Tunneling spectra for \((d_{x^2-y^2} + is)\)-wave superconductors versus tunneling spectra for \((d_{x^2-y^2} + id_{xy})\)-wave superconductors

N. Stefanakis

Department of Physics, University of Crete, P.O. Box 2208, GR-71003, Heraklion, Crete, Greece

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Abstract

The tunneling conductance spectra of a normal metal / insulator / singlet superconductor is calculated from the reflection amplitudes using the Blonder-Tinkham-Klapwijk (BTK) formulation. The pairing symmetry of the superconductor is assumed to be \(d_{x^2-y^2} + is\), or \(d_{x^2-y^2} + id_{xy}\). It is found that in the \((d_{x^2-y^2} + is)\)-wave case there is a well defined conductance peak in the conductance spectra, in the amplitude of the secondary \(s\)-wave component. In the \((d_{x^2-y^2} + id_{xy})\)-wave case the tunneling conductance has residual values within the gap, due to the formation of bound states. The bound state energies depend on the angle of the incident quasiparticles, and also on the boundary orientation. On the basis of this observation an electron focusing experiment is proposed to probe the \((d_{x^2-y^2} + id_{xy})\)-wave state.
I. INTRODUCTION

Two decades ago, Blonder, et. al. [1] used the Bogoliubov-de Gennes (BdG) equations to calculate the tunneling conductance of normal metal / s-wave superconductor contacts, with a barrier of arbitrary strength between them, in terms of the probability amplitudes of Andreev [2] and normal reflection. In the Andreev reflection process an electron incident, in the barrier can be reflected as an electron (normal reflection), reflected as a hole without changing its momentum (Andreev reflection), it can also be transmitted into the superconductor as an electron-like, hole-like quasiparticle.

Recently the BTK theory was extended by several groups to consider the anisotropy of the pair potential. In $d$-wave superconductors the pair potential changes sign under a $90^\circ$-rotation. So under appropriate orientation of the $a$-axis of $d$-wave superconductor the transmitted quasiparticle feel different sign of the pair potential. This results in the formation of bound states within the energy gap, which are detected as peaks in the conductance spectra. In $d$-wave superconductor the peak exists at $E = 0$ for a great range of angles of incidence of the incoming electron. This range depends on the surface orientation. [3] In particular for (110) surfaces the peak exists at $E = 0$ for all angles of incidence, and disappears for the (010) or (100) surface.

In the presence of another barrier inside the normal metal additional subgap bound states exist due to multiple Andreev reflections [4,5]. The same phenomenon occurs in $d$-wave superconductor / insulator / $d$-wave superconductor. In these systems the quasiparticle current has been examined by several groups [6–8], using BTK formalism with recursive relations for the determination of the probability amplitudes.

There is a competition between different pairing symmetries in the bulk. The coexistence of a subdominant order parameter in bulk depends on the strength of the secondary order parameter attractive interaction relative to the attractive interaction in the dominant pairing channel. When the secondary order parameter is strong enough a second phase transition occurs at a temperature $T_{c1} < T_c$ which depends on the strength of the secondary order
parameter. Numerical results show that when such coexistence is realized the relative phase of the order parameters is $\pi/2$ leading to $d_{x^2-y^2} + is$ or $d_{x^2-y^2} + id_{xy}$ pairing state in the bulk. The temperature dependence of the various thermodynamic quantities and transport properties change from power lows to exponential below $T_{c1}$. \[9,10\] When the secondary order parameter is not strong enough, only the $d_{x^2-y^2}$-wave order parameter appears in the bulk. For (110) surfaces the $d_{x^2-y^2}$-wave order parameter changes sign under reflection at the surface and vanishes at the surface. On the other hand the $s$ or $d_{xy}$ does not change sign and are not effeected by the presence of the surface, so there is the possibility of their presence near the surface even when their attractive interaction is not strong enough for them to exist in the bulk \[11,12\].

The presence of the secondary order parameter near a surface is manifested in tunneling spectra as a splitting of the zero energy conductance peak (ZEP) at low temperatures at zero external field and further non-linear splitting with increasing external field. \[13\] The field dependence of the splitting of the ZEP in the tunneling spectra of YBCO has been examined \[14,15\]. The observation is consistent with a $d_{x^2-y^2} + is$ surface order parameter or a $d_{x^2-y^2} + id_{xy}$ order parameter.

In this paper we extend the BTK formula to calculate the tunneling conductance in a normal metal / insulator / $(d_{x^2-y^2} + is)$-wave, or $(d_{x^2-y^2} + id_{xy})$-wave superconductor. In particular we find that in the $d_{x^2-y^2} + is$-state the conductance peak remains rigid at the energy of the subdominant ($s$) order parameter. \[16,17\] Besides in the $d_{x^2-y^2} + id_{xy}$ state, there is a plateau region inside the gap due to the formation of bound states at discreet values of the quasiparticle trajectory angle $\theta$, for all junction orientations. Also the evolution of the tunneling conductance with temperature depends on the nature of the subdominant order parameter. These features can be used to distinguish between states with broken time-reversal symmetry.
II. THE MODEL FOR THE NS INTERFACE

We consider the normal metal / insulator / superconductor junction shown in Fig. I. We choose the $y$ direction to be parallel to the interface, and the $x$ direction to be normal to the interface. The insulator is modeled by a delta function, located at $x = 0$, of the form $V\delta(x)$. The temperature is fixed to 0K.

The motion of quasiparticles in inhomogeneous superconductors is described by the BdG equations

$$\mathcal{H}_e(r)u(r) + \int dr'\Delta(s, x)v(r') = Eu(r),$$
$$\int dr'\Delta^*(s, x)u(r') - \mathcal{H}_e^*(r)v(r) = Ev(r),$$

where the single-particle Hamiltonian is given by $\mathcal{H}_e(r) = -\hbar^2 \nabla_r^2 / 2m_e + V(r) - E_F$, $E$ is the energy measured from the Fermi energy $E_F$. $\Delta(s, x)$ is the pair potential, after a transformation from the position coordinates $r, r'$ to the center of mass coordinate $x = (r + r')/2$ and the relative vector $s = r - r'$. After Fourier transformation the pair potential depends on the related wave vector $k$ and $x$. In the weak coupling limit $k$ is fixed on the Fermi surface ($|k| = k_F$), and only its direction $\theta$ is a variable. Also we neglect any spatial variation near the interface, e.g. the pair potential does not depend on $x$. The pair potential has the form:

$$\Delta(x, \theta) = \begin{cases} 
0, & x < 0 \\
\Delta(\theta), & x > 0
\end{cases},$$

where $\theta$ is the angle of the quasiparticle trajectory measured from $x$-axis. When a beam of electrons is incident from the normal metal to the insulator, with an angle $\theta$, the general solution of Eqs. (1), is the two component wave function, which for $x < 0$ is written

$$\Psi_I = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{iqx \cos \theta} + a \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{iqx \cos \theta} + b \begin{pmatrix} -1 \\ 0 \end{pmatrix} e^{-iqx \cos \theta},$$

while for $x > 0$, the solution is
\[ \Psi_{II} = c \begin{pmatrix} u_+ \phi_+ \\ v_+ \end{pmatrix} e^{ik_c x \cos \theta} + d \begin{pmatrix} v_- \phi_- \\ u_- \end{pmatrix} e^{-ik_h x \cos \theta}, \quad (4) \]

where \( a, b \) are the amplitudes for Andreev and normal reflection, and \( c, d \) are the amplitudes for transmission into the superconductor as electron-like and hole-like quasiparticles respectively. In the following we assume that \( q_e \approx q_h \approx k_e \approx k_h \approx k_F \). The latter approximation is valid within the BCS weak coupling theory. The BCS coherence factors are given by

\[ u^2_\pm = \left[ 1 + \sqrt{E^2 - |\Delta_\pm(\theta)|^2}/E \right]/2, \quad (5) \]

and

\[ v^2_\pm = \left[ 1 - \sqrt{E^2 - |\Delta_\pm(\theta)|^2}/E \right]/2, \quad (6) \]

The internal phase coming from the energy gap is given by \( \phi_\pm = |\Delta_\pm(\theta)|/|\Delta_\pm(\theta)| \), where \( \Delta_+ (\theta) = \Delta (\theta) \) (\( \Delta_- (\theta) = \Delta (\pi - \theta) \)), is the pair potential experienced by the transmitted electron-like (hole-like) quasiparticle respectively. Using the matching conditions of the wave function at \( x = 0 \), \( \Psi_I (0) = \Psi_{II} (0) \) and \( \Psi_{II}' (0) - \Psi_I' (0) = (2mV/\hbar^2) \Psi_I (0) \), the magnitude of the Andreev and normal reflection \( R_a = |a|^2 \) and \( R_b = |b|^2 \), are obtained as

\[ R_a = \frac{\sigma_N^2 |n_+|^2}{|1 + (\sigma_N - 1)n_+ n_- \phi_+ \phi_-^*|^2}, \quad (7) \]

\[ R_b = \frac{(1 - \sigma_N)|1 - n_+ n_- \phi_+ \phi_-^*|^2}{|1 + (\sigma_N - 1)n_+ n_- \phi_+ \phi_-^*|^2}, \quad (8) \]

where \( n_\pm = v_\pm/u_\pm \). The tunneling conductance, normalized by that in the normal state is given by

\[ \sigma(E) = \frac{\int_{-\pi/2}^{\pi/2} d\theta \sigma_s(E, \theta)}{\int_{-\pi/2}^{\pi/2} d\theta \sigma_N}, \quad (9) \]

according to the BTK formula the conductance of the junction, \( \sigma_s(E, \theta) \), is expressed in terms of the probability amplitudes \( a \), and \( b \): \( \sigma_s(E, \theta) = 1 + R_a - R_b \). The transparency of the junction \( \sigma_N \) is connected to the barrier height \( V \) by the relation
where \( Z = 2mV/\hbar^2k_F \), denotes the strength of the barrier. In the \( Z = 0 \) (large \( \sigma_N \)) limit the interface is regarded as a weak link, showing metallic behavior while for large \( Z (\sigma_N = 0) \) values the interface becomes insulating.

We consider the following cases:

a) In case of \( d_{x^2-y^2} \)-wave superconductor

\[
\Delta(\theta) = \Delta_1(T) \cos[2(\theta - \beta)],
\]

where \( \beta \) denotes the angle between the normal to the interface and the \( x \)-axis of the crystal. The temperature dependence of the gap follows the usual BCS relation \( \Delta_1(T) = \Delta_d\sqrt{1-T/T_d} \), where \( T_d \) is the transition temperature.

b) In the \( (d_{x^2-y^2} + i) \)-wave case

\[
\Delta(\theta) = \Delta_1(T) \cos[2(\theta - \beta)] + i\Delta_2(T),
\]

where \( \Delta_2(T) = \Delta_s\sqrt{1-T/T_s} \), and \( T_s \) is the transition temperature for the \( s \)-wave component.

c) In the \( (d_{x^2-y^2} + id_{xy}) \)-wave case

\[
\Delta(\theta) = \Delta_1(T) \cos[2(\theta - \beta)] + i\Delta_2(T) \sin[2(\theta - \beta)],
\]

where the angular form of the secondary component is obtained by the substitution of \( \beta \) in the \( d_{x^2-y^2} \)-wave order parameter by \( \beta + \pi/4 \). \( \Delta_2(T) = \Delta_{d_{xy}}\sqrt{1-T/T_{d_{xy}}} \), follows the BCS relation, and \( T_{d_{xy}} \) is the transition temperature for the \( d_{xy} \)-wave component.

III. TUNNELING CONDUCTANCE CHARACTERISTICS

In Figs. 2-4 we plot the tunneling conductance \( \sigma(E) \) as a function of \( E/\Delta_0 \) for various values of \( Z \), for different orientations (a) \( \beta = 0 \), (b) \( \pi/8 \), (c) \( \pi/4 \). The pairing symmetry of the superconductor is \( d_{x^2-y^2} \)-wave, with \( \Delta_d = 0.7\Delta_0 \), in Fig. 2, \( (d_{x^2-y^2} + i) \)-wave, with
\[ \Delta_d = 0.7\Delta_0, \Delta_s = 0.3\Delta_0, \text{ in Fig. 3}, \] 

\( (d_{x^2-y^2} + id_{xy})\)-wave, with \( \Delta_d = 0.7\Delta_0, \Delta_{dxy} = 0.3\Delta_0 \) in Fig. 4. It is clear from these figures that the peaks are narrowed by the increase of \( Z \). In this section the temperature is fixed to 0K.

For \( \beta = 0 \) e.g. when the lobes of the dominant \( d \)-wave component point towards the junction interface the position of the conductance peak, is near the energy gap \( \Delta_d \), in all the above pairing symmetries. This peak is mainly effected from the bulk density of states.

For \( \beta \neq 0 \) another peak exists in the conductance spectra, for the \( d_{x^2-y^2} \)-wave, \( (d_{x^2-y^2} + is)\)-wave cases, but its physical origin is different than that found near \( \Delta_d \). For the \( d \)-wave case this peak exists at \( E = 0 \) for all the non zero values of \( \beta \), due to the different sign of the pair potential that the transmitted quasiparticles feel. However, the height of the conductance peak (ZEH) depends on the orientation angle \( \beta \). For a given angle \( \beta \) the ZEH is proportional to the range of \( \theta \) angles for which sign change occurs. This is seen in Fig. 2 (c) for \( \beta = \pi/4 \) where the ZEH is maximum since for this orientation the transmitted quasiparticles feel different sign of the pair potential for all angles \(-\pi/2 < \theta < \pi/2 \). On the other hand for \( \beta = \pi/8 \) in Fig. 2 (b) the range of angles is reduced and the ZEH takes a lower value.

For the \( (d_{x^2-y^2} + is)\)-wave case in Fig. 3, the position of the conductance peak is shifted to the energy \( E = \Delta_s \), for all values of \( \beta \). For each value of \( \beta \), its height depends on the range of \( \theta \) angles where the transmitted quasiparticles feel different sign of the pair potential. For \( \beta = \pi/4 \) the conductance peak as seen in Fig. 3 (c) at \( E = \Delta_s \), has its maximum value since the transmitted quasiparticles feel the sign change of the pairing potential for all angles \( \theta \). This range is reduced for other orientations and for \( \beta = 0 \) it goes to zero, as we can see in Fig. 3 (a). Also a subgap opens within the conductance spectra due to the imaginary \( s \)-wave component. Within the subgap in the tunneling limit, the tunneling conductance is zero, \( \sigma(E) = 0 \) while in the metallic limit \( (Z = 0) \), \( \sigma(E) = 2 \) independently from the orientation, as in the \( s \)-wave case. In the \( Z = 0 \) case the normal reflection coefficient is zero while the Andreev reflection coefficient is unit. In this case the charge transport into the superconductor is twice as large as in the normal state, for energies within the subgap
region.

In the $d_{x^2-y^2} + id_{xy}$ case, seen in Fig. 4, the tunneling conductance has residual values within the gap for all orientations $\beta$. In particular for $\beta = 0$, as seen in Fig. 4 (a) in the tunneling limit, the conductance $\sigma(E = 0)$, at $E = 0$ has a non zero value contrary to the $(d_{x^2-y^2} + is)$-wave case where it is zero. In the $d_{x^2-y^2} + is$ case for $\beta = 0$, there is no angle $\theta$ for which the transmitted quasiparticles to experience the sign change of the pair potential, and the tunneling conductance goes to zero. This is different for the $d_{x^2-y^2} + id_{xy}$ where for $\beta = 0$ the transmitted quasiparticles feel the sign difference due to the secondary order parameter $d_{xy}$.

Also the zero energy conductance height evolves very differently with the orientation of the superconductor, for the three pairing symmetries. This is seen in Fig. 5 where the dependence of zero-energy conductance height on $\beta$ is plotted, for $Z = 2.5$, for the three pairing symmetries. It is seen that for the $(d_{x^2-y^2} + id_{xy})$-wave case (dashed line), for $\beta$ close to $\pi/4$, the height representing the plateau like feature seen in Fig. 4 is enhanced. Besides for angles close to zero, the height of the ZEP for the $(d_{x^2-y^2} + id_{xy})$-wave case is reduced, but is not zero. Note that the height for $\beta = 0$, remains finite even in the large $Z$-limit, while the height in the $(d_{x^2-y^2} + is)$-wave case goes to zero.

IV. BOUND STATE ENERGIES

These features are explained if we calculate the energy of the midgap state, which is given for large $Z$ by the value in which the denominator of Eq. (7,8) vanishes. The equation giving the energy peak level is written as

$$\phi_- \phi_+^* n_+ n_- |_{E=\Ep} = 1.0.$$  (14)

In the $d_{x^2-y^2}$-wave case, for a given angle $\beta$, this equation has solution $E = 0$, for a finite range of angles $\theta$. For $\beta = \pi/4$ the solution is $E = 0$ for $-\pi/2 < \theta < \pi/2$, since $n_+ n_- |_{E=0} = -1$, and also the transmitted quasiparticles feel different sign of the pair potential i.e. $\phi_- \phi_+^* |_{E=0} = -1$. In the $(d_{x^2-y^2} + is)$-wave case for $\beta = \pi/4$, the solution is $E = \Delta_s$
in the $\theta$ interval $[0 : \pi/2]$. In this case the $n_+, n_-$ and the internal phases are varied in a way that Eq. [3] is satisfied for $E = \Delta$, and a midgap state is formed. When a midgap state exists the tunneling conductance $\sigma_s(E, \theta)$ is equal to 2 for all $\theta$ and the peek in $\sigma(E)$ seen in Fig. 2 is due to the normal state conductance $\sigma_N$ in Eq. [10], which depends inversely on the $Z^2$ for large $Z$. For intermediate angles $\beta$, the peak height of the tunneling conductance $\sigma(E)$ is proportional to $8\beta$, for $0 < \beta < \pi/4$, [3] and for $\beta = 0$ the range of $\theta$ angles for which Eq. [4] has solutions collapses to zero in both symmetry states, and no bound states are formed. Then $\sigma(E)$ goes to zero as $1/Z^2$ and there is no conductance peak. For energies different than the bound state energy $E_p$, for large $Z$, $\sigma_s(E, \theta)$ is inversely proportional to $Z^2$ as the $\sigma_N$ is and the tunneling conductance has a constant value as we can see in Fig. 4, for $E > 0$. In the $(d_{x^2-y^2} + id_{xy})$-wave case for fixed $\beta$ the solutions of [4] depend both on $E$, and $\theta$, as seen in Fig. 3, where the bound state energy $E_p$ is plotted for $\beta = 0, \pi/16, \pi/8, \pi/4$, as a function of $\theta$. In this case the midgap state for a given $\beta$ is formed for a pair of angles $\theta$, for energies within the gap. This observation can be used to explain the residual values of the tunneling conductance within the gap, seen in Fig. 4 as follows. When a bound state is formed the conductance $\sigma_s(E, \theta)$ is equal to 2 exactly at the bound state energy for the two discreet values of $\theta$ and the peak in the $\sigma(E)$ should be proportional to the $Z^2$ for large $Z$ for these values of $\theta$. For the rest of the quasiparticle trajectory angles $\theta$ the tunneling conductance $\sigma(E)$, has a constant value. Thus the height for a given energy, and angle $\beta$ is determined from the interplay of two competitive factors, i.e., the bound state energy formed at a couple of $\theta$ angles which gives a contribution proportional to $Z^2$, and the rest of $\theta$ angles which give a constant value contribution independent of $Z$. Also the steps in $\theta$, in evaluating the integral in Eq. [4] are very much crucial since the calculation of the tunneling conductance has to be performed exactly at the bound state energy. If this is not the case then the peak due to the bound states in the tunneling conductance would have a smaller value which would depends on $Z$ in general. We conclude that in the $d_{x^2-y^2} + id_{xy}$ the discreet values of the quasiparticle trajectory angle $\theta$, over which a bound state is formed, compared to the interval of $\theta$ angles in the other two pairing states explains
the reduced height of the tunneling conductance within the gap. However if we calculate the conductance $\sigma_s(E, \theta)$, for the $d_{x^2-y^2} + id_{xy}$ at a given $\beta$ for a value of $\theta$ for which bound state occurs then the conductance should develop a peak at the bound state energy, where $\sigma_s(E, \theta)$ is equal to 2. For the rest of the energies, $\sigma_s(E, \theta)$, goes to zero as $1/Z^2$. This is seen in Fig. 7 where the conductance $\sigma_s(E, \theta)$ for $Z = 2.5$ is plotted for fixed $\beta = \pi/4$ as a function of the energy $E$, for different values of the angle $\theta = \pi/4, 3\pi/8, \pi/2$ for which bound state occurs. We see that for $\theta = \pi/4$ the peak is at $E = 0$. However as we change the angle $\theta$ towards $\pi/2$ the peak level moves from $E = 0$ to $E = \Delta_{d_{xy}}$.

The occurrence of residual density of states in the $(d_{x^2-y^2} + id_{xy})$-wave case is unaffected by the calculation of $\sigma(E)$ including the self-consistency of the order parameter. In this calculation an enhancement appears at $E = \Delta_{d_{xy}}$, for $\beta = \pi/4$. In our calculation we also observed a similar enhancement at $E = \Delta_{d_{xy}}$ when the definition

$$\sigma(E) = \frac{\int_{-\pi/2}^{\pi/2} d\theta \sigma_s(E, \theta) \cos \theta}{\int_{-\pi/2}^{\pi/2} d\theta \sigma_N \cos \theta},$$

was used for the calculation of the tunneling conductance. The $\cos \theta$ factor was included in the integration formula to calculate the $x$-component of the tunneling spectra. Within this definition the bound state at $\theta = 0$ contributes more (due to the $\cos \theta$ factor) that the bound state at $\theta$ close to $\pi/4$. As seen in figure 6 the bound state at $\theta = 0$ corresponds to energy $E = \Delta_{d_{xy}}$ causing the peak in $\sigma(E)$ at $E = \Delta_{d_{xy}}$. Also in a self consistent calculation the bound state at $(\theta = \pi/4, E = 0)$ contribute less in $\sigma(E)$ that that at $(\theta = \pi/4, E = \Delta_{d_{xy}})$ due to the depletion near the interface. In any case the peak near $E = \Delta_{d_{xy}}$ in $(d_{x^2-y^2} + id_{xy})$-wave pairing state is much more suppressed that that at $E = \Delta_s$ in $(d_{x^2-y^2} + id)$-wave state.

The angular dependence of the bound state energy for fixed boundary orientation at the $xy$ plane can be used to identify the $(d_{x^2-y^2} + id_{xy})$-wave pairing state. The method we propose here is the two point spectroscopy described by Benistant et. al. [19]. They measured the reflected hole distribution along the boundary $y$-direction, when electrons are injected with certain distribution $P(\phi)$, through a point contact, at $y = 0$, into a normal metal of
thickness $d$ attached to an $s$-wave superconductor. The presence of a magnetic field parallel to the $z$-axis deflects the trajectories of the electrons and leads to an asymmetric distribution of angles of incidence in the normal metal / superconductor interface. Also the magnetic field focuses the reflected holes into a second point contact which acts as a hole collector. Moving the second point contact around the first one or using several point contacts along the direction parallel to the interface we are able to measure the intensity of the Andreev reflected holes as a function of the $y$ direction. In the $s$-wave case one observes a single peak called 'focusing peak' at $y = y_0$ from the injection point at $y = 0$, since the Andreev reflected probability amplitudes are independent of the injection angle. For the $(d_{x^2-y^2} + id_{xy})$-wave case the bound state energies, for which the reflection coefficient is equal to one, occurs at angles $\theta_1 < 0, \theta_2 > 0$, for a given boundary orientation and large barrier strength $Z$. These bound states will give rise to a second peak in the hole distribution, at a different position, besides the one due to the focusing. The presence of the magnetic field leads to an asymmetric distribution of angles of incidence in the interface and the trajectory which corresponds to bound state at $\theta_1$ has shorter path from that at $\theta_2$ and the corresponding injected electrons have smaller angle $\phi$. If the angular distribution probability $P(\phi)$ of the injected particles is peaked at small injection angles, this will lead to larger contribution to the secondary peak from the bound state at $\theta_1$ then that at $\theta_2$ This new peak would be observed for all energies for which bound states exist in a $(d_{x^2-y^2}+id_{xy})$-wave superconductor. In the case of a $d_{x^2-y^2}$-wave superconductor, and a $(d_{x^2-y^2} + is)$-wave superconductor the resonance exist only for $E = 0, E = \Delta_s$ correspondingly. Experiments of this kind require high quality normal conducting crystal and point contacts for the electron injection. Any voltage drop has to occur at the point contact for the electrons to move ballistically in the normal metal. Similar procedure has been proposed from Honerkamp and Sigrist [20] to discriminate between unitary and nonunitary triplet states for the superconductor Sr$_2$RuO$_4$. 
V. TEMPERATURE DEPENDENCE OF THE TUNNELING SPECTRA

At finite temperatures the tunneling conductance is calculated from the relation

$$\sigma(eV) = \int_{-\infty}^{\infty} dE \left[ -\frac{\partial f(E + eV)}{\partial E} \right] \frac{\int_{-\pi/2}^{\pi/2} d\theta \sigma_s(E, \theta)}{\int_{-\pi/2}^{\pi/2} d\theta \sigma_N},$$

(16)

$eV$ is the electron energy and $f(E)$ is the Fermi function $f(E) = 1/(e^{\beta E} + 1)$, $\beta = 1/k_B T$. In the case of a two component order parameter, we assume that below a surface transition temperature a subdominant order parameter can develop which breaks spontaneously the time reversal symmetry. Its amplitude is below the value for the formation of spontaneously broken time reversal symmetry state in the bulk. [12] The temperature dependence of the pair potential amplitude is assumed to obey the usual BCS relation. As a consequence under the coexistence of the secondary component the $T_c$'s for the dominant $d$-wave $T_d$ and the subdominant $s(d_{xy})$ components, $T_s(T_{d_{xy}})$ directly correspond to the amplitude of the attractive interaction in each case.

Fig. 8 shows the tunneling conductance $\sigma(eV)$ for different temperatures $T/T_d = 0.1, 0.2, 0.3, 0.4$, in the large barrier strength limit $Z = 10$, $\beta = \pi/4$. The pairing symmetry of the superconductor is $d_{x^2-y^2}$-wave in Fig. 8 (a), $(d_{x^2-y^2} + is)$-wave, with $T_s = 0.3T_d$, in Fig. 8 (b), $(d_{x^2-y^2} + id_{xy})$-wave, with $T_{d_{xy}} = 0.3T_d$ in Fig. 8 (c). It is seen that due to the thermal occupation of states contributing to the tunneling current, the peaks are getting broadened as the temperature increases. In the $d_{x^2-y^2}$-wave case, as seen in Fig. 8 (a) the ZEP is suppressed when the temperature increases and disappears almost at the critical temperature. This feature of the calculated spectra is consistent with the experimental results of YBa$_2$Cu$_3$O$_{7-\delta}$ observed by low-temperature scanning tunneling spectroscopy. [4] The evolution of the conductance spectra with temperature is qualitatively similar with the calculation including the self-consistency. [22] On the other hand in the $(d_{x^2-y^2} + is)$-wave, seen in Fig. 8 (b) the tiny subgap of the order of $\Delta_s = 0.3\Delta_0$ at $T = 0$ disappears with the increase of the temperature. For $T > T_s$ it follows the usual $d_{x^2-y^2}$-wave like dependence. In the $(d_{x^2-y^2} + id_{xy})$-wave, shown in Fig. 8 (c) the zero energy height is suppressed with
the increase of the temperature. For $T > T_{d_{xy}}$ the temperature dependence of the spectra for the $(d_{x^2-y^2} + id_{xy})$-wave state is similar to the $d_{x^2-y^2}$-wave.

In Fig 9 we plot the ZEH as a function of temperature for the three pairing states. For the $d_{x^2-y^2}$-wave case the ZEH behaves as $T^{-1}$. For the $(d_{x^2-y^2} + is)$-wave case the ZEH increases up to $T = 0.2T_d$ and then decreases with increasing the temperature. For $T > T_s$ it follows the $d_{x^2-y^2}$-wave behavior. The downturn of the ZEH at low temperatures in the $(d_{x^2-y^2} + is)$-wave case corroborates with the ZEP splitting and has also been observed experimentally (see Fig.1 in Ref. [13]). In the $(d_{x^2-y^2} + id_{xy})$-wave case the ZEH decreases with $T$ in different scales for $T < T_{d_{xy}}$ and $T > T_{d_{xy}}$ indicating the different pairing states. In all cases the transition from the $d_{x^2-y^2}$-wave to the $(d_{x^2-y^2} + is)$-wave or $(d_{x^2-y^2} + id_{xy})$-wave is continuous.

In the metallic limit ($Z = 0$) (not presented in the figure) the tunneling conductance at $eV = 0$ decreases, as the temperature increases, from its zero temperature value $\sigma(eV) = 2$, to the normal state value $\sigma(eV) = 1$ at the transition temperature. The variation with $T$ for the $d_{x^2-y^2} + is$ $(d_{x^2-y^2} + id_{xy})$-wave for $T < T_s(T_{d_{xy}})$ deviates from the $d_{x^2-y^2}$-wave behavior. In both cases where time reversal symmetry is broken, a change of slope exists in the $\sigma(eV = 0)$ vs $T$ diagram, at the subdominant order parameter transition temperature. However in this case the variation with $T$ is similar for $d_{x^2-y^2} + is$, $d_{x^2-y^2} + id_{xy}$ and thus it can not be used to discriminate between the two pairing states.

VI. CONCLUSIONS

We calculated the tunneling conductance in normal metal / insulator / anisotropic superconductor, using the BTK formalism. We showed that the conductance peak for (110) surface orientation, in a $d_{x^2-y^2}$-wave superconductor, appears in zero energy, and is shifted according to the amplitude of the secondary order parameter in the $(d_{x^2-y^2} + is)$-wave case. In the $(d_{x^2-y^2} + id_{xy})$-wave case the tunneling conductance has residual states within the energy gap. These are due to the formation of bound states at discreet values of the tra-
jectory angle $\theta$ for each boundary orientation angle $\beta$, for energies within the gap. These bound states explain both the residual states within the subgap and also the small height of the conductance within the subgap region. The calculation of the conductance $\sigma_s(E, \theta)$ for given boundary orientation at an incident angle $\theta$ for which bound state occurs shows an enhancement at the bound state energy. The energy dependence of the bound state on $\theta$ can be used within the method of electron focusing to detect the $(d_{x^2-y^2} + id_{xy})$-wave state. In such a case besides the focusing peak another peak exists in the reflected hole distribution spectrum for all energies of the injected electrons less than the amplitude of the secondary order parameter. This peak should also be observed for the $d_{x^2-y^2}$-wave and $(d_{x^2-y^2} + is)$-wave cases but only at the energy $E = 0, E = \Delta_s$ respectively.

The zero energy conductance peak decreases as $T^{-1}$ with increasing the temperature and disappears almost at the transition temperature for the $d_{x^2-y^2}$-wave case. The temperature dependence of the ZEH deviates from the usual $T^{-1}$ behavior of the $d_{x^2-y^2}$, in the case where a subdominant surface order parameter is developed, for $T < T_{c1}$, where $T_{c1}$ is the transition temperature for the subdominant order parameter. These features can be used to distinguish between time-reversal broken symmetry states.

Throughout this paper the spatial variation of the dominant order parameter near the surface which depends on the boundary orientation is ignored for simplicity. As a consequence, since the nucleation of the secondary order parameter near the surface depends on the strength of the dominant one, the spatial variation of the secondary order parameter is also ignored. We expect more drastic changes when the orientation is $\beta = \pi/4$ where the suppression of the dominant order parameter is more significant. However, since the features presented here are intrinsic and are generated by the existence of surface bound states, the essential results do not change qualitatively.

Also we assumed perfectly flat interfaces in the clean limit, so any impurity scattering and the effect of the surface roughness are ignored. Generally surface roughness will lead to a statistical distribution of the outgoing trajectories, and will alter the results presented. The effect of surface roughness on the tunneling effect in interfaces between normal metals and
superconductors with time reversal symmetry broken, has been studied.\[23\] It is found that in the $d_{x^2-y^2} + id_{xy}$ case additional bound states are formed due to the surface roughness. Also in $d_{x^2-y^2}$-wave superconductor, the ZEP may appear even for (100) interfaces with surface roughness \[12\].

Also in a more realistic treatment of the problem, one has to take into account also the thickness of the barrier. In that case additional resonances are expected in the tunneling spectra due to multiple Andreev reflections within the barrier, besides the ones due to the bound states.

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FIG. 1. The geometry of the normal metal / insulator / superconductor interface. The vertical line along the $y$-axis represents the insulator. The arrows illustrate the transmission and reflection processes at the interface. In this figure, $\beta$ is the angle between the normal to the interface and the $a$-axis of superconductor, and $\theta$ is the angle of the incident electron beam and the normal. On the top, the $d$-wave order parameter is shown.
FIG. 2. Normalized tunneling conductance $\sigma(E)$ as a function of $E/\Delta_0$ for $Z = 0$ (solid line), $Z = 2.5$ (dotted line), $Z = 10$ (dashed line), for different orientations (a) $\beta = 0$, (b) $\pi/8$, (c) $\pi/4$. The pairing symmetry of the superconductor is $d_{x^2-y^2}$, $\Delta_d = 0.7\Delta_0$. The temperature is $T = 0$. 
FIG. 3. The same as in Fig. 2. The pairing symmetry of the superconductor is $d_{x^2-y^2} + is$, $\Delta_d = 0.7\Delta_0$, $\Delta_s = 0.3\Delta_0$. 
FIG. 4. The same as in Fig. 2. The pairing symmetry of the superconductor is $d_{x^2-y^2} + id_{xy}$, $\Delta_d = 0.7\Delta_0$, $\Delta_{d_{xy}} = 0.3\Delta_0$. 
FIG. 5. Normalized tunneling conductance $\sigma$ for $E = 0$ as a function of $\beta$ for $Z = 2.5,$ and $T = 0$. The pairing symmetry of the superconductor is $d_{x^2-y^2}$ (solid line), $\Delta_d = 0.7\Delta_0,$ $d_{x^2-y^2} + is$ (dotted line), $\Delta_d = 0.7\Delta_0$, $\Delta_s = 0.3\Delta_0$, and $d_{x^2-y^2} + id_{xy}$ (dashed line), $\Delta_d = 0.7\Delta_0$, $\Delta_{dxy} = 0.3\Delta_0$.

FIG. 6. Bound state energy $E_p$, for $T = 0$, versus the quasiparticle angle $\theta$ for different orientations $\beta = 0, \pi/16, \pi/8, \pi/4$. The pairing symmetry of the superconductor is $d_{x^2-y^2} + id_{xy}$ with $\Delta_d = 0.7\Delta_0$, $\Delta_{dxy} = 0.3\Delta_0$. 

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FIG. 7. Conductance $\sigma_s(E, \theta)$ for $Z = 2.5$, and $T = 0$, as a function of $E$ for fixed angle $\beta = \pi/4$, at different angles $\theta = \pi/4, 3\pi/8, \pi/2$, for which a bound state is formed at a different value of $E$. The pairing symmetry of the superconductor is $d_{x^2-y^2} + id_{xy}$ with $\Delta_d = 0.7\Delta_0$, $\Delta_{dxy} = 0.3\Delta_0$. 
Normalised tunneling conductance $\sigma$ versus the applied voltage $eV$, for different temperatures $T/T_d = 0.1, 0.2, 0.3, 0.4$. The barrier strength is $Z = 10$, and the junction orientation is fixed to $\beta = \pi/4$. The pairing symmetry of the superconductor is $d_{x^2-y^2}$ in a), $d_{x^2-y^2} + is$ with $T_s = 0.3T_d$ in b), and $d_{x^2-y^2} + id_{xy}$ with $T_{dxy} = 0.3T_d$ in c).
FIG. 9. Normalized tunneling conductance $\sigma$ for $eV = 0$ as a function of the temperature $T/T_d$ for $Z = 10$, and $\beta = \pi/4$. The pairing symmetry of the superconductor is $d_{x^2-y^2}$ (solid line), $d_{x^2-y^2} + is$ with $T_s = 0.3T_d$ (dotted line), and $d_{x^2-y^2} + id_{xy}$ with $T_{d_{xy}} = 0.3T_d$ (dashed line).