π phase in magnetic-layered superconductors

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We show that in a system composed of alternating superconducting and magnetic layers the ground state may be the so-called "π phase," wherein the superconducting order parameter changes its sign as we go from one superconducting layer to another. This phase is similar to the Larkin-Ovchinnikov-Fulde-Ferrell phase. We find that the π phase exists, under certain conditions, in the presence of both ferro- and antiferromagnetism.

I. INTRODUCTION

It has recently become possible to produce artificially an entire family of layered compounds, in which superconducting (S) layers alternate with magnetic (M) [ferromagnetic (F) or antiferromagnetic (AF)] layers. Examples of such systems are superstructures of the S-F type,[1] layered superconductors intercalated with magnetic atoms,[2] and high-temperature superconductors of the type $R\mathrm{Ba_2Cu_3O_7}$, where nonmagnetic $R=Y$ layers alternate with magnetic R layers, such as the nonsuperconducting $R=\mathrm{Pr}$.[3] Sputtering technology now permits the artificial growing of an S-M structure with layer thicknesses as small as one lattice constant. Such systems are interesting because they illustrate the interplay of magnetism and superconductivity.[4]

The case of thick, alternating magnetic and superconducting layers was investigated in Ref. 5; the authors used quasiclassical Usadel equations to calculate the parallel and perpendicular critical fields. Systems of alternating superconducting-metallic layers with thicknesses of the order of one interatomic length [where microscopic Bardeen-Cooper-Schrieffer (BCS) theory is applicable] have also attracted considerable theoretical attention.[6,7] In this work, we use microscopic theory to investigate a system of alternating superconducting-magnetic layers. We show below that the ground state of this system may be the so-called "π phase," characterized by a superconducting order parameter that changes its sign as we go from one superconducting layer to another.

One noted case of an inhomogeneous order parameter is the Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) phase,[8,9] which occurs in a three-dimensional superconductor with an exchange field h that acts only on electron spins. There is a small region of h-T phase diagram in which it is energetically favorable to form Cooper pairs with total momentum not equal to zero (see Ref. 10). At the transition line, the order parameter takes the form $\Delta=|\Delta|e^{i\mathbf{k}\cdot\mathbf{r}}$, where $|\mathbf{k}|\sim\xi_0^{-1}$, and ξ_0 is the superconducting coherence length.

We present in Sec. II a model for the study of thin (on the order of an interatomic length) alternating superconducting and magnetic layers. We use the standard BCS approach to investigate the existence of the π phase. In Sec. III we present our results in the case of ferromagnetic and antiferromagnetic conducting layers, and also in the case of insulating magnetic layers. In Sec. IV we consider the effect of impurities, both with and without the exchange field h. In Sec. V, we interpret the excitation spectrum and show how it differs from the usual BCS case and the results of Ref. 6. In Sec. VI, we discuss our results and suggestions for experimental verification.

II. FORMULATION OF THE PROBLEM

We consider the model of an elementary cell consisting of one superconducting and one magnetic layer. Movement of quasiparticles within the layers is, for simplicity, described by one and the same energy spectrum $\xi(\mathbf{p})$, and movement perpendicular to the layers is characterized by the transfer integral t of the tight-binding model (we consider the layers to be linked only by Josephson coupling, so that $t \ll T_c$). We assume that the pairing constant between electrons Λ is equal to zero in the M layers, and that the exchange field h, which we consider to be a constant in the case of a ferromagnet, exists only on the M layer. The exchange field on the M layer will affect T_c only by acting on the electrons which tunnel between the layers.

We note that orbital effects of magnetic induction may often be neglected in comparison with the effects of the exchange field in magnetic superconductors; see Ref. 11. We now concentrate on the model with exchange field only.

We write down the Hamiltonian of the system:

$$H=\sum_{\mathbf{p},n,i,\sigma}\xi(\mathbf{p})a^\dagger_{ni\sigma}(\mathbf{p})a_{ni\sigma}(\mathbf{p}) +t[a^\dagger_{ni\sigma}(\mathbf{p})a_{n,-i,\sigma}(\mathbf{p})+a^\dagger_{n+1,-i,\sigma}(\mathbf{p})a_{ni\sigma}(\mathbf{p})+\mathrm{H.c.}] +H_{\mathrm{int1}}+H_{\mathrm{int2}}\ , \tag{1a}$$

$$H_{\mathrm{int1}}=\frac{\Lambda}{2}\sum_{\mathbf{p}_1\mathbf{p}_2 n\sigma}a^\dagger_{n1\sigma}(\mathbf{p}_1)a^\dagger_{n1-\sigma}(-\mathbf{p}_1) \times a_{n1-\sigma}(-\mathbf{p}_2)a_{n1\sigma}(\mathbf{p}_2)\ , \tag{1b}$$

$$H_{\text{int2}} = -\sum_{\mathbf{p},n,\sigma} h\sigma a^{\dagger}_{n,-1,\sigma}(\mathbf{p}) a_{n,-1,\sigma}(\mathbf{p}) \ , \tag{1c}$$

where $a^{\dagger}_{ni\sigma}(\mathbf{p})$ is the creation operator of an electron with spin σ in the nth elementary cell and momentum $\mathbf{p}$ on the layer i. $i=1$ in the case of an S layer and $i=-1$ in the case of an M layer.

We write down the equations of motion for the operators $a_{ni\sigma}(\mathbf{p})$ and $a^{\dagger}_{ni\sigma}(\mathbf{p})$, and from them derive the Gor'kov equations describing the normal $[G_{\alpha\beta ij}(\mathbf{p},q,q',\omega)]$ and anomalous $[F^{\dagger}_{\alpha\beta ij}(\mathbf{p},q,q',\omega)]$ Green's functions, where we have made a Fourier transform from the discrete layer indices n and m to quasimomenta q and q' ($0 \le q, q' \le 2\pi$). α and β are spin indices, and i and j are layer indices (1 or -1). We assume that the order parameter changes from cell to cell in the following manner: $\Delta = |\Delta| e^{ikn}$. Noting that $F^{\dagger}_{\alpha\beta ij}(\mathbf{p},q,q',\omega) = F^{\dagger}_{\alpha\beta ij}(\mathbf{p},q,\omega)\delta(q+k-q')$, we may write the Green's functions as functions of only q, instead of both q and q', but we must include the functions $G_{\alpha\beta ij}(\mathbf{p},q+k,\omega)$ in our calculations.

We may write a matrix equation for either $G_{\downarrow\downarrow ij}(\mathbf{p},q-k,\omega)$ and $F^{\dagger}_{\uparrow\downarrow ij}(\mathbf{p},q,\omega)$, or for $G_{\uparrow\uparrow ij}(\mathbf{p},q-k,\omega)$ and $F^{\dagger}_{\downarrow\uparrow ij}(\mathbf{p},q,\omega)$. We choose the former here, omitting the arrows for brevity below. This choice determines the sign before the term h in the Green's function. As will be seen below, this choice is in the end not important; h appears in all final expressions only as h^2. Following Ref. 6, we write the Gor'kov equations in matrix form:

$$\begin{bmatrix} \omega_- & -T_k & |\Delta| & 0 \\ -T_k^* & \omega_- + h & 0 & 0 \\ |\Delta| & 0 & \omega_+ & T \\ 0 & 0 & T^* & \omega_+ + h \end{bmatrix} \begin{bmatrix} G_{1j}(q+k) \\ G_{1j}(q+k) \\ F^{\dagger}_{1j}(q) \\ F^{\dagger}_{1j}(q) \end{bmatrix} = \begin{bmatrix} \delta_{1j} \\ \underline{\delta}_{1j} \\ 0 \\ 0 \end{bmatrix} , \tag{2}$$

where we have omitted the explicit dependence of the Green's functions on $\mathbf{p}$ and ω, as well as spin, for brevity.

We define $\omega_{\pm} = i\omega \pm \xi(\mathbf{p})$, $T = 2t\cos(q/2)e^{iq/2}$, $T_k = 2t\cos[(q+k)/2]e^{i(q+k)/2}$, $\omega = \pi T(2n+1)$, and j is a layer index. We may reduce this 4×4 matrix into 2×2 submatrices, and write in abbreviated form

$$\hat{G}_0^{-1}(\mathbf{p},q+k,\omega)\hat{G}(\mathbf{p},q+k,\omega) + \hat{\Delta}\hat{F}^{\dagger}(\mathbf{p},q,\omega) = 1 \ , \tag{3a}$$

$$\hat{G}_0^{-1}(\mathbf{p},q,-\omega,-h)\hat{F}^{\dagger}(\mathbf{p},q,+\omega) - \hat{\Delta}^*\hat{G}(\mathbf{p},q+k,+\omega,+h) = 0 \ , \tag{3b}$$

where $\hat{F}^{\dagger}(\mathbf{p},q,\omega)$ is the matrix $F^{\dagger}_{ij}(\mathbf{p},q,\omega)$, $\hat{G}(\mathbf{p},q,\omega)$ the matrix $G_{ij}(\mathbf{p},q,\omega)$ (i and j are layer indices), and

$$\hat{\Delta} = \begin{bmatrix} |\Delta| & 0 \\ 0 & 0 \end{bmatrix}, \quad \hat{G}_0^{-1} = \begin{bmatrix} \omega_- & -T_q \\ -T_q^* & \omega_- + h \end{bmatrix} . \tag{4}$$

Note that above we have written the Green's function as an explicit function of h. The signs of h and ω in the expression $\hat{G}_0^{-1}(\mathbf{p},q,-\omega,-h)$ are the opposite of those in the expression $\hat{G}(\mathbf{p},q+k,+\omega,+h)$.

III. π PHASE IN F AND AF CASES

A. Ferromagnet: $T - T_c/T_c \ll 1$

Near T_c we can eliminate the term $\Delta F^{\dagger}(\mathbf{p},q,\omega)$ in the above system of equations because it is second order in Δ; this allows us to rewrite Eq. (3b) above as

$$\hat{G}_0^{-1}(\mathbf{p},q,-\omega,-h)\hat{F}^{\dagger}(\mathbf{p},q,\omega) = \hat{\Delta}^*\hat{G}_0(\mathbf{p},q+k,+\omega,+h) \ . \tag{5}$$

We must choose the value of k that corresponds to the highest T_c. We find the anomalous Green's function $F^{\dagger}_{11}(\mathbf{p},q,\omega)$ for the S layer,

$$F^{\dagger}_{11}(\mathbf{p},q) = \frac{-|\Delta|(\omega_- + h)(\omega_+ + h)}{[(\omega_-)(\omega_- + h) - 4t^2\cos^2(q+k)/2][(\omega_+)(\omega_+ + h) - 4t^2\cos^2 q/2]} \ , \tag{6}$$

from which we calculate T_c. Expanding in the small parameter t/T_c and integrating over momenta, we arrive at the following equation for the critical temperature T_c:

$$\ln\frac{T_c}{T_{c0}} = -\pi T_c t^2 \sum_{\omega} \frac{4}{|\omega|(4\omega^2 + h^2)} + \pi T_c t^4 \cos k \sum_{\omega} \frac{12\omega^4 - 7\omega^2 h^2 - h^4}{|\omega|^3(\omega^2 + h^2)(4\omega^2 + h^2)^2} \ , \tag{7}$$

where T_{c0} is T_c defined at $t=0$ in the mean-field approximation.

As is seen from (7), for $h=0$, maximal T_c corresponds to $k=0$. For $h \gg T_{c0}$, the coefficient of $\cos k$ has a negative sign and the π phase becomes energetically favorable ($k=\pi$). Numerical calculations give for the critical value of the exchange field (h, at which k changes from 0 to π) $h_{\text{crit}} = 3.77T_{c0}$ (we note that T_c is equal to T_{c0} to second order in t/T_{c0}). These and other numerical results are summarized in Table I.

We note that tunneling between layers results in a small (second order in t) reduction in T_c, as is usually the case.[12] This can be interpreted as the fact that the electrons which tunnel into the M layer "feel" a zero pairing potential, and the average Λ (coupling constant of the BCS theory) of the system is lowered. It is interesting to note that as the exchange field on the M layer grows, tunneling becomes energetically more costly, so that the term second order in t falls as $1/h^2$ for large h. For very large exchange fields, the effective transfer integral becomes zero, the layers uncouple, and T_c returns to T_{c0}.

If the M layer has a narrow energy band that we model as a constant $\xi = E$ (i.e., infinite effective mass), we find that $h_{\text{crit}}/T_c = 31.6$ for $|E|/(\pi T_c) = 10$, and $h_{\text{crit}}/T_c = 4.5$ for $|E|/(\pi T_c) = 1$. As the band on the M layer moves farther and farther away from the Fermi level, the transfer of electrons from one layer to the next becomes energetically less favorable and the field necessary to bring about the π phase, h_{crit}, increases. The sign of E (i.e., whether the M-layer band lies above or below the Fermi energy) does not enter into the result.

In the case of the narrow-band M layer, the term second order in t also slightly suppresses T_c. The suppression disappears at large h and/or large E.

B. Ferromagnet: $T \ll T_c$

At low temperatures, we calculate the free energy directly. We represent the free energy of the system by a functional $\mathcal{F}$, obtained by integration over Δ of the self-consistency equation. We now write the anomalous Green's function $F_{ij}^{\dagger}(\mathbf{p},q,\omega,\Delta)$ as an explicit function of the variable Δ, because we must integrate $F_{ij}^{\dagger}(\mathbf{p},q,\omega,\Delta)$ over Δ to get the free energy $\mathcal{F}$. We integrate the equation of self-consistency for the order parameter:

$$\frac{\partial \mathcal{F}}{\partial \Delta} = \frac{\Delta}{\Lambda} - T \sum_{\mathbf{p},q,\omega} F_{11}^{\dagger}(\mathbf{p},q,\omega,\Delta) \tag{8}$$

from $\Delta = 0$ to $\Delta = \Delta(T)$. Integrating first by Δ, we get

$$\mathcal{F} = \mathcal{F}_0 + \mathcal{F}_k \ , \tag{9a}$$

$$\mathcal{F}_0 = -\tfrac{1}{2} N(0) \Delta^2 \ln \frac{e\Delta_0^2}{\Delta^2} + O(t^2) \ , \tag{9b}$$

$$\mathcal{F}_k = -N(0)\pi T_c t^4 \cos k \sum_{\omega} \left[\frac{10h^4|\omega| + 2h^2|\omega|\Delta^2 - 8|\omega|^3 h^2 + 2|\omega|\Delta^4}{[(h^2+\Delta^2)^2 + 4h^2\omega^2]^2 (h^2+\omega^2)} + \frac{-(\Delta^2+h^2)}{(\omega^2+\Delta^2)^{3/2}[(\Delta^2+h^2)^2+4h^2\omega^2]} + \frac{(-2)(h^4+\Delta^4-4h^4\omega^2+2h^2\Delta^2)}{(\omega^2+\Delta^2)^{1/2}[(h^2+\Delta^2)^2+4h^2\omega^2]^2} \right] , \tag{9c}$$

where $N(0)$ is the density of states at the Fermi surface, Δ_0 is the value of the order parameter at $T=0$ for an isolated superconducting layer, $\Delta_0 = 1.76 T_{c0}$. We assume, due to the smallness of the term (t/T_c), that $\Delta(T=0) = \Delta_0$. To obtain $\mathcal{F}_k$, we have obtained the k-dependent term of lowest order in the small parameter (t/T_c).

To calculate h_{crit}, we find it necessary to evaluate the sum above. Numerical calculations give $h_{\text{crit}} = 0.87 T_{c0}$. In the case of an M layer with a narrow band, we get for $E/(\pi T_c) = 1$, $h_{\text{crit}} = 3.1 T_{c0}$, and for $E/(\pi T_c) = 10$, $h_{\text{crit}} = 31.4 T_{c0}$.

A schematic phase diagram of this system is shown in Fig. 1. The transition region between the 0 phase and the

TABLE I. Numerically obtained values of h_{crit}/T_c for $T \cong 0$ and $T \cong T_c$, where h_{crit} is the value of the exchange field on the M layer needed to produce a nonzero k such that $\Delta = |\Delta| e^{ikn}$. Δ is the order parameter on the nth S layer. E is a constant, ξ_m and ξ_s are the electronic spectra on the M and S layers, respectively, and τ is the scattering time. Note that h_{crit} is always lower at low temperatures than at T_c, and that a "narrow band" model of the M-layer's electronic spectrum will make it harder to bring about the π phase in the case of a ferromagnet, while being essential to the existence of the π phase in the case of the antiferromagnet. Note also that both magnetic and nonmagnetic impurities raise h_{crit}. The ratio h_{crit}/T_{c0} was calculated in the case of the ferromagnet and antiferromagnet, but T_c/T_{c0} is unity to second order in t/T_c.

h_{crit}/T_c	$T \cong 0$	$T \lesssim T_c$
Ferromagnet		
Tight-binding ($\xi_m = \xi_s$)	0.87	3.77
Narrow band ($\xi m = E$)		
$E = 10\pi T_c$	31.4	31.6
$E = \pi T_c$	3.1	4.5
Antiferromagnet		
$E \cong T_c$		$\left[\frac{\varepsilon_F}{T_c}\right]^{1/2}$
Impurities		
Magnetic		
$\tau_2 \pi T_c = 100$		3.8
$\tau_2 \pi T_c = 0.1$		20.0
Nonmagnetic		
$\tau_1 \pi T_c = 100$		3.79
$\tau_1 \pi T_c = 0.1$		18.34

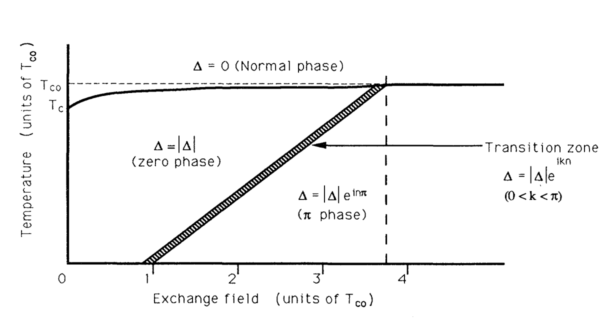

FIG. 1. Schematic phase diagram of a system composed of alternating superconducting (S) and ferromagnetic (M) layers. Shown are the possible phases of the order parameter Δ of the nth superconducting layer as a function of the temperature T and the exchange field h on all the ferromagnetic layers. For $T = T_c$, the π phase (where the sign of Δ reverses as one moves from one S layer to the next) appears at $h = 3.77 T_{c0}$; for $T=0$, at $h = 0.87 T_{c0}$.

π phase (that is, the region in which k changes smoothly from 0 to π) is a narrow zone of width $\Delta h \approx t^4/T_{c0}^3$, the cross-hatched region in Fig. 1. The horizontal dashed line in Fig. 1 is T_{c0}, the value of T_c for the transfer integral t equal to zero. Also shown in Fig. 1 is the dependence of T_c of the system on the exchange field h. To find the dependence of the wave vector k on the exchange field in the transition region, it is necessary to keep all terms up to eighth order in t. It is then seen that k changes smoothly in the transition region. We note that the narrow transition zone is an analogy of the inhomogenous LOFF phase[8,9] in our quasi-two-dimensional system. As in the case of the LOFF phase, $0<k<\pi$ does not necessarily imply that current flows. If a "current-carrying solution" $\Delta_c = |\Delta| e^{ikn}$ has a higher free-energy cost than a "zero-current solution" ($\Delta_z = |\Delta| \cos kn$), then there will be no uniform movement of the condensate.

C. Antiferromagnet

In the case of an antiferromagnetic magnetic layer, we assume that the magnetic field inside the M layer varies spatially as $he^{i\mathbf{Q}\cdot\rho}$, where $\mathbf{Q}$ is the antiferromagnetic ordering vector, and that $2\mathbf{Q}=\mathbf{K}$, where $\mathbf{K}$ is the inverse lattice vector. We write the Gor'kov equations (for $T \lesssim T_c$) for the normal Green's functions $G_{ij}(\mathbf{p},q+k,\omega)$ and $G_{ij}(\mathbf{p}+\mathbf{Q},q+k,\omega)$, and for the anomalous Green's functions $F_{ij}^{\dagger}(\mathbf{p},q,\omega)$ and $F_{ij}^{\dagger}(\mathbf{p}+\mathbf{Q},q,\omega)$. (We are again using the spin convention of the Green's functions mentioned earlier.) We get 4×4 matrices for both pairs of Green's functions, since we assume that $G(\mathbf{p}+2\mathbf{Q},q,\omega)=G(\mathbf{p},q,\omega)$. We calculate the anomalous Green's function on the S layer $[F_{11}^{\dagger}(\mathbf{p},q,\omega)]$ and from it derive the equations of self-consistency and obtain an expression for T_c.

If the electronic spectra ξ of the M and S layers are identical, the π phase does not appear for any reasonable value of h (i.e., less than ε_F). The electron, tunneling from the S to the M layer, "feels" an effective field (averaged over the path of the electron) $h=0$ on the M layer. But if we take the energy to wave-vector relationship (ε versus k) on the antiferromagnetic layer to be a constant E (i.e., infinite effective mass), then the π phase will appear (for E of the order of T_c) when $h=(T_c\varepsilon_F)^{1/2}$, which is reachable for real materials.

IV. IMPURITIES

We consider the effect of impurities on the M layer on the critical temperature T_c and field that brings about the π phase, h_{crit}. In the coordinate representation the interaction between impurities and electrons is described by the matrix operator:

$$\hat{V}_n(\boldsymbol{\rho}) = \sum_j \begin{bmatrix} 0 & 1 \\ 0 & U(\boldsymbol{\rho}-\boldsymbol{\rho}_j) \end{bmatrix} \delta_{nn_j}\,, \tag{10}$$

where the sum is taken over all impurities, n_j is the number of the elementary cell where the jth impurity is located, and ρ_j is its coordinate within the layer. In the case of magnetic impurities, we write $U(\boldsymbol{\rho}-\boldsymbol{\rho}_j)=u_1(\boldsymbol{\rho}-\boldsymbol{\rho}_j)+u_2(\boldsymbol{\rho}-\boldsymbol{\rho}_j)\mathbf{s}_j\cdot\boldsymbol{\sigma}$,[13] where $\boldsymbol{\sigma}$ are the Pauli matrices and $\mathbf{s}_j$ is the spin of the jth impurity. The first term describes the potential scattering, and the second describes magnetic scattering.

We shall use the first Born approximation and will assume that $U(\boldsymbol{\rho}-\boldsymbol{\rho}_j)=(u_1+u_2\mathbf{s}_j\cdot\boldsymbol{\sigma})\delta(\boldsymbol{\rho}-\rho_j)$. Thus, transforming to the quasimomentum representation, we get the operator of the impurity potential:

$$\hat{V}(q,\mathbf{p}) = \sum_j e^{-iqn_j - i\mathbf{p}\cdot\rho_j} \begin{bmatrix} 0 & 0 \\ 0 & u_1+u_2\mathbf{s}_j\cdot\boldsymbol{\sigma} \end{bmatrix}. \tag{11}$$

Below we follow the method of Abrikosov and Gor'kov.[14]

After averaging over all impurity positions and the directions of their spins $\mathbf{s}$, momentum will be conserved, i.e., we can introduce $\hat{G}_{\alpha\beta}(\mathbf{p},q,\omega)$ and $\hat{F}^{\dagger}_{\alpha\beta}(\mathbf{p},q,\omega)$ as

$$\hat{G}_{\alpha\beta}(\mathbf{p},q;\mathbf{p}',q',\omega) = (2\pi)^3\delta(q-q')\delta(\mathbf{p}-\mathbf{p}')\hat{G}(\mathbf{p},q,\omega)\,, \tag{12a}$$

$$\hat{F}_{\alpha\beta}(\mathbf{p},q;\mathbf{p}',q',\omega) = (2\pi)^3\delta(q+k-q')\delta(\mathbf{p}-\mathbf{p}')\hat{F}^{\dagger}(\mathbf{p},q,\omega)\,, \tag{12b}$$

where we have written anew the spin dependence of these functions explicitly (the $\alpha\beta$ subscript). The notation $\hat{G}_{\alpha\beta}(\mathbf{p},q,\omega)$ means the matrix $G_{\alpha\beta ij}(\mathbf{p},q,\omega)$, where i and j are layer indices as before.

For $(T-T_c)/T_c \ll 1$, using the standard notation, we write the following diagram equations [where we have retained terms up to first order in $\hat{F}^{\dagger}(\mathbf{p},q,\omega)$]:

$$\Rightarrow \;=\; \rightarrow \;+\; \rightarrow \overset{\cdot\cdot\cdot\cdot\cdot}{\times \Rightarrow \times} \Rightarrow \,, \tag{13a}$$

$$\overset{q\;\;q+k}{\Leftrightarrow} \;=\; \overset{q\;\;q+k}{\leftrightarrow} \;+\; \overset{q\;\;q+k}{\leftrightarrow} \overset{\cdot\cdot\cdot\cdot\cdot}{\times \Rightarrow \times} \overset{q+k}{\Rightarrow} \;+\; \overset{q}{\leftarrow} \overset{\cdot\cdot\cdot\cdot\cdot}{\times \Leftarrow \times} \overset{q\;\;q+k}{\Leftrightarrow} \;+\; \overset{q}{\leftarrow} \overset{\cdot\cdot\cdot\cdot\cdot}{\times \Leftrightarrow \times} \overset{q+k}{\Rightarrow} \,, \tag{13b}$$

where q and $q+k$ in the above diagrams are arguments of the Green's functions (quasimomentum perpendicular to the layers). We have also used in (13a) and (13b) the following notation:

$$\overset{\cdot\cdot\cdot\cdot\cdot}{\times \Rightarrow \times} = -\hat{\hat{G}}_{\alpha\beta}(\vec{p},q,\omega) = -\left\langle \int \frac{d\vec{p}\,' dq'}{(2\pi)^3} \hat{V}(\vec{p}-\vec{p}\,')\; \hat{G}_{\alpha\beta}(\vec{p}\,',q',\omega)\; \hat{V}(\vec{p}-\vec{p}\,') \right\rangle, \tag{14a}$$

$$\overset{\cdot\cdot\cdot\cdot\cdot}{\times \Leftrightarrow \times} = -\hat{\hat{F}}^{+}_{\alpha\beta}(\vec{p},q,\omega) = -\left\langle \int \frac{d\vec{p}\,' dq'}{(2\pi)^3} \hat{V}(\vec{p}-\vec{p}\,')\; \hat{F}^{+}_{\alpha\beta}(\vec{p}\,',q',\omega)\; \hat{V}(\vec{p}-\vec{p}\,') \right\rangle. \tag{14b}$$

The brackets $\langle\ \rangle$ here indicate an averaging over all impurities.

We must take into account that the spin dependence of the Green's functions in the presence of the exchange field h may be expressed as $\hat{G}_{\alpha\beta}(\mathbf{p},q,\omega)=\hat{G}^{1}(\mathbf{p},q,\omega)\delta_{\alpha\beta}+\hat{G}^{2}(\mathbf{p},q,\omega)\sigma^{z}_{\alpha\beta}$, while the anomalous Green's function conserves its spin dependence $\hat{F}^{\dagger}_{\alpha\beta}(\mathbf{p},q,\omega)=i\sigma^{y}_{\alpha\beta}\hat{F}^{\dagger}(\mathbf{p},q,\omega)$. We obtain the following equations:

$$\hat{\hat{G}}_{\alpha\beta}(\mathbf{p},q,\omega)=n\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}\left[\begin{bmatrix}0&0\\0&u_1\end{bmatrix}\hat{G}^{1}(\mathbf{p}',q',\omega)\begin{bmatrix}0&0\\0&u_1\end{bmatrix}\delta_{\alpha\beta}+\begin{bmatrix}0&0\\0&u_2\end{bmatrix}\hat{G}^{1}(\mathbf{p}',q',\omega)\begin{bmatrix}0&0\\0&u_2\end{bmatrix}\frac{S(S+1)}{3}\delta_{\alpha\beta}\right.$$
$$\left.+\begin{bmatrix}0&0\\0&u_1\end{bmatrix}\hat{G}^{2}(\mathbf{p}',q',\omega)\begin{bmatrix}0&0\\0&u_1\end{bmatrix}\sigma^{z}_{\alpha\beta}-\frac{S(S+1)}{9}\begin{bmatrix}0&0\\0&u_2\end{bmatrix}\hat{G}^{2}(\mathbf{p}',q',\omega)\begin{bmatrix}0&0\\0&u_2\end{bmatrix}\sigma^{z}_{\alpha\beta}\right], \tag{15a}$$

$$\hat{\hat{F}}^{\dagger}_{\alpha\beta}(\mathbf{p},q,\omega)=n\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}\left[\begin{bmatrix}0&0\\0&u_1\end{bmatrix}\hat{F}^{\dagger}(\mathbf{p}',q',\omega)\begin{bmatrix}0&0\\0&u_1\end{bmatrix}-\begin{bmatrix}0&0\\0&u_2\end{bmatrix}\hat{F}^{\dagger}(\mathbf{p}',q',\omega)\begin{bmatrix}0&0\\0&u_2\end{bmatrix}\frac{S(S+1)}{3}\right]i\sigma^{y}_{\alpha\beta}, \tag{15b}$$

where n is the concentration of impurities.

The integral

$$\int\frac{d\mathbf{p}'dq'}{(2\pi)^3}\hat{G}^{2}(\mathbf{p}',q',\omega)$$

is equal to zero, so

$$\hat{\hat{G}}_{\alpha\beta}(\mathbf{p},q,\omega)=\begin{bmatrix}0&0\\0&-\dfrac{i\,\mathrm{sgn}\omega}{2}\left[\dfrac{1}{\tau_1}+\dfrac{1}{\tau_2}\right]\end{bmatrix}\delta_{\alpha\beta},$$

where

$$\frac{1}{\tau_1}=nmu_1^2\quad\frac{1}{\tau_2}=nm[S(S+1)/3]u_2^2$$

are the reciprocal times of potential and magnetic scattering, respectively.

Equation (13) is written in analytical form as follows:

$$\hat{G}(\mathbf{p},q,\omega)=\hat{G}^{0}(\mathbf{p},q,\omega)+\hat{G}^{0}(\mathbf{p},q,\omega)\hat{\hat{G}}(\mathbf{p},q,\omega)\hat{G}(\mathbf{p},q,\omega), \tag{16a}$$

$$\hat{F}^{\dagger}(\mathbf{p},q,\omega)=\hat{F}^{\dagger 0}(\mathbf{p},q,\omega)+\hat{F}^{\dagger 0}(\mathbf{p},q,\omega)\hat{\hat{G}}(\mathbf{p},q,\omega)\hat{G}_{\uparrow\uparrow}(\mathbf{p},q+k,\omega)$$
$$+\hat{G}^{0}_{\downarrow\downarrow}(\mathbf{p},q,-\omega)\hat{\hat{G}}(\mathbf{p},q,-\omega)\hat{F}^{\dagger}(\mathbf{p},q,\omega)+\hat{G}^{0}_{\downarrow\downarrow}(\mathbf{p},q,-\omega)\hat{\hat{F}}^{\dagger}(\mathbf{p},q,\omega)\hat{G}_{\uparrow\uparrow}(\mathbf{p},q+k,\omega). \tag{16b}$$

Using Eqs. (15) and (16), we obtain the following expressions:

$$\hat{G}_{\uparrow\uparrow}(\mathbf{p},q,\omega)=\begin{bmatrix}i\omega-\xi&-T_q\\-T_q^{*}&i\tilde{\omega}-\xi-h\end{bmatrix} \tag{17}$$

and

$$\hat{\hat{F}}^{\dagger}(\mathbf{p},q,\omega)=\hat{G}_{\downarrow\downarrow}(\mathbf{p},q,-\omega)[\hat{\Delta}^{*}+\hat{\hat{F}}^{\dagger}(\mathbf{p},q,\omega)]\hat{G}_{\uparrow\uparrow}(\mathbf{p},q+k,\omega), \tag{18}$$

where $\tilde{\omega}=\omega+(\mathrm{sgn}\omega/2\tau_1)+(\mathrm{sgn}\omega/2\tau_2)$ and we have used the relation

$$\hat{F}^{\dagger 0}(\mathbf{p},q,\omega)=\hat{G}^{0}_{\downarrow\downarrow}(\mathbf{p},q,-\omega)\hat{\Delta}^{*}\hat{G}^{0}_{\uparrow\uparrow}(\mathbf{p},q+k,\omega). \tag{19}$$

Substituting (18) into (15b) and introducing b as the matrix element

$$\hat{\hat{F}}^{\dagger}=\begin{bmatrix}0&0\\0&b\end{bmatrix}, \tag{20}$$

we get (including terms up to second order in t/T_c)

$$b=-\frac{t^2(1+e^{ik})\Delta^{*}}{\omega(\omega+\tilde{\omega}+ih)\{[2\tau_1\tau_2/(\tau_1-\tau_2)]\mathrm{sgn}\omega(\tilde{\omega}+ih)+1\}}. \tag{21}$$

Substituting b back into Eq. (18), we get an expression for the anomalous Green's function on the S-layer $F^{\dagger}_{11}(\mathbf{p},q,\omega)$:

$$F^{\dagger}_{11}(\mathbf{p},q,\omega)=\frac{-\Delta^*}{[(\omega_-)(\tilde{\omega}_- - h)-|T_k|^2][(\omega_+)(\tilde{\omega}_+ - h)-|T|^2]}\times\left[(\omega_+ - h)(\omega_- - h)+\frac{T_k^* T t^2(1+e^{ik})}{\omega(\omega+\tilde{\omega}+ih)\{[2\tau_1\tau_2/(\tau_1-\tau_2)]\mathrm{sgn}\omega(\tilde{\omega}+ih)+1\}}\right], \tag{22}$$

where

$$\tilde{\omega}_- = \omega_- + (\mathrm{sgn}\omega/2\tau_1)+(\mathrm{sgn}\omega/2\tau_2)$$

and

$$T_k = 2te^{i(q+k)/2}\cos(q+k)/2\ ,$$
$$T=2te^{iq/2}\cos q/2\ .$$

The difference between magnetic and nonmagnetic impurities manifests itself only in the second term of this equation, as τ_1 and τ_2 enter with different signs. Thus, the difference between the two types of impurities exists only in terms of order $(t/T_c)^4$ and higher.

From (22) we get the equation that defines T_c. To order $(t/T_c)^2$ we have

$$\ln\frac{T_c}{T_{c0}}=-\pi T_c t^2\sum_{\omega}\frac{\omega+\tilde{\omega}}{2\omega^2[(\omega+\tilde{\omega})^2+h^2]}\ . \tag{23}$$

We consider first the case when the exchange field h is absent. In the case of weak scattering ($T_c\tau \gg 1$) we obtain

$$\ln\frac{T_c}{T_{c0}}=-\pi T_c t^2\sum_{\omega}\frac{1}{4\omega^3}+\frac{\pi T_c t^2}{16(\tau_1+\tau_2)}\sum_{\omega}\frac{1}{4\omega^4}\ . \tag{24}$$

In the opposite limit ($T_c\tau \ll 1$) we obtain

$$\ln\frac{T_c}{T_{c0}}=-\pi T_c t^2\frac{\tau_1\tau_2}{(\tau_1+\tau_2)}\sum_{\omega}\frac{1}{\omega^2}\ ; \tag{25}$$

i.e., we see that in the case of strong scattering the term $[\tau_1\tau_2/(\tau_1+\tau_2)]t^2$ plays the role of the effective hopping integral. This coincides with the results of Bulaevskii and Kuzii.[15]

We note that both magnetic and non magnetic impurities increase T_c. This can be explained in the following way: superconducting electrons feel a pairing potential which is "averaged" over their path of motion. The presence of impurities, both magnetic and nonmagnetic, leads to the reduction of the effective transfer integral. Therefore, in the presence of impurities, superconducting electrons are localized on the S layer and feel a greater coupling constant than when impurities are absent.

If we retain terms of order $(t/T_c)^4$ in the self-consistency equation, we can find the dependence of T_c on k, the wave vector of the order parameter, as well as h_{crit}, the critical field for the appearance of the π phase. The calculation is quite lengthy and involved, so we shall proceed directly to results obtained numerically.

Impurities both magnetic and nonmagnetic enhance h_{crit} (i.e., make the π phase energetically favorable at higher fields than in their absence). Calculations give $h_{\mathrm{crit}}/T_c=3.80$ for $\tau_2\pi T_c=100$ and $h_{\mathrm{crit}}/T_c=20$ for $\tau_2\pi T_c=0.1$ (purely magnetic scattering); in the case of nonmagnetic scattering, we obtain $h_{\mathrm{crit}}/T_c=3.79$ for $\tau_1\pi T_c=100$ and $h_{\mathrm{crit}}/T_c=18.34$ for $\tau_1\pi T_c$.

V. EXCITATION SPECTRUM

As was shown in Ref. 6, for layered systems of the type superconductor-normal metal (S-N), the density of superconducting electrons [obtained by summing $F^{\dagger}_{-1-1}(\mathbf{p},q,\omega)$ over momenta and frequency] in the normal layers rises abruptly at temperatures less than t^2/T_c, which results in the reduction of the London penetration depth.

We obtain the following expression for the anomalous Green's function on the M layer:

$$F^{\dagger}_{-1-1}(\mathbf{p},q,\omega)=\frac{-|\Delta|T^*T_k}{D}\ , \tag{26}$$

where

$$D=(\omega_+\omega_- - \Delta^2)(\omega_+ + h)(\omega_- + h)-(\omega_-)(\omega_- + h)|T|^2 -(\omega_+)(\omega_+ + h)|T_k|^2+|T|^2|T_k|^2\ .$$

In the case of the π phase, the density of superconducting electrons on the M layer is strictly equal to zero, because $F^{\dagger}_{-1-1}(\mathbf{p},q,\omega)$ becomes an odd function of q, which when integrated over q gives zero.

The authors of Ref. 6 also showed that at low temperatures ($T \gtrsim 0$) for $h=0$, the quasiparticle excitation spectrum is gapless on both layers. The density of states on the normal layer at temperatures lower than t^2/T_c was shown to rise as $\sqrt{\varepsilon}$ from $\varepsilon=0$. For h small ($h \ll T_c$) but not equal to zero, the spectrum on both layers is gapless, but the density of states at $\xi=0$ is finite (i.e., not zero), unlike the case of Ref. 6.

This is calculated in the following manner:

$$\rho_i(\omega)=-\frac{1}{\pi}\sum_{\mathbf{p},q}\mathrm{Im}[G_{ii}(\mathbf{p},q,\omega)|_{i\omega\to\omega+i\delta}]\ , \tag{27}$$

where $\rho_i(\omega)$ is the density of quasiparticle states of energy ω on layer i [note that there is no sum over i in Eq.

(28)].

The general case cannot be solved because finding the poles of the Green's function exactly requires solving a quartic equation in ω. For $h=0$ and $T \ll t^2/T_c$, we regain the Green's function of Ref. 6:

$$G_{-1-1}(\mathbf{p},q,\omega) \cong \frac{\omega_+}{(\omega_- \omega_+ - \tilde{\Delta}_2^2)} , \tag{28}$$

where $\tilde{\Delta}_2 = (4t^2 \cos^2 q/2)/T_c$. Thus, a gapless spectrum is obtained (due to the fact that $\tilde{\Delta} \to 0$ for $q \to \pi$).

For small h, we may expand the denominator in powers of h/Δ (for $T \ll T_c$) and obtain a different expression for the Green's function:

$$G_{-1-1}(\mathbf{p},q,\omega=0) = \frac{(\xi+h)}{(\xi^2-\xi_1^2)} , \tag{29}$$

where $\xi_1^2 = h^2 - (2|T|^4/\Delta^2)$. We get for the density of states on the M layer at $\omega=0$ (evaluated at $h \ll \Delta$ and $T \ll T_c$)

$$\rho_2(\omega=0) \propto N(0) \frac{1}{\pi} \frac{(h\Delta)^{1/2}}{t(2)^{1/4}} \int_0^1 \frac{dx}{(1-x^4)^{1/2}} . \tag{30}$$

If h is on the order of the "gap" on the M layer, t^2/Δ, the density of states at the Fermi level becomes on the order of that of a regular metal. The M layer enters the normal state smoothly as h increases. This can be explained as follows: in our case, there is a whole range of electrons that "feel" a "gap" $\tilde{\Delta}$ between zero and t^2/Δ. Those with a "gap" $\tilde{\Delta} < h$ become normal. The number of such electrons, and therefore the density of available states at $\omega=0$, increase smoothly with h.

For $h \gg T_c$, the layers decouple and the S layer becomes a regular BCS superconductor with gap Δ, while the density of states on the M layer becomes that of a regular metal, a constant.

VI. DISCUSSION

We have calculated the properties of our system in the mean-field approximation, which is applicable to quasi-two-dimensional systems in the case $[T_c^2/\varepsilon_F(T_c - T)]\ln(t/T_c) \ll 1$.[2] Thus, even for $t \ll T_c$, fluctuations of the phase of the order parameter are important only in a very narrow temperature region close to T_c.

Characteristic values of the exchange field in magnetic metals are $h = 100-1000$ K (the Curie temperature for the RKKY mechanism $\theta \sim h^2/\varepsilon_F$ and the superconducting transition temperature are both of the order 10–100 K), so that conditions for the appearance of the π phase are realizable.

If the superlattice consists of an even number of superconducting layers, then the phase of the order parameter at the ends will differ by π, and the entire system will function as a Josephson π contact (see Ref. 16). As indicated in Ref. 16, spontaneous current will flow in a circuit containing such a π contact, and this could be observed experimentally.

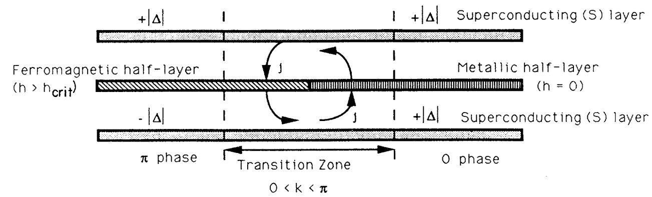

FIG. 2. Experimental measurement of the π phase. The superconducting layers on the ferromagnet side have an alternating order parameter, while those on the side of the normal metal have a constant order parameter. The smooth change of the phase of the order parameter in the transition region allows the possibility of current flow, as indicated in the figure by the label j.

Another possibility of detecting the π phase would be to introduce an inhomogenous normal layer between superconducting layers. One-half of the layer would be a ferromagnet with large exchange field $h > h_{\text{crit}}$, and the other half would be a regular metal (see Fig. 2). The superconducting layers on the side of the ferromagnetic half of the "sandwich" would have an order parameter that alternates its sign as we go from one layer to the next. The superconducting layers on the other side of the "sandwich" would have a constant order parameter. This implies that within every other superconducting layer, the order parameter would change its phase from 0 to π. The smooth change in phase of the order parameter might create intralayer currents near the ferromagnet-metal boundary that could be experimentally observable.

In conclusion, we have shown that a nonhomogenous "π phase," with a superconducting order parameter that changes its sign as we move from one superconducting layer to another, exists in a system composed of alternating S and M (both insulating and conducting) layers with thicknesses on the order of an intratomic length. This phase appears when h, the exchange field in the ferromagnet, is larger than T_c. This phase will disappear if the F layers are replaced by AF ones, except if the energy spectrum of the AF is a single band of constant energy close to the Fermi level. We find that both magnetic and nonmagnetic impurities cannot bring about the π phase, their only effect being to increase the field necessary to bring it about, h_{crit}. Our numerical results are listed in Table I. We find that the transition from π phase to 0 phase is a continuous one, and that the density of states on both layers is not only gapless, but also finite at the Fermi level.

We note that some of these results have been published in Ref. 17.

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