

## Andreev Spectra and Subgap Bound States in Multiband Superconductors

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A theory of Andreev conductance is formulated for junctions involving normal metals (N) and multiband superconductors (S) and applied to the case of superconductors with nodeless extended  $s_{\pm}$ -wave order parameter symmetry, as possibly realized in the recently discovered ferropnictides. We find qualitative differences from tunneling into  $s$ -wave or  $d$ -wave superconductors that may help to identify such a state. First, interband interference leads to a suppression of Andreev reflection in the case of a highly transparent N/S interface and to a current deficit in the tunneling regime. Second, surface bound states may appear, both at zero and at nonzero energies.

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The recent discovery of high- $T_c$  superconductivity in ferropnictides has been a major event in solid state physics. The first theoretically proposed pairing symmetry for this compound,  $s$ -wave with a sign-reversing order parameter ( $s_{\pm}$ ), has been followed by a number of theoretical papers substantiating this proposal at various degrees of sophistication and exploring the ramifications of the proposed state [1]. Within this proposal, two sets of Fermi surfaces are distinguished: the hole Fermi surfaces around  $\Gamma$  and the electron Fermi surfaces around  $M$ . The  $\pi$  phase difference between the superconducting condensates is thought to be induced by spin fluctuations. Experimental evidence has been favorable to the  $s_{\pm}$  model so far, but is still ambiguous.

Andreev spectroscopy is a strong experimental probe of the superconducting order parameter. But in the case of the ferropnictides, both nodeless as well as nodal superconductivity have been inferred from the absence [2] or presence [3] of zero-bias conductance peaks. Also, point-contact spectroscopy has provided evidence for both a single gap as well as multiple gaps [2,3]. One of many questions to be asked in this connection is how possible interference between the two bands in the ferropnictides may affect the Andreev conductance spectra. Can the interference phenomenon be used to distinguish the  $s_{\pm}$  state from other scenarios? To address these questions, a generalized theory of Andreev conductance is needed, relevant also to other multiband systems.

Surface phenomena in  $s_{\pm}$  superconductors have attracted considerable recent attention [4–8]. Certain limiting cases were considered, but no general calculation of Andreev and tunneling current, properly accounting for the effect of interference between the two relevant bands, has been published so far. This we provide in this Letter. The formation of bound states at a free surface of an  $s_{\pm}$  superconductor, at an  $S_{\pm}/N/S$ , and at an  $N/S/S_{\pm}$  junction

was found in Refs. [4–6], respectively. However, the conditions for such a bound state and its effect on Andreev and tunneling conductance were not addressed in these papers. Reference [7] found an enhancement of the density of states at zero energy in a thin N layer on the top of an  $s_{\pm}$  superconductor, but it is unclear whether this numerical result is related to bound states or not, since *finite energy* rather than *zero energy* bound states were predicted in [4–6]. Finally, Ref. [8] considered the same problem as ours, the conductance spectra in an  $N/S_{\pm}$  junction, but did not find any new effects compared to regular Andreev reflection. This may be related to not properly accounting for any interference effect. At the moment, a general analytical unrestricted treatment of an interface in an arbitrary  $s_{\pm}$  superconductor seems necessary to clarify the existing confusion.

We have studied Andreev conductance in an  $N/S_{\pm}$  junction by including in the classical “BTK” model [9] the interference between the excitations in a two-band superconductor at arbitrary interface transparency. Applying our extended BTK model to the  $s_{\pm}$  scenario we find qualitatively new effects. For a fully transparent interface, the destructive interband interference leads to a strong suppression of Andreev reflection, in striking contrast to the conventional case. In the tunneling regime, two new effects are found: (a) a current deficit at high bias voltage, which is also due to destructive interband interference, and (b) Andreev bound states similar to those responsible for the zero-bias anomaly (ZBA), a well-known fingerprint of  $d$ -wave superconductors [10]. However, instead of a ZBA, a peak of similar origin may appear (depending on the parameters) at a finite energy, that can easily be mistaken for an extra gap.

A ballistic Andreev contact can be modeled by a one-dimensional conductor, whose right half ( $x > 0$ ) is a two-band metal (two different states at the Fermi level, one with

the wave vector  $p$  and the other with  $q$ ), and the left half is a simple metal. The wave function at the energy  $E_F$  in the left half is  $\Psi_L(x) = \psi_k(x) + b\psi_{-k}(x)$ , where the first term is the incident Bloch wave and the second term the reflected Bloch wave. The wave function on the right-hand side is  $\Psi_R(x) = c[\phi_p(x) + \alpha_0\phi_q(x)]$ . Here  $p$  and  $q$  are the Fermi vectors for the two bands,  $\phi$  is the Bloch function in the two-band metal, and the mixing coefficient  $\alpha_0$  defines the ratio of probability amplitudes for an electron crossing the interface from the left to tunnel into the first or second band on the right. Similar problems have been studied in the theory of the tunneling magnetoresistance, where the leads are usually multiband  $d$  metals.

The main conceptual pitfall here is that the standard approaches to tunneling assume the wave functions to be plane waves. However, there cannot be two different plane waves propagating in the same direction with the same energy. This may only occur when the wave functions are *Bloch* waves—which they are in reality. It has been realized in the past that there is not a single factor that defines the relative tunneling probability of the two Bloch waves. If the wave vector parallel to the interface is not conserved (it usually is not, except perhaps for epitaxially grown contacts), one factor is the number of tunneling channels in each band, proportional to  $\langle Nv_\perp \rangle$ , where  $N$  is the density of states and  $v_\perp$  is the Fermi-velocity component normal to the interface. Even more important is the character of these Bloch wave functions. For example, states of different parity on the right and on the left sides of the interface hardly overlap, so that even a weak interface barrier will strongly suppress tunneling from particular bands. With this in mind, we keep  $\alpha_0$  arbitrary and present the results for different cases. One implication is that the observable tunneling spectra may actually change drastically from contact to contact, as the interface properties change. Indeed, there are indications that this may be the case [11].

At a normal metal (N)–superconductor (S) contact, in the case of the two-gap model with unequal  $s$ -wave gaps, one can write

$$\begin{aligned}\Psi &= \Psi_N\theta(-x) + \Psi_S\theta(x), \\ \Psi_N &= \psi_k \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a\psi_k \begin{pmatrix} 0 \\ 1 \end{pmatrix} + b\psi_{-k} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\ \Psi_S &= c \left[ \phi_p \begin{pmatrix} u_1 \\ v_1 e^{-i\varphi_1} \end{pmatrix} + \alpha_0 \phi_q \begin{pmatrix} u_2 \\ v_2 e^{-i\varphi_2} \end{pmatrix} \right] \\ &+ d \left[ \phi_{-p} \begin{pmatrix} v_1 \\ u_1 e^{-i\varphi_1} \end{pmatrix} + \alpha_0 \phi_{-q} \begin{pmatrix} v_2 \\ u_2 e^{-i\varphi_2} \end{pmatrix} \right].\end{aligned}\quad (1)$$

Here  $\varphi_{1,2}$  are the phases of the gaps  $\Delta_{1,2}$  in both bands,  $u$  and  $v$  are the standard Bogoliubov coefficients  $u_{1,2}^2 = \frac{1}{2} + \sqrt{E^2 - \Delta_{1,2}^2}/2E$ ,  $v_{1,2}^2 = \frac{1}{2} - \sqrt{E^2 - \Delta_{1,2}^2}/2E$ . In the case of the  $s_\pm$  gap model with unequal  $s$ -wave gaps of opposite sign, we have  $\varphi_1 - \varphi_2 = \pi$ , while in the standard two-band model with the gaps of the same sign we have  $\varphi_1 = \varphi_2$ . The amplitudes  $a$ ,  $b$  describe Andreev and normal re-

flection, and the amplitudes  $c$ ,  $d$  describe transmission without branch crossing and with branch crossing, respectively.

The total wave function must satisfy the following boundary conditions at the interface ( $x = 0$ ):

$$\Psi(0) = \Psi_S(0) = \Psi_N(0), \quad (3)$$

$$\frac{\hbar^2}{2m} \frac{d}{dx} \Psi_S(0) - \frac{\hbar^2}{2m} \frac{d}{dx} \Psi_N(0) = H\Psi(0), \quad (4)$$

where  $H$  is the strength of the (specular) barrier.

The boundary conditions on the wave function derivatives are usually expressed in terms of Fermi velocities. However, a closer look reveals that this is actually incorrect for Bloch waves. Therefore, in the following, we introduce an “interface velocity.” For a given Bloch function, say,  $\psi_k(x) = \sum_G A_{G,k} \exp[i(k + G)x]$ , it is defined as

$$v_k = -\frac{i\hbar}{m} \frac{1}{\psi_k(x)} \frac{d\psi_k(x)}{dx} \Big|_{x=0}. \quad (5)$$

The so-defined  $v_k$  is real and has the same symmetry properties as the Fermi velocity (this can be shown by expanding the wave functions in terms of the plane waves), but it coincides with the actual group velocity only for free electrons. For general Bloch waves it is different, and even dependent on the position of the interface plane in the crystal. We leave the interesting and important issue of the relationship between the interface velocity and the group velocity [12] for a further study, and proceed with the problem at hand.

Now, introducing the barrier strength  $Z = H/\hbar v_N$ , where  $v_N$  is the velocity on the N side, defined according to Eq. (5), and using the boundary conditions Eqs. (3) and (4), we find the general solution for  $a$ ,  $b$ ,  $c$ , and  $d$ . It depends on  $Z$  and on the ratios of the interface velocities. To keep the expressions compact, we present them below for the case of equal interface velocities on the N side and in both bands on the S side.

For the  $s_\pm$  model where  $\varphi_1 - \varphi_2 = \pi$ , this gives

$$\begin{aligned}\gamma a &= u_1 v_1 - \alpha(u_1 v_2 + u_2 v_1) + \alpha^2 u_2 v_2, \\ \gamma b &= (Z^2 + iZ)[v_1^2 - u_1^2 + \alpha^2(u_2^2 - v_2^2)],\end{aligned}\quad (6)$$

$$\gamma c = (1 - iZ)(u_1 - \alpha u_2)\delta, \quad \gamma d = iZ(v_1 - \alpha v_2)\delta,$$

where  $\gamma = (1 + Z^2)(u_1^2 - \alpha^2 u_2^2) - Z^2(v_1^2 - \alpha^2 v_2^2)$ ,  $\delta = \psi_k(0)/\phi_p(0)$ , and  $\alpha = \alpha_0 \phi_q(0)/\phi_p(0)$ . Note that for plane waves  $\delta = 1$  and  $\alpha = 0$ .

For the  $s_{++}$  model with  $\varphi_1 = \varphi_2$ , we obtain

$$\begin{aligned}\gamma a &= u_1 v_1 + \alpha(u_1 v_2 + u_2 v_1) + \alpha^2 u_2 v_2, \\ \gamma b &= (Z^2 + iZ)[(v_1 + \alpha v_2)^2 - (u_1 + \alpha u_2)^2],\end{aligned}\quad (7)$$

$$\gamma c = (1 - iZ)(u_1 + \alpha u_2)\delta, \quad \gamma d = iZ(v_1 + \alpha v_2)\delta,$$

with  $\gamma = (1 + Z^2)(u_1 + \alpha u_2)^2 - Z^2(v_1 + \alpha v_2)^2$ .

In a single-band case ( $\alpha = 0$ ) and for plane waves the standard BTK results are recovered. Below we shall discuss new effects arising in the  $s_\pm$  model. First, we consider a transparent interface,  $Z = 0$ . In the  $s_\pm$  case,  $b = d = 0$ ,

$a = (v_1 - \alpha v_2)/(u_1 + \alpha u_2)$ ,  $c = 1/(u_1 + \alpha u_2)$ . At  $E = 0$  we get  $a = (\sqrt{\Delta_1} - \alpha\sqrt{\Delta_2})/(\sqrt{\Delta_1} + \alpha\sqrt{\Delta_2}) < 1$ ; i.e., Andreev reflection is suppressed. On the other hand, in the  $s_{++}$  case  $b = d = 0$ ,  $a = (v_1 + \alpha v_2)/(u_1 + \alpha u_2)$ ,  $c = 1/(u_1 + \alpha u_2)$  resulting in  $a = 1$  at zero energy, as expected in the standard BTK model. This effect is due to the destructive interference between the transmitted waves in the  $s_{\pm}$  superconductor, which was missing in the previous works [4–8].

If

$$\Psi = \begin{pmatrix} f \\ g \end{pmatrix},$$

then the probability current  $J_P$  is given by

$$J_P = \frac{\hbar}{m} [\text{Im}(f^* \nabla f) - \text{Im}(g^* \nabla g)], \quad (8)$$

properly taking electron and hole contributions into account. Using Eq. (2) for  $\Psi$  at the superconducting side of the interface,  $J_P = (C + D)J_k$ , where  $J_k = v_N |\psi_k(0)|^2$  is the probability current of a normal electron in the state  $\psi_k$ , and the transmission probabilities  $C$  and  $D$  depend on the velocities in the two bands. For equal band velocities they are given by

$$C = |c/\delta|^2 [w_1 + \alpha^2 w_2 + 2\alpha \text{Re}(u_1 u_2^* \pm v_1 v_2^*)], \quad (9)$$

$$D = |d/\delta|^2 [w_1 + \alpha^2 w_2 + 2\alpha \text{Re}(u_1 u_2^* \pm v_1 v_2^*)], \quad (10)$$

for the  $s_{\pm}$  and  $s_{++}$  models, respectively, where  $w_{1,2} = |u_{1,2}|^2 - |v_{1,2}|^2$ .

At the normal side of the interface the probability current is  $(1 - A - B)J_k$ , where  $A = |a|^2$  and  $B = |b|^2$  are Andreev and normal reflection probabilities. From Eqs. (6), (7), (9), and (10), it can be verified that  $A + B + C + D = 1$ . Thus we have proven that the probability current is conserved. The electric current  $I$  across the contact is given by the standard expression [9]

$$I = \frac{1}{eR_N} \int_{-\infty}^{\infty} [f_0(E - eV) - f_0(E)] [1 + A - B] dE, \quad (11)$$

where  $f_0$  is the Fermi function,  $R_N$  is the normal state interface resistance, and  $V$  the voltage bias across the interface. Below, we present calculations of the angle-resolved conductance  $dI/dV$  in the full transparency regime  $Z = 0$  and in the tunneling regime  $Z \gg 1$ .

The  $T = 0$  conductance at  $Z = 0$  is shown in Fig. 1. In the  $s_{++}$  case, there is a standard enhancement of conductance at low bias  $eV < \Delta_1$  due to Andreev reflection, followed by a decrease of conductance and a weaker feature at  $eV = \Delta_2$ . At the same time, as discussed above, a striking suppression of the zero-bias conductance occurs in the  $s_{\pm}$  case. The strongest suppression occurs at  $\alpha = \sqrt{\Delta_1/\Delta_2}$ .

Figure 2 shows the zero-temperature conductance for large  $Z$  in the  $s_{\pm}$  case. Sharp conductance peaks appear at certain values of  $\alpha$ . These peaks have a clear interpretation as Andreev bound states. Indeed, for large  $Z$ , a bound state

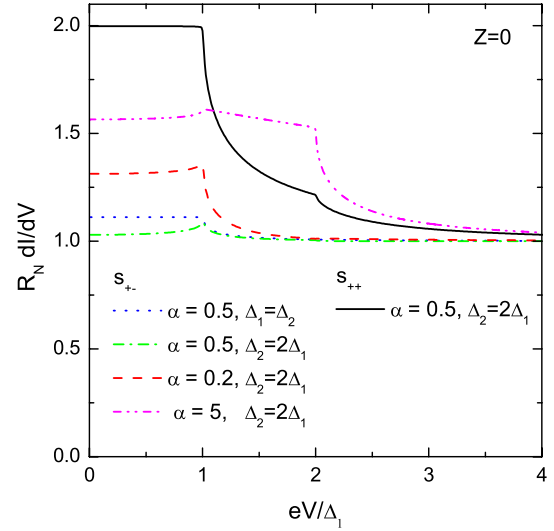


FIG. 1 (color online). Conductance in the case of fully transparent interface,  $Z = 0$ : comparison of the  $s_{\pm}$  and  $s_{++}$  models.

exists if  $\gamma = 0$ , that is, if  $u_1^2 - v_1^2 = \alpha^2(u_2^2 - v_2^2)$ . The energy of the bound state is

$$E_B = \sqrt{(\Delta_1^2 - \alpha^4 \Delta_2^2)/(1 - \alpha^4)}. \quad (12)$$

If  $\Delta_1 = \Delta_2$ , this gives the trivial  $E_B = \Delta$  solution, that is, no subgap bound states. If  $\alpha = 0$ , similarly,  $E_B = \Delta_1$ . However, when  $0 \leq \alpha^2 \leq \Delta_1/\Delta_2$  bound state solutions exist (see Fig. 3), most notably a zero-bound state  $E_B = 0$  if  $\alpha^2 = \Delta_1/\Delta_2$ . Note the bound states for  $\alpha = 0.5$  and  $0.7$  in Fig. 2.

Further, it is also seen from Fig. 2 (e.g., for  $\alpha = 0.9$ ) that there is a current deficit at high bias. This feature is due to a destructive interband interference and is in contrast with the properties of N/S junctions known so far, irrespective of whether S is an  $s$  or a  $d$  wave. The only known case is a

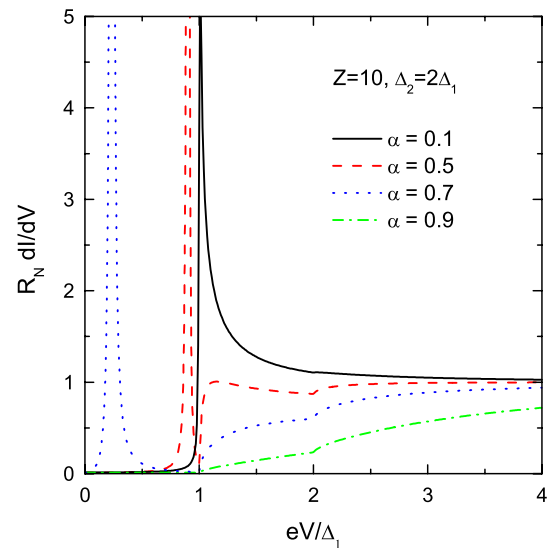


FIG. 2 (color online). Conductance in the low transparency regime,  $Z = 10$ , in the  $s_{\pm}$  model.

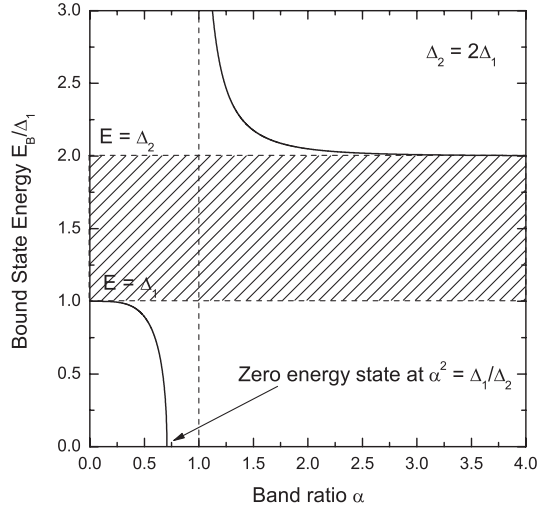


FIG. 3. Bound state energy at contacts to  $s_{\pm}$  superconductors as function of the band ratio parameter  $\alpha$  for  $\Delta_2 = 2\Delta_1$ . No bound states exist at energies between the two gaps (shaded region). Also, for band ratios  $\sqrt{\Delta_1/\Delta_2} < \alpha < 1$  no surface bound states exist.

double-barrier junction, where current deficit occurs due to nonequilibrium quasiparticle distribution [13].

For comparison, we also present the results for the  $s_{++}$  model in Fig. 4, where bound states are absent, as expected. Still, interference effects at  $\alpha \sim 1$  result in a complex  $dI/dV$  behavior, where the conductance is not a simple sum over two individual bands. Presently, the conductance spectra of contacts with the multiband superconductor  $\text{MgB}_2$  are usually fitted by the sum of two single-band tunneling probabilities [14]. With the increased level of sophistication in the realization of epitaxial magnesium

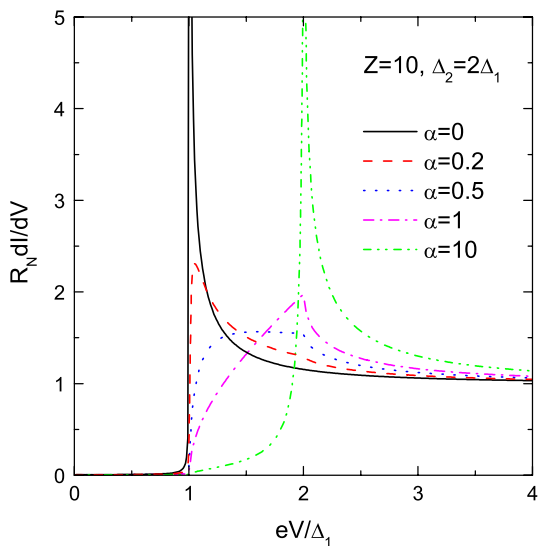


FIG. 4 (color online). Conductance in the low transparency regime,  $Z = 10$ , in the  $s_{++}$  model.

diboride junctions and single crystalline point contacts, one can expect that the present predictions for multiband interference effects can be observed there as well.

In order to demonstrate the main features of the model, we have concentrated on the discussion of the angle-resolved conductance. The total conductance depends on the orientation of the interface and on the type of scattering, specular or diffusive, which determines whether an electronic trajectory crosses both bands or only one. Thus, knowledge of the junction geometry and interface properties should make it possible to compare the model with experimental data. Qualitatively, one can see already that the observation of a zero-bias conductance peak can be consistent with nodeless superconductivity, and that a non-zero energy surface bound state, that can exist at subgap as well as supergap energies, can easily be mistaken for a gap feature when interpreting conductance spectra.

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