{F} \frac{d}{dx} F_{F}(-d_{N}) = 0, \tag{11}$$

$$\xi_{S} \frac{d}{dx} F_{S}(0) - \gamma_{SN} \xi_{N} \frac{d}{dx} F_{N}(0) = 0, \tag{12}$$

$$F_{F}(-d_{N}) - F_{F}(-d_{N}) = \gamma_{b}^{NF} \xi_{F} \frac{d}{dx} F_{F}(-d_{N}). \tag{13}$$

$$\frac{d}{dx} F_{N}(0) = \gamma_{SN} \xi_{N} \frac{d}{dx} F_{N}(0), \tag{14}$$

$$\frac{d}{dx} F_{S}(d_{S}) = 0, \tag{15}$$

where

$$\gamma_{NF} \equiv \frac{\rho_{N} \xi_{N}}{\rho_{F} \xi_{F}}, \quad \gamma_{SN} \equiv \frac{\rho_{S} \xi_{S}}{\rho_{N} \xi_{N}}. \tag{16}$$

The $\gamma_{b}^{SN}$ and $\gamma_{b}^{NF}$ are dimensionless quantities characterizing S/N and N/F interfaces, respectively, given by

$$\gamma_{b}^{NF} \equiv \frac{R_{b}^{NF} A}{\rho_{F} \xi_{F}}, \quad \gamma_{b}^{SN} \equiv \frac{R_{b}^{SN} A}{\rho_{N} \xi_{N}}, \tag{17}$$

The $R_{b}^{SN}$ and $R_{b}^{NF}$ are dimensionless quantities characterizing S/N and N/F interfaces, respectively, given by.

FIG. 1: Schematic drawing of an S/N/F trilayer. The coordinate $x$ is taken as perpendicular to the interfaces.
where $R_b^{NF}$ and $R_b^{SN}$ are the interface resistances between N and F and S and N, respectively, and $A$ is the interface area. $\gamma_b^{SN}$ and $\gamma_b^{NF}$ are modeled in terms of spin conserving potential barriers, and do not introduce any spin modifying mechanism. On the other hand, the boundary of the F can be spin dependent or spin active, and the BC of Eq. (13) should be modified accordingly. The spin-active interface can induce the long range triplet components. One possible description of the spin-active interface is that the parameter $\gamma_b^{NF}$ is given by a $4 \times 4$ matrix instead of a scalar with the state $|\gamma_b^{NF}|$.

Then, utilizing the BC at $x = -d_N$ of Eq. (11) and (13), the $F_N(-d_N)$ and $\frac{d}{dx}F_N(-d_N)$ can be written in terms of $F_F(-d_N)$ and $\frac{d}{dx}F_F(-d_N)$. Then, using Eq. (21), we find

$$\xi_N \frac{d}{dx} F_N(-d_N) = \hat{A}_{NF} F_N(-d_N),$$

where

$$\hat{A}_{NF} \equiv \left( 1 + \hat{A}_F \gamma_b^{NF} \right)^{-1} \gamma_{NF} \hat{A}_F.$$ (25)

B. Boundary condition in terms of $F_S$

The Usadel equation (4), (5), (6) together with the BC (10), (11), (12), (13), (14), (15) and self-consistency equation (9) forms a complete set of equations to describe an S/N/F trilayer near $T \approx T_c$. It is solved by extending the numerically exact Green’s function technique developed by Fominov et al. for the S/F bilayers. To utilize the technique, everything should be written in terms of $F_S$ alone in the S region. The Usadel equation and the self-consistency relation are already written in terms of $F_S$ alone in the S region, and the remaining task is to write the BC at $x = 0$ and $x = d_S$ in terms of $F_S$ only. The BC at $x = d_S$ is already given by Eq. (15), and the one at $x = 0$ can be derived by writing the Usadel equation with the corresponding BC successively starting from the F to N regions. The procedure is very similar to Fominov et al. (22).

First, for the F region we solve the homogeneous equation (6) with BC (10) to obtain

$$F_F = \left( \begin{array}{cc} \cosh k_F(x_{NF}) & \cosh k_F^*(x_{NF}) \\ - \cosh k_F(x_{NF}) & \cosh k_F^*(x_{NF}) \end{array} \right) \left( \begin{array}{c} C_F^+(i\omega_n) \\ C_F^-(i\omega_n) \end{array} \right),$$

where

$$x_{NF} = x + d_N + d_F, \quad k_F = \frac{1}{\xi_F} \sqrt{\frac{|\omega_n| + iE_{ex}}{\pi T_c}}.$$

Note that the $k_F$ implies another length scale $\xi_F$ much shorter than $\xi_F$ alluded earlier. Because $E_{ex} \gg |\omega_n|$ for relevant Matsubara frequencies, one has

$$\xi_F \frac{d}{dx} F_F(-d_N) = \hat{A}_F F_F(-d_N),$$

where

$$\hat{A}_F = \left( \begin{array}{cc} \Re A_F & -\Im A_F \\ -\Im A_F & \Re A_F \end{array} \right),$$

$$A_F \equiv k_F \xi_F \tanh k_F d_F.$$ (23)

where

$$\hat{A}_{NF} \equiv \left( 1 + \hat{A}_F \gamma_b^{NF} \right)^{-1} \gamma_{NF} \hat{A}_F.$$ (25)

Second, the anomalous function $F_N$ in the N region described by Eq. (6) may be written as

$$F_N(x, i\omega_n) = F_N(-d_N) \cosh k_N(x + d_N) + \xi_N \frac{d}{dx} F_N(-d_N) \frac{\sinh k_N(x + d_N)}{k_N \xi_N},$$

where

$$k_N = \frac{1}{\xi_N} \sqrt{\frac{|\omega_n|}{\pi T_c}}.$$ (27)

Then, we use Eqs. (20) and (24) to obtain

$$\xi_N \frac{d}{dx} F_N(0) = \hat{A}_{NS} F_N(0),$$

where

$$\hat{A}_{NS} \equiv \left( A_N + \hat{A}_{NF} \right) \left( 1 + \frac{\hat{A}_{NF} A_N}{k_N^2 \xi_N^2} \right)^{-1},$$

$$A_N = k_N \xi_N \tanh k_N d_N.$$ (30)

Third, using BC at $x = 0$ given by Eqs. (12) and (13), and Eq. (28), we can finally obtain the BC in terms of $F_S(0)$ and $\frac{d}{dx} F_S(0)$ such as

$$\xi_S \frac{dF_S(0)}{dx} = \hat{A}_S F_S(0),$$

where

$$\hat{A}_S \equiv \left( 1 + \hat{A}_{NS} \gamma_b^{SN} \right)^{-1} \gamma_{SN} \hat{A}_{NS}.$$ (32)

Eq. (31) connects $\frac{dF_F(0)}{dx}$ and $\frac{dF_S(0)}{dx}$ with $F_F(0)$ and $F_S(0)$ only to solve the Usadel equation in S region for $0 < x < d_S$ given by Eq. (4).

$$\pi T_c \xi_S^2 \frac{\partial^2}{\partial x^2} F_S^+(x, i\omega_n) - |\omega_n| F_S^+(x, i\omega_n) = -\Delta(x).$$ (33)
We write from BC of (15)

\[ F_S(x, i\omega_n) = C_S(i\omega_n) \cosh k_S(x - d_s), \quad (34) \]

where

\[ k_S = \frac{1}{\xi_S} \sqrt{\frac{[\omega_n]}{\pi T_c}}. \quad (35) \]

Using this to eliminate the \( F_S(0) \) from (31) for \( \frac{dF_S(0)}{dx} \), we obtain

\[ \xi_S \frac{dF_S^+(0)}{dx} = W(i\omega_n)F_S^+(0), \quad (36) \]

where

\[ W(i\omega_n) = \gamma_{SN} \frac{A_S(\gamma_b^{SN} + ReB_{SN}) + \gamma_{SN}}{A_S[\gamma_b^{SN} + B_{SN} + \gamma_{SN}(\gamma_b^{SN} + ReB_{SN})]}. \quad (37) \]

and \( A_S \) and \( B_{SN} \) are defined by

\[ A_S = k_S \xi_S \tanh k_S d_S, \quad (38) \]

\[ B_{SN} = [k_N \xi_N \tanh k_N (d_N + x_0)]^{-1}, \quad (39) \]

\[ \tanh k_N x_0 = \frac{1}{k_N \xi_N \gamma_{NF} + \alpha_f}. \quad (40) \]

C. Green’s function method

Now, the problem is reduced to solving Eq. (33) with BC (15) and (36). To do it by the Green’s function technique, one needs to solve the following source equation:

\[ \pi T_c \xi_S \frac{\partial^2}{\partial x^2} G(x, y) - |\omega_n| G(x, y) = -(x - y), \quad (41) \]

with the BC corresponding to (30) and (15)

\[ \xi_S \frac{\partial}{\partial x} G(0, y) = W(i\omega_n)G(0, y), \quad (42) \]

\[ \xi_S \frac{\partial}{\partial x} G(d_s, y) = 0. \quad (43) \]

The Green’s function can be constructed as follows:

\[ G(x, y; i\omega_n) = \frac{k_S[|\omega_n|]}{\sinh k_S d_S + \frac{W(i\omega_n)}{\xi_S} \cosh k_S d_S} \times \begin{cases} v_1(x)v_2(y), & 0 < x < y \\ v_1(y)v_2(x), & y < x < d_s \end{cases}, \quad (44) \]

where

\[ v_1(x) = \cosh k_S x + \frac{W(i\omega_n)}{k_S \xi_S} \sinh k_S x, \quad (45) \]

\[ v_2(x) = \cosh k_S(x - d_s). \quad (46) \]

The solution of (33) is then

\[ F_S^+(x, i\omega_n) = \int_0^dS dy G(x, y; i\omega_n)\Delta(y). \quad (47) \]

The gap function \( \Delta(x) \) is determined by Eq. (8).

Substituting (17) into (8) gives the self-consistency equation,

\[ \Delta(x) = V g(\epsilon_F)\pi T_c \sum_{\omega_n>0} \int_0^dS dy G(x, y; i\omega_n)\Delta(y). \quad (48) \]

From this self-consistency equation, we can write down the equation for \( T_c \) with respect to \( T_{c0} \).

\[ \Delta(x) \ln \left( \frac{T_{c0}}{T_c} \right) = \int_0^dS dy M(x, y)\Delta(y), \]

\[ M(x, y) = \pi T_c \sum_{\omega_n>0} \left| \delta(x-y) - G(x, y; i\omega_n) \right|. \quad (49) \]

The above integral equation can be reduced to an eigenvalue problem after we change the integration over \( y \) into a summation by discretization. The \( T_c \) is determined by the smallest eigenvalue of the discretized \( M(x, y) \) matrix, which yields the highest \( T_c \). One plugs an arbitrary initial \( T_c \) into the right-hand side of Eq. (49) and calculates a new \( T_c \), and iterates until the input and output are equal within a tolerance. After a convergence is reached, \( T_c \) is obtained, and the corresponding eigenvector to the smallest eigenvalue gives \( \Delta(x) \). Then, the anomalous function \( F^+ \) can be obtained from Eq. (17), and the singlet and triplet pair functions \( \Psi^+(x) \) and \( \Psi^-(x) \) can be calculated from

\[ \Psi^\pm(x) = \pi T_c \sum_{\omega_n>0} F^\pm(x, i\omega_n). \quad (50) \]

Technical details for calculating SPC and TPC are collected in Appendix.

III. RESULTS: \( T_c \) AND PAIR FUNCTIONS OF S/N/F TRILAYERS

A. Perfect interfaces

\( T_c \) of S/N/F trilayers were calculated by self-consistently solving Eq. (19) by numerical iterations. And \( T_c \) of S/N bilayers were calculated for comparison. The singlet and triplet pair functions were also calculated as detailed in Appendix. Let us first consider the ideal case of perfect interfaces with \( \gamma_{SN} = \gamma_{NF} = 0 \). We take \( \rho_S = 15.9627 \mu \Omega cm, \rho_N = 2.0 \mu \Omega cm, \rho_F = 40.0 \mu \Omega cm, \xi_S = 7.0 nm, \xi_N = 110 nm, \xi_F = 10.241 nm, E_{ex} = 1235 K, \) and \( T_{c0} = 7.927 K \), which are appropriate for S = 23 nm Nb, N = Au, and F = CoFe as reported in the reference. Recall that the condition \( E_{ex} \tau \ll 1 \) should be satisfied for the diffusive Usadel equation to be
applicable. Using $D = \frac{1}{4}v_F^2\tau$, and the $\xi_F$ and $T_{c0}$ values, we obtain $E_{ex}\tau = 10^{-2}$ so that the Usadel equation is applicable to Nb/CoFe systems.

We show in Fig. 2(a) $T_c$ as a function of $N$ layer thickness, $d_N$, for $d_S = 23$ nm and $d_F = 23$ nm S/N and S/N/F. For S/N bilayers $T_c(d_N)$ decreases as $d_N$ is increased, but for S/N/F trilayers $T_c(d_N)$ increases as $d_N$ is increased. The length scale of both decrease and increase is given by the N coherence length $\xi_N$. As $d_N \to \infty$ the two $T_c$ approach each other as expected. In Fig. 2(b) we show $T_c$ as a function of $F$ for S/F and S/N/F. Note the different length scales between (a) and (b) given by $\xi_N$ and $\xi_{ex}$, respectively. $T_c(d_F)$ for S/F shows the well known behavior of an exponential decrease with a shallow dip. For S/N/F, we took $d_N = 50$ nm. The presence of the N layer weakens the effects of exchange energy of F. Consequently, $T_c(d_F)$ for S/N/F, compared with S/F, is lower at $d_F = 0$ but higher as $d_F \to \infty$, and has a shallower dip.

We may also calculate the pair functions as well as $T_c$ from the Usadel equation for various S-N-F layers. In Fig. 3(a) we show the SPC $\Psi^+(x)$ for S/N and S/N/F for $d_S = 23$ nm, $d_N = 50$ nm, and $d_F = 23$ nm, normalized by the value at $x = 23$ nm. It decreases monotonically in N but non-monotonically in F. The non-monotonicity of $\Psi^+(x)$ and $T_c(d_F)$ results from the same physics. It may be understood as originating from the non-zero net momentum of a Cooper pair. In (b) we show both SPC and TPC for an S/N/F. While SPC is maximum at the S outer surface of $x = 23$ nm, TPC is maximum near the N/F interface. The position of TPC peak is roughly $\xi_{ex}$ from the N/F interface.

To see the TPC more clearly, we plot in Fig. 4 the SPC and TCP of S/F bilayers for several values of $E_{ex}$. Note that for $E_{ex} = 0$ F becomes like an N; the length scale $\xi_{ex}$ becomes $\xi_F$ and TPC vanishes. The TPC becomes small also for large $E_{ex}$ because TPC decays rapidly for small $\xi_{ex} \propto E_{ex}^{-1/2}$. The TPC $\to 0$ as $E_{ex} \to 0$ or $\to \infty$, and is fully induced for an intermediate $E_{ex}$, as can be seen from figure (b). For each $E_{ex}$, the peak of TPC is determined by the competition between the exponential decrease of length scale $\xi_{ex}$ and linear increase determined by the BC

$$\xi_S \frac{d}{dx} F(0) - \gamma_{SF} \xi_F \frac{d}{dx} F(0) = 0. \quad (51)$$

The TPC, therefore, has a peak at around $\xi_{ex}$ away from S/F interface, which can be seen from Fig. 4.

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**FIG. 2:** (a) Numerical results of $T_c/T_{c0}$ of S/N/F and S/N as a function of $d_N$, shown by dashed and solid curves, respectively. Both curves have the coherence length $\xi_N$ and merge as $d_N \to \infty$ as expected. (b) $T_c/T_{c0}$ of S/N/F and S/F as a function of $d_F$, shown by the dashed and solid curves. Note the different length scales $\xi_N$ and $\xi_{ex}$ between (a) and (b).

**FIG. 3:** (a) SPC of S/N/F and S/N shown by the solid and dashed lines, respectively. $\Psi(x)$ is normalized by the value at the outer surface of the S layer. (b) SPC and TPC of an S/N/F trilayer shown by solid and dashed lines, respectively. TPC is magnified by 10 times for clarity.

**FIG. 4:** The SPC and TCP of S/F bilayers for several values of $E_{ex}$. Note that for $E_{ex} = 0$ F becomes like an N; the length scale $\xi_{ex}$ becomes $\xi_F$ and TPC vanishes. The TPC becomes small also for large $E_{ex}$ because TPC decays rapidly for small $\xi_{ex} \propto E_{ex}^{-1/2}$. The TPC $\to 0$ as $E_{ex} \to 0$ or $\to \infty$, and is fully induced for an intermediate $E_{ex}$, as can be seen from figure (b). For each $E_{ex}$, the peak of TPC is determined by the competition between the exponential decrease of length scale $\xi_{ex}$ and linear increase determined by the BC

$$\xi_S \frac{d}{dx} F(0) - \gamma_{SF} \xi_F \frac{d}{dx} F(0) = 0. \quad (51)$$

The TPC, therefore, has a peak at around $\xi_{ex}$ away from S/F interface, which can be seen from Fig. 4.
is the largest value of $\Psi^+$ decreases in F region as shown in Figs. 6 and 7. An 
$\mathbf{F} \gamma$ increased. $\mathbf{T}$ figures (a) and (b), however, $\Psi^+$ shows 
the same $\gamma$ seen from Fig. 5. Figure (a) shows 
an S/N/F trilayers. This can be 
10 1.0 0.2 0.0 -20 -10 0 10 20 $x$ (nm) 
(a) SPC 
(b) TPC 
FIG. 4: SPC and TPC of S/F bilayers for several $E_{ex}$. The 
peak position of TPC is given by the decay length scale $\xi_{ex}$ of 
SPC. Note that the TPC vanishes as F becomes an N ($E_{ex} = 0$).

B. Effects of interface resistances

We now turn to the more realistic case with non-zero interface resistances. There are two interfaces in 
an S/N/F, between S and N, and N and F, parameterized by $\gamma_{SN}^b$ and $\gamma_{NF}^b$, respectively. The main effect of the interface resistances is to weaken the proximity effects and increase the $T_c$ of S/N/F trilayers. This can be seen from Fig. 6. Figure (a) shows $T_c$ vs. $d_N$ of S/N/F for several $\gamma_{SN}^b$ with $\gamma_{NF}^b = 0$. $T_c$ vs. $d_N$ of S/N with the same $\gamma_{SN}^b$ are also shown for comparison. Figure (b) shows $T_c$ vs. $d_N$ for several $\gamma_{NF}^b$ with $\gamma_{SN}^b = 0$. In both figures (a) and (b), $T_c$ of a given $d_N$ increases as $\gamma_b$ is increased.

Another, perhaps more technical, way of saying this is from BC of Eqs. (11), (12), (13), and (14). Non-zero $\gamma_{SN}^b (\gamma_{NF}^b)$ introduces the discontinuity of the anomalous function $F^\pm$ at the interface. The anomalous function $F^+$ and pair function $\Psi^+$, therefore, increases in S but decreases in F region as shown in Figs. 6 and 7. An increase of $\Psi^+(x)$ in S means an increase of $T_c$ because it is the largest value of $\Psi^+(x)$ that determines $T_c$. (In the figures, however, $\Psi^+(x)$ is normalized at $x = d_S$ and this point is not manifested clearly.) We plot in Fig. 6 $\Psi^+(x)$ for S/N/F for several $\gamma_{SN}^b$ values with $\gamma_{NF}^b = 0$. And in Fig. 7 $\Psi^+(x)$ for several $\gamma_{NF}^b$ values with $\gamma_{SN}^b = 0$. Note that $\Psi^+(x)$ in S region is increased as $\gamma_{SN}^b$ or $\gamma_{NF}^b$ is increased.

Now, let us look at in more detail how $T_c$ behaves as a function of $d_N$ for non-zero $\gamma_{SN}^b$ or $\gamma_{NF}^b$. When $\gamma_{NF}^b = 0$ and $\gamma_{SN}^b$ is increased for S/N/F, as shown in Fig. 5(a), $T_c$ always increases as $d_N$ is increased. However, when $\gamma_{SN}^b$ is increased with $\gamma_{NF}^b = 0$, $T_c(d_N)$ increases with $d_N$ for $\gamma_{SN}^b = 0$ but decreases for $\gamma_{NF}^b = 1.0$, and the two curves merge together as $d_N \to \infty$. This is simple to understand. When $\gamma_{NF}^b = 0.0$, the pair breaking effects of the exchange field of F fully influences S for small $d_N$, and its effect is weakened as $d_N$ is increased. $T_c$, therefore, increases as $d_N$ is increased. When $\gamma_{NF}^b = 1.0$, on the other hand, the effects of F is almost blocked out and it behaves like S/N. Consequently, $T_c$ of $\gamma_{NF}^b = 1.0$ is much larger compared with that of $\gamma_{NF}^b = 0.0$ as $d_N \to 0$ and decreases as $d_N$ is
increased. When $d_N \gtrsim 200$ nm, the effects of F are also blocked out irrespective of $\gamma_{NF}$, and all $T_c$ curves merge together.

\textbf{FIG. 6}: The SPC and TPC of S/N/F for several $\gamma_{SN}$ with $\gamma_{NF} = 0$. The inset shows TPC in detail in F region. Non-zero $\gamma_{SN}$ produces a discontinuity in SPC and TPC at the S/N interface.

We now turn to the calculations of pair functions for S/N/F. In Fig. 6 we took $\gamma_{NF} = 0$ and plot SPC and TPC for several $\gamma_{SN}$. Non-zero $\gamma_{SN}$ introduces the discontinuity in both SPC and TPC. The inset shows the peak and dip structure of TPC more closely. As discussed for Fig. 4 the TPC has a peak around $\xi_{ex}$ away from the N/F interface. In Fig. 7 we plot SPC and TPC for several $\gamma_{NF}$ with $\gamma_{SN} = 0$. The discontinuity is at the N/F interface in this case.

\textbf{C. $T_c$ discontinuity due to boundary condition mismatch}

An interesting point for $T_c(d_N)$ of S/N/F trilayers appears when we consider $d_N \to 0$ limit. $T_c$ of this limit, of course, ought to coincide with that of the corresponding S/F of $d_N = 0$. For example, $T_c$ of Nb/Au/CoFe trilayers must approach that of Nb/CoFe as Au thickness goes to 0. Also, the change of $T_c$ with $d_N$ should have the length scale of $\xi_N$ simply because there is no other length scale in the N region. We therefore expect that $T_c(d_N)$ of Nb/Au/CoFe trilayers should behave like the curve shown by the long dashed line beginning with the $T_c$ of Nb/CoFe represented by the solid square at the low left corner of the main plot in Fig. 8. The experimental $T_c(d_N)$ measurements, however, show quite different behavior as shown by the solid squares reproduced in Fig. 8. There is an abrupt increase of $T_c$ with the length scale of approximately 2 nm as $d_N$ is increased as shown in the inset, and $T_c$ increases with the expected length scale $\xi_N$ as $d_N$ is further increased.

One may understand this experimental $T_c$ vs. $d_N$ behavior as follows. Recall that in the present formalism the interfaces are modeled in terms of the two parameters $\gamma_{SN}$ and $\gamma_{NF}$ irrespective of N thickness. S/N/F trilayers, as $d_N \to 0$, still have two interfaces characterized by $\gamma_{SN}$ and $\gamma_{NF}$, but the corresponding S/F bilayer has one interface characterized by $\gamma_{SF}$. Unless the three $\gamma_b$s satisfy a special match condition, $T_c(d_N = 0)$ of the bilayer and $\lim_{d_N \to 0} T_c(d_N)$ of the trilayers need not be
the same. This condition may be derived from the BC of Eqs. (11), (13), and (14). We add (13) and (14), and take $d_N \to 0$. We then obtain using (11)

$$F_S(0) - F_F(0) = (\gamma_b^{NF} + \gamma_b^{SN} \gamma_{NF}) \frac{d}{dx} F_F(0).$$ (52)

For this to agree with the corresponding S/F bilayer, it is required that

$$\gamma_b^{SF} = \gamma_b^{NF} + \gamma_b^{SN} \gamma_{NF}.$$ (53)

This condition need not be satisfied. The $\gamma_b^{SF}$ may take an arbitrary value irrespective of $\gamma_b^{NF}$ or $\gamma_b^{SN}$. In case of a mismatch, $T_c(d_N)$ then shows a discontinuity at $d_N = 0$. The right hand side is usually larger as is the case with the Nb/Au/CoFe trilayers, and $T_c$ of $d_N \to 0$ S/N/F should be larger than that of S/F.

![FIG. 8: $T_c(d_N)$ of Nb/Au/CoFe trilayers and Nb/Au bilayers, represented by the solid and empty squares, respectively. Nb and CoFe layers are fixed at $d_N = 23$ and $d_F = 10$ nm. The inset is the detailed plot of the short length scale. The long dashed curve in the main plot is the expected behavior of $T_c(d_N)$ without the BC mismatch. The dotted line connecting empty squares is a guide to eyes. Reproduced from the reference 22.](image)

Note, however, that in experiments $d_N \to 0$ has a single interface of course, and $T_c$ of Nb/Au/CoFe as $d_N \to 0$ must agree with that of Nb/CoFe. As $d_N$ is increased from 0 in Nb/Au/CoFe, there begin to form two distinct interfaces. For the electrons to feel the two interfaces as the theoretical model assumed, a finite width of $N$ region is necessary. This width of about 2 nm is the length which is needed to interpolate the $T_c$ of Nb/CoFe and that of $d_N \to 0$ Nb/Au/CoFe. The theoretical step function behavior of $T_c(d_N)$ then should appear as a short length scale of $\approx 2$ nm observed in the experiments.22 This length scale is not the material width of the Nb/Au interface which is approximately an order of magnitude smaller. The same short length of $\approx 2$ nm has also been observed for $N = Cu$, Al.22 The sudden increase of $T_c(d_N)$ as $d_N$ is increased was also observed in the epitaxial Nb(110)/Au(111)/Fe(110) trilayers by Yamazaki and his coworkers.22

IV. SUMMARY AND CONCLUDING REMARKS

In this paper, we have extended the Green’s function method developed for S/F bilayers by Fominov et al. to S/N/F trilayer systems. We have calculated the superconducting transition temperature $T_c$ and the singlet and triplet pairing components near $T \approx T_c$ for S/N/F trilayers. The interface between S and N (N and F) was modeled in terms of $\gamma_b^{SN} (\gamma_b^{NF})$. They represent spin independent interface resistances. As have been and will be reported separately, the experimental $T_c$ measurements could be fit by the present formalism.23,29,30,31

There seems, however, a room to improve the present formalism. One possible route might be to model the N/F interface with two spin dependent parameters as was done for example in ref. 27 or to model it in terms of a spin-active interface.18,19,20,21 The latter route will be an interesting problem in connection with the long range odd frequency triplet pairing components because they are induced even when the exchange field in F region is uniform if the N/F interface in spin-active.

Also noteworthy in the S/N/F system is the observation of the length scale of $\approx 20$ nm in the $T_c$ vs. $d_N$ measurements in Nb/Au/CoFe trilayers.22 The natural length scale in N region is the coherence length $\xi_N \approx 100$ nm as shown, for instance, in Figs. 6 and 8. In addition, the short length of $\approx 2$ nm was observed because of the boundary condition mismatch. In the same experiments the $T_c$ as a function of $d_N$ also exhibited a small oscillation with the length scale of $\approx 20$ nm. The origin of this is not clear. It seems difficult to understand this oscillation within the current Usadel formalism because there is only one length scale of $\xi_N$ in the theory. It is interesting that this $T_c$ oscillation was also observed in the epitaxial Nb(110)/Au(111)/Fe(110) trilayers.22 In the epitaxially grown Nb(110)/Au(111)/Fe(110) trilayers the $T_c$ oscillation length scale was $\approx 2$ nm, which is an order of magnitude smaller than that of the sputtering grown Nb/Au/CoFe trilayers. More experiments with different conditions will be necessary to clarify the origin of the $T_c$ oscillations as a function of $d_N$.

We have calculated the singlet pairing component and short range odd frequency triplet pairing components in the present paper. The triplet pairing component is induced on top of the dominant singlet component by the proximity effects and time reversal symmetry breaking exchange field. In the present work, the exchange field is unidirectional over the F region, and only the short range triplet component was induced. If the orientation of the exchange field changes in the F region, or if the inner-interface of F is spin active, then the other long range triplet components will also appear. In the latter...
We also have
where

V. APPENDIX: CALCULATION OF SINGLET AND TRIPLET PAIR FUNCTIONS

We will in this Appendix present the procedure to calculate the singlet and triplet pair functions using the Usadel formalism developed in Sec. II. As discussed there, the anomalous function $F_S(x, i\omega_n)$ in the S region can be written as

$$\left( \begin{array}{cc} F_S^+ & F_S^- \\ F_S^- & C_S^-(i\omega_n) \cosh k_S(x-d_S) \end{array} \right). \tag{54}$$

The BC at $x = 0$ in terms of $F_S$ alone is given by Eq. (31).

$$\xi_S \frac{dF_S(0)}{dx} = \hat{A}_S F_S(0). \tag{55}$$

We also have

$$\xi_S \frac{dF_S(0)}{dx} = \hat{A} F_S(0), \tag{56}$$

where

$$\hat{A} = \left( \begin{array}{cc} W(i\omega_n) & 0 \\ 0 & -\hat{A}_S \end{array} \right), \tag{57}$$

where $W(\omega_n)$ and $\hat{A}_S$ are given by Eq. (37). We therefore write

$$\hat{A}_S - \hat{A} \left[ \begin{array}{c} F_S^+(0, i\omega_n) \\ C_S^-(i\omega_n) \cosh k_S d_S \end{array} \right] = 0. \tag{58}$$

Dividing this by $F_S^+$, we obtain

$$\hat{A}_S \left[ \begin{array}{c} 1 \\ 0 \end{array} \right] = \left[ \begin{array}{c} 1 \\ 0 \end{array} \right] - k_S \xi_S \sinh k_S d_S$$

$$- \hat{A} \left[ \begin{array}{c} 1 \\ 0 \end{array} \right] \left[ \begin{array}{c} W(i\omega_n) \\ C_S^-(i\omega_n)/F_S^+(0, i\omega_n) \end{array} \right]. \tag{59}$$

Note that $\Delta(x)$ is the eigenvector corresponding to the smallest eigenvector $M(x, y)$ of Eq. (19), and $F_S^\pm(x, i\omega_n)$ can be obtained from Eq. (17). We can therefore find $C_S^-(i\omega_n)$ from Eq. (59), and calculate $F_S^-(s, i\omega_n)$ using Eq. (44). This completes the calculation of the SPC and TPC in the S region.

We now turn to calculation of the pairing functions in the N region. The function $F_N^\pm$ can be written as

$$F_N^\pm(x, i\omega_n) = F_N^\pm(0, i\omega_n) \cosh k_N x + \xi_N \frac{d}{dx} F_N^\pm(0, i\omega_n) \sinh k_N x. \tag{60}$$

From the BC (12), we get

$$F_N^\pm(x) = F_N^\pm(0) \left[ (1 - \frac{\gamma_{SN}}{\gamma_{SN}} \hat{A}_S) \cosh k_N x + \frac{1}{\gamma_{SN}} \hat{A}_S \sinh k_N x \right]. \tag{61}$$

Therefore we get

$$F_N^\pm(-d_N) = F_N^\pm(0) \left[ (1 - \frac{\gamma_{SN}}{\gamma_{SN}} \hat{A}_S) \cosh k_N d_N \right.$$

$$- \frac{1}{\gamma_{SN}} \hat{A}_S \sinh k_N d_N \right] \tag{62}$$

$$\xi_N \frac{d}{dx} F_N^\pm(-d_N) = F_N^\pm(0) \left[ \frac{1}{\gamma_{SN}} \hat{A}_S \cosh k_N d_N \right.$$

$$- \xi_N k_N \left( 1 - \frac{\gamma_{SN}}{\gamma_{SN}} \hat{A}_S \sinh k_N d_N \right] \tag{63}$$

$$F_N^\pm(-d_N)$$

We subtract and add (63) and (64) to obtain

$$C_F^+ = \frac{\xi_N \frac{d}{dx} F_N^+(d_N) - \xi_N \frac{d}{dx} F_N^-(d_N)}{2 \gamma_{NF} \xi_F k_F \sinh k_F d_F}, \tag{65}$$

$$C_F^- = \frac{\xi_N \frac{d}{dx} F_N^+(d_N) + \xi_N \frac{d}{dx} F_N^-(d_N)}{2 \gamma_{NF} \xi_F k_F \sinh k_F d_F} \tag{66}$$

We then obtain $F_F^\pm$ by plugging $C_F^\pm$ into Eq. (18).
\[(\cosh k_F(x + d_N) + \sinh k_F(x + d_N) \tanh k_FD_F)\]. (67)

\[F^\mp(x, i\omega_n) = -\text{Im} \left[ \frac{\xi_N \frac{d}{dx} F_N(-d_N) - \xi_N \frac{d}{dx} F_N(-d_N)}{2\gamma N \xi_F k_F \tanh k_F d_F} \right]. (68)\]

We can therefore calculate the anomalous functions $F$ in trilayers. The pair functions $\Psi(x)$ are given by

\[\Psi^\pm(x) = \pi T_c \sum_{\omega_n > 0} F^\pm(x, i\omega_n). \] (69)

This completes the calculation of the singlet and triplet pairing components over the entire region of an S/N/F trilayer.