Theory of proximity effect in superconductor/ferromagnet heterostructures

A. Bagrets and C. Lacroix
Laboratoire Louis Néel, CNRS, Boîte Postale 166, 38042 Grenoble cedex 9, France

A. Vedyayev
CEA/Grenoble, Département de Recherche Fondamentale sur la Matiŕe Condensée, SP2M/NM, 38054 Grenoble, France and Department of Physics, M. V. Lomonosov Moscow State University, 119899 Moscow, Russia

(Received 2 April 2003; published 29 August 2003)

We present a microscopic theory of the proximity effect in the ferromagnet/superconductor/ferromagnet (F/S/F) nanostructures where S is an *s*-wave low-T_c superconductor and F's are layers of 3*d* transition ferromagnetic metal. Our approach is based on the direct analytical solution of Gor'kov equations for the normal and anomalous Green's functions together with a self-consistent evaluation of the superconducting order parameter. We take into account the elastic spin-conserving scattering of the electrons assuming *s*-wave scattering in the S layer and *s*-*d* scattering in the F layers. In accordance with previous quasiclassical theories, we found that due to exchange field in the ferromagnet the anomalous Green's function $F(z)$ exhibits the damping oscillations in the F layer as a function of distance z from the S/F interface. In the given model, a half of the period of oscillations is determined by the length $\xi_m^0 = \pi v_F/\varepsilon_{\mathrm{ex}}$, where v_F is the Fermi velocity and $\varepsilon_{\mathrm{ex}}$ is the exchange field, while damping is governed by the length $l_0 = (1/l_\uparrow + 1/l_\downarrow)^{-1}$, with $l_\uparrow$ and $l_\downarrow$ being spin-dependent mean free paths in the ferromagnet. The superconducting transition temperature $T_c(d_F)$ of the F/S/F trilayer shows the damping oscillations as a function of the F-layer thickness d_F with period $\xi_F = \pi/\sqrt{m\varepsilon_{\mathrm{ex}}}$, where m is the effective electron mass. The oscillations of $T_c(d_F)$ are a consequence of the oscillatory behavior of the superconducting order parameter at the S/F interface vs thickness d_F, which in turn is caused by the oscillations of $F(z)$ in the F region. We show that strong spin-conserving scattering either in the superconductor or in the ferromagnet significantly suppresses these oscillations. The calculated $T_c(d_F)$ dependences are compared with existing experimental data for Fe/Nb/Fe trilayers and Nb/Co multilayers.

DOI: 10.1103/PhysRevB.68.054532 PACS number(s): 74.78.Fk, 74.50.+r, 74.62.Bf, 74.78.−w

I. INTRODUCTION

The artificially fabricated layered nanostuctures with alternating superconducting (S) and ferromagnetic (F) layers provide a possibility to study the physical phenomena arising due to the proximity of two materials (S and F) with two antagonistic types of long-range ordering. One such interesting effect is the existence of the so-called π-phase superconducting state in which the order parameter in adjacent S layers has opposite sings. The π junctions were originally predicted to be possible due to spin-flip processes in magnetic layered structures containing paramagnetic impurities in the barrier between S layers.[1] Later on, Buzdin *et al.*[2,3] and Radović *et al.*[4] showed that, due to the oscillatory behavior of the Cooper pair wave function in the ferromagnet, π coupling can be realized also for S/F multilayers. The π coupling leads to a nonmonotonic oscillatory dependence of the superconducting transition temperature T_c as a function of ferromagnetic layer thickness d_F.[2–4] The effect occurs because of periodically switching of the ground state between 0 and π phases, so that the system chooses the state with higher transition temperature T_c.

These theoretical predictions stimulated a considerable interest to proximity effect in S/F structures also from experimental point of view. First, the oscillatory behavior of $T_c(d_F)$ was observed by Wong *et al.*,[5] in V/Fe multilayers and later on these results were well explained by theoretical calculations of Radović *et al.*[4] However, in subsequent experiments with V/Fe multilayers,[6] the oscillatory $T_c(d_F)$ dependence was not observed. The following experiments[7–13] revealed the different and even controversial behavior of $T_c(d_F)$ for different structures. The nonmonotonic oscillationlike behavior of $T_c(d_F)$ was reported by Jiang *et al.*[7] for Nb/Gd multilayers and Nb/Gd/Nb trilayers, by Mühge *et al.*[8] for Fe/Nb/Fe trilayers, and recently by Obi *et al.*[9] for Nb/Co and V/Co multilayers. However, negative results were reported for Nb/Gd/Nb trilayers by Strunk *et al.*,[10] for $V/V_{1-x}Fe_x$ multilayers by Aarts *et al.*,[11] for Fe/Nb bilayers by Mühge *et al.*,[12] and Nb/Fe multilayers by Verbanck *et al.*[13] For interpretation of experimental results, along with mechanisms of π coupling and suppression of T_c due to strong exchange field in the ferromagnet, other mechanisms were suggested such as the complex behavior of the "magnetically dead" interfacial S/F layer (for details, see Ref. 8), the effects of a finite interface transparency,[11] and spin-orbit scattering.[14]

The original theory of the proximity effect proposed by Buzdin *et al.*[3,4] is based on the quasiclassical Usadel equations[15] applied for S/F structures. In this case the Usadel equations must be supplemented by boundary conditions for the quasiclassical Green's functions at the S/F interface. This essential point was recently discussed in Ref. 16. On the other hand, the boundary conditions for microscopic Green's functions can be written obviously for ideal S/F interfaces if one uses Gor'kov equations.[17] These equations, however, are more complex to resolve than the quasiclassical ones. In the given paper, we present a theoretical investigation of the $T_c(d_F)$ behavior for F/S/F trilayer structures based on

Gor'kov equations. We consider that F layers are $3d$ transition metals and assume that the main mechanism of spin-conserving electron scattering in F layers is the s-d scattering, while S layer is an s-wave superconductor with s-s scattering. We find the characteristic lengths determining the periods of oscillations and damping of critical temperature T_c and Cooper pair wave function, and show that in the given model these lengths differ from length scales predicted by quasiclassical theories.[3,4,16,18] We show that strong spin-conserving scattering either in the superconductor or in the ferromagnet significantly suppresses the oscillations of T_c. We compare our results with the existing data on $T_c(d_F)$ for Fe/Nb/Fe trilayers[8] and V/Co multilayers,[9] where F's are $3d$ ferromagnets, and find reasonable agreement between theory and experiment.

II. GOR'KOV EQUATIONS AND GREEN'S FUNCTIONS

We consider a trilayer structure $F_1/S/F_3$, where S is a low-T_c superconductor and F's are $3d$-metal ferromagnetic layers. The thicknesses d_S and d_F of the S and F layers are assumed to be much smaller than the in-plane dimension of the structure, so that the system can be considered as homogeneous in the xy plane (parallel to the interfaces). We denote the axis perpendicular to the xy plane as the z axis. Let $z=\pm a$ be the positions of the outer boundaries of the F layers and $z=\pm d$ be the positions of S/F interfaces, then $d_S=2d$ and $d_F=a-d$. We adopt that S is a simple s-wave superconductor with s-s mechanism of electron scattering. According to Ref. 19, for superconducting Nb which is usually used in preparing the S/F heterostructures, s-wave scattering is indeed prevailing. Concerning the ferromagnetic layers, we adopt the simplified model[20] considering that two types of electrons form the total band structure of $3d$ transition metals: almost freelike spin-up and spin-down electrons from sp bands (these electrons are referred to as s electrons) and localized d electrons from narrow strongly exchange-split bands. The main mechanism of spin-conserving electron scattering in $3d$ ferromagnetic metals is the s-d scattering[21] because of a dominant contribution of d density of states (DOS) to the total DOS at the Fermi energy ε_F. The mean free path of the conduction s electrons depends on the spin due to the s-d scattering and the different d density of states at ε_F for majority- and minority-spin bands. In the present work, we consider only the scattering by nonmagnetic impurities.

As a starting point, we take the system of Gor'kov equations[17] for the normal and anomalous Green's functions $G^{ss}_{\uparrow\uparrow}(x_1,x_2)=-\langle T_\tau\psi_\uparrow(x_1)\psi^\dagger_\uparrow(x_2)\rangle$ and $F^{ss}_{\downarrow\uparrow}(x_1,x_2)=\langle T_\tau\psi^\dagger_\downarrow(x_1)\psi^\dagger_\uparrow(x_2)\rangle$, where $x=(\tau,\mathbf{r})$ is a four-component vector and the creation and annihilation field operators are associated with s electrons. By carrying out the Fourier transformation in the xy plane and over the imaginary time τ, we get the following system for the Green's functions.

(i) For the F layers,

$$\left[i\omega+\frac{1}{2m}\left(\frac{\partial^2}{\partial z^2}-\kappa^2\right)+\varepsilon_F+h(z)-x_0\gamma_{sd}^2G^{dd}_{\uparrow\uparrow}(z,z)\right]\times G^{ss}_{\uparrow\uparrow}(z,z')+\Delta(z)F^{ss}_{\downarrow\uparrow}(z,z')=\delta(z-z'),$$

$$\Delta^*(z)G^{ss}_{\uparrow\uparrow}(z,z')+\left[i\omega-\frac{1}{2m}\left(\frac{\partial^2}{\partial z^2}-\kappa^2\right)-\varepsilon_F+h(z)-x_0\gamma_{sd}^2G^{dd}_{\downarrow\downarrow}(z,z)\right]F^{ss}_{\downarrow\uparrow}(z,z')=0. \qquad (1)$$

(ii) For the S layer,

$$\left[i\omega'+\frac{1}{2m}\left(\frac{\partial^2}{\partial z^2}-\kappa^2\right)+\varepsilon_F\right]G^{ss}_{\uparrow\uparrow}(z,z')+\Delta_\omega(z)F^{ss}_{\downarrow\uparrow}(z,z')=\delta(z-z'),$$

$$\Delta^*_\omega(z)G^{ss}_{\uparrow\uparrow}(z,z')+\left[i\omega'-\frac{1}{2m}\left(\frac{\partial^2}{\partial z^2}-\kappa^2\right)-\varepsilon_F\right]F^{ss}_{\downarrow\uparrow}(z,z')=0 \qquad (2)$$

with

$$\omega'=\omega+icu_0^2G^{ss}_{\uparrow\uparrow}(z,z),$$

$$\Delta_\omega(z)=\Delta(z)+cu_0^2F^{*ss}_{\downarrow\uparrow}(z,z). \qquad (3)$$

In Eqs. (1) and (2), κ is the in-plane momentum, parallel to the S/F interface, m is the effective electron mass which is assumed to be the same for both metals, $h(z)$ is the exchange field in the ferromagnet, and $\omega=\pi T(2n+1)$ are Matsubara frequencies (the units are $\hbar=1=k_B$). The scattering processes are introduced in the Born approximation. The parameters u_0 and γ_{sd} are the strengths of impurity potentials, and c and x_0 are impurity concentrations in the S and F layers. We assume that a BCS coupling constant is zero for the ferromagnet, therefore $\Delta(z)=0$ in the F layers. We also neglect the possible deviation of $\Delta(z)$ from zero in the F region due to scattering, since this correction is of the order of γ_{sd}^4 which is small.

The superconductor order parameter has to be found self-consistently,

$$\Delta(z)=\lambda T\sum_\omega\int_0^{k_F}\frac{\kappa d\kappa}{2\pi}F^*(\omega,\kappa,z=z'), \qquad (4)$$

where summation over ω goes up to Debye frequency ω_D, $\lambda>0$ is the BCS coupling constant in a superconductor, and $F=F^{ss}_{\downarrow\uparrow}$. The critical temperature T_c is defined as the first zero of equation $\Delta(z)=0$ when T decreases from high temperatures.

Below, in this section and in Sec. III we present a scheme to evaluate the Green's functions considering as the first step the non-self-consistent solution of Eqs. (1) and (2), where $\Delta(z)=\Delta$ is a real number which does not depend on z. Section IV is devoted to the self-consistent evaluation of $\Delta(z)$. We will assume that the mutual orientation of magnetizations in the F layers is antiparallel (AP), therefore $h(z)=h>0$ in the F_1 layer and $h(z)=-h$ in the F_3 layer. The advantage of the AP configuration is that in this case the self-consistency can be achieved for real values of $\Delta(z)$ in the S region. The study of the influence of the mutual orientation of magnetizations on T_c (Refs. 22–24) in the framework of the given model requires considering $\Delta(z)$ as a complex-valued function. This question is beyond the present study and will be discussed in a forthcoming paper. However, as can be seen further, the general conclusions of the given paper are not sensitive to the particular configuration of the magnetizations.[25] At the first step we also suppose that there is no scattering in the S layer. The scattering processes in the S layer [Eq. (3)] are taken into account at the last step of the evaluation of the critical temperature (Sec. V).

By introducing the Green's functions $\tilde{G}^{ss}_{\downarrow\downarrow}(x_1,x_2) = -\langle T_\tau \psi^\dagger_\downarrow(x_1)\psi_\downarrow(x_2)\rangle$ and $\tilde{F}^{ss}_{\uparrow\downarrow}(x_1,x_2) = \langle T_\tau \psi_\uparrow(x_1)\psi_\downarrow(x_2)\rangle$ the system of Gor'kov equations can be written in the matrix form[26]

$$[i\omega\hat{I}-\hat{\mathcal{A}}]\begin{pmatrix} G & \tilde{F} \\ F & \tilde{G}\end{pmatrix} = \hat{I}\delta(z-z'), \tag{5}$$

where $\hat{I}$ is the unit matrix and $\hat{\mathcal{A}}$ is the (2×2)-matrix differential operator, the components of which can be found by comparing the Eqs. (1) and (2) and Eq. (5).

In order to find the matrix Green's function, consider Schrödinger's equation with Hamiltonian $\hat{\mathcal{A}}$:

$$[i\omega\hat{I}-\hat{\mathcal{A}}]\psi(z)=0. \tag{6}$$

This equation has four linear independent solutions

$$\varphi_\mu(z) = \begin{pmatrix}\varphi^+_\mu(z)\\ \varphi^-_\mu(z)\end{pmatrix} \quad (\mu=\uparrow,\downarrow),$$

and

$$\psi_\rho(z) = \begin{pmatrix}\psi^+_\rho(z)\\ \psi^-_\rho(z)\end{pmatrix} \quad (\rho=\uparrow,\downarrow).$$

We require that $\psi_\mu(z)$ and $\psi_\rho(z)$ obey zero boundary conditions at points $z=\pm a$, and choose these independent solutions in such a way that two functions $\varphi_\uparrow(z)$ and $\psi_\uparrow(z)$ describe spin-up electrons in the ferromagnetic layers, and functions $\varphi_\downarrow(z)$ and $\psi_\downarrow(z)$ describe spin-down holes in the F layers. Namely, in the layer F_1 $(-a<z<-d)$ the solutions $\varphi_\mu(z)$ have the form

$$\varphi_\uparrow(z) = \begin{pmatrix}1\\0\end{pmatrix}\sin[p^\uparrow_1(z+a)], \tag{7}$$

$$\varphi_\downarrow(z) = \begin{pmatrix}0\\1\end{pmatrix}\sin[p^\downarrow_1(z+a)],$$

and in the F_3 layer $(d<z<a)$ the solutions $\psi_\rho(z)$ are

$$\psi_\uparrow(z) = \begin{pmatrix}1\\0\end{pmatrix}\sin[p^\uparrow_3(a-z)], \tag{8}$$

$$\psi_\downarrow(z) = \begin{pmatrix}0\\1\end{pmatrix}\sin[p^\downarrow_3(a-z)].$$

Here $p_1^{\uparrow(\downarrow)}$ is an electron (hole) momenta in the F_1 layer,

$$p_1^{\uparrow(\downarrow)} = \sqrt{2m\left(\varepsilon_F - \frac{\kappa^2}{2m} \pm h \pm \frac{i}{2}\tau^{-1}_{\uparrow(\downarrow)} \pm i\omega\right)}, \tag{9}$$

and $p_3^{\uparrow(\downarrow)}$ are momenta in the F_3 layer,

$$p_3^{\uparrow(\downarrow)} = \sqrt{2m\left(\varepsilon_F - \frac{\kappa^2}{2m} \mp h \pm \frac{i}{2}\tau^{-1}_{\downarrow(\uparrow)} \pm i\omega\right)}. \tag{10}$$

The inverse lifetimes of quasiparticles are given by $\tau^{-1}_{\uparrow(\downarrow)} = -2x_0\gamma^2_{sd}\mathrm{Im}G^{dd}_{\uparrow\uparrow(\downarrow\downarrow)} = k_F^{\uparrow(\downarrow)}/(ml_{\uparrow(\downarrow)})$, where $k_F^{\uparrow(\downarrow)} = \sqrt{2m(\varepsilon_F \pm h)}$ being Fermi momenta in the ferromagnet and $l_{\uparrow(\downarrow)}$ being mean free paths which are considered as parameters.

In the S region $(-d<z<d)$ the solutions of Eq. (6) are

$$\varphi_\mu(z) = A^\mu_+\begin{pmatrix}1\\ \alpha\end{pmatrix}e^{ik_+(z+d)} + A^\mu_-\begin{pmatrix}1\\ \alpha\end{pmatrix}e^{-ik_+(z+d)} + B^\mu_+\begin{pmatrix}\alpha\\ 1\end{pmatrix}e^{ik_-(z+d)} + B^\mu_-\begin{pmatrix}\alpha\\ 1\end{pmatrix}e^{-ik_-(z+d)}, \tag{11}$$

$$\psi_\rho(z) = C^\rho_+\begin{pmatrix}1\\ \alpha\end{pmatrix}e^{ik_+(z-d)} + C^\rho_-\begin{pmatrix}1\\ \alpha\end{pmatrix}e^{-ik_+(z-d)} + D^\rho_+\begin{pmatrix}\alpha\\ 1\end{pmatrix}e^{ik_-(z-d)} + D^\rho_-\begin{pmatrix}\alpha\\ 1\end{pmatrix}e^{-ik_-(z-d)},$$

where the wave vectors $k_\pm$ are defined as

$$k_\pm = \sqrt{2m\left(\varepsilon_F - \frac{\kappa^2}{2m} \pm i\sqrt{\omega^2+\Delta^2}\right)}$$

and

$$\alpha = \frac{i}{\Delta}[\sqrt{\omega^2+\Delta^2}-\omega].$$

We neglect the interfacial roughness, thus the coefficients $A^\mu_\pm$, $B^\mu_\pm$, $C^\rho_\pm$, and $D^\rho_\pm$ have to be found from the conditions of continuity of the functions $\varphi_\mu(z)$ and $\psi_\rho(z)$ and their derivatives at the points $z=\pm d$, which can be found easily by solving the system of algebraic linear equations.

To evaluate the matrix Green's function, let us introduce the matrices

$$\Phi(z) = \begin{pmatrix}\varphi^+_\uparrow(z) & \varphi^+_\downarrow(z)\\ \varphi^-_\uparrow(z) & \varphi^-_\downarrow(z)\end{pmatrix},$$

$$\Psi(z') = \begin{pmatrix}\psi^+_\uparrow(z') & \psi^+_\downarrow(z')\\ \psi^-_\uparrow(z') & \psi^-_\downarrow(z')\end{pmatrix},$$

and let J be the matrix of "currents,"

$$J = \begin{pmatrix} j_{\uparrow\uparrow} & j_{\uparrow\downarrow}\\ j_{\downarrow\uparrow} & j_{\downarrow\downarrow}\end{pmatrix},$$

with components

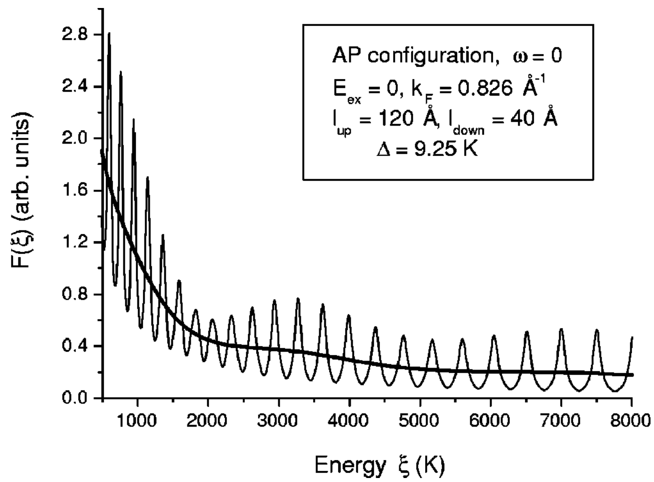

FIG. 1. The typical dependence of the anomalous Green's function $F(\omega,\xi,z)$ on the energy $\xi=\kappa^2/2m-\varepsilon_F$ under given $\Delta=9.25$ K, $\omega=0$, $z=0$, $\varepsilon_{\rm ex}=0$, mean free paths in the F layer are $l_\uparrow=120$ Å and $l_\downarrow=40$ Å, and Fermi momentum $k_F=0.826$ Å^{-1}. $F(\xi)$ exhibits quantum oscillations; the smooth line shows function $F(\xi)$ averaged over oscillations, i.e., $F_0(\xi)$ (see text for the details).

$$j_{\mu\rho}=\varphi_\mu^+(z)\overleftrightarrow{\nabla}_z\psi_\rho^+(z)-\varphi_\mu^-(z)\overleftrightarrow{\nabla}_z\psi_\rho^-(z). \quad (12)$$

Here $\mu,\rho=\uparrow,\downarrow$ and $\overleftrightarrow{\nabla}_z=(\overrightarrow{\nabla}_z-\overleftarrow{\nabla}_z)$ is the antisymmetric gradient operator. The matrix J is the Wronskian of system (6), which does not depend on z, i.e., $\partial J(z)/\partial z=0$. Finally, the matrix Green's function introduced in Eq. (5) is given by

$$\hat{G}(z,z')=2m\Phi(z)[J^{-1}]^T\Psi(z'). \quad (13)$$

Here T denotes the transposition operation. The obtained expression allows one to evaluate the normal and anomalous Green's functions in both layers (S and F).

III. ANOMALOUS GREEN'S FUNCTION

A. S layer

Consider first the anomalous Green's function (Cooper pair wave function) $F(\omega,\kappa,z=z')$ in the S region. Denote $\theta_\pm=2ik_\pm d$ and $\theta_\pm=\theta\pm i\delta$, i.e., θ and δ are real and imaginary parts of phases $\theta_\pm$. Using solutions (11) in Eq. (6) in the superconductor, we get the exact expressions for currents

$$j_{\mu\rho}=(1-\alpha^2)j_{\mu\rho}^0,$$

where

$$j_{\mu\rho}^0=2ik_+[A_-^\mu C_+^\rho e^{-i\theta_+}-A_+^\mu C_-^\rho e^{i\theta_+}]$$
$$-2ik_-[B_-^\mu D_+^\rho e^{-i\theta_-}-B_+^\mu D_-^\rho e^{i\theta_-}]. \quad (14)$$

Since the currents $j_{\mu\rho}$ do not depend on z, the same expressions can be obtained using the solutions of Eq. (6) in the ferromagnetic layers.

It is convenient to introduce an energy variable $\xi=\varepsilon_F-\kappa^2/2m$. The typical dependence of $F(\xi)$ on ξ under given arguments ω and Δ at the point $z=z'=0$ is shown in Fig. 1. Function $F(\xi)$ exhibits the quantum oscillations which are the result of exponentials $e^{\pm i\theta_\pm}$ in Eq. (14) with rapidly varying phases. Since the superconducting order parameter is determined by the integral of $F(\xi)$ over ξ, one can average $F(\xi)$ over the oscillations.

Denote $a_{\mu\rho}$ $(\mu,\rho=\uparrow,\downarrow)$ as the components of the matrix

$$[J^{-1}]^T=\begin{pmatrix} a_{\uparrow\uparrow} & a_{\uparrow\downarrow} \\ a_{\downarrow\uparrow} & a_{\downarrow\downarrow} \end{pmatrix}.$$

For $a_{\mu\rho}$ we get

$$a_{\mu\rho}=\frac{\mathrm{sgn}(\mu\rho)}{(1-\alpha^2)\tilde{D}}j_{-\mu,-\rho}^0=\frac{1}{\tilde{D}}[a_{\mu\rho}^-e^{-i\theta}+a_{\mu\rho}^+e^{i\theta}],$$

where

$$a_{\mu\rho}^-=\frac{\mathrm{sgn}(\mu\rho)}{(1-\alpha^2)}[2ik_+A_-^{-\mu}C_+^{-\rho}e^{\delta}-2ik_-B_-^{-\mu}D_+^{-\rho}e^{-\delta}],$$

$$a_{\mu\rho}^+=-\frac{\mathrm{sgn}(\mu\rho)}{(1-\alpha^2)}[2ik_+A_+^{-\mu}C_-^{-\rho}e^{-\delta}-2ik_-B_+^{-\mu}D_-^{-\rho}e^{\delta}], \quad (15)$$

where $\theta\pm i\delta=\theta_\pm=2ik_\pm d$ and $\tilde{D}=\det J/(1-\alpha^2)^2$ is the determinant of the matrix of currents:

$$\tilde{D}=-D_0+\Gamma_+e^{2i\theta}+\Gamma_-e^{-2i\theta}.$$

The expressions for D_0 and $\Gamma_\pm$ are given in Appendix A.

By carrying out the Fourier transformation of $a_{\mu\rho}$, we can write the first terms of the expansion

$$\langle a_{\mu\rho}\rangle=b_{\mu\rho}^+e^{i\theta}+b_{\mu\rho}^-e^{-i\theta}+\cdots, \quad (16)$$

where $b_{\mu\rho}^\pm$ are defined by the following integrals:

$$b_{\mu\rho}^\pm=\frac{1}{2\pi}\int_{-\pi}^{+\pi}d\phi\,\frac{a_{\mu\rho}^\mp e^{-i\phi}+a_{\mu\rho}^\pm}{\Gamma_+e^{i\phi}+\Gamma_-e^{-i\phi}-D_0}.$$

Using Eq. (13), we get an expression for $F(\omega,\xi,z=z')$:

$$F(\omega,\xi,z=z')=2m\sum_{\mu,\rho=\uparrow\downarrow}\varphi_\mu^-(z)\langle a_{\mu\rho}\rangle\psi_\rho^+(z),$$

where $\varphi_\mu^-(z)$ and $\psi_\rho^+(z)$ are the components of solutions $\varphi_\mu(z)$ and $\psi_\rho(z)$ in the S layer. Denote

$$\theta_1\pm i\delta_1=k_\pm(d+z),\qquad \theta_2\pm i\delta_2=k_\pm(d-z),$$

then $\theta_1+\theta_2=\theta$, $\delta_1+\delta_2=\delta$, and

$$\varphi_\mu^-(z)=\Lambda_+^\mu e^{i\theta_1}+\Lambda_-^\mu e^{-i\theta_1},$$

$$\psi_\rho^+(z)=\Sigma_+^\rho e^{i\theta_2}+\Sigma_-^\rho e^{-i\theta_2},$$

where

$$\Lambda_+^\mu=\alpha A_+^\mu e^{-\delta_1}+B_+^\mu e^{\delta_1},\qquad \Lambda_-^\mu=\alpha A_-^\mu e^{\delta_1}+B_-^\mu e^{-\delta_1},$$

$$\Sigma_+^\rho=C_-^\rho e^{-\delta_2}+\alpha D_-^\rho e^{\delta_2},\qquad \Sigma_-^\rho=C_+^\rho e^{\delta_2}+\alpha D_+^\rho e^{-\delta_2}.$$

The higher-order terms with $e^{\pm in\theta}$, where $n\geqslant 2$, can be dropped in expansion (16) because they are responsible for rapid oscillations of $F(\xi)$. Finally, we arrive at the following expression for the anomalous Green's function in the S layer:

$$F(\omega,\xi,z=z')=F_0(\omega,\xi,z)+F_1(\omega,\xi,z),$$

where

$$F_0(\omega,\xi,z)=2m\sum_{\mu\rho}\{\Lambda_+^{\mu}\Sigma_+^{\rho}b_{\mu\rho}^{-}+\Lambda_-^{\mu}\Sigma_-^{\rho}b_{\mu\rho}^{+}\},\quad(17)$$

$$F_1(\omega,\xi,z)=2m\sum_{\mu\rho}\{\Lambda_+^{\mu}\Sigma_-^{\rho}[b_{\mu\rho}^{+}e^{2i\theta_1}+b_{\mu\rho}^{-}e^{-2i\theta_2}]+\Lambda_-^{\mu}\Sigma_+^{\rho}[b_{\mu\rho}^{+}e^{2i\theta_2}+b_{\mu\rho}^{-}e^{-2i\theta_1}]\}.$$

Contribution F_1 to function F is essential only in the vicinity of S/F interfaces, $z=\pm d$, as far as $\theta_1\sim(z+d)$ and $\theta_2\sim(d-z)$. At the point $z=z'=0$ (the middle of the S layer), the anomalous Green's function is determined by the function $F_0(\omega,\xi,z)$ which is shown by the thick smooth line in Fig. 1. The obtained result is used below in Sec. IV where we discuss the self-consistent evaluation of the order parameter.

B. F layer

Due to the proximity effect, the correlations between electrons are induced in the ferromagnet close to the supercoducting layer. Instead of a simple decay, as it would be for the superconductor/normal-metal interface, in the case of ferromagnetic layer the Cooper pair wave function exhibits the damping oscillatory behavior in the ferromagnet by increasing the distance from the S/F interface.[3,4,18] The reason is that exchange splitting of bands in the F region changes the pairing conditions for electrons; therefore, the Cooper pairs are formed from quasiparticles with equal energies, but with difference in modulus momenta $p_\uparrow$ and $-p_\downarrow$. Due to the nonzero center of mass momentum Δp, the Cooper pair wave function obtains the spatially dependent phase in the ferromagnetic layer. In the "clean" limit (no scattering in the ferromagnet) one can find[18] that the Cooper pair wave function oscillates with distance z into the F layer as $\sim\sin(z/\xi_F^0)/(z/\xi_F^0)$, where $\xi_F^0=v_F/\varepsilon_{\rm ex}$.

This result holds also in the case of "dirty" ferromagnet. The microscopic theory of S/F multilayers based on the quasiclassical Usadel equations[3,4] predicts that the anomalous Green's function behaves in the ferromagnet as $\sim\exp\{-(1+i)\sqrt{h/D_M}z\}$, where $D_M=v_Fl/3$ is the diffusion coefficient and l is the electron mean free path in the F layer. Therefore, a length scale for oscillations and damping is the same and this scale is set by the length $\xi_M=\sqrt{2l\xi_F^0/3}$. Below, in this section it is shown that in the framework of our model the scales for oscillations and damping of the anomalous Green's function are determined by different lengths.

We can find the anomalous Green's function $F(\omega,\xi,z=z')$ in the F region $(d<z<a)$ following the same approach that was used to evaluate the F function in the superconductor. The solutions $\psi_{\uparrow(\downarrow)}(z)$ in the layer F_3 $(d<z<a)$ are given by Eq. (8). For solutions $\varphi_\mu(z)$ $(\mu=\uparrow,\downarrow)$ we can write

$$\varphi_\mu(z)=X_+^{\mu}\begin{pmatrix}1\\0\end{pmatrix}e^{ip_3^{\uparrow}(a-z)}+X_-^{\mu}\begin{pmatrix}1\\0\end{pmatrix}e^{-ip_3^{\uparrow}(a-z)}+Y_+^{\mu}\begin{pmatrix}0\\1\end{pmatrix}e^{ip_3^{\downarrow}(a-z)}+Y_-^{\mu}\begin{pmatrix}0\\1\end{pmatrix}e^{-ip_3^{\downarrow}(a-z)},$$

where $X_\pm^{\mu}$ and $Y_\pm^{\mu}$ can be found from conditions of continuity of functions $\varphi_\mu(z)$ and their derivatives at $z=d$, assuming the perfect S/F interface.

The anomalous Green's function averaged over oscillations is

$$F(\omega,\xi,z=z')=2m\sum_{\mu}\varphi_\mu^{-}(z)\langle a_{\mu\uparrow}\rangle\psi_\uparrow^{+}(z)=2m\sum_{\mu}F_\mu\langle a_{\mu\uparrow}\rangle.\quad(18)$$

It turns out that function $\varphi_\mu^{-}(z)$ contains four terms with multipliers $e^{\pm\theta_+}$ and $e^{\pm\theta_-}$. Denoting $\theta_\pm=\theta\pm i\delta$, we can write F_μ in the form

$$F_\mu=\Phi_\mu^{+}e^{i\theta}+\Phi_\mu^{-}e^{-i\theta},\quad(19)$$

where

$$\Phi_\mu^{+}=[\Theta_+^{\mu}\cos(p_3^{\downarrow}z_1)+\Xi_+^{\mu}\sin(p_3^{\downarrow}z_1)]\sin[p_3^{\uparrow}(d_F-z_1)],\quad(20)$$

$$\Phi_\mu^{-}=[\Theta_-^{\mu}\cos(p_3^{\downarrow}z_1)+\Xi_-^{\mu}\sin(p_3^{\downarrow}z_1)]\sin[p_3^{\uparrow}(d_F-z_1)].$$

Here $z_1=z-d$ is the distance from the S/F interface, and

$$\Theta_+^{\mu}=B_+^{\mu}e^{\delta}+\alpha A_+^{\mu}e^{-\delta},$$

$$\Theta_-^{\mu}=\alpha A_-^{\mu}e^{\delta}+B_-^{\mu}e^{-\delta},$$

$$\Xi_+^{\mu}=\frac{ik_-}{p_3^{\downarrow}}B_\mu^{+}e^{\delta}+\alpha\frac{ik_+}{p_3^{\downarrow}}A_+^{\mu}e^{-\delta},$$

$$\Xi_-^{\mu}=-\left(\alpha\frac{ik_+}{p_3^{\downarrow}}A_-^{\mu}e^{\delta}+\frac{ik_-}{p_3^{\downarrow}}B_-^{\mu}e^{-\delta}\right).$$

Using Eqs. (16), (18), and (19) we get the expression for function F averaged over the rapid oscillations

$$F(\omega,\xi,z=z')=2m\sum_{\mu}[\Phi_\mu^{-}b_{\mu\uparrow}^{+}+\Phi_\mu^{+}b_{\mu\uparrow}^{-}].$$

It follows from Eq. (20) for $\Phi_\mu^{\pm}$ that the dependence of function $F(\omega,\xi,z)$ on variable z or $z_1=z-d$ is given by a sum of the terms with sine and cosine from arguments $(p_3^{\uparrow}+p_3^{\downarrow})z_1$ and $(p_3^{\uparrow}-p_3^{\downarrow})z_1$. The terms with phases $(p_3^{\uparrow}+p_3^{\downarrow})z_1$ determine the short-periodic oscillations with respect to oscillations with a larger period $\sim(p_3^{\uparrow}-p_3^{\downarrow})^{-1}$. Ne-

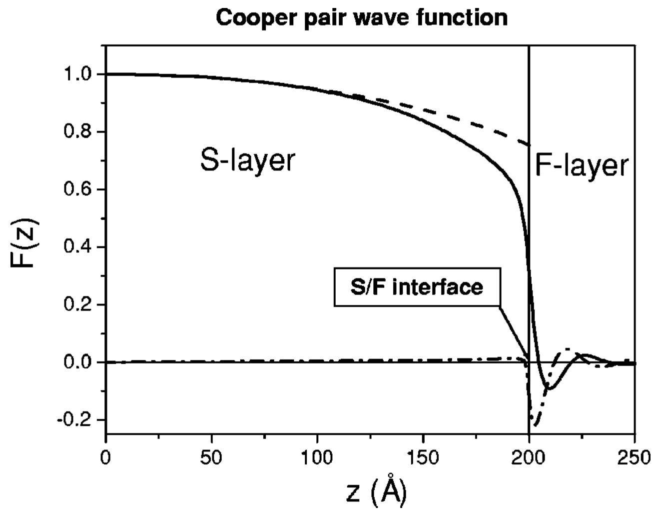

FIG. 2. The behavior of the anomalous Green's function $F(z)$ along the F/S/F structure with $d_S = 400$ Å, $d_F = 50$ Å, $\varepsilon_{\rm ex} = 1.156$ eV, $l_\uparrow = 133$ Å, $l_\downarrow = 35$ Å. The point $z = 200$ Å is the S/F interface. Solid line — Re $F(z)$ and dashed dotted line — Im $F(z)$. The contribution Re $F_0(z)$ [see Eq. (17)] to the function Re $F(z)$ in the S layer is shown by the dashed line.

glecting the nonessential terms with short-periodic oscillations, the anomalous Green's function can be presented in the form

$$F(\omega,\xi,z=z') = \tilde{\Theta}(\omega,\xi)\cos(\Delta p_3 z_1) + \tilde{\Xi}(\omega,\xi)\sin(\Delta p_3 z_1), \tag{21}$$

where $z_1 = z - d$, $\Delta p_3 = p_3^\uparrow - p_3^\downarrow$, and $p_3^{\uparrow(\downarrow)}$ are given by Eqs. (9) and (10).

The real and imaginary parts of the function

$$F(z) = T\sum_\omega \int_0^{\varepsilon_F} d\xi \;\; F(\omega,\xi,z)$$

normalized on the value of its real part at the point $z=0$ (the middle of the S layer) are shown in Fig. 2. The dashed line in Fig. 2 shows the contribution $F_0(z)$ [see Eq. (17)] to the function $F(z)$ in the S layer. We can estimate the lengths responsible for the oscillations and decay using Eq. (10) for momenta $p_3^\uparrow$ and $p_3^\downarrow$. Neglecting $\pm i\omega$ in Eq. (10), since $|\omega| \leqslant \omega_D$, we obtain

$$p_3^{\uparrow(\downarrow)} = \sqrt{2m(\xi \pm h)}\left[1 \pm \frac{i}{4}\tau^{-1}_{\downarrow(\uparrow)}\frac{1}{\xi \pm h} + \cdots\right].$$

As far as the integration over ξ goes from 0 to ε_F, then the damping of oscillations is determined by the value

$$\sim \frac{1}{l_0} = \frac{1}{l_\uparrow} + \frac{1}{l_\downarrow}.$$

Neglecting $\pm i\tau^{-1}_{\downarrow(\uparrow)}$ and $\pm i\omega$ in Eq. (10), we get

$$p_3^{\uparrow(\downarrow)} = \sqrt{2m\xi}\left[1 \pm \frac{h}{2\xi} + \cdots\right].$$

If $\xi \sim \varepsilon_F$, then

$$\Delta p_3 z_1 \sim \frac{\varepsilon_{\rm ex}}{v_F} z_1 = \frac{\pi z_1}{\xi_m^0},$$

where $\xi_m^0 = \pi v_F/\varepsilon_{\rm ex} = \pi \xi_F^0$ is the half-period of oscillations of $F(z)$ (the distance between the nearest zeros). Note that $\xi_m^0 \neq \pi l_0$ in contrast to what is found by using a quasiclassical approach.

The oscillatory terms in Eq. (21) arise due to quantum interference between two plane waves describing an electron and a hole propagating in the ferromagnetic layer with different momenta $p_3^\uparrow$ and $-p_3^\downarrow$ along the z axis. If $h \neq 0$ then $\Delta p_3 \neq 0$, and the oscillatory dependence of the Cooper pair wave function occurs due to the exchange field in the ferromagnet. If $h=0$, then $F(z)$ exhibits only the exponential decay into the F layer with characteristic length l_0. As it was already pointed out by many authors, the physical picture of the proximity effect is similar to the nonuniform Fulde-Ferrel-Larkin-Ovchinnikov state[27,28] which is characterized by the oscillatory dependent order parameter and arises in a homogeneous superconductor in the presence of a strong enough uniform exchange field.

IV. SELF-CONSISTENT EVALUATION OF THE ORDER PARAMETER

In this section we proceed further by constructing the self-consistent solution of Eqs. (1), (2), and (4). In the case of antiparallel orientation of magnetizations in the ferromagnetic layers the self-consistency can be reached if the order parameter $\Delta(z)$ takes the real values. We will search the self-consistent solution of Eq. (4) in the S layer assuming that in this equation the function $F(\omega,\xi,z)$ is replaced by its first contribution $F_0(\omega,\xi,z)$ given by Eq. (17). Function $F_0(z)$ is shown by a dashed line in Fig. 2 and can be approximated by a simple analytical function on z, such as $\propto \cos(qz)$, where q is a parameter. In order to take into account the correction $F_1(z)$ one has to choose a more complex class of sample functions for $\Delta(z)$. However, this will not change the results significantly.

Let us look for $\Delta(z)$ in the form

$$\Delta(z) = \Delta\cos(qz) \simeq \Delta\left(1 - \frac{q^2 z^2}{2}\right),$$

where the wave vector q (which has to be found) is small. The magnitude $\Delta(d) = (1-\delta_0)\Delta$ defines the amplitude of the superconducting order parameter at the S/F interface (see Fig. 2); here $\delta_0 = q^2 d^2/2 \sim 0.1$ is a small parameter. Following the well-known WKB approximation,[29] we search the solutions of Schrödinger's equation (6) in the form

$$\psi(z) = \begin{pmatrix} e^{i\xi_+(z)} \\ e^{i\xi_-(z)} \end{pmatrix}.$$

For $\xi_\pm$ we get the system of equations

$$\left[i\omega+\xi+\frac{1}{2m}(i\xi_+''-\xi_+'^2)\right]e^{i\xi_+}+\Delta(z)e^{i\xi_-}=0,$$
$$\Delta^*(z)e^{i\xi_+}+\left[i\omega-\xi-\frac{1}{2m}(i\xi_-''-\xi_-'^2)\right]e^{i\xi_-}=0, \tag{22}$$

where $\xi=\varepsilon_F-\kappa^2/2m$ and primes above $\xi_\pm$ denote the derivatives by z.

In the case of $q=0$, $\Delta(z)=\Delta$, four solutions of system (22) are $\xi_+^0=\pm k_+z$, $\xi_-^0=\pm k_+z+i\ln\alpha$ and $\xi_+^0=\pm k_-z+i\ln\alpha$, $\xi_-^0=\pm k_-z$ which give four initial eigenfunctions of the nonperturbed equation (6) $(q=0)$:

$$u_\pm^0(z)=\begin{pmatrix}1\\ \alpha\end{pmatrix}e^{\pm ik_+z},\quad v_\pm^0(z)=\begin{pmatrix}\alpha\\ 1\end{pmatrix}e^{\pm ik_-z}.$$

Consider, for example, the perturbed solution $u_+(z)$ which corresponds to $u_+^0(z)$ in the case of $q\neq0$. We look for the phases $\xi_\pm$ in the form $\xi_\pm=\xi_\pm^0+\eta_\pm$, where $\xi_+^0=k_+z$, $\xi_-^0=k_+z+i\ln\alpha$ for $u_+^0(z)$. The typical order of $\eta_\pm$ is $\sim qz\sim qd=\sqrt{2\delta_0}<1$. By linearizing system (22) with respect to $\eta_\pm$ we arrive at the following equations:

$$-\frac{1}{\alpha}\frac{k_+}{m}\ \eta_+'+i\Delta(\eta_--\eta_+)=\Delta\frac{q^2z^2}{2}, \tag{23}$$
$$\alpha\frac{k_+}{m}\eta_-'-i\Delta(\eta_--\eta_+)=\Delta\frac{q^2z^2}{2}.$$

We have also dropped the terms with $\eta_\pm'^2$ and $\eta_\pm''$ which are small as compared to $k_\pm\eta_\pm'$, since $\eta_\pm'^2\sim\eta_\pm'\eta_\pm/d\sim\eta_\pm'\sqrt{2\delta_0}/d\ll k_\pm\eta_\pm'$ if $d\sim200$ Å, $k_\pm\sim0.5$ Å^{-1}, and $\eta_\pm''\sim\eta_\pm'/d\ll k_\pm\eta_\pm'$. The equations similar to Eqs. (23) can be written also for phases $\eta_\pm$ which determine other three solutions $u_-(z)$ and $v_\pm(z)$. Solving these equations we get

$$u_\pm(z)=\begin{pmatrix}e^{\pm i[k_+z+\eta_+^{(\pm)}(z)]}\\ \alpha e^{\pm i[k_+z+\eta_-^{(\pm)}(z)]}\end{pmatrix},$$

with

$$\eta_\pm^{(+)}(z)=\tau_3^\pm z^3+\tau_2^\pm z^2+\tau_1^\pm z+\tau_0^\pm,$$
$$\eta_\pm^{(-)}(z)=\tau_3^\pm z^3-\tau_2^\pm z^2+\tau_1^\pm z-\tau_0^\pm;$$

and

$$v_\pm(z)=\begin{pmatrix}\alpha e^{\pm i[k_-z+\zeta_+^{(\pm)}(z)]}\\ e^{\pm i[k_-z+\zeta_-^{(\pm)}(z)]}\end{pmatrix},$$

where

$$\zeta_\pm^{(+)}(z)=\rho_3^\pm z^3+\rho_2^\pm z^2+\rho_1^\pm z+\rho_0^\pm,$$
$$\zeta_\pm^{(-)}(z)=\rho_3^\pm z^3-\rho_2^\pm z^2+\rho_1^\pm z-\rho_0^\pm.$$

The expressions for coefficients $\tau_i^\pm$ and $\rho_i^\pm$ of polynomials are given in Appendix B.

Next, the procedure of evaluation of the anomalous Green's function in the S layer is similar to one described in detail in Secs. II and III for the case of $\Delta(z)=\Delta$. By representing the solutions $\varphi_\mu(z)$ and $\psi_\mu(z)$ of Eq. (6) as a linear combination of eigenfunctions $u_\pm(z)$ and $v_\pm(z)$ similar to representation (11), we can find the new coefficients $A_\pm^\mu$, $B_\pm^\mu$, $C_\pm^\mu$, and $D_\pm^\mu$ solving the system of four linear equations. By evaluating the currents $j_{\mu\rho}$ at the point $z=0$ ($j_{\mu\rho}$ do not depend on z), we obtain the expressions for $j_{\mu\rho}$ similar to Eq. (14), where $k_\pm$ should be replaced by

$$\tilde{k}_+=k_++\frac{\tau_1^+-\alpha^2\tau_1^-}{1-\alpha^2},\quad \tilde{k}_-=k_-+\frac{\rho_1^--\alpha^2\rho_1^+}{1-\alpha^2},$$

and $\theta_\pm=2ik_\pm d=\theta\pm i\delta$. The substitutions $k_\pm\to\tilde{k}_\pm$ also have to be made in Eq. (15) for $a_{\mu\rho}$ and in the expression for det J (see Appendix A). Finally, the anomalous Green's function $F(\omega,\xi,z)$ is given by Eqs. (17), where $\Lambda_\pm^\mu$ and $\Sigma_\pm^\rho$ are replaced by new functions $\tilde{\Lambda}_\pm^\mu$ and $\tilde{\Sigma}_\pm^\rho$:

$$\tilde{\Lambda}_+^\mu=\alpha A_+^\mu e^{-\delta_1+i\eta_-^{(+)}}+B_+^\mu e^{\delta_1+i\zeta_-^{(+)}},$$
$$\tilde{\Lambda}_-^\mu=\alpha A_-^\mu e^{\delta_1-i\eta_-^{(-)}}+B_-^\mu e^{-\delta_1-i\zeta_-^{(-)}},$$
$$\tilde{\Sigma}_+^\rho=C_-^\rho e^{-\delta_2-i\eta_+^{(-)}}+\alpha D_-^\rho e^{\delta_2-i\zeta_+^{(-)}},$$
$$\tilde{\Sigma}_-^\rho=C_+^\rho e^{\delta_2+i\eta_+^{(+)}}+\alpha D_+^\rho e^{-\delta_2+i\zeta_+^{(+)}},$$

where δ_1, δ_2, $\eta_\pm^{(\pm)}$, and $\zeta_\pm^{(\pm)}$ are functions on z. The fixed point $q=q_*$ which determines the order parameter $\Delta(z)$ has to be found numerically by solving Eq. (4) using the iterative procedure.

V. CRITICAL TEMPERATURE T_c

If the anomalous Green's function in the S region $F(\omega,\xi,z)=F(\omega,\xi,z=0)\cos(q_*z)$ is known, the superconducting transition temperature T_c can be found. Up to now we assume the "clean" limit for a superconductor. Corrections (3) due to scattering will be taken into account further. Let us introduce the function

$$F_\omega=\frac{1}{k_F}\int_0^{\varepsilon_F}d\xi F(\omega,\xi,z=0),$$

where k_F is Fermi momentum in the S layer. This integral can be evaluated only numerically. However, we can approximate F_ω by the analytical function of argument ω. Let us represent F_ω in the form

$$F_\omega=\frac{\Delta}{\sqrt{\omega^2+\Delta^2}}F_\omega^{(1)}.$$

For the bulk superconductor $F_\omega^{(1)}=1$. Let $T\to T_c$, therefore $\Delta\ll\Delta(0)$, where $\Delta(0)$ is the order parameter at $T=0$. If ω takes values from 0 till $\sim5\omega_D$, $F_\omega^{(1)}$ can be well approximated by the following function:

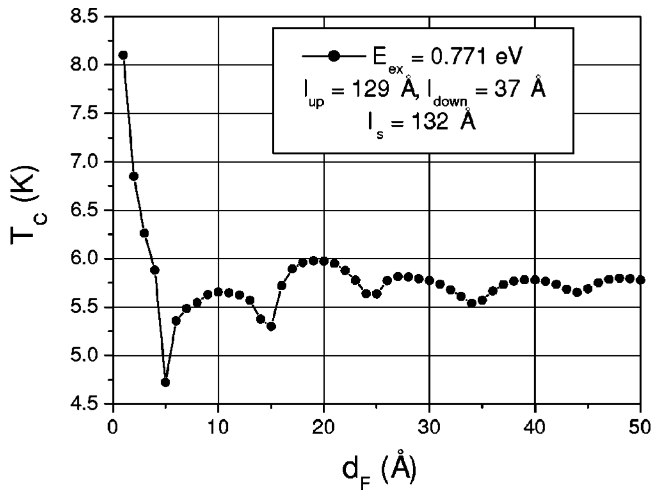

FIG. 3. Critical temperature T_c for the F/S/F trilayer as a function of the ferromagnetic layer thickness d_F. The parameters are $\varepsilon_{ex}=0.771$ eV (exchange field in the ferromagnet), $l_\uparrow=129$ Å, $l_\downarrow=37$ Å, $l_s=132$ Å (mean free paths in the F and S layers), $k_F=0.826$ Å^{-1} (Fermi momentum in the superconductor), $\omega_D=275$ K, and $T_c^0=9.25$ K.

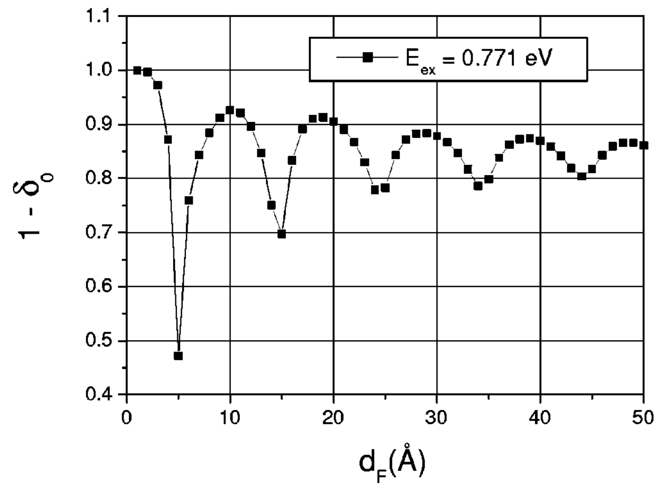

FIG. 4. The dependence of the normalized amplitude $(1-\delta_0)$ of the superconducting order parameter at the S/F interface as a function of the F-layer thickness d_F for the same parameters as in Fig. 3.

$$F_\omega^{(1)} \simeq A_0 \tanh\left(\frac{\gamma_0|\omega|}{2\omega_D}\right). \tag{24}$$

The coefficients A_0 and γ_0 are found numerically by minimizing the norm of a difference between the exact and the approximate function. These coefficients are nonmonotonic functions of the F-layer thickness d_F when d_S is fixed. For typical values of the parameters describing the F/S/F structure the magnitudes of A_0 and γ_0 are $A_0\sim 0.9$ and $\gamma_0\sim 4.0$.

The scattering in the S layer is introduced by Eq. (3). Numerical analysis shows that in Eq. (3) the Green's function $G_{\uparrow\uparrow}^{ss}(z,z)$ does not depend on z in the S region and its real part is negligibly small. Obviously, $\Delta_\omega(z)=\Delta_\omega\cos(q_* z)$. From numerical analysis it follows that G_ω in the S layer can be represented as

$$G_\omega=\frac{1}{k_F}\int_0^{\varepsilon_F} d\xi \;\; G_{\uparrow\uparrow}^{ss}(\omega,\xi,z=0)\approx -A_0\frac{i\omega}{\sqrt{\omega^2+\Delta^2}}. \tag{25}$$

Taking into account Eqs. (24) and (25), Eqs. (3) can be written in the form similar to the case of the bulk superconductor:[26]

$$\omega' \approx \omega + \frac{A_0}{2\tau_0}\frac{\omega'}{\sqrt{\omega'^2+\Delta_\omega^2}},$$

$$\Delta_\omega \approx \Delta + \frac{A_0}{2\tau_0}\frac{\Delta_\omega}{\sqrt{\omega'^2+\Delta_\omega^2}}, \tag{26}$$

where $\tau_0^{-1}=2\pi c u_0^2 N(\varepsilon_F)$ is the inverse lifetime of quasiparticles in the superconductor, and $N(\varepsilon_F)=mk_F/2\pi^2$ is density of states at the Fermi energy. Deriving Eq. (26) we took into account that if $\frac{1}{2}\tau_0^{-1}\sim\omega_D\sim 300$ K corresponding to mean free path $l_s\sim 130$ Å, then for $\omega'\simeq\omega+A_0/2\tau_0$ and $\gamma_0\sim 4.0$ we have $\tanh(\gamma_0|\omega'|/2\omega_D)\approx 1$.

Equations (26) can be written as[26]

$$\omega'=\omega\,\eta(\omega), \quad \Delta_\omega=\Delta\,\eta(\omega),$$

$$\eta(\omega)=1+\frac{A_0}{2\tau_0\sqrt{\omega^2+\Delta^2}}. \tag{27}$$

Using Eqs. (27) and (4) we come to the equation for T_c:

$$\pi\rho T_c\sum_\omega \frac{1}{|\omega|}\tanh\left(\frac{\gamma_0|\omega'|}{2\omega_D}\right)=1, \tag{28}$$

where

$$\omega'=\omega+\frac{A_0}{2\tau_0}, \qquad \rho=\rho_0 A_0<\rho_0,$$

and $\rho_0=\lambda N(\varepsilon_F)$ is the renormalized coupling constant. By carrying out the summation over Matsubara frequencies $\omega=\pi T_c(2n+1)$ in Eq. (28), we get the equation for the reduced critical temperature $\tau=T_c/T_c^0$:

$$\tau=\exp\left\{\left(\frac{1}{\rho_0}-\frac{1}{\rho}\right)-\Phi[\,\eta_0(\tau)]\right\}, \tag{29}$$

where

$$\Phi(\eta_0)=\sum_{n=0}^{+\infty}\frac{4\Gamma_0 e^{-(2n+1)\eta_0}}{(2n+1)(1+\Gamma_0 e^{-(2n+1)\eta_0})},$$

$$\eta_0(\tau)=\frac{\gamma_0\pi T_0}{\omega_D}\tau, \quad \tau=T_c/T_c^0,$$

$$\Gamma_0=\exp\left(-\frac{\gamma_0 A_0}{2\tau_0\omega_D}\right),$$

TABLE I. The comparison of the periods of oscillations ξ_F predicted by formula (30) with the period $\tilde{\xi}_F$ obtained from numerical analysis for different values of exchange field $\varepsilon_{\rm ex}$, effective electron mass m, and a superconductor layer thickness d_S. Other model parameters are the same as in Fig. 3. The accuracy of determining of $\tilde{\xi}_F$ is restricted by a finite step for d_F in numerical calculations.

$\varepsilon_{\rm ex}$ (eV)	m (m_e)	d_S (Å)	ξ_F (Å)	$\tilde{\xi}_F$ (Å)
0.385	1.0	400	13.97	14.0
0.771	1.0	400	9.98	10.0
1.156	1.0	400	8.06	8.0
2.027	1.0	400	6.09	6.0
0.610	0.45	600	16.55	16.5

and $T_c^0=2\pi^{-1}\omega_D\gamma e^{-1/\rho_0}$ ($\gamma=e^C$, $C=0.577\ldots$) is transition temperature of the bulk superconductor.

VI. RESULTS AND DISCUSSION

In this section we present the results of numerical calculation of the critical temperature T_c. We first focus on the general features of a behavior of the system. Next, we consider selected experimental data which can be interpreted in the framework of the given model.

A. Oscillatory behavior of T_c

The typical dependence of critical temperature $T_c(d_F)$ with respect to ferromagnetic layer thickness d_F with $d_S=400$ Å is shown in Fig. 3 where the model parameters are given in the figure caption. The effective electron mass is $m=m_e$ (m_e is a bare electron mass). For the superconductor we took $\omega_D=276$ K and $T_c^0=9.25$ K which are the parameters of bulk Nb. The corresponding normalized magnitude $(1-\delta_0)$ of the order parameter at the S/F interface as a function of d_F is shown in Fig. 4.

Both functions $(1-\delta_0)$ and $T_c(d_F)$ show the pronounced damping oscillatory behavior with the same period. The oscillatory behavior of $T_c(d_F)$ is a consequence of oscillations of the amplitude $\Delta(d)=\Delta(1-\delta_0)$ of the order parameter at the S/F interface when d_F is varying. The minima of $\Delta(d)$ correspond to minima of T_c and the maxima of $\Delta(d)$ correspond to the maxima of T_c, as they should. The oscillations of $\Delta(d)$ in turn are caused by the oscillations of the anomalous Green's function $F(z)$ in the F layer. Function $F(z)$ must satisfy the zero boundary condition at the ferromagnet/vacuum interface. Because of oscillations of $F(z)$ in the F region, the order parameter at the S/F interface is forced to adjust in such a way that the condition $F(a)=0$ is fulfilled at the outer boundary $z=a$ of the F layer.

The results of numerical analysis, presented in Table I for different values of exchange field $\varepsilon_{\rm ex}$ and effective electron mass m, show that the period ξ_F of T_c oscillations is defined as

$$\xi_F=\frac{\pi}{\sqrt{m\varepsilon_{\rm ex}}}=\sqrt{\pi\xi_m^0 k_F^{-1}}, \tag{30}$$

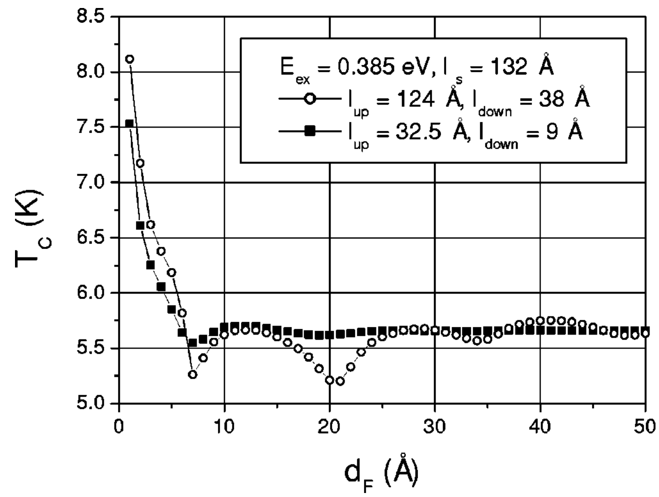

FIG. 5. The critical temperature $T_c(d_F)$ for the case of weak and strong scattering in the ferromagnetic layers; $\varepsilon_{\rm ex}=0.385$ eV, $l_s=132$ Å. Dots (weak scattering)—$l_\uparrow=124$ Å, $l_\downarrow=38$ Å; squares (strong scattering)—$l_\uparrow=32.5$ Å, $l_\downarrow=9$ Å.

where k_F is the Fermi momentum in a superconductor. The period ξ_F, therefore, does not depend on the electron mean free paths in the S and F layers. The first minimum of $T_c(d_F)$ occurs at the thickness $\xi_F/2$, while the location of first maximum is ξ_F.

As can be seen from Fig. 5, the strong scattering in the ferromagnetic layers significantly damps the oscillations of T_c, but their period remains unchanged for any values of the mean free paths $l_\uparrow$ and $l_\downarrow$. As it follows from the analysis presented in Sec. III, the reason of such a behavior is that the strong scattering in the F region affects only the length l_0 of decay of the Cooper pair wave function $F(z)$ but not the period $\sim\xi_m^0$ of its oscillations. The less pronounced are the oscillations of $F(z)$ with respect to $z_1=z-d$ in the case of strong electron scattering, the less is the amplitude of oscillations of $\Delta(d)$ and T_c with respect to the ferromagnetic layer thickness d_F. In the case of extremely strong scattering, the coherent coupling which was established due to these oscillations between two boundaries of the ferromagnetic layer is destroyed and thus the oscillations of T_c are suppressed completely.

We also observed that strong scattering in the S layer (small mean free path l_s) suppresses the amplitude of T_c oscillations (look at Fig. 6). The critical temperature is higher for smaller values of l_s. The reason for it is that in the thin superconducting films T_c is reduced with respect to T_c^0 due to dimensional effect, and the magnitude of T_c depends on d_S only via the dimensionless thickness d_S/ξ_S, where $\xi_S\propto\sqrt{\xi_0 l_s}$ is a coherence length for the dirty superconductor, and ξ_0 is a BCS coherence length. Small mean free path l_s, therefore, corresponds to large value of the effective film thickness d_S/ξ_S.

B. Comparison with experiment

The experimental situation regarding the oscillatory behavior of $T_c(d_F)$ in the S/F structures is known to be con-

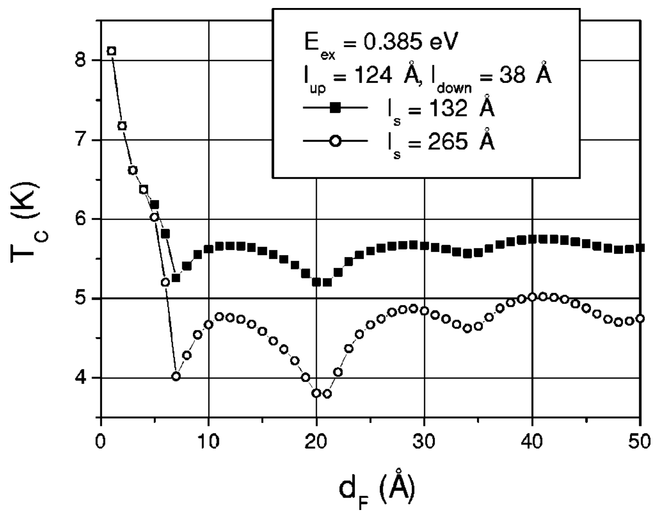

FIG. 6. The critical temperature $T_c(d_F)$ for different values of the mean free paths in the S layer; $\varepsilon_{ex}=0.385$ eV, $l_\uparrow=124$ Å, $l_\downarrow=38$ Å. Squares: $l_s=132$ Å; dots: $l_s=265$ Å.

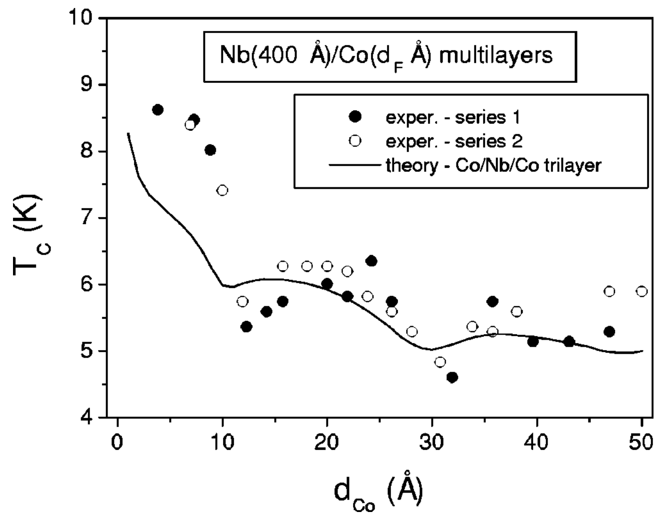

FIG. 8. The comparison of the theoretical $T_c(d_F)$ curve with experiment by Obi *et al.* (Ref. 9) for Nb(400 Å)/Co multilayers. The fitting parameters are $l_\uparrow=240$ Å, $l_\downarrow=80$ Å, and $l_s=188$ Å.

troversial. Nevertheless, there are two groups of experiments described in the literature where oscillations of $T_c(d_F)$ were clearly observed and the 3d ferromagnets were used as F layers—these are reports on Fe/Nb/Fe trilayers by Mühge *et al.*[8] and Nb/Co and V/Co multilayers by Obi *et al.*[9]

In Fig. 7 the fitting is shown to experimental data by Mühge *et al.*[8] for Fe(d_F)/Nb(400 Å)/Fe(d_F) trilayers prepared by rf sputtering. According to formula (30) the period ξ_F of oscillations is determined by exchange-splitting energy in the ferromagnet. If we take the value $\varepsilon_{ex}^d \simeq 0.149$ Ry $=2.03$ eV (Ref. 30) of exchange splitting of the Fe d bands near the Fermi energy and put $m=m_e$, we obtain $\xi_F^{(d)}=6.09$ Å (see Table I) which is too small as compared to the location of a maximum at $d_F\sim 10$–15 Å in Fig. 7. However, we can assume that in the S and F layers the Cooper pairs are formed by s electrons of Nb and Fe. The value of exchange

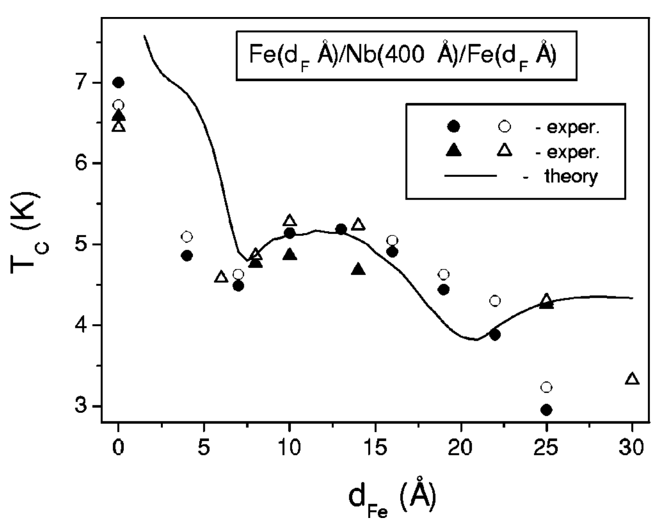

FIG. 7. The comparison of the theoretical $T_c(d_F)$ curve with experiment by Mühge *et al.* (Ref. 8) for Fe/Nb(400 Å)/Fe trilayers. The fitting parameters are $l_\uparrow=120$ Å, $l_\downarrow=40$ Å, $l_s=269$ Å.

splitting $\varepsilon_{ex}^s=0.028$ Ry $=0.381$ eV at the bottom of Fe s bands (Γ point, Ref. 30) together with $m=m_e$ gives the period $\xi_F=14.05$ Å. Thus, the first minimum of $T_c(d_F)$ is at the point $\xi_F/2\approx 7$ Å and the first maximum is at $\xi_F\approx 14$ Å. From Fig. 7 it follows that these values correlate with positions of minimum and maximum of T_c which can be roughly determined from the scattered experimental points. We have put $\varepsilon_F=0.387$ Ry corresponding to the s band of Nb (Ref. 30) which gives the Fermi momentum value $k_F=1.18$ Å^{-1} for $m=m_e$. We used $\omega_D=276$ K and $T_c^0=9.25$ K for Nb. The fitting parameters are the values of mean free paths in Fe and Nb which were estimated approximately as $l_\uparrow=120$ Å, $l_\downarrow=40$ Å, and $l_s=269$ Å. Note that magnetic measurements by Mühge *et al.* showed that thin Fe layers were not magnetic for $d_F\leqslant 7$ Å, and it was assumed that magnetically dead Fe-Nb alloy of a thickness about 7 Å was formed at the interfacial S/F region for all samples with different d_F. Mühge *et al.* qualitatively explained the observed nonmonotonic behavior of $T_c(d_F)$ in terms of a rather complex behavior of this magnetically dead Fe-Nb layer when d_F was varying (for details, see Ref. 8). They also argued that a nonmonotonic $T_c(d_F)$ behavior in their case could not be possible due to the mechanism of π coupling as it was predicted for the S/F multilayers because of a single S layer in the trilayer system. Indeed, the well-known theoretical prediction by Buzdin *et al.*[3,4] ascribes the oscillatory behavior of $T_c(d_F)$ to the periodical switching of the ground state energy between 0 and π phases of the order parameter if the neighboring S layers in the S/F multilayer are coupled. However, it follows from the above analysis that the oscillatory behavior of $T_c(d_F)$ does not necessary require π coupling and can occur also for a trilayer (or bilayer) F/S/F structure.

Let us consider the experiments on Nb/Co multilayers by Obi *et al.*[9] The theoretical curve $T_c(d_F)$ in comparsion with experimental data is shown in Fig. 8. The exchange splitting of Co spin-up and -down s bands at Γ point is $\varepsilon_{ex}=0.014$ Ry (Ref. 30) which gives $\xi_F=19.87$ Å ($m=m_e$).

The first and second minimum of $T_c(d_F)$ should, therefore, be placed at points $d^1_{\rm min}=10$ Å and $d^2_{\rm min}=30$ Å. These values correlate with values 12 Å and 32 Å obtained from experiment. The fitting mean free paths are $l_\uparrow=240$ Å, $l_\downarrow=80$ Å, and $l_s=188$ Å. We have to note that in experiment Nb/Co structures are multilayers. A qualitative resemblance of theoretical T_c curve calculated for a trilayer structure with experimental points for a multilayer and the agreement between theoretical and experimental values of $d^1_{\rm min}$ and $d^2_{\rm min}$ allows us to assume that neighboring S layers were decoupled in the experiment. As it was observed by Strunk *et al.*[10] for similar Nb/Fe multilayered system (where the F layer is 3*d* transition metal), the decoupling regime is set when d_F is larger than some critical value $d_c^{\rm dc}$ which in turn is less than the critical thickness d_c^F of the onset of ferromagnetism. This threshold value was $d_c^F\approx 7$ Å in experiments by Obi *et al.*[9] In Ref. 9 it was noted that d_c^F was less than the first minimum of T_c at $d^1_{\rm min}\approx 12$ Å, so that for Nb/Co system the first minimum could not be ascribed to the onset of ferromagnetism as it was argued by Mühge *et al.* for the Fe/Nb/Fe system.[8] Our theoretical explanation assuming the decoupling regime is incorrect only for very thin Fe layers with $d_F<d_c^{\rm d}$ when, probably, the Fe films are nonmagnetic due to alloying effect.

Note also that experiments by Obi *et al.*[9] on $Nb_{1-x}Ti_x$/Co multilayers with $Nb_{1-x}Ti_x$ alloy being the superconductor with small coherence length did not reveal the oscillatory behavior of T_c, but showed only a small reduction of the critical temperature $T_c\approx 8$ K for large d_F as compared to the bulk value $T_c^0\approx 9.2$ K (see Fig. 3 in Ref. 9). Therefore, the observation of increasing T_c when the scattering is strong in the S layer together with damping of oscillations for small l_s (see Fig. 6) is in a qualitative agreement with these experimental observations.

VII. SUMMARY

In conclusion, we have presented a theory of proximity effect in F/S/F trilayer nanostructures where S is a superconductor, and F are layers of 3*d* transition ferromagnetic metal. As a starting point of our calculations, we took the system of Gor'kov equations, which determine the normal and anomalous Green's functions. The solution of these equations was found together with a self-consistent evaluation of the superconductor order parameter. In accordance with the known quasiclassical theories of proximity effect for S/F multilayers,[3,4,16,18] we found that due to the presence of an exchange field in the ferromagnet the anomalous Green's function $F(z)$ exhibits damping oscillations in the F layer as a function of a distance z from the S/F interface. In the presented model, a half-period of oscillations of $F(z)$ is determined by the length $\xi_m^0=\pi v_F/\varepsilon_{\rm ex}$, where v_F is the Fermi velocity, $\varepsilon_{\rm ex}$ is the exchange field, and the length of damping is given by $l_0=(1/l_\uparrow+1/l_\downarrow)^{-1}$, where $l_\uparrow$ and $l_\downarrow$ are spin-dependent mean free paths in the ferromagnetic layer. The oscillations of the anomalous Green's function (Cooper pair wave function) in the F region and a zero boundary condition at the ferromagnet/vacuum interface give rise to the oscillatory dependence of the superconductor order parameter at the S/F interface vs the F-layer thickness d_F. These oscillations result in oscillations of the superconductor transition temperature $T_c(d_F)$ with a period $\xi_F=\pi/\sqrt{m\varepsilon_{\rm ex}}$. Thus, we have demonstrated that the nonmonotonic oscillatory dependence of critical temperature $T_c(d_F)$ does not necessarily require the mechanism of π coupling between neighboring superconducting layers as it takes place in the S/F multilayers.[3,4] The strong electron scattering either in the superconductor or in the ferromagnet significantly suppresses the oscillations. In the case of extremely strong scattering in the ferromagnet, the length of damping l_0 becomes very short and the oscillations of T_c are suppressed completely. The reason for this is the loss of coherent coupling between two boundaries of the ferromagnetic layer that was established due to oscillations of Cooper pair wave function $F(z)$. We compared our results with the existing data on $T_c(d_F)$ for Fe/Nb/Fe trilayers[8] and V/Co multilayers,[9] where F's are 3*d* ferromagnets, and found reasonable agreement with theory and experiment.

ACKNOWLEDGMENTS

This work was partially supported by the Russian Foundation for Basic Research under Grant No. 01-02-17378. A.B. is grateful to NATO for financial support.

APPENDIX A

The determinant $\tilde{D}=\det J/(1-\alpha^2)^2$ of the matrix of currents [Eq. (12)] is given by the expression

$$\tilde{D}=-D_0+\Gamma_+e^{2i\theta}+\Gamma_-e^{-2i\theta},$$

where

$$D_0=4k_+^2\begin{vmatrix}A_+^\uparrow & A_+^\downarrow\\ A_-^\uparrow & A_-^\downarrow\end{vmatrix}\begin{vmatrix}C_+^\uparrow & C_+^\downarrow\\ C_-^\uparrow & C_-^\downarrow\end{vmatrix}+4k_-^2\begin{vmatrix}B_+^\uparrow & B_+^\downarrow\\ B_-^\uparrow & B_-^\downarrow\end{vmatrix}\begin{vmatrix}D_+^\uparrow & D_+^\downarrow\\ D_-^\uparrow & D_-^\downarrow\end{vmatrix}$$
$$+4k_+k_-e^{2\delta}\begin{vmatrix}A_-^\uparrow & A_-^\downarrow\\ B_+^\uparrow & B_+^\downarrow\end{vmatrix}\begin{vmatrix}C_+^\uparrow & C_+^\downarrow\\ D_-^\uparrow & D_-^\downarrow\end{vmatrix}$$
$$+4k_+k_-e^{-2\delta}\begin{vmatrix}A_+^\uparrow & A_+^\downarrow\\ B_-^\uparrow & B_-^\downarrow\end{vmatrix}\begin{vmatrix}C_-^\uparrow & C_-^\downarrow\\ D_+^\uparrow & D_+^\downarrow\end{vmatrix},$$

$$\Gamma_+=4k_+k_-\begin{vmatrix}A_+^\uparrow & A_+^\downarrow\\ B_+^\uparrow & B_+^\downarrow\end{vmatrix}\begin{vmatrix}C_-^\uparrow & C_-^\downarrow\\ D_-^\uparrow & D_-^\downarrow\end{vmatrix},$$

$$\Gamma_-=4k_+k_-\begin{vmatrix}A_-^\uparrow & A_-^\downarrow\\ B_-^\uparrow & B_-^\downarrow\end{vmatrix}\begin{vmatrix}C_+^\uparrow & C_+^\downarrow\\ D_+^\uparrow & D_+^\downarrow\end{vmatrix},$$

and $A_\pm^\mu$, $B_\pm^\mu$, $C_\pm^\mu$, $D_\pm^\mu$ are coefficients introduced in Eq. (11).

APPENDIX B

Let us define the quantities

$$\lambda_{\pm}^{-1}=\frac{2m}{k_{\pm}}\sqrt{\omega^2+\Delta^2},$$

$$W_{\pm}=\frac{\Delta^2}{3}\left(\frac{m}{k_{\pm}}\right)^2 q^2,$$

$$V_{\pm}=\frac{q^2}{2}\left(\frac{m}{k_{\pm}}\right)\left[\frac{\omega^2}{\sqrt{\omega^2+\Delta^2}}\mp\omega\right].$$

In the case of $q\neq 0$ four linear independent solutions of Eq. (6) have the following forms.

(i) Solution $u_+(z)$:

$$u_+(z)=\begin{pmatrix} e^{ik_+z+i\eta_+^{(+)}(z)} \\ \alpha e^{ik_+z+i\eta_-^{(+)}(z)}\end{pmatrix},$$

where

$$\eta_+^{(+)}(z)=-i\lambda_+W_+z^3+i\lambda_+V_+z^2+2i\lambda_+^2V_+z+2i\lambda_+^3V_+$$
$$\equiv\tau_3^+z^3+\tau_2^+z^2+\tau_1^+z+\tau_0^+,$$

$$\eta_-^{(+)}(z)=\frac{1}{\alpha^2}\eta_+^{(+)}(z)+\frac{\Delta}{3\alpha}\left(\frac{m}{k_+}\right)q^2z^3$$
$$\equiv\tau_3^-z^3+\tau_2^-z^2+\tau_1^-z+\tau_0^-.$$

(ii) Solution $u_-(z)$:

$$u_-(z)=\begin{pmatrix} e^{-ik_+z-i\eta_+^{(-)}(z)} \\ \alpha e^{-ik_+z-i\eta_-^{(-)}(z)}\end{pmatrix},$$

where

$$\eta_{\pm}^{(-)}(z)=-\eta_{\pm}^{(+)}(-z)=\tau_3^{\pm}z^3-\tau_2^{\pm}z^2+\tau_1^{\pm}z-\tau_0^{\pm}.$$

(iii) Solution $v_+(z)$:

$$v_+(z)=\begin{pmatrix} \alpha e^{ik_-z+i\zeta_+^{(+)}(z)} \\ e^{ik_-z+i\zeta_-^{(+)}(z)}\end{pmatrix},$$

where

$$\zeta_+^{(+)}(z)=i\lambda_-W_-z^3+i\lambda_-V_-z^2-2i\lambda_-^2V_-z+2i\lambda_-^3V_-$$
$$\equiv\rho_3^+z^3+\rho_2^+z^2+\rho_1^+z+\rho_0^+,$$

$$\zeta_-^{(+)}(z)=\alpha^2\zeta_+^{(+)}(z)+\frac{\alpha\Delta}{3}\left(\frac{m}{k_-}\right)q^2z^3$$
$$\equiv\rho_3^-z^3+\rho_2^-z^2+\rho_1^-z+\rho_0^-.$$

(iv) Solution $v_-(z)$:

$$v_-(z)=\begin{pmatrix} \alpha e^{-ik_-z-i\zeta_+^{(-)}(z)} \\ e^{-ik_-z-i\zeta_-^{(-)}(z)}\end{pmatrix},$$

where

$$\zeta_{\pm}^{(-)}(z)=-\zeta_{\pm}^{(+)}(-z)=\rho_3^{\pm}z^3-\rho_2^{\pm}z^2+\rho_1^{\pm}z-\rho_0^{\pm}.$$

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