Coexistence of superconductivity and band antiferromagnetism in layered contacts

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The spatial coexistence of a superconducting order and a magnetic order in thin-film contacts of a band antiferromagnet with a superconductor is analyzed in the tunneling model of the proximity effect. The change in the spectra of one-particle excitations of these metals due to an interaction of the superconducting pairing and the antiferroamgnetic exchange field is calculated.

The coexistence of two different cooperative phenomena—superconductivity and magnetism—in one volume has been the topic of a lively discussion for a long time now (see, e.g., a monograph[1] and a recent review[2]). There are various ways to produce structures in which two types of order are realized simultaneously: introduce impurity paramagnetic ions which retain their localized moments in a superconductor,[1] study layered compounds with alternating superconducting and antiferromagnetic planes (in particular, the RE–Cu–O, RE–Ba–Cu–O, etc., high-T_c compounds, where RE is a rare-earth ion[2]), and, finally, study thin-film structures which are formed by putting a superconductor in direct contact with a magnetic material. The latter structures have the advantage that, under certain experimental conditions, they make it possible to observe the behavior of a superconductor in an exchange field in a "purer" form and to clarify the effect of superconducting pairing on the properties of a magnetic material. The overwhelming majority of studies in this direction have focused on superconductor–ferromagnet contacts (see, in particular, Refs. 3–5 and the papers cited there). Superconductor–antiferromagnetic-metal (SC–AFM) structures, on the other hand, hold promise for research at this point both from a fundamental standpoint (to identify the role played by antiferromagnetic fluctuations in high-T_c superconductivity) and for applications (to develop Josephson junctions with an interlayer of a conducting antiferromagnet[6]).

In this letter we report a study of the changes in the spectra of elementary excitations of superconducting and band antiferromagnetic metals put in direct contact. We work from the tunneling model of the proximity effect proposed by McMillan.[7] The reason for selecting McMillan's model is the desire to use the results to study high-T_c superconductivity. On the one hand, there are reasons[8] to believe that this approach gives a satisfactory description of the internal proximity effect in the superconducting metal oxides. On the other, the presence of a poorly conducting layer on the surface of a high-T_c superconductor makes this model directly applicable to the properties of contacts of high-T_c cuprates with ordinary metals.[9,10]

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In the spirit of the tunneling formalism (see, for example, Chap. 3 in Ref. 11) we write the Hamiltonian of the superconducting–antiferromagnetic system as a sum of two complete multiparticle Hamiltonians H_S and H_{AF}, which describe the superconductor and the antiferromagnet when isolated from each other, and also a perturbation H_T, which leads to transitions of individual electrons from one layer to the other:

$$H_T = \sum_{\mathbf{kp}\sigma} T_{\mathbf{kp}}\{c^+_{\mathbf{p}\sigma}(a_{\mathbf{k}\sigma}+b_{\mathbf{k}\sigma})+\text{H.c.}\}, \quad \sigma=\pm 1. \tag{1}$$

The parameter $T_{\mathbf{kp}}$ in (1) is proportional to the corresponding transition matrix elements, the operator $c^+_{\mathbf{p}}$ creates electron states in the superconductor, and the operator $a_{\mathbf{k}}$ ($b_{\mathbf{k}}$) annihilates Bloch electron states in sublattice A (B) of the antiferromagnet. It is assumed here that the N layer is a transition d-metal, in which the itinerant electrons are described by band theory and exhibit properties characteristic of systems with localized magnetic moments. In the simplest case of a two-sublattice antiferromagnetic metal, the corresponding Hamiltonian can be written[12]

$$H_{AF} = \sum_{\mathbf{p}\sigma}\left\{\left(\gamma_{\mathbf{p}}+\frac{1}{2}\sigma h_s\right)a^+_{\mathbf{p}\sigma}a_{\mathbf{p}\sigma}+\left(\gamma_{\mathbf{p}}-\frac{1}{2}\sigma h_s\right)b^+_{\mathbf{p}\sigma}b_{\mathbf{p}\sigma}+t_{\mathbf{p}}(a^+_{\mathbf{p}\sigma}b_{\mathbf{p}\sigma}+b^+_{\mathbf{p}\sigma}a_{\mathbf{p}\sigma})\right\}.$$

Here $\gamma_{\mathbf{p}}$ ($t_{\mathbf{p}}$) is the intrasublattice (intersublattice) electron hopping integral. The intraatomic interaction is dealt with in the random-phase approximation. It reduces to the effect of an alternating field $\frac{1}{2}h_s = 2MU/N_0$, where U is an intraatomic repulsion parameter, N_0 is the number of sublattices, and $M=M_A=-M_B$ is the sublattice magnetization.

A standard canonical transformation puts the Hamiltonian H_{AF} in diagonal form:

$$H_{AF} = \sum_{\mathbf{p}\sigma} E_{\mathbf{p}\sigma}(\alpha^+_{\mathbf{p}\sigma}\alpha_{\mathbf{p}\sigma}+\beta^+_{\mathbf{p}-\sigma}\beta_{\mathbf{p}-\sigma}) \tag{2}$$

with a dispersion relation

$$E_{\mathbf{p}\sigma}=\gamma_{\mathbf{p}}+\sigma\left(t^2_{\mathbf{p}}+\frac{1}{2}h^2_s\right)^{-1/2}$$

for the conduction electrons. In other words, a gap opens up at the edge of the Brillouin zone of the new (doubled) unit cell in the electron spectrum in the magnetically ordered state. We wish to stress that the action of the antiferromagnetic field h_s is not the same as that of a ferromagnetic exchange field. The latter splits the spectrum of electrons (first) with the opposite spin direction and (second) at the center of the Brillouin zone.

The tunneling Hamiltonian in the quasiparticle operators α and β transforms into an expression of the type

$$H_T = \sum_{\mathbf{kp}\sigma}\{T^\sigma_{\mathbf{kp}}(c^+_{\mathbf{p}\sigma}\alpha_{\mathbf{k}\sigma}+c^+_{\mathbf{p}-\sigma}\beta_{\mathbf{k}-\sigma})+\text{H.c.}\}, \tag{3}$$

where the tunneling matrix elements are explicit functions of the spin variable σ:

$$T^\sigma_{\mathbf{kp}}=T_{\mathbf{kp}}(\cos\theta_{\mathbf{k}}+\sigma\sin\theta_{\mathbf{k}}), \quad \tan 2\theta_{\mathbf{k}}=2t_{\mathbf{k}}/h_s.$$

The origin of this dependence can be understood easily on the basis of (2). It involves the splitting of the charge carrier spectrum at the boundary of zone.

Following Éliashberg's strong-coupling theory (see, for example, Chap. 4 in Ref. 11), we write the eigenenergy part of the electron energy in matrix form:

$$\hat{\Sigma}(\mathbf{p},\omega)=[1-Z(\mathbf{p},\omega)]\omega\hat{I}+Z(\mathbf{p},\omega)\Delta(\mathbf{p},\omega)\hat{\tau}_1,$$

where $Z(\mathbf{p},\omega)$ is a renormalization function, $\Delta(\mathbf{p},\omega)$ is an energy-gap parameter, $\hat{I}$ is the unit matrix, and $\hat{\tau}_1$ is the Pauli spin matrix. When the perturbation H_T is taken into account by the standard self-consistency procedure,[7] we find that the pairing potential $\Delta_s(\mathbf{p},\omega)$ in the superconducting film is different from the seed quantity $\Delta_s^0(\mathbf{p},\omega)$, and a nonzero order parameter $\Delta_{n\pm}(\mathbf{p},\omega)$ arises in the antiferromagnetic layer. For the functions $\Delta_s(\omega)$ and $\Delta_{n\pm}(\omega)$ averaged over the Fermi surface of these metals we have

$$\begin{aligned}\Delta_s(\omega)=\{&Z_s^0(\omega)\Delta_s^0(\omega)+\Gamma_s^+\Delta_{n+}(\omega)[\Delta_{n+}^2(\omega)-\omega^2]^{-1/2}+\Gamma_s^-\Delta_{n-}(\omega)\\ &\times[\Delta_{n-}^2-\omega^2]^{-1/2}\}\{Z_s^0(\omega)+\Gamma_s^+[\Delta_{n+}^2(\omega)-\omega^2]^{-1/2}\\ &+\Gamma_s^-[\Delta_{n-}^2(\omega)-\omega^2]^{-1/2}\}^{-1},\end{aligned} \tag{4a}$$

$$\Delta_{n\pm}(\omega)=\Gamma_n^\pm\Delta_s(\omega)\{\Gamma_n^\pm+[\Delta_s^2(\omega)-\omega^2]^{1/2}\}^{-1}, \tag{4b}$$

where the parameters $\Gamma_s^\pm\sim(T^\pm)^2d_nN_s(0)$ and $\Gamma_n^\pm\sim(T^\pm)^2d_sN_n(0)$ describe the finite lifetime of an electron because of its tunneling into the opposite film. Here $d_s(d_n)$ is the thickness of the superconducting (antiferromagnetic) film, and $N_s(0)$ $[N_n(0)]$ is the corresponding density of electron states at the Fermi surface. The derivation of (4) made use of the fact that the tunneling of electrons in real solid-state structures is not a selective process,[11] so an average can be taken over the Fermi surface of the contact layer. As a result, constants $(T^\pm)^2$ arise [an average of $(T_{\mathrm{kp}}^\pm)^2$ over angle on the Fermi surface]. The values of these constants are not known, strictly speaking; they are determined by the particular nature of the scattering of electrons at the superconductor–antiferromagnet interface.

Equations (4) have been derived in second order in tunneling Hamiltonian (3). In contrast with a single-band N metal, for which the tunneling is taken into account in higher-order perturbation theory by simply a renormalization of the parameters $\Gamma_{s,n}$ (Ref. 13), in the case at hand the result is a "mixing" of the band states of the N layer. The first nonvanishing corrections of this sort are of fourth-order perturbation theory, and we will ignore them.

Solving self-consistent equations (4), we find the density of one-particle states in the superconducting and N layers:

$$N_{s,n\pm}(\omega)=\mathrm{Re}\{|\omega|[\omega^2-\Delta_{s,n\pm}^2(\omega)]^{-1/2}\}. \tag{5}$$

This density can be found directly in tunneling measurements (see, for example, Ref. 11).

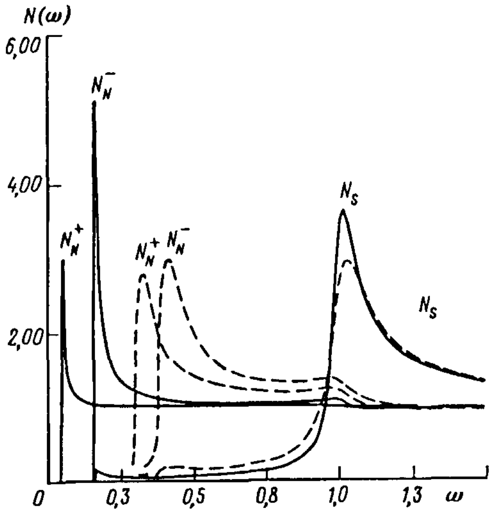

FIG. 1. Normalized electron density of states in the SC and AFM layers for the following parameter values of the contact. Dashed curves—$\Gamma_s^+=0.02$, $\Gamma_s^-=0.03$, $\Gamma_n^+=0.5$, $\Gamma_n^-=0.7$; solid curves—$\Gamma_s^+=0.0$, $\Gamma_s^-=0.02$, $\Gamma_n^+=0.05$, $\Gamma_n^-=0.2$. The energy is expressed in units of Δ_s^0.

Let us list the basic features of the superconducting properties of a superconductor–antiferromagnetic-metal contact which follow from an analysis of expressions (4) and (5) for the case of a weak-coupling superconductor, with $\Delta_s^0(\omega)=\Delta_s^0=\text{const}$ and $Z_s^0(\omega)=1$.

1. In the paramagnetic state we have $h_s=0$, $\theta_{\mathbf{k}}=\pm\pi/2$, and, for example, $T^-=T$ and $T^+=0$. Equations (4) reduce to McMillan's original equations[7] with the standard characteristics of an SN contact.

2. In the antiferromagnetic phase one observes a splitting of the order parameter of the induced superconducting state. This splitting should be seen experimentally in data on electron tunneling in the N direction, as structural features on the current-voltage characteristics near the energies Δ_{n+} and Δ_{n-}. These features are separated in energy by an amount $\Delta_{n+}-\Delta_{n-}\sim d_sN_n(0)\sin 2\theta$ (θ is the value of $\theta_{\mathbf{k}}$ averaged over the Fermi surface).

3. In a thin normal metal ($d_n \ll d_s$) and for small transmission coefficients, with $\Gamma_s^\pm \ll \Gamma_n^\pm \ll \Delta_s^0$, the energy gaps in the antiferromagnetic metal are $\Delta_n(\omega)\simeq\Gamma_n^+$ and $\Delta_n(\omega)\simeq\Gamma_n^-$, and the tunneling density of states is of the BCS form for each band. In the superconducting layer we have

$$\Delta_s(\omega)=\Delta_s^0[1+i\Gamma_s^+(\omega^2-\Delta_{n+}^2)^{-1/2}+i\Gamma_s^-(\omega^2-\Delta_{n-}^2)^{-1/2}]^{-1},$$

and additional structural features appear in the density of electron states at points at which the gaps $\Delta_{n\pm}(\omega)$ open up:

$$N_s(\omega)\simeq(\Gamma_s^+/\Delta_s^0)N_{n+}(\omega)+(\Gamma_s^-/\Delta_s^0)N_{n-}(\omega). \quad (6)$$

In the limit $\Gamma_s^\pm=0$ ($d_n\to 0$) system (4) can be solved explicitly:

$$\Delta_{n\pm}(\omega)=\Delta_s^0\Gamma_n^\pm[(\Delta_s^{02}-\omega^2)^{1/2}+\Gamma_n^\pm]^{-1}.$$

Figure 1 shows the results of a numerical calculation of the tunneling density of states (5) for the superconducting layer, $N_s(\omega)$, and for the antiferromagnetic layer, $N_{n\pm}(\omega)$, for contacts with the following properties: a) $\Gamma_s^+=0.02$, $\Gamma_s^-=0.03$, $\Gamma_n^+=0.5$, $\Gamma_n^-=0.7$; b) $\Gamma_s^+=0.0$; $\Gamma_s^-=0.02$, $\Gamma_n^+=0.05$, $\Gamma_n^-=0.2$. The curves demonstrate the features listed above: the splitting of the tunneling density of states in the antiferromagnetic film and the appearance of a shoulder in $N_{n\pm}(\omega)$ in the region in which the superconducting gap $\Delta_s(\omega)$ opens up. In the case of tunneling in the superconductor direction we observe a smearing of the BCS peak, an extended tail in $N_s(\omega)$ stretching to the values of the minimum gap in the antiferromagnetic layer, and small structural features in the density of states of the superconducting film at $\omega\simeq\Delta_{n\pm}$. Incorporation of effects of a strong electron–phonon coupling leads to an even greater attenuation of the structural features near Δ_s^0 and to the appearance of a structure in $N_{n\pm}(\omega)$, as in $N_s(\omega)$, which reflects the phonon density of states of the superconductor. In addition, in real contacts we would expect effects stemming from a spatial nonuniformity.

McMillan's model assumes that the order parameter remains constant over the entire thickness of the layer. This uniformity is not always achievable experimentally. Incorporating a spatial variation requires a different approach, e.g., an analysis of the semiclassical Gor'kov equations, as in Ref. 14 for superconductor–ferromagnetic-metal superstructures. In the latter case, the pronounced paramagnetic splitting of the electron spectrum by the exchange field causes the variations in the order parameter in the ferromagnetic N layer to be much greater than in a corresponding nonmagnetic metal.[14] There is no paramagnetic exchange splitting in an antiferromagnetic metal, and the question of the spatial variations in the order parameter Δ_n requires a separate study. Such a study goes beyond the scope of the present letter.

We would like to stress once more that the most direct way to observe changes in the spectrum of elementary excitations in superconducting and antiferromagnetic metals in direct contact is tunneling spectroscopy.[11] Measurements of the differential conductance of M–I–SC/AFM or M–I–AFM/SC tunnel structures, where M is a metal injector, and I is a layer of insulator, can be used to determine the structure of the density of one-particle excitations in the superconducting and antiferromagnetic layers, respectively. Experiments of this sort on the spin splitting of the density of states N_s of a superconductor in an external magnetic field are well known,[15] but a splitting of this sort caused by an antiferromagnetic exchange field has yet to be observed. It may be that the anomalously large number of gap features in several tunneling characteristics of high-T_c superconductors is pertinent to the problem discussed above. It may also be that incorporating effects of an inelastic tunneling between conducting layers involving antiferromagnetic fluctuations (as was done in Ref. 8) will make it possible to explain certain characteristic features of superconducting metal oxides.

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