

# Effects of Anomalous Andreev Reflection in High $T_c$ Layered Structures

Alexander A. Golubov and Francesco Tafuri

**Abstract**—Andreev reflection is investigated in layered anisotropic normal metal / superconductor (N/S) systems in the case of an energy gap in S not negligible respect to the Fermi energy, as probably occurring in high critical temperature superconductors (HTS). We find that in these limits retro-reflectivity, which is a fundamental feature of Andreev reflection, is broken modifying sensitively transport across S/N interfaces. This study is extended to aspects proper of HTS junctions to investigate both the supercurrents in S-N-S Josephson structures and zero bound states in S-N contacts respectively. Such an investigation provides a new insight into the effects that anisotropy determines into the phenomenology of HTS grain boundary junctions.

**Index Terms**— Andreev reflection, Grain boundaries Josephson junctions, High temperature superconductors.

## I. INTRODUCTION

ANDREEV reflection (AR) is a scattering process occurring at superconductor / normal metal (S/N) interfaces that converts an electron incident on a superconductor into a hole, while a Cooper pair is added to the superconducting condensate. 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. Retro-reflection occurs whenever the Fermi energy ( $E_F$ ) is much larger than the gap value ( $\Delta$ ) (Andreev approximation). Such an approximation neglects that the retro-reflected hole has in reality a different momentum  $\Delta k$  in the direction perpendicular to the S/N interface, which is proportional to the ratio  $\Delta/E_F$ . This means that retro-reflectivity is broken in some conditions and this may be the case for high-critical temperature superconductor (HTS) junctions with important consequences on their phenomenology.

While predictions based on the Andreev approximation provide accurate explanations in systems employing low critical temperature superconductors, in HTS 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 the gap in traditional superconductors) and that the Fermi energy is roughly one order of magnitude less than  $E_F$  of traditional superconductors [1], it is interesting to go beyond the Andreev approximation for systems employing HTS. Concepts based on AR have been widely used to interpret properties of HTS grain boundary (GB) Josephson junctions (JJ) [2]. Some new interesting arguments have been developed by taking into account unconventional order parameter symmetry. Examples are given by the presence of zero bound states (ZBA) in the density of states of  $YBa_2Cu_3O_7$  in the (110) crystallographic direction [3,4].

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 and an enhancement of ordinary scattering at S/N interfaces. These effects also influence on bound states at interfaces employing superconductors with d-wave order parameter symmetry and can reveal several important features in charge transport in HTS Josephson junctions. 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 [5], we consider a layered normal metal facing an isotropic superconductor with a high value of the order parameter typical for HTS ( $\approx 20$  meV), as illustrated in the junction scheme of Fig.1a and in 3-dimensional view in Fig. 1b. An electron moving along the planes tilted of an angle  $\theta_1$  with respect to the junction interface is reflected as a hole at an angle  $\theta_2$ . Locally Andreev reflection tends to move quasi-particles out of planes and to favorite in some way transport across c-axis. This counterbalances the fact that quasi-particles transport in HTS is much favored along the a-b planes. We will present calculations for the layered structures reported in Fig.1c and Fig.1d. The results we obtain can be considered representative of (100) and non-ideal (001) tilt GB JJs respectively [6,7].

## II. GENERAL FORMALISM

We first describe the main formalism and introduce the basic equations in the most general case of a d-wave superconductor, that will be simplified and discussed for the different problems we consider.

Let us consider a normal metal - superconductor (N/S) interface in the case of anisotropic normal metal (N) and large

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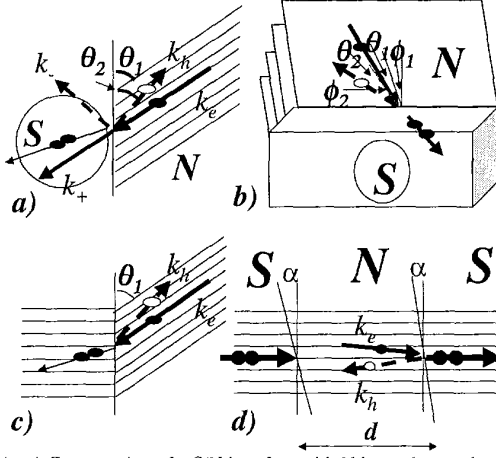


Fig. 1. a) Cross section of a S/N interface with N layered normal metal and S isotropic superconductor with a high value of the order parameter. An electron moving along the planes tilted of an angle  $\theta_1$  with respect to the junction interface is reflected as a hole at an angle  $\theta_2$ ; b) 3-dim. View of (a); c) cross section of a S/N interface like in (a) being both electrodes layered; d) non-ideal (001) GB JJ along with the supercurrent transport mechanism.

$\Delta/E_F$  ratio in a superconductor (S). In order to describe the Andreev reflection processes in this regime, we use the Blonder-Tinkham-Klapwijk (BTK) approach [8] introducing some significant modifications. Solutions of the Bogoliubov – de Gennes equations are the incoming, reflected and transmitted waves (see Fig.1a):

$$\psi_{inc} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_e x}, \quad \psi_{refl} = a \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_h x} + b \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_e x}, \quad (1a)$$

$$\psi_{trans} = c \begin{pmatrix} u_+ \\ v_+ e^{-i\varphi_+} \end{pmatrix} e^{ik_+ x} + d \begin{pmatrix} v_- e^{-i\varphi_-} \\ u_- \end{pmatrix} e^{-ik_- x}, \quad (1b)$$

where we keep the terms of the order of  $\Delta/E_F$  in the expressions for the electron (hole) wave vectors  $k_{e,h}$  in N metal and  $k_{\pm}$  in S metal:

$$u_{\pm} = \frac{1}{2} (1 + \sqrt{E^2 - |\Delta_{\pm}^2|} / E), v_{\pm} = \frac{1}{2} (1 - \sqrt{E^2 - |\Delta_{\pm}^2|} / E), \Delta_{\pm} = |\Delta_{\pm}| e^{i\varphi_{\pm}},$$

$$k_{e,h} = \sqrt{k_{Fn}^2 \pm 2mE/\hbar^2} = k_{Fn} \sqrt{1 \pm E/E_F}, k_{\pm} = k_{Fs} \sqrt{1 \pm \sqrt{E^2 - |\Delta_{\pm}^2|} / E_F}.$$

Here  $\Delta_{\pm}$  is the gap function along the directions  $k_{\pm}$  is S.

We also generalize the matching conditions for the waves the waves (1) at the N/S interface

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

where generally different barrier strengths for electrons and holes,  $Z_{1,2} = H_{1,2} / \hbar v_{Fs}$ , respectively are introduced. A difference between  $Z_1$  and  $Z_2$  corresponds to the fact that holes and electrons may have different kinetic energy to overcome the barrier especially if we model transmission through rectangular barrier, rather than through delta-barrier.

We may expect  $Z_1 < Z_2$  since the hole has somewhat less kinetic energy to overcome the barrier [9].

The matching conditions (2) provide the solutions for the coefficients  $a, b, c, d$  in eq.(1) and for the probabilities of Andreev reflection  $A(E)$  and normal reflection  $B(E)$  respectively

$$A(E) = |a(E)|^2 = \frac{2(\alpha_1 + \alpha_2)^2 \beta_1 \beta_2 |u_- v_+^2|}{|e^{i\varphi_+} u_- u_+ \gamma_1 \gamma_2 - e^{i\varphi_-} v_- v_+ \delta_1 \delta_2|^2}, \quad (3a)$$

$$B(E) = |b(E)|^2 = \frac{|e^{i\varphi_+} u_- u_+ \eta_1 \gamma_2 - e^{i\varphi_-} v_- v_+ \delta_1 \eta_2|^2}{|e^{i\varphi_+} u_- u_+ \gamma_1 \gamma_2 - e^{i\varphi_-} v_- v_+ \delta_1 \delta_2|^2}, \quad (3b)$$

$$\text{where } \gamma_{1,2} = \alpha_{1,2} + \beta_{1,2} \mp 2Z_{1,2}, \delta_{1,2} = \alpha_{2,1} - \beta_{1,2} \pm 2Z_{1,2},$$

$$\eta_{1,2} = \alpha_{1,2} \mp \beta_{1,2} \mp 2Z_1, \alpha_1 = ik_+ / k_{Fs}, \alpha_2 = ik_- / k_{Fs},$$

$$\beta_1 = k_e / k_{Fs}, \beta_2 = k_h / k_{Fs}.$$

More details can be found in ref.10. We will give a few examples of how this general formalism can be applied to cases of practical interest. We will demonstrate how it follows from eqs.(1)-(3) that by increasing the mismatch between the Fermi momenta in planes and across the planes the contribution of Andreev reflection to the current is reduced due to the loss of retroreflectivity.

### III. S (ISOTROPIC)/N INTERFACE: CONDUCTANCE

We first consider conductance  $G$  as a function of voltage  $V$  for the SN junction, being N a layered normal metal and S a s-wave superconductor characterized by large gap values and low Fermi energy (Fig.1a). We also suppose the same barrier strength for electrons and holes,  $Z_1 = Z_2$ .

Let an electron has an angle  $\alpha_e$  relative to the planes. As discussed in the introduction, the Andreev reflected hole moves at an angle  $\alpha_h$  different from  $\alpha_e$ . The relation between these angles follows from the conservation of the electron and hole Fermi momenta parallel to the interface  $k_e \sin(\alpha - \alpha_e) = k_h \cos(\alpha - \alpha_h)$ , where  $\alpha = \pi/2 - \theta_1$  is the angle between the planes and the interface normal. The electron and hole momenta are related by

$$(1 \pm \tilde{E}/E_F) k_{e,h}^{-2} = \cos^2(\alpha_{e,h} - \alpha) k_{\max}^{-2} + \sin^2(\alpha_{e,h} - \alpha) k_{\min}^{-2}. \quad (4)$$

We have approximated the highly anisotropic Fermi surface by an ellipsoid with axes  $k_{\max}, k_{\min}$  (or  $k_{\parallel}, k_{\perp}$ ). Here  $\tilde{E}$  is an energy difference between electrons and holes, which in most physical situations is of the order of  $\Delta$ . To illustrate the effect of conductance, we will assume for simplicity  $E = \Delta$ . Equations for  $k_{e,h}$  are easily solved numerically in order to calculate  $k_{e,h}$  as a function of the angle  $\theta_1$ . According to the BTK model, the low-temperature

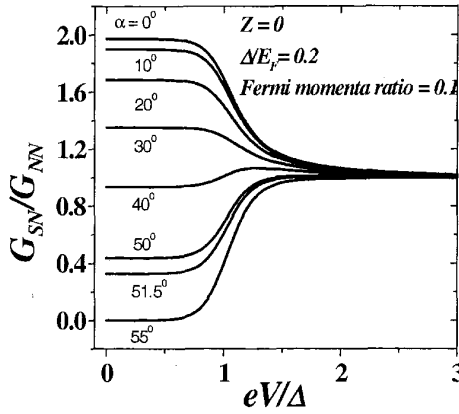


Fig.2. Conductance across the NS interface in the geometry of Fig.1a.

conductance  $G(V)$  at the subgap voltages  $eV < \Delta$  is given by

$$G(V)/G_N = 2|a|^2 \sim 2T_e T_h \frac{(1 + \beta^2) k_h^2 \cos^2 \alpha_h}{(1 - r_e r_h)^2 + \beta^2 (1 + r_e r_h)^2}, \quad (5)$$

where  $G_N$  is the normal state conductance of a contact,  $\beta = \sqrt{\Delta^2 - (eV)^2} / eV$ , and the probabilities of transmission  $T_{e,h}$  and reflection  $r_{e,h}$  are given by  $r_{e,h} = \sqrt{1 - T_{e,h}}$ ,  $T_e = \cos^2 \alpha / (\cos^2 \alpha + Z^2)$ , and  $T_h = \cos \alpha_h \cos \alpha / ((\cos \alpha_h + \cos \alpha)^2 / 4 + Z^2)$ .

It follows from eq.(5) that the conductance scales with the hole momentum  $k_h$  which vanishes with increasing angle  $\alpha$ . In Fig.2 the conductance is shown for various values of  $\alpha$ , fixed ratio  $\Delta/E_F = 0.2$  and anisotropy  $k_\perp/k_\parallel = 0.1$ , which can be considered reasonable for HTS systems. Most of changes occur for energies less than the gap value. For  $Z=0$  it is possible to pass from a regime with excess current to a regime characterized by complete absence of current at  $eV < \Delta$ . The latter approximately occurs for angles  $\alpha > 55^\circ$ , when Andreev reflection is fully suppressed.

#### IV. 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.1d). 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,  $Z_1=Z_2=Z$  and both electrodes as s-wave superconductors.

The relation between angles  $\alpha_h$  and  $\alpha_e$  is again given by

eq. (4) with  $\tilde{E} = E_B$ , where  $E_B = \Delta$  is the Andreev bound state energy in a tunnel junction. According to the formalism of Furusaki *et al.* [11], the Josephson current per conduction channel is proportional to the amplitude of Andreev reflection  $a(\varphi)$  in the junction ( $\varphi$  is the phase difference). This amplitude is found from the solution of BdG equations and describes the multiple scattering in the barrier region. For the  $\delta$ -barrier the angle dependence of the Andreev amplitude is given by  $a \propto k_e k_h k_{F_n}^{-2} (1 + Z^2)^{-1}$ . The normal state conductance is given by  $G_N \propto k_e^2 k_{F_n}^{-2} (1 + Z^2)^{-1}$ . As follows from eq.(4), no real solution exists for  $k_h$  for the angles  $\alpha_e > \alpha_e^{th}$ , the threshold angle  $\alpha_e^{th}$  being controlled by the anisotropy ratio and  $\Delta/E_F$  [10].

$I_c$  and  $G_N$  are obtained by the integration over the angle  $\alpha$ . The final result depends on the barrier shape, which controls the relation between  $\alpha_h$ ,  $\alpha_e$  and trajectories in S regions. We consider below an extended barrier for strong directional tunneling around the normal direction (the tunneling cone effect [9]). The results of the numerical calculations of  $I_c$  and  $G_N$  are shown in Fig.3 for different values of the  $\Delta/E_F$  ratio and Fermi mismatch. We give evidence of a remarkable decrease of  $I_c$  with the increase of the angle  $\alpha$ . The reason for this drop is the existence of both a threshold angle  $\alpha_e^{th}$  and a narrow tunneling cone. This result is in qualitative agreement with experimental data obtained on GB JJs [6]. 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.1c providing the same qualitative behavior.

The interplay between the effect of loss retro-reflectivity considered in this paper and well established effects such as interface roughness or the co-existence of order parameters

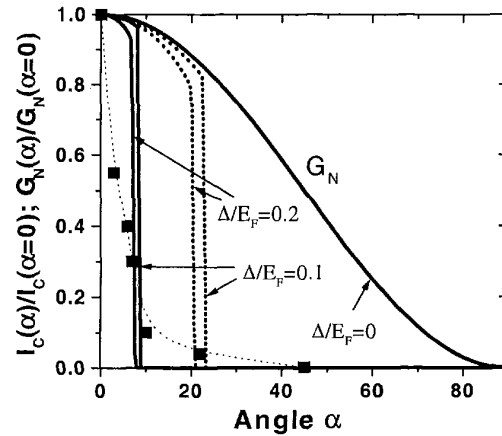


Fig.3. Dependence of  $I_c$  and  $G_N$  on the angle  $\alpha$  between the planes and the interface for different values of  $\Delta/E_F$  ratio and Fermi mismatch  $k_\perp/k_\parallel = 0.1$  (solid lines) and 0.3 (dashed lines). Experimental data for (100) tilt grain boundaries from ref.7 are shown by dots.

with different symmetry close to junction interfaces [2,12,13] deserves further investigations. Interface roughness produces a smooth dependence of  $I_c$  on the angle  $\alpha$  in contrast to the sharp dependences shown above [10].

#### V. S (ANISOTROPIC)/N INTERFACE: CONDUCTANCE AND THE PROBLEM OF ZERO BOUND STATE

We consider another aspect typical of HTS 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. 4, 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  $45^\circ$ ). 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 manifests itself as a zero bias anomaly (ZBA) in the density of states in S [3,14].

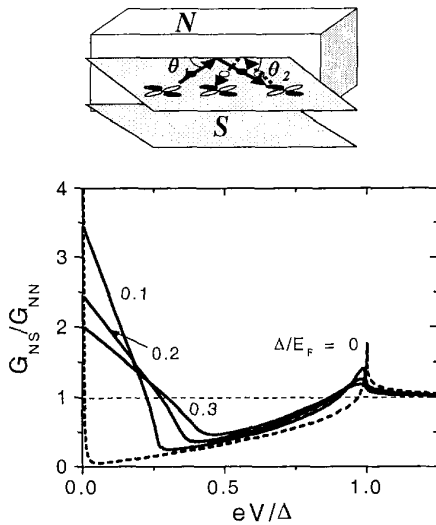


Fig.4. The normalized conductance of a tunnel NIS junction for  $\alpha = 45^\circ$  and different values of  $\Delta/E_F$ . The origin of the resonance state at the interface of a d-wave superconductor (S) facing a normal metal N along the (110) direction is demonstrated.

This constructive interference breaks down for high values of  $\Delta/E_F$  since 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 due to the loss of the retroreflectivity [10].

We have calculated the conductance of a tunnel NIS junction selfconsistently by the method developed in [13],

taking into account the angle mismatch of electrons and holes and the reduction of the pair potential at the interface. The results of calculations are presented in Fig.4 for  $\alpha = 45^\circ$  and different values of the  $\Delta/E_F$  ratio, giving the evidence of broadening of the ZBA.

#### VI. CONCLUSIONS

Andreev reflection has been theoretically investigated in layered anisotropic normal metal / superconductor systems in the case of not negligible  $\Delta/E_F$  ratio. 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 HTS Josephson junctions, as experimentally observed. A damping of the resonances originating the zero bound states has been also predicted.

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