

# $\pi$ phase in layered magnetic superconductors

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In layered superconductors with alternating superconducting and magnetic layers, a  $\pi$  phase in which the superconductivity order parameter changes sign in the transition to the neighboring layer may correspond to the ground state of the system.

A large number of layered compounds, in which superconducting ( $S$ ) layers alternate with magnetic ( $M$ ) layers, have now been produced [the magnetic layer may be either ferromagnetic ( $F$ ) or antiferromagnetic ( $AF$ )]. Examples are  $S/F$  superlattices,<sup>1</sup> layered superconductors with intercalated magnetic atoms,<sup>2</sup> and, finally, high- $T_c$  superconductors of the  $(RE)Ba_2Cu_3O_7$  type, in which layers with a nonmagnetic  $Re = Y$  alternate with layers with a magnetic  $RE$ , including nonsuperconducting layers with  $RE = Pr$  (Ref. 3). Sophisticated techniques make it possible to develop  $S/M$  structures with layer thicknesses as small as one lattice constant.

In the present letter we show that the exchange interaction of conduction electrons with the atoms of the magnetic interlayer can give rise to an inhomogeneous superconducting  $\pi$  phase, in which the sign of the order parameter changes in the transition to the neighboring superconducting layer.

We consider the following model: The unit cell consists of two layers, one superconducting and one magnetic. For simplicity, the motion of the quasiparticles along the layers is described by the same spectrum  $\xi(\mathbf{p})$ , while the motion across the layers is described in the tight-binding approximation with a transfer integral  $t$  (we are considering the case of a Josephson interaction of the layers, i.e.,  $t \ll T_c$ ). We assume that the pairing of electrons occurs only in the  $S$  layer, while in the  $M$  layer there is an exchange field  $h$ , which we assume to be constant in the case of a ferromagnet (the orbital effect is almost always negligible in comparison with the exchange effect in magnetic superconductors<sup>4</sup>). We write the Hamiltonian of this system as follows:

$$\begin{aligned}
 H = & \sum_{\mathbf{p}n\alpha\sigma} \xi(\mathbf{p})a_{n\alpha\sigma}^+(\mathbf{p})a_{n\alpha\sigma}(\mathbf{p}) + t(a_{n\alpha\sigma}^+(\mathbf{p})a_{n-\alpha\sigma}(\mathbf{p}) + a_{n+\alpha,-\alpha,\sigma}^+(\mathbf{p})a_{n\alpha\sigma}(\mathbf{p}) \\
 & + \text{h.c.}) + H_{int1} + H_{int2} \\
 H_{int1} = & \frac{\lambda}{2} \sum_{\mathbf{p}_1\mathbf{p}_2n\sigma} a_{n1\sigma}^+(\mathbf{p}_1)a_{n1-\sigma}^+(\mathbf{p}_1)a_{n1-\sigma}(-\mathbf{p}_2)a_{n1\sigma}(\mathbf{p}_2), \\
 H_{int2} = & \sum_{\mathbf{p}n\sigma} h\sigma_z a_{n,-1,\sigma}^+(\mathbf{p})a_{n,-1,\sigma}(\mathbf{p}),
 \end{aligned} \tag{1}$$

where the operator  $a_{n\alpha\sigma}^+(\mathbf{p})$  creates an electron with a spin  $\sigma$  in unit cell  $n$  with momentum  $\mathbf{p}$  along the layers, with  $\alpha = 1$  for an  $S$  layer or  $\alpha = -1$  for an  $M$  layer.

Under the assumption that the phase of the superconductivity order parameter varies from layer to layer in accordance with  $\Delta = \Delta_0 e^{ikn}$ , in this system, we can switch from a discrete representation in terms of  $n$  to a quasimomentum representation, by introducing a momentum  $q$ , in the direction perpendicular to the layers. We then find an anomalous Green's function  $F^+(\mathbf{p}, q)$  for an  $S$  layer:

$$F^+(\mathbf{p}, q) = \frac{\Delta_0^*(\xi_- + h)(\xi_+ - h)}{[\xi_-(\xi_- + h) - 4t^2 \cos^2 q/2][\xi_+(\xi_+ - h) - 4t^2 \cos^2 \frac{(q+k)}{2}]}, \quad (2)$$

where  $\xi_{\pm} = \xi_p \pm i\omega$ , and  $\omega = \pi T(2n + 1)$ . Carrying out an expansion in  $t/T_c$ , and integrating over the momentum, we then find the following equation for the superconducting transition temperature:

$$\ln \frac{T_c}{T_{c0}} = -\pi T_c t^2 \sum_{\omega} \frac{1}{\omega(4\omega^2 + h^2)} + \pi T_c t^4 \cos k \sum_{\omega} \frac{12\omega^4 - 7\omega^2 h^2 - h^4}{\omega^3(\omega^2 + h^2)(4\omega^2 + h^2)^2}, \quad (3)$$

where  $T_{c0}$  is the transition temperature in the mean-field approximation for  $t = 0$ , and where we have retained only terms  $\sim t^4$ , which depend on  $k$ .

It follows from (3) that the transition temperature  $T_c$  depends on  $k$  and that the value of  $k$  which is realized is evidently the one which corresponds to the highest value of  $T_c$ . With  $h = 0$ , there is of course a uniform state with  $k = 0$ . At  $h \gg T_c$ , the coefficient of  $\cos(k)$  in (3) is negative, and a phase with  $k = \pi$  (a  $\pi$  phase) is favored. In this phase, the sign of the order parameter changes in the transition to the neighboring superconducting layer.

A numerical calculation yields  $h_c = 3.77T_c$  as the critical value of the exchange field (i.e., the field at which there is a transition from a uniform phase to a nonuniform phase).

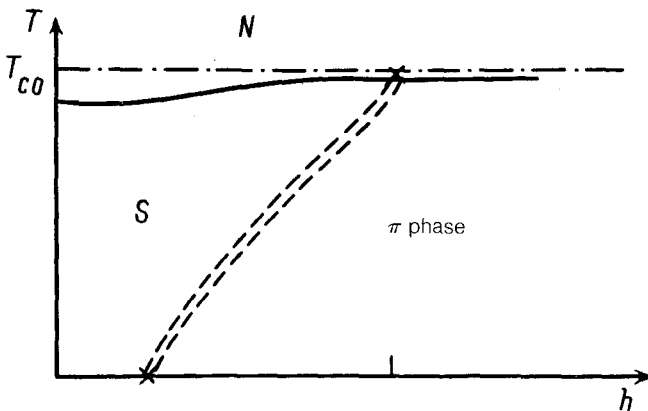


FIG. 1.

A calculation of the free energy at  $T = 0$  reveals  $h_c = 0.87T_{c0}$  in this case. Figure 1 is a schematic phase diagram of this system. As  $h$  increases, the coupling of the  $S$  and  $M$  layers weakens, causing a slight increase in  $T_c$  [see Eq. (3)].

The transition from the 0 phase to the  $\pi$  phase occurs smoothly in a narrow region of width  $h \sim t^4/T_{c0}^3$ , outlined by the dashed lines in Fig. 1. In order to determine how the wave vector  $k$  depends on the exchange field  $h$  in this region, we need to retain terms on the order of  $t^8$  in (3). The narrow transition region with  $0 < k < \pi$  is essentially an analog of a Larkin-Ovchinnikov-Fulde-Ferrell nonuniform superconducting phase.<sup>5,6</sup>

If the  $M$  layer is antiferromagnetic, and if the electron spectra are the same in the  $S$  and  $M$  layers, a  $\pi$  phase does not appear. If the electron spectrum at the  $AF$  layer is a very narrow band near the Fermi level (at a distance  $E$  above or below the Fermi level), on the other hand, then a  $\pi$  phase may appear at  $E \lesssim T_c$ , and we would have  $h_c \sim \sqrt{\epsilon_F T_{c0}}$ . In the case of  $F$  layers with a narrow band  $\xi(\mathbf{p}) = E$ , a numerical calculation yields the following values of the critical field  $h_c$  at  $T = T_c$ :  $h_c/T_c = 4.5$  if  $E/(\pi T_c) = 1$  or  $h_c/T_c = 31.6$  if  $E/(\pi T_c) = 10$ .

As was shown in Ref. 7, in superconductor-(normal metal) ( $S/N$ ) layered systems the density of superconducting electrons at the  $N$  layers increases sharply at temperatures below  $t^2/T_c$ , leading to, for example, a decrease in the London penetration depth. In contrast, the density of superconducting electrons at the  $M$  layer for the  $\pi$  phase always remains identically equal to zero.

The typical exchange fields for magnetic metals are  $h \sim 100\text{--}1000$  K (the Curie temperature for the RKKY mechanism is  $\Theta \sim h^2/\epsilon_F$ , and we would have  $\Theta \sim 10\text{--}100$  K), so the conditions for the occurrence of the  $\pi$  phase,  $h \gtrsim T_c$ , are easily arranged. If the entire superlattice contains an odd number of superconducting layers, the phases of the order parameter at the edges should differ by  $\pi$ , so the system should constitute a Josephson  $\pi$  junction.<sup>8</sup> According to Ref. 8, a closed loop including a  $\pi$  junction has a spontaneous current and a magnetic flux in the ground state. It might be possible to establish this fact experimentally.

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