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Andreev reflection in layered structures: Implications for high-T_c grain-boundary Josephson junctions

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Andreev reflection is investigated in layered anisotropic normal-metal–superconductor (N/S) systems in the case of an energy gap (Δ) in S not negligible with respect to the Fermi energy (E_F), as it probably occurs with high critical temperature superconductors (HTSC's). We find that in these limits retroreflectivity, which is a fundamental feature of Andreev reflection, is broken modifying sensitively transport across S/N interfaces. We discuss the consequences for supercurrents in HTSC Josephson junctions and for the midgap states in S-N contacts.

Andreev reflection (AR) is a scattering process occurring at superconductor–normal-metal (S/N) interfaces which convert an electron incident on a superconductor into a hole, while a Cooper pair is added to the superconducting condensate.[1] Because of conservation of momentum, the hole is reflected back in the direction of the incoming electron and all components of the velocity are substantially inverted if the exchange momentum in the scattering process is much less than the Fermi momentum. Retroreflection occurs whenever the Fermi energy (E_F) is much larger than the gap value (Δ) (Andreev approximation). Such an approximation neglects that the retroreflected hole has in reality a different momentum $\delta\mathbf{k}$ in the direction perpendicular to the S/N interface, which is proportional to the ratio Δ/E_F.[1,2] This means that retroreflectivity is broken in some conditions and this will be one of the main issues of this paper.

While predictions based on the Andreev approximation provide accurate explanations in systems employing low critical temperature superconductors, in high-critical temperature superconductor (HTSC) structures the situation is more questionable. If we consider that the gap value could be in some directions of the order of 20 meV (one order of magnitude larger than Δ of traditional superconductors) and that the Fermi energy is roughly one order of magnitude less than E_F of traditional superconductors,[3] it is interesting to go beyond the Andreev approximation for systems employing HTSC. Concepts based on AR have been widely used to interpret properties of HTSC grain-boundary (GB) Josephson junctions (JJ's).[4] Some interesting arguments have been developed by taking into account unconventional order-parameter symmetry. Examples are given by the presence of zero bound states in the density of states of $YBa_2Cu_3O_7$ in the (110) crystallographic direction[5,6] and more generally by phenomena associated with broken time-reversal symmetry.[7]

In this paper we demonstrate that the effects neglected in the Andreev approximation may determine an extreme depression of Andreev reflection processes in some directions at S/N interfaces and an enhancement of ordinary scattering. The implications of these effects on bound states at interfaces employing superconductors with d-wave-order-parameter symmetry are also considered. These phenomena can reveal several important features in charge transport in HTS JJ's and enlighten some aspects of the phenomenology of the junctions within the framework of fundamental issues of HTSC's, such as anisotropy. We stress that the effect we consider, being intrinsically related to Andreev reflection, provides a microscopic explanation of an intrinsic enhanced scattering at the S/N interface.

Before taking into account an order parameter with a d-wave symmetry,[8] we consider a layered normal metal facing an isotropic superconductor with a high value of the order parameter typical for HTSC's. This is illustrated in the junction cross section scheme of Fig. 1(a) and in the three-dimensional view in Fig. 1(b). An electron moving along the planes tilted at an angle θ_1 with respect to the junction interface is reflected as a hole at an angle θ_2. Locally Andreev reflection tends to move quasiparticles out of plane and to favor in some way transport along the c axis. This counter-

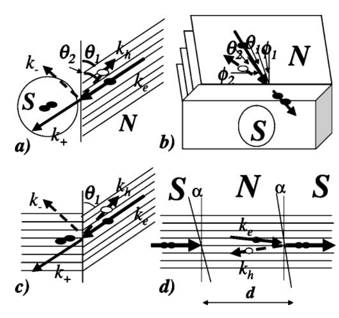

FIG. 1. (a) Cross section of a S/N interface with N layered normal metal and S isotropic superconductor with a high value of the order parameter. An electron moving along the planes tilted of an angle θ_1 with respect to the junction interface is reflected as a hole at an angle θ_2; (b) three-dimensional view of (a); (c) cross section of a S/N interface as in (a) being both electrodes layered. (d) Scheme of nonideal (001) GB JJ's along with the supercurrent transport mechanism.

balances the fact that quasiparticle transport in HTSC's is much favored along the *a*-*b* planes. We will present calculations and phenomenological predictions for the layered structures reported in Figs. 1(c) and 1(d). These can be considered representative of (100) and nonideal (001) tilt GB JJ's, respectively.[9,10]

General formalism: Andreev reflection probability for large values of the Δ/E_F *ratio.* In order to describe charge transport through a normal-metal–superconductor (N/S) interface, we have used the Blonder-Tinkham-Klapwijk (BTK) approach[11] introducing some significant modifications. In solving the Bogoliubov–de Gennes (BdG) equations for the wave functions $\psi_{n,s}$ in the N, S regions, we consider the terms of the order of Δ/E_F in the expressions of the wave vectors along the incoming (electronic) and reflected (hole) trajectories in N, $k_{e,h}=k_{Fn}\sqrt{1\pm E/E_F}$, and along the transmitted trajectories without and with branch crossing in S, $k_{\pm}=k_{Fs}\sqrt{1\pm\sqrt{E^2-|\Delta_{\pm}|^2}/E_F}$ [see Fig. 1(a)]. The expression for $k_{\pm}$ is extended to the general anisotropic case, when the magnitude $|\Delta_{\pm}|$ and the phase $\varphi_{\pm}$ of the gap function in S are specified on the trajectories $k_{\pm}$. We also generalize the BTK matching conditions for $\psi_{n,s}$ at the N/S interface:

$$\psi_n=\psi_s,\frac{\hbar^2}{2m}(\psi_s'-\psi_n')=\begin{pmatrix}H_1\\H_2\end{pmatrix}\psi(0).$$

Here $H_{1,2}=\int(U(x)-E_{e,h})dx$, $U(x)$ is the interface barrier potential, $E_{e,h}$ are the kinetic energies of the electrons and the holes. In the WKB approximation barrier transmission coefficients $D_{e,h}\propto\exp[-2\int\sqrt{U(x)-E_{e,h}}/\hbar\,dx]$ and $D_h<D_e$, since the hole has less kinetic energy to overcome the barrier.[12] In analogy with the BTK model, the dimensionless barrier strengths for electrons and holes can be introduced $Z_{1,2}=\sqrt{(1-D_{e,h})/D_{e,h}}$ and generally $Z_1<Z_2$. This effect may only hold for a realistic extended barrier[12] rather than for a δ-barrier.

With these modifications, we solve the BdG equations and find the probability of the Andreev and normal reflection process for an electron incoming from the N side, respectively,

$$A(E)=\frac{2(\alpha_1+\alpha_2)^2\beta_1\beta_2|u_-^2v_+^2|}{|\gamma_1\gamma_2u_-u_+e^{i\varphi_+}-\delta_1\delta_2v_-v_+e^{i\varphi_-}|^2},\qquad(1)$$

$$B(E)=\left|\frac{u_-u_+\gamma_2\eta_1e^{i\varphi_+}-v_-v_+\delta_1\eta_2e^{i\varphi_-}}{\gamma_1\gamma_2u_-u_+e^{i\varphi_+}-\delta_1\delta_2v_-v_+e^{i\varphi_-}}\right|^2.\qquad(2)$$

Here $\gamma_{1,2}=\alpha_{1,2}+\beta_{1,2}\mp2Z_{1,2}$, $\delta_{1,2}=\alpha_{2,1}-\beta_{1,2}\pm2Z_{1,2}$, $\eta_{1,2}=\alpha_{1,2}\mp\beta_1\mp2Z_1$, $\alpha_1=i(k_+/k_{Fs})$, $\alpha_2=i(k_-/k_{Fs})$, $\beta_1=i(k_e/k_{Fs})$, $\beta_2=i(k_h/k_{Fs})$, $u_{\pm}^2=\frac{1}{2}(1+i\sqrt{|\Delta_{\pm}^2|-E^2}/E)$, $v_{\pm}^2=\frac{1}{2}(1-i\sqrt{|\Delta_{\pm}^2|-E^2}/E)$.

This approach formally presents some analogies with the formulation of the problem of spin-polarized tunneling in ferromagnet-superconductor (F/S) junctions.[13,14] A formal analogy can be established, for example, between the Fermi momenta in the spin subbands and the Fermi momenta in the planes ($k_{\|}=k_{n+}$) and across the planes ($k_{\perp}=k_{n-}$), respectively. By increasing the mismatch between them, in both cases the contribution to the current due to Andreev reflection is reduced. The effects considered in the present paper arise from the loss of retroreflectivity due to large gap values, while in the F/S interfaces they are due to an exchange field in F.

Josephson current: comparison with HTS JJ. The modification of the probability of the Andreev reflection process has direct consequences on the calculation of the Josephson current carried by Andreev bound states [see Fig. 1(d)]. Andreev bound states are localized in the barrier region and are formed by an electron and a hole moving in opposite directions. As a consequence the momenta mismatch between an electron and a hole leads to a depression of the Josephson current. As a generic case, we consider tunnel SIS junction, $Z_1=Z_2=Z\gg1$ and both electrodes as *s*-wave superconductors.

Let an electron have an angle α_e relative to the planes. As discussed in the Introduction, the Andreev reflected hole moves at an angle α_h different from α_e. The angles $\alpha_{e,h}$ are related by the conservation of the momenta parallel to the interface $\sin(\alpha-\alpha_e)k_e=\sin(\alpha-\alpha_h)k_h$, where $\alpha=(\pi/2-\theta_1)$ is the angle between the planes and the interface normal and the electron (hole) momenta, $k_{e,h}$ are given by $(1\pm E_B/E_F)k_{e,h}^{-2}=\cos^2(\alpha_{e,h}-\alpha)k_{\|}^{-2}+\sin^2(\alpha_{e,h}-\alpha)k_{\perp}^{-2}$. Here E_B is the Andreev bound-state energy, and the anisotropic Fermi surface is approximated by an ellipsoid with axes $(k_{\perp},\ k_{\|})$. The results do not depend qualitatively on this choice.

According to the formalism of Furusaki *et al.*[15] the Josephson current per conductance channel is expressed via the amplitude of Andreev reflection $a(\varphi,\omega_n)$ in the barrier region (N)

$$I_s=\frac{e\Delta}{2\hbar}\sum_n\left[\frac{a(\varphi,\omega_n)}{k_e}-\frac{a(-\varphi,\omega_n)}{k_h}\right]\frac{k_e+k_h}{\sqrt{\omega_n^2+\Delta^2}}.\qquad(3)$$

Here $\omega_n=\pi T(2n+1)$ and φ is the phase difference. The amplitude $a(\varphi,\omega_n)$ is found from the solution of BdG equations and describes the multiple scattering in the barrier region. In a tunnel junction $E_B=\Delta$. We neglect here a weak energy dependence of Δ due to nonconstant density of states in the relevant energy range.

The angle dependence of $a(\varphi,\omega_n)$ in Eq. (3) is mainly controlled by the scattering amplitude t_{eh} in the electron-hole channel, $a\propto t_{eh}(\alpha,\alpha_e,\alpha_h)$. The normal-state conductance of the junction G_N per channel is determined by the scattering amplitude t_{ee} in the electron-electron channel $G_N\propto t_{ee}(\alpha,\alpha_e)$. The explicit form of t_{eh}, t_{ee} depends on a choice of the shape of a potential barrier. For the δ barrier the BdG solution yields $a\propto t_{eh}\propto k_ek_hk_{Fn}^{-2}(1+Z^2)^{-1}$, $G_N\propto_e k_e^2k_{Fn}^{-2}(1+Z^2)^{-1}$. As it follows from the above set of equations for $k_{e,h}$, no real solution exists for k_h for the angles $\alpha_e>\alpha_e^{th}$, where the Andreev reflection process is prohibited. The threshold angle α_e^{th} sensitively depends on $k_{\perp}/k_{\|}$ and Δ/E_F.

I_c and G_N are obtained by considering all conductance channels, i.e., integration over the angle α_e. The final result depends on the barrier shape, which controls the relation between α_e,α_h and trajectories in S regions. We consider below an extended barrier for strong directional tunneling around the normal direction (the tunneling cone effect).[12]

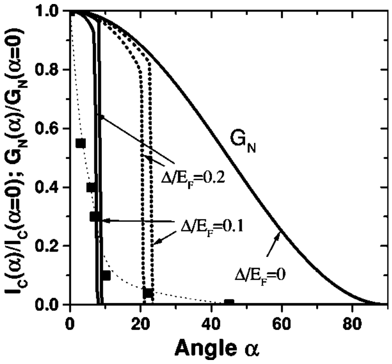

FIG. 2. Dependence of I_C and G_N on the angle α between the planes and the interface for different values of the Δ/E_F ratio and the Fermi mismatch $(k_\perp/k_\parallel)=0.1$ (solid lines) and 0.3 (dashed lines). Experimental data for (100) tilt grain boundaries are shown by dots.

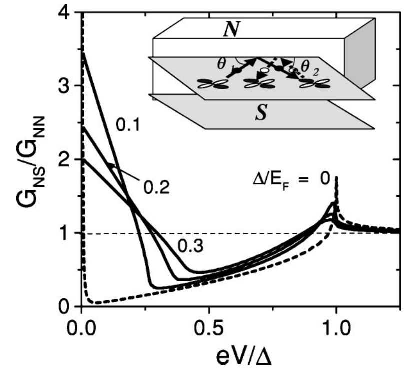

FIG. 3. The conductance for different values of the Δ/E_F ratio in a tunnel NIS junction. Inset: resonant state originating at the interface of a d-wave S facing an insulator or a normal metal N′ along the (110) orientation.

The results of the numerical calculations of $I_C(\alpha)$ and $G_N(\alpha)$ are shown in Fig. 2 for different values of the Δ/E_F ratio and Fermi mismatch $k_\perp/k_\parallel$. We give evidence of a remarkable decrease of I_C with the increase of the angle α. The reason for this drop is the existence of both a threshold angle α_e^{th} and a narrow tunneling cone. This result is in qualitative agreement with experimental data obtained on GB JJ's.[9] An account of the distribution of tunnel angles in a real interface would broaden the sharp transitions in Fig. 2.

The general picture considered above can be also applied to the geometry shown in Fig. 1(c) providing the same qualitative behavior. A rigorous treatment would require some further hypothesis on Cooper pair transport in the c direction that is beyond the scope of this paper.

The interplay between the effect of loss retroreflectivity considered in this paper and well established effects such as interface roughness or the coexistence of order parameters with different symmetry close to junction interfaces,[4,16,18,19] deserves further investigation. Interface roughness produces a smooth dependence of I_C on the angle α, in contrast to the sharp dependences shown above.

S (anisotropic superconductor) / N interface: conductance and the problem of zero bound state. We consider another aspect typical of HTSC junctions related to Andreev reflection by introducing a d-wave order parameter for the S and investigating the origin of zero bound states (ZBS). The basic process is shown in Fig. 3, where a d-wave S faces an insulator or a normal metal N' along the (110) orientation (the a-b planes can be, in principle, rotated of an angle with respect the S/N interface different from 45°). An electron, coming, for instance, along the direction of the positive lobe of the order parameter, first suffers an ordinary scattering at the interface with a normal metal (N′) and then is Andreev reflected towards the negative lobe of the order parameter. Then the hole will experience an ordinary scattering at the S/N′ interface and will be reflected towards the positive lobe of the order parameter, where it will be Andreev reflected again. This process produces a constructive interference and as a consequence a resonant state, formally described by a pole in the Andreev amplitude Eq.(1). This manifests itself as a zero-bias peak in the density of states in S (zero-bias anomaly) (ZBA).[5,17]

These arguments are essentially based on the retroreflection property of Andreev reflection. On the other hand, the constructive interference breaks down for high values of Δ/E_F: the electronic state created after two Andreev and two normal reflections will not propagate along the same trajectory as the initial one. As a consequence ZBS will be damped and the low voltage conductance will be decreased.

We have calculated the conductance of a tunnel NIS junction ($Z_1=Z_2\gg 1$) self-consistently by the method of Ref. 19, taking into account the angle mismatch of electrons and holes and the self-consistent reduction of the pair potential at the interface. The angle averaging was performed by choosing a δ-function potential barrier with an angular dependence of the transmission coefficient $D(\theta)=D(0)\cos^2\theta$. The results of calculations are presented in Fig. 3 for misorientation angle $\alpha=45^0$ and different values of the Δ/E_F ratio, giving some evidence of broadening of the ZBA. We also point out that in contrast with ZBS broadening due to surface roughness,[18–20] the mechanism we propose has an intrinsic nature mainly controlled by the Δ/E_F ratio.

The problem of the ZBA has also been investigated in the case that Z_1 is different from Z_2. This difference is particularly meaningful in the formation of the ZBS, where both electron and hole scattering processes across the same interface are involved. In Fig. 4 we report the conductance in the regime $\Delta/E_F=0$ for fixed value of $Z_1=0.5$ and for different values of Z_2 at temperature $T=0$ K. We notice the appearance of peaks at finite voltages and the removal of the ZBA for some values of $Z_2>Z_1$. This means that the crossover

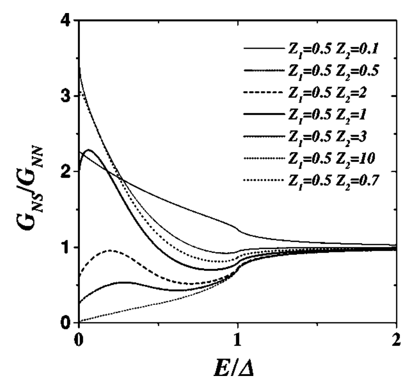

FIG. 4. The conductance for a fixed value of $Z_1=0.5$ and for different values of Z_2 at temperature T = 0 K.

from ZBA to bound states at finite voltages can also take place due to a different transparency of electrons and holes at the S/N interface. Such a crossover has been also predicted for ferromagnet-insulator–superconductor junctions by Kashiwaya *et al.*[14] Our result is obviously independent of any ferromagnetic electrode or barrier and only relies on a possible barrier asymmetry for holes and electrons. Barrier asymmetry acts as a kind of filter which creates an electron-hole imbalance, thus reducing the probability of the formation of the ZBA.

In conclusion, Andreev reflection has been theoretically investigated in layered anisotropic normal-metal-superconductor (N/S) systems in the case of an energy gap (Δ) in S not negligible with respect to the Fermi energy (E_F). We have demonstrated that the combination of large gap and strong anisotropy leads to an intrinsic decrease of the critical current density as a function of the tilt angle in HTSC Josephson junctions, as experimentally observed. A damping of the resonances originating the zero bound states has been also found.

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