Andreev reflection in layered structures: implications for high $T_c$ grain boundary Josephson junctions

Alexander Golubov
Department of Applied Physics, University of Twente, 7500 AE Enschede, The Netherlands

Francesco Tafuri
Dipartimento di Ingegneria dell’Informazione, Seconda Università di Napoli, 81031 Aversa (CE) and INFM-Dipartimento Scienze Fisiche dell’Università di Napoli “Federico II”, 80125 Napoli (ITALY)

Andreev reflection is investigated in layered anisotropic normal metal / superconductor (N/S) systems in the case of an energy gap ($\Delta$) in S not negligible with respect to the Fermi energy ($E_F$), as it probably occurs with 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. We discuss the consequences for supercurrents in HTS Josephson junctions and for the midgap states in S-N contacts.

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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 $\delta \mathbf{k}$ 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 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 (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 $\Delta$ of traditional superconductors) and that the Fermi energy is roughly one order of magnitude less than $E_F$ of traditional superconductors, 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). 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 in the density of states of $\text{YBa}_2\text{Cu}_3\text{O}_y$ in the (110) crystallographic direction and more generally by phenomena associated with broken time reversal symmetry (BTRS).

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 and enlighten some aspects of the phenomenology of the junctions within the framework of fundamental issues of HTS, 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, we consider a layered normal metal facing an isotropic superconductor with a high value of the order parameter typical for HTS. This is illustrated in the junction cross section scheme of Fig.1a and in 3-dimensional view in Fig.1b. An electron moving along the planes tilted at 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 plane and to favor in some way transport along the c-axis. This counterbalances the fact that quasi-particle transport in HTS is much favored along the a-b planes. We will present calculations and phenomenological predictions for the layered structures reported in Fig.1c and Fig.1d. These can be considered representatives of (100) and non-ideal (001) tilt GB JJs respectively.

General formalism: Andreev reflection probability for large values of the $\Delta/E_F$ ratio. In order to describe charge transport through a normal metal - superconductor (N/S) interface, we have used the Blonder-Tinkham-Klapwijk (BTK) approach 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 $\Delta/E_F$ in the expressions of the wave vectors along the incoming (electronic) and reflected (hole) trajectories in
Here $\gamma_{1,2} = \alpha_{1,2} + \beta_{1,2} + 2Z_{1,2}$, $\delta_{1,2} = \alpha_{2,1} - \beta_{1,2} + 2Z_{1,2}$, $\eta_{1,2} = \alpha_{1,2} - \beta_{1,2} + 2Z_{1,2}$, $\alpha_{1} = i\frac{k_{1}}{k_{F_{e}}}$, $\alpha_{2} = i\frac{k_{2}}{k_{F_{e}}}$, $\beta_{1} = i\frac{k_{1}}{k_{F_{h}}}$, $\beta_{2} = i\frac{k_{2}}{k_{F_{h}}}$, $u\alpha_{1} = \frac{1}{2}(1+i\sqrt{\Delta_{1}^{2} - E^{2}/E})$, $v\alpha_{2} = \frac{1}{2}(1 - i\sqrt{\Delta_{2}^{2} - E^{2}/E})$.

This approach formally presents some analogies with the formulation of the problem of spin- polarized tunneling in ferromagnet / superconductor (F/S) junctions [1][2]. A formal analogy can be established for example between the Fermi momenta in the spin subbands and the Fermi momenta in the planes ($k_{\parallel} = k_{n_{e}}$) and across the planes ($k_{\perp} = k_{n_{h}}$) 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.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, $Z_{1} = Z_{2} = Z \gg 1$ and both electrodes as s-wave superconductors.

Let an electron have 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 angles $\alpha_{e,h}$ are related by the conservation of the momenta parallel to the interface $\sin(\alpha - \alpha_{e})k_{n_{e}} = \sin(\alpha - \alpha_{h})k_{n_{h}}$, 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 $(1 \pm E_{F}/E_{F})k_{0}^{2} = \cos^{2}(\alpha_{e,h} - \alpha)k_{\parallel}^{2} + \sin^{2}(\alpha_{e,h} - \alpha)k_{\perp}^{2}$. Here $E_{B}$ is the Andreev bound state energy, and the anisotropic Fermi surface is approximated by an ellipsoid with axes ($k_{\parallel}, k_{\perp}$). The results do not depend qualitatively on this choice.

According to the formalism of Furusaki et al. [3][4][5] the Josephson current per conductance channel is expressed via the amplitude of Andreev reflection $a(\varphi, \omega_{n})$ in the barrier region (N)

$$I_{s} = \frac{e\Delta}{2\hbar} \sum_{n} \left[ \frac{a(\varphi, \omega_{n})}{k_{e}} - \frac{a(-\varphi, \omega_{n})}{k_{h}} \right] \frac{k_{e} + k_{h}}{\sqrt{\omega_{n}^{2} + \Delta^{2}}}.$$  \hspace{1cm} (3)

Here $\omega_{n} = \pi T(2n+1)$ and $\varphi$ 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 $\Delta$ due to non-constant 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 $t_{eh}(\alpha_{e}, \alpha_{h})$. The normal state
As it follows from the above set of equations for the Andreev reflection process is prohibited. The threshold barrier. For the δ-barrier the BdG solution yields
\[ a \propto t_{eh} k_{0e}^2 (1 + Z^2)^{-1}, \]
\[ G_N \propto k_{0h}^2 k_{Fn}^2 (1 + Z^2)^{-1}. \]

It follows from the above set of equations for \( k_{0e,h} \), no real solution exists for \( k_{0h} \) for the angles \( \alpha_e > \alpha_{th} \), where the Andreev reflection process is prohibited. The threshold angle \( \alpha_{th} \) sensitively depends on \( k_{\perp}/k_{||} \) and \( \Delta/E_F \).

The general picture considered above can be also applied to the geometry shown in Fig. 1c providing the same interface roughness produces a smooth dependence of \( I_C \) on the angle \( \alpha \), 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 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. 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. (6). This manifests itself as a zero bias peak in the density of states in S (zero bias anomaly) (ZBA).

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 \( \Delta/E_F \): 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 \((Z_1 = Z_2 \gg 1)\) selfconsistently by the method
of Ref.\cite{19} taking into account the angle mismatch of electrons and holes and the selfconsistent reduction of the pair potential at the interface. The angle averaging was performed by choosing a $\delta$-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 $\Delta/E_F$ ratio, giving some evidence of broadening of the ZBA. We also point out that in contrast with ZBS broadening due to surface roughness, the mechanism we propose has an intrinsic nature mainly controlled by the $\Delta/E_F$ 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 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 ferromagnetic insulator - superconductor junctions by Kashiwaya et al.\cite{19} 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 ($\Delta$) 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 HTS Josephson junctions, as experimentally observed. A damping of the resonances originating the zero bound states has been also found.

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

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