Superconducting-Quasiparticle Interface States

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We describe superconducting-quasiparticle interface states which are produced by a certain class of local potentials at interfaces involving superconductors. These states penetrate at least a coherence distance into the superconductor and arise even when the pair potential is uniform throughout the superconductor. We specifically predict such a state at the interface between an insulating ferromagnet below its Curie temperature and a thin superconductor.

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The occurrence of quasiparticle states at energies within the gap of a superconductor is a phenomenon of continuing and long-standing interest in the physics of superconductors. Such states typically appear in situations wherein the energy gap varies spatially, because of inhomogeneities[1] or the presence of a magnetic field.[2] We report here the prediction of subgap quasiparticle states which can appear in response to a certain class of local potentials at interfaces involving superconductors. These states will play an important role in the determination of the properties of materials in which interfaces between superconductors and other materials are involved, such as in tunnel junctions or artificially produced superconducting multilayers. Furthermore, these states may make it possible to "design" the gap-region density of states via the introduction of interfaces at which potentials of this class are present.

As a specific example of a member of this class, we discuss the local exchange-field polarization at an interface between an insulating ferromagnet below its Curie temperature and a superconductor in which the gap does not (necessarily) vary spatially. The new states arising from this potential are quasiparticle *interface* states because their amplitude decays exponentially into the superconductor, over a length scale which is *greater* than a coherence length. Their existence indicates that the influence of a ferromagnetic layer on superconducting quasiparticles extends *at least* a coherence length into the superconductor.

The spins in the ferromagnet are assumed to have a net polarization in the plane of the interface, so that there is *no consequent magnetic induction in the neighboring superconductor.* Thus *the exchange field acts as a local potential,* coupling spins in the ferromagnet to quasiparticle spins in the superconductor at the interface. Depending upon the sign of the exchange, this local potential is attractive for quasiparticles of one spin, repulsive for those of the opposite spin. In the quasi-one-dimensional geometry of the ferromagnet/superconductor (F/S) interface (with translational invariance assumed in the plane of the interface) the attractive potential yields bound states (i.e., poles in the Green's function) at an energy $E_0 > 0$ (relative to the Fermi energy) and beneath the energy gap (Δ) of the bulk superconductor. A corresponding state is located at $-E_0$ for quasiparticles of the opposite spin.

A simple but relatively general mathematical derivation of these results now follows. Assume translational invariance in the y and z directions. The equations for the retarded Green's function then become quasi one dimensional in character.[3] Next, assume that the Green's function in the absence of the perturbation of interest, $G_0(x,x')$, can be found (the dependence on k_y, k_z, and energy E is implicit in all functions here and below). This Green's function is in general a 4×4 matrix,[4] in order to account for particlelike and holelike excitations of each spin. We further consider only single-particle perturbations. If we designate the single-particle perturbation as $V(x)$ (also a 4×4 matrix), then the exact Green's function obeys

$$G(x,x') = G_0(x,x') + \int dx''\, G_0(x,x'')\, V(x'')\, G(x'',x'). \tag{1}$$

Finally, we assume that the perturbation is a local surface or interface perturbation, confined to the plane $x=0$, with, for simplicity,

$$V(x'') = U\delta(x''). \tag{2}$$

The assumption of a delta-function potential is not essential, but it does greatly simplify the mathematics. We now easily obtain

$$G(x,x') = G_0(x,x') + G_0(x,0)\, U[1-G_0(0,0)\,U]^{-1} G_0(0,x'). \tag{3}$$

We next consider a class of perturbations, U, such that there exist projection operators $P_\pm$ satisfying

$$P_\pm U = Z_\pm P_\pm, \tag{4}$$

$Z_\pm$ being proportional to the unit matrix, and the Green's functions can be decomposed into the orthogonal subspaces

$$G = G_+P_+ + G_-P_-, \quad G_0 = G_{0+}P_+ G_{0-}P_-. \tag{5}$$

A wide variety of single-particle perturbations is encompassed by this class. Using the result

$$P_\pm MM^{-1} = M_\pm P_\pm M^{-1} = P_\pm \rightarrow P_\pm M^{-1} = (M_\pm)^{-1} P_\pm, \tag{6}$$

where M is any 4×4 matrix which is invertible, we find

$$G_\pm(x,x') = G_{0\pm}(x,x') \pm G_{0\pm}(x,0) Z_\pm [1 - G_{0\pm}(0,0) Z_\pm]^{-1} G_{0\pm}(0,x'). \tag{7}$$

Therefore, when we have

$$\det[G_{0\pm}(0,0)^{-1} - Z_\pm] = 0 \tag{8}$$

for real energy E, there exists a bound state (here, an *interface* state).

Quite generally speaking, the spatial variation of $G_{0\pm}(x,x')$ in the x coordinates is governed by the wave vectors[5]

$$K_\pm = \left[k_F^2 \cos^2\theta \pm \frac{2m}{\hbar^2}(E^2 - \Delta^2)^{1/2} \right]^{1/2}, \tag{9}$$

where θ is the angle relative to the interface normal and Δ is the superconductor gap. For $E < 0$, these wave vectors contain an imaginary part, of approximate magnitude (for most values of θ)

$$\mathrm{Im} K_+ \approx \frac{(\Delta^2 - E^2)^{1/2}}{\hbar v_F \cos\theta} < \frac{2\Delta}{\hbar v_F} = \xi_0^{-1}, \tag{10}$$

where ξ_0 is the coherence length. States contributing to $G(x,x')$ at $E < \Delta$ must therefore decay exponentially with x into the superconductor, over a length given by the inverse of $\mathrm{Im} K_+$.

Now specialize to the case in which $G_{0\pm}(0,0)$ is the Green's function for a semi-infinite superconductor, occupying the half-space $x > 0$, evaluated at $x = x' = 0$ in k_y, k_z, and E space[6] (in the notation of Maki[7]):

$$G_{0\pm}(0,0)^{-1} = -i(\epsilon - \delta\rho_2\sigma_2), \tag{11}$$

where

$$\epsilon = E/(E^2 - \Delta^2)^{1/2}, \quad \delta = \epsilon\Delta/E. \tag{12}$$

The matrices σ_j are the usual Pauli matrices, while the 4×4 matrices ρ_j are, for example,

$$\rho_2 = \begin{bmatrix} 0 & -iI \\ iI & 0 \end{bmatrix}, \quad \rho_3 = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}, \tag{13}$$

where I is the 2×2 identity matrix. The product $\rho_j\sigma_k$ is interpreted as the direct product. For notational convenience, we have normalized G_0 by a factor of $2/\hbar v_F \cos\theta$, with a corresponding normalization understood for $Z_\pm$.

Using this function, and assuming that U is *not* proportional to $\rho_2\sigma_2$, we find for (8)

$$\det[G_{0\pm}(0,0)^{-1} - Z_\pm] = (\epsilon - iZ_\pm)^2 - \delta^2 = 1 - 2iZ_\pm\epsilon - Z_\pm^2 = 0. \tag{14}$$

So we obtain a bound state at energy E given by

$$E/(\Delta^2 - E^2)^{1/2} = (1 - Z_\pm^2)/2Z_\pm. \tag{15}$$

If $Z_\pm = \pm Z$, $1 > Z > 0$, then the positive-E state is associated with the upper sign, the negative-E state with the lower sign.

If the interface at $x = 0$ contains polarized spins which are coupled via a local exchange interaction (J) to superconducting quasiparticles, then U is a local proper self-energy, given by an expansion in powers of J. If we keep only the term which is linear in J, then

$$U = p\rho_3\sigma_3, \tag{16}$$

where p is equal to J, divided by the Fermi energy, times the average value of the z component of spin in the ferromagnet. The projection operators for this case are $P_\pm = \frac{1}{2}(1 \pm \rho_3\sigma_3)$. Thus $Z_\pm = \pm p$, and the interface states are found at

$$E_0 = \pm \left| \frac{1-p^2}{1+p^2} \right| \mathrm{sgn}\left(\frac{1-p^2}{2p} \right) \Delta, \tag{17}$$

located symmetrically about the Fermi energy ($E = 0$), within the gap of the superconductor. If we keep terms of second order in J, then the pole in the Green's function becomes a resonance at E_0, with width governed by the magnitude of the second-order term.

A potentially serious deficiency is the neglect of spatial variation in the gap function as a result of pair breaking at the interface. This would cause the gap to be depressed at the F/S interface. A bound state due to Andreev scattering[8] must then form in this pair-potential depression, potentially masking the polarization-induced interface state. The pair-potential depression may be avoided experimentally by making the superconductor thin compared to a coherence length. The average gap Δ would then be approximately constant, lower than the bulk value, and E_0 would be located at a fraction of this gap, according to Eq. (17).

Tunneling is an ideal probe of this interface state, because it directly reflects the density of states for quasiparticles propagating nearly normal to the interface. The analogous tunneling observation of bound states in a pair-potential well (formed by interfaces between a strong- and a weak-coupling superconductor) was first reported by Rowell and McMillan.[9] In the situation of interest here, the ferromagnetic insulator acts as a tunneling barrier itself. Of course, one must assume that a thin ferromagnetic layer can exhibit a net polarization, and that spin-spin interactions at the interface in this layer are not profoundly affected by the proximate superconductor. There is strong evidence that these conditions have been achieved by Stageberg *et al.*[10] in a recent experiment. We shall presently discuss the relevance of our results to this experiment.

In Fig. 1 we display the calculated quasiparticle density of states at the F/S interface for a superconductor with a gap of 1.4 meV, a polarization parameter at the interface, p, equal to -0.23, an elastic magnetic scattering rate equal to $8.0\times10^{-5}\ E_F/\hbar$ (E_F is the Fermi energy), and negligible nonmagnetic interface scattering. For comparison the BCS density of states is also shown as a dashed line. Note that the divergence at the energy gap remains, but that states are less dense above the gap than in the BCS case. Evidently, the interface state removes density from regions above the gap, while maintaining the divergence at the gap. The inset in Fig. 1 displays the same density of states averaged over a Gaussian distribution of energies, the Gaussian of width 0.03 meV. This is an approximate way of accounting for a distribution of polarizations, p, over the interfacial area.

In Fig. 2 we display the I-V curve and its derivative (the normalized differential conductance) for a superconductor/insulating ferromagnet/superconductor tunnel junction. The curve is obtained by numerical integration of

$$I(V)=\int_0^{eV} dE\, N(E)N(E-eV), \tag{18}$$

where $N(E)$ is the density of states in the inset of Fig. 1, V is the voltage, and e the electronic charge. Because $N(E)$ is the density of states *for both spins,* we have implicitly assumed the existence of domains, so that there is no unique spin-up or -down direction. If

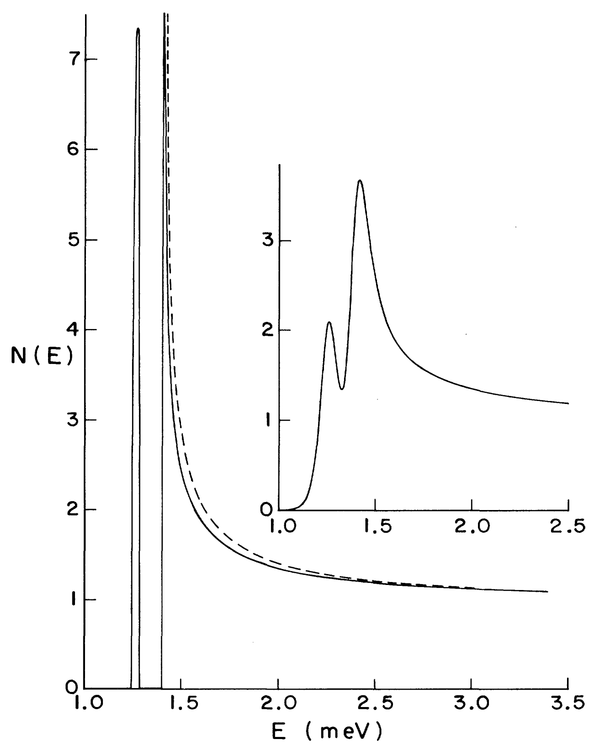

FIG. 1. Total quasiparticle density of states vs energy at an insulating ferromagnet/superconductor interface for a superconductor gap of 1.4 meV, polarization parameter $p=-0.23$, and elastic magnetic scattering rate of $8\times10^{-5}E_F/\hbar$. The bound-state peak occurs at 1.26 meV for one spin. The dashed line is the BCS density of states. The inset is the density of states averaged over a Gaussian of width 0.03 meV, to simulate a distribution of polarizations.

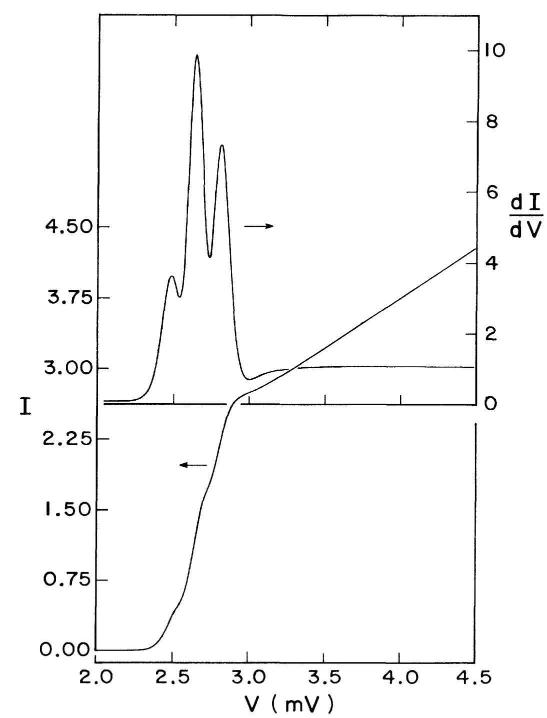

FIG. 2. Lower curve: Current vs voltage obtained with use of density of states from inset of Fig. 1. Upper curve: Derivative of current-vs-voltage curve. The peaks in the upper curve are located at 2.48, 2.64, and 2.8 mV.

there were such a unique direction, tunneling would not be allowed between the interface states on opposite sides of the Fermi level, because these states have opposite spins. Note the dramatic three-peak structure in the derivative curve. If the spin selection rule were operative, there would be only two peaks.

The three-peak structure has been observed by Stageberg *et al.*[10] in a junction consisting of Pb and $Ho(OH)_3$, a ferromagnet with a Curie temperature of about2 K.[11] As noted in Ref. 10, the three-peak structure can arise from the formation of a quasiparticle bound state in the depression of the Pb pair potential created by the magnetic material at the interface. Such a state can occur in this experiment because both Pb layers are thick compared to the coherence length of Pb, so that spatial variations are not suppressed as they would be in thin Pb layers.

Yet there are certain qualitative features of the experimental result which cannot be explained solely by the formation of an Andreev bound state in a pair-potential depression at the interface. First, theoretically the spectral density in the Andreev bound state should dominate over that at the gap edge, because such a bound state removes the divergence at the gap edge.[5] Experimentally, however, the peak in the vicinity of the gap edge remains dominant over the lower-energy peak. Further, theoretically there should be a *depression* in the normalized differential conductance at twice the gap. Experimentally, there is a depression, but it is located *above* the energy 2Δ. In Figs. 1 and 2, one notes that these two qualitative experimental observations apparently agree with the interface state model. An *unambiguous* observation of the interface state could be achieved if the two Pb layers were less than a coherence length thick. Then, perhaps, theory and experiment could be compared in detail, and relevant parameters extracted.

Measurement of the infrared absorption of a thin layer of Pb on an insulating magnetic substrate should also reveal the interface state, because this state influences the superconductor over a length scale at least as large as a coherence length. We predict an aborption which, in the threshold region, resembles the I-V curve in Fig. 2, exhibiting thresholds at energies $2E_0$, $E_0+\Delta$, and 2Δ.

In conclusion, we have demonstrated that local single-particle potentials of a certain class can produce quasiparticle bound states at interfaces involving superconductors. We have presented a specific example, that of the F/S interface, to illustrate a member of this class which has not previously been considered. Some evidence has been given that the tunneling experiment of Stageberg *et al.*[10] provides an example of this phenomenon. We predict that such states will also be observable in the infrared absorption by a thin superconductor on an insulating magnetic substrate.

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