Theory of the electrical transport in tilted layered superconductive Josephson junctions

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We present a theory of the Josephson effect in a twofold-tilted Josephson junction made by d-wave anisotropic layered superconductors. We find the appearance of an intrinsic electrical resistance that arises from the misalignment of the superconductive planes (the CuO2 planes in YBCO) in the two electrodes. This intrinsic contribution to the tunnel barrier has several non-trivial consequences. The result is relevant for understanding the electric transport properties of [100] tilt and [100] tilt-tilt Josephson junctions based on d-wave superconductors.

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Grain boundary Josephson junctions (GBJs) have been fabricated and studied immediately after the discovery of High Tc superconductors\(^1\). Nonetheless the mechanism of the supercurrent transport in these devices is still matter of scientific investigation and argument of general physical interest\(^2, 3\). It is well known that the dc Josephson effect can be described by means of a scattering theory using the Bogoliubov-de Gennes (BdG) equations\(^4\). Characteristic localized states of quasi-particles, known as Andreev bound states, are found in the superconductive energy gap region through which the Josephson supercurrent flows between the two electrodes\(^5\). This kind of theoretical approach has been successfully used in describing analytically the physics of in-plane grain boundary cuprate Josephson junctions\(^[001]\) where a two-dimensional scattering theory\(^6–8\) finely incorporates both the propagation of the quasi-particles along the Cu-O planes and the anisotropic d-wave-induced symmetry of the pair potential\(^9\). Moreover in ref\(^2\) a numerical approach, also based on the BdG equations, has enriched the understanding of the role of charge inhomogeneities in limiting supercurrents in \([001]\) GBJs.

However, a number of experiments have been carried out on \([100]\) YBCO GBJs\(^[10–12]\), where the Cu-O planes of one or both electrodes are tilted by an arbitrary angle \(\phi_1\) and \(\phi_2\) in Fig. 1, with respect to the substrate surface, implying that the relevant geometry of the junction is no longer in-plane. In particular, relatively high values of the \(L_R\) products\(^[12–14]\) have been observed in such YBCO GBJs. \([100]\) junctions seem to be very promising for developing new sensors of radiation in the terahertz band\(^[14–17]\) and observing macroscopic quantum properties\(^15\). Indeed Kawabata et al\(^18\) have pointed out that macroscopic quantum effects in YBCO devices may be better observed in junctions showing electrodes with pair potential lobes aligned each other (\(d_0/d_0\) junctions). This configuration can be obtained with out-of-plane \([100]\) GBJs geometries, whereas \([001]\) GBJs are not suitable for fabricating \(d_0/d_0\) junctions\(^9\).

In spite of all these circumstances, as of today, and differently from the \([001]\) tilt junction case, a specific theoretical treatment of the transport properties in \([100]\) junctions is lacking\(^15\). One can probably individuate emblematically the obstacle of developing a model theory for this case in the non-trivial modification suffered by the quasiclassical trajectories of the excitations. Indeed such trajectories are no longer confined to a single plane as in \([001]\) layered junctions\(^2, 8, 15\), but lay in planes tilted with respect to the substrate plane by the misorientation angles \(\phi_1, \phi_2\), see Fig. 1.

In this Letter we take an important step towards the effective evaluation of the peculiar transport properties of YBCO \([100]\) tilt junction (\(\alpha_L=\alpha_R=0\) in Fig. 1) and \([100]\) tilt-tilt junctions (junctions in which one or both angles \(\alpha_L, \alpha_R\) are different from zero).

We focus on the dc Josephson effect and find that the influence of the different tilting of the conduction planes with respect to the barrier plane (on passing from one electrode to the others) brings about an enhanced normal state electric resistance of the junction. The key result is an analytical expression for the Andreev spectrum for the quasiparticles, which retains the influence of the tilting of the Cu-O planes as well as the effects of the d-wave anisotropic symmetry of the pair potential.

In order to describe charge transport in a mesoscopic \([100]\) YBCO grain boundary Josephson junction, we assume a superconductor-normal-insulator-normal-superconductor (SNINS) model\(^8, 21, 23\). The superconductive material considered is a d-wave anisotropic cuprate. The presence of normal regions of the order \(\sim \xi_0 = \hbar v_F/\pi \Delta_0\), the ballistic coherence length\(^24\), is introduced for modeling the mechanism of the Andreev reflection and a possible suppression of the order parameter near the junction.

Furthermore we suppose that the quasiparticles are
2d quasiclassical Bogoliubov de Gennes equations [27]. For the plane \(x’ - y\) and \(x > 0\) they write (analogous equations hold in the plane \(x'' - y\) for \(x < 0\))

\[
\begin{align*}
Eu(x', y) &= \hat{h}(x', y)u(x', y) + \Delta_R(\hat{k})\Theta(x' - b)v(x', y) \\
Ev(x', y) &= -\hat{h}(x', y)v(x', y) + \Delta_R(\hat{k})\Theta(x' - b)u(x', y)
\end{align*}
\]

where \(\hat{h}(x', y) = -\hbar^2(\partial^2/\partial x'^2 + \partial^2/\partial y^2)/2m + V(x) - E_F\). \(\Theta(z)\) is the Heaviside step function and \(E_F = \hbar^2k_F^2/2m\) is the Fermi energy. The insulating barrier is modeled by a delta function, \(V(x) = U_0\delta(x)\), \(U_0\) being the Hartree potential. The spatial dependence of the pair potential is assumed to have a step-functional form described by \(\vartriangle(k, r) = \Theta(-a - x)\vartriangle L(\hat{k}) + \Theta(x - b)\vartriangle R(\hat{k})\). The bound states solutions of Eqs (1) for \(|\Psi(x')\rangle\) and \(|\Psi(x'')\rangle = \Psi(x') \exp(ik_y y), |\Psi(x'', y)\rangle = \Psi(x'') \exp(ik_y y)\) in the \(SL, NL, NR\) and \(SR\) regions, including normal and Andreev reflections of holes and electrons, are respectively

\[
\begin{align*}
\Psi^{SL}(x'') &= a_B(E) \left( u_{0L}^- e^{-ikL^-x''} + v_{0L}^- e^{-ivL^-x''} \right) \\
&\quad + b_B(E) \left( u_{0L}^+ e^{-ivL^+x''} + v_{0L}^+ e^{-ikL^+x''} \right) \\
\Psi^{NL}(x'') &= \left\{ \begin{array}{ll} 
1 & \text{if } x'' < a \\
0 & \text{if } a < x'' < b \\
1 & \text{if } x'' > b
\end{array} \right.
\left( U_1 e^{ik_1 x''} + U_2 e^{-ik_1 x''} \right)
+ \left( V_1 e^{ik_2 x''} + V_2 e^{-ik_2 x''} \right)
\Psi^{NR}(x'') &= \left\{ \begin{array}{ll} 
1 & \text{if } x'' < a \\
0 & \text{if } a < x'' < b \\
1 & \text{if } x'' > b
\end{array} \right.
\left( U_3 e^{ik_1 x''} + U_4 e^{-ik_1 x''} \right)
+ \left( V_3 e^{ik_2 x''} + V_4 e^{-ik_2 x''} \right)
\Psi^{SR}(x'') &= c_B(E) \left( u_{0R}^+ e^{-ivR^+x''} + v_{0R}^+ e^{-ivR^+x''} \right) \\
&\quad + d_B(E) \left( u_{0R}^- e^{-ivR^-x''} + v_{0R}^- e^{-ivR^-x''} \right)
\end{align*}
\]

with

\[
\begin{align*}
u_{00}^{\beta, \pm} &= \left[ \frac{1}{2} \left( 1 + i \frac{\Omega_0^\beta}{E} \right) \right]^{1/2}, \quad v_{00}^{\beta, \pm} = \left[ \frac{1}{2} \left( 1 - i \frac{\Omega_0^\beta}{E} \right) \right]^{1/2} \\
k_{\pm}^{\beta, e} &= \left( k_F^2 - k_y^2 + i \frac{2m\Omega_{\pm}^\beta}{\hbar^2} \right)^{1/2}, \\
k_{\pm}^{\beta, h} &= \left( k_F^2 - k_y^2 - i \frac{2m\Omega_{\pm}^\beta}{\hbar^2} \right)^{1/2}, \quad \Omega_{\pm}^\beta = \left( |\Delta_{L}^\beta|^2 - E^2 \right)^{1/2} \\
k_1^\beta &= \left( k_F^2 - k_y^2 + 2mE/\hbar^2 \right)^{1/2}, \quad k_h^\beta = \left( k_F^2 - k_y^2 - 2mE/\hbar^2 \right)^{1/2}
\end{align*}
\]

\(\beta\) denoting right (R) or left (L), \(k_{\pm}^{\beta, e}, k_{\pm}^{\beta, h}\) are the wave numbers of the electron-like and hole-like quasiparticles.

FIG. 1: a) z axis view of a layered SNINS [100] tilt-tilt junction. The thickness of the normal region is \(a+b\), the d-wave superconducting regions occupy the space defined by \(x < -a\) and \(x > b\). The insulating barrier (I) is located at \(x = 0\). b) 3d view of the conducting planes with the indicated tilt angles \(\varphi_1\) and \(\varphi_2\). The d-symmetry pair potential is represented by \(\Delta L(\hat{k}) = \Delta_0 \cos(2\theta - 2\alpha_L); \Delta R(\hat{k}) = e^{i\varphi} \Delta_0 \cos(2\theta - 2\alpha_R)\), \(\varphi = \varphi_R - \varphi_L\) is the global phase difference between the two superconducting regions. The solid and dashed lines represent the electron-like and the hole-like elementary excitation trajectories extending over the two planes, respectively.
respectively, see Fig 1, that move in the superconducting regions, \( k_F^\pm, k_F^\mp \) the wave numbers of the electrons and holes in the normal regions respectively, and \( E \leq |\Delta|^0 \).

The conducting layers in the electrodes are treated as planes parallel to the \( x'' - y \) plane or to the \( x' - y \) plane. The propagation coordinates \( x'', x' \) in the left and right electrode are given by \( x' = x \cos \phi_1 + z \sin \phi_1, x'' = x \cos \phi_2 - z \sin \phi_2 \), respectively. For d-wave symmetry the effective barrier parameter is modeled as \( \Delta_L^0 = \Delta_0 |\cos(2(\theta_\perp + \alpha_L))| e^{i\phi_m^L}, \Delta_R^0 = \Delta_0 |\cos(2(\theta_\perp + \alpha_R))| e^{i(\phi_m^R + \alpha_L) \mp} \) [\( \phi_m \)], where \( \phi_m^L, \phi_m^R \) are the phases as felt in a normal reflection by the electrons (+) and holes (-), \( \phi \) is the global phase difference between the two superconducting regions and \( \alpha_L, \alpha_R \) are the angles between the crystallographic a-axis of the left and right superconductors and the normal to the y axis. \( \theta \) is the incident angle of the quasiparticle trajectory into the normal plane or to the y axis.

\[ Z_{\text{eff}}(\theta, \phi_1, \phi_2) = \sqrt{4Z(\theta)^2 + (\cos \phi_1 - \cos \phi_2)^2} \]  

with \( Z(\theta) = Z_0/\cos \theta \) and \( Z_0 = k_F U_0/2 E_F \) the usual barrier parameter. With the definition \ref{eq:Zeff}, we may write the spectral equation in the same form which holds for the [001] case described in [\ref{20}] and [\ref{23}]. However Eq. \ref{eq:Gn} shows a new contribution to the barrier, coming from the specific geometrical configuration depending on the angles \( \phi_1 \) and \( \phi_2 \). Equation \ref{eq:Gn} provides the quasiparticle energy levels as a function of the superconducting phase difference \( \phi \) for the case of layered SNINS d-wave [100] tilt-tilt junctions and other limits (SIS, SNS, INS). When the junction is in the clean limit, \( (Z_0 = 0) \) the transparency of [100] junctions does not reach the unitary value but it is still limited to

\[ T_{\text{eff}}^0 = \frac{4 \cos \phi_1 \cos \phi_2}{(\cos \phi_1 + \cos \phi_2)^2} \]  

\[ \frac{d\Psi}{dx''}, \]  

across the clean interfaces \( x = -a, x = b \), respectively. Moreover, at the normal-insulator-normal interface (plane \( x = 0 \)) where the change in the propagation direction from \( x'' \) to \( x' \) occurs, boundary conditions are the continuity of \( \Psi \) and the discontinuity of \( d\Psi/dx \) imposed by the presence of the \( \delta \)-function barrier insulator. Then, since \( d/dx = \cos \phi_1 d/dx' \) and \( d/dx = \cos \phi_2 d/dx'' \), we write the matching conditions at \( x = 0 \) as

\[ \Psi_N(0) = \Psi_{N_A}(0) \]  

\[ \cos \phi_2 \frac{d\Psi_{N_A}(0)}{dx''} - \cos \phi_1 \frac{d\Psi_N(0)}{dx'} = \frac{2mU_0}{\hbar^2} \Psi_N(0) \]  

Using Eq. \ref{eq:Zeff} and imposing the above conditions, under the assumption of perfect retro-reflectivity \( (E_F \gg |\Delta|^0) \) of the Andreev reflections [\ref{24}], we derive an homogeneous linear system of equations for the twelve unknown coefficients. The condition of existence of solutions, in addition to the trivial one, provides the following spectral equation:

\[ (\Gamma_L^R e^{-i(\gamma_+ + \phi)} e^{-iDr}) (\Gamma_L^R e^{-i(\gamma_+ + \phi)} e^{-iDr}) + Z_{\text{eff}}^2 (\Gamma_L^R e^{-i(\gamma_+ + \phi)} e^{-iDr}) (\Gamma_L^R e^{-i(\gamma_+ + \phi)} e^{-iDr}) = 0 \]  

where \( \gamma_+ = \pi/2 \) is the \( \theta \)-independent. Eq. \ref{eq:Zeff} embodies the pure effect on the junction transparency of the misalignment of the conducting planes between the two electrodes. The zero-temperature normal-state conductance \( G_n \) is evidently also affected by the angles \( \phi_1 \) and \( \phi_2 \) and can be written, in terms of the average transparency \( T_{\text{eff}} \), as

\[ G_n = \frac{2e^2 k_F L_u}{\hbar} (T_{\text{eff}}) \]  

\[ \langle T_{\text{eff}} \rangle = T_{\text{eff}}^0 \left[ 1 - \frac{C^2 \coth^{-1} (\sqrt{1 + C^2})}{\sqrt{1 + C^2}} \right] \]  

where \( C = 2Z_0/|\cos \phi_1 + \cos \phi_2|, \) and \( 2(T_{\text{eff}}) = \int_{-\pi/2}^{\pi/2} d\theta \cos(\theta) T_{\text{eff}}(\theta, \phi_1, \phi_2) \). Therefore, the effect of the tilting of the planes in SNINS junction manifests as an excess of electrical resistance in the normal state. This effect persists also in the limit of zero size normal regions \( (a = b = 0) \).

One of the consequences is that the Andreev level spectra are strongly modified. Indeed, in Fig 2 the Andreev spectra for two different GBJ configurations are reported. In particular we have considered, most representatively, the case of [100] tilt-tilt mirror \( (\alpha_L = -\alpha_R) = GBJ, \) with \( \phi_1 = 0, \phi_2 = \pi/4, \) and \( \alpha = \pi/8 \) (dashed line) and the analogous mirror [001] junction (solid line) both in the clean limit \( (Z_0 = 0) \). As it well known, in mirror junctions, for a given symmetric rotation \( \alpha (0 < \alpha < 45^\circ) \) around the c-axes, depending on the quasiparticle inci-
The sign of the critical current $I_0$, which is the zero temperature maximum Josephson current, is sensitive to the modifications derived so far. In the short junction limit, for which $a + b < < \xi_0$, the discrete Andreev levels determine all the Josephson current through the expression [8, 30]

$$I_0(\phi_1, \phi_2) = \frac{2e}{h} k_f L_y \sum_n \int_{-\pi/2}^{\pi/2} d\theta \cos(\theta) \frac{dE_n(\theta, \phi_1, \phi_2)}{d\phi} f(E_n(\theta))$$

(10)

where the index $n$ labels the bound Andreev energy levels and $f(E_n, \theta)$ is the Fermi function. As a matter of fact it turns out that the Josephson current shows a dependence on the angles $\phi_1$ and $\phi_2$ in [100] geometries. Fig. 3 shows a comparison of the dependence on the temperature of the maximum Josephson current between asymmetric [100] and [001] mirror junctions. The current is normalized with respect to $I_0 = 2e k_f L_y/\hbar$, which is the zero temperature maximum Josephson current through an s-wave SNS junction in the clean limit [30]. The superconducting gaps in the two electrodes are assumed to obey a Bardeen-Cooper-Schrieffer (BCS) temperature dependence. It is well known that in this kind of junction the interplay between midgap and edgegap states may lead to a temperature sign inversion of the maximum Josephson current (Fig. 3b), i.e. to a temperature dependent $0 - \pi$ crossover [22, 23] (arrow in Fig. 3). For the chosen value of the barrier strength parameter $Z_0 = 0.7$, the modifications for increasing values of the tilt angle $\phi_2$ are evident, showing a shift towards higher temperatures of the $0 - \pi$ crossover as $\phi_2$ increases from 0° to 45°, see curves b) in Fig. 3.

In this Letter we have presented a theoretical model for the description of electrical transport in YBCO [100] tilt valley type GBJs based on the quasiclassical BdG equations. We have compared our results with the well studied [001] tilt case. We have derived the spectral rela-
tion in the case of [100] tilt-tilt junctions. The Andreev bound states calculated through this equation show modifications analogous to those caused by the presence of an insulating layer. However the nature of this modifications is different: it depends on the geometrical mismatch between conducting planes. We have evaluated the temperature dependence of the maximum Josephson current in the case of [100] mirror junctions and found a dependence of the 0-to-π crossover temperature on the inter-electrode misorientation angles.

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