Theory of Andreev reflection in a two-orbital model of iron-pnictide superconductors

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Abstract. A recently developed theory for the problem of Andreev reflection between a normal metal (N) and a multiband superconductor (MBS) assumes that the incident wave from the normal metal is coherently transmitted through several bands inside the superconductor. Such splitting of the probability amplitude into several channels is the analogue of a quantum waveguide. Thus, the appropriate matching conditions for the wave function at the N/MBS interface are derived from an extension of quantum waveguide theory. Interference effects between the transmitted waves inside the superconductor manifest themselves in the conductance. We provide results for a FeAs superconductor, in the framework of a recently proposed effective two-band model and two recently proposed gap symmetries: in the sign-reversed s-wave ($\Delta \cos(k_x)\cos(k_y)$) scenario resonant transmission through surface Andreev bound states (ABS) at nonzero energy is found as well as destructive interference effects that produce zeros in the conductance; in the extended s-wave ($\Delta [\cos(k_x) + \cos(k_y)]$) scenario no ABS at finite energy are found.

1. Introduction

Electronic scattering at the interface between a normal metal and a superconductor has been used as a probe to investigate the electronic properties of FeAs superconductors (FAS) [1, 2]. FAS have a complex band structure, with a Fermi surface (FS) consisting of four sheets, two of them hole-like (labeled as $\alpha_1, \alpha_2$), and the other two electron-like (labeled as $\beta_1, \beta_2$) [3, 4, 5, 6]. S-wave, d-wave and p-wave pairing scenarios have been proposed to describe the superconducting state [7, 8, 9, 10], as well as extended s-wave [11].

Recently, two of the suggested pairing scenarios have been in dispute [5, 11]. In the "sign-reversed s-wave state" ($s^\pm$-state), the gap function has no nodes on any of the FS sheets but takes on opposite signs on the hole-like and the electron-like sheets of the FS. Throughout the unfolded BZ, the gap function can be approximated as $\Delta(k) = \Delta \cos(k_x)\cos(k_y)$. The other pairing symmetry is the extended s-wave, in which the gap function has four nodes on the electron FS sheets, no nodes on the hole sheets, and has the same sign on both hole FS’s. We shall approximate the gap function as $\Delta(k) = \Delta [\cos(k_x) + \cos(k_y)]$. On the experimental side, the results for lanthanum based superconductors (LaFeAsO family) seem to be mostly consistent with unconventional gap functions with nodes on the FS, while the experiments with superconductors containing rare-earth atoms ([Re]FeAsO family) as well as the Fe$_2$As$_2$ family tend to suggest a nodeless nearly isotropic gap across the FS. We note, however, that Andreev...
reflection studies have lead to different conclusions on the pairing symmetry for the same (rare-earth based) material [1, 2].

Existing theories of Andreev scattering [12, 13] apply to one band superconductors and, in the analysis of experimental data for multiband superconductors, the bands are usually treated as separate conduction channels with (classically) additive conductances. Such theories neglect the quantum mechanical nature of the scattering problem at the interface, where interference effects between the transmission channels (bands) inside the MBS are expected.

2. Matching conditions at the N/MBS interface

We recently addressed [14] the problem of interface scattering between a one-band metal a MBS. A two-orbital model that reproduces the FS’s of iron pnictides assumes two orbitals on each site, the $d_{xz}$ and the $d_{yz}$ orbitals (although a larger number of bands has also been argued necessary [15]). A one-dimensional model of the N/MBS interface is a tight-binding chain with a bifurcation because the electron on the normal metal atom that is closest to the interface can hop to either one of the two Fe orbitals (see Figure 1). This is the same quantum mechanical problem as in a quantum waveguide. In the two dimensional case, the tight-binding chain is repeated along the $y$ (interface) direction. The appropriate matching conditions for the wave function at the interface then follow as an extension of quantum waveguide theory to this problem [14]. While an incoming plane wave state in the normal metal, with energy $\varepsilon(k)$, takes the simple form $e^{ik \cdot r}$, a plane wave in the MBS has a two-component form:

$$\phi_k(x > 0) = \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} e^{ik \cdot r},$$

(1)

where $\alpha_k$ and $\beta_k$ denote projections on the $d_{xz}$ and $d_{yz}$ branches, respectively, and are obtained from the two orbital model Hamiltonian, $\hat{H}_S$, for the FAS that has been described in Ref [16]. In the superconducting state, we assume that an elementary excitation is a linear combination of plane waves with opposite momenta with Bogolubov-deGennes amplitudes $u$ and $v$. The transmitted part of the wave function, $\psi(x > 0)$, is a superposition of plane waves of the form (1). The first matching condition establishes that the wave function must be single-valued at the node $O$ where the three branches meet:

$$\psi(x = 0^-) = (1, 0) \cdot \psi(x = 0^+) = (0, 1) \cdot \psi(x = 0^+).$$

(2)

The probability current conservation at the circuit node is guaranteed by the second matching condition:

$$\left[ \frac{\partial \varepsilon}{\partial k_x} \psi \right]_{x=0^-} = (1, 1) \cdot \left[ \frac{\partial \hat{H}_S}{\partial k_x} \psi \right]_{x=0^+},$$

(3)
where the Hamiltonian is written in momentum space and the operator \( \hat{k} = -i\nabla \) in the continuum limit. The left multiplication by \((1, 1)\) gives the sum of the transmitted currents through branches \(d_{xz}\) and \(d_{yz}\), which is equal to the incoming current from the normal metal.

3. Results
3.1. \(s^{\pm}\)-wave gap symmetry

The gap function \(\Delta(k) = 0.02\cos(k_x)\cos(k_y)\) is used, which takes on different sign on the hole and electron FS sheets. The Fermi velocity and momentum in the normal metal are taken as \(p_F = \pi\) and \(v_F = 1.83\). A potential \(h v_F Z \delta(x)\) simulates interface disorder [12]. For each transverse momentum (or angle of incidence), the superconducting state conductance, \(g_s\), may be compared to the normal state conductance, \(g_n\). Figure 2 shows angle resolved relative conductances. Andreev bound states make \(g_s\) become disorder independent and therefore produce a peak in \(g_s/g_n\) for strong disorder, because \(g_n\) decreases. The energy of the ABS depends on the transverse momentum, unlike the usual case of single band d-wave superconductors, where it is zero. It has a non monotonic dependence on transverse momentum displayed in Figure 3.

Figure 2. Relative conductance, \(g_s/g_n\), for \(s^{\pm}\)-wave symmetry, for different disorder values, \(Z\), at normal incidence \((p_y = 0)\) and for a finite transverse momentum, \(p_y\). Destructive interference effects between the transmitted plane waves produce a zero in the conductance at normal incidence.

Figure 3. Energy of the surface Andreev bound state as function of the transverse momentum, for \(s^{\pm}\)-wave symmetry. The dispersion for the smaller momenta is remarkably different from that obtained using a constant gap function [14].
3.2. Extended s gap symmetry

We use the gap function $\Delta(k) = 0.01 [\cos(k_x) + \cos(k_y)]$ which produces nodes on the electron FS sheets. In contrast with the above, we find no ABS at finite energy for this symmetry. In principle, the usual zero energy ABS should exist for a different orientation of the interface relative to the gap function [13]. In Figure 4 we show the relative conductance.

![Figure 4](image1.png)

**Figure 4.** Relative conductance, $g_s/g_n$, for different disorder values, $Z$, at normal incidence ($p_y = 0$) and for a finite transverse momentum, $p_y$, for extended s-wave symmetry.

In an experiment, the integrated differential conductance over the transverse momenta of incoming particles, $\sigma_{S,N} = \int dp_y g_{s,n}$ is observed. Figure 5 compares the integrated relative differential conductance for each gap symmetry.

![Figure 5](image2.png)

**Figure 5.** The integrated relative differential conductance for each gap symmetry.

4. References

[1] Chen T Y, Tesanovic Z, Liu R H, Chen X H and Chien C L 2008 Nature 453, 1224
[2] Wang Y L, Shan L, Fang L, Cheng P, Ren C and Wen H H 2009 Supercond. Sci. Technol. 22, 015018
[3] Singh D J and Du M H 2008 Phys. Rev. Lett. 100, 237003
[4] Xu G, Ming W, Yao Y, Dai X, Zhang S C and Fang Z 2008 Europhysics Letters 82, 67002
[5] Mazin I I, Singh D J, Johannes M D and Du M H 2008 it Phys. Rev. Lett. 101, 057003
[6] Haule K, Shim J H and Kotliar G 2008 Phys. Rev. Lett. 100, 226402
[7] Chubukov A V, Efremov D V and Eremin I 2008 Phys. Rev B 78, 134512
[8] Qi X L, Raghu S, Liu C X, Scalapino D J, Zhang S C 2008 Preprint 0804.4332
[9] Lee P A and Wen X G 2008 Phys. Rev B 78, 144517
[10] Yao Z J, Li J X, Wang Z D 2009 New J. Phys. 11, 025009
[11] Graser S, Maier T A, Hirschfeld P J, Scalapino D J 2009 New J. Phys. 11, 025016
[12] Blonder G E, Tinkham M and Klapwijk T M 1982 Phys. Rev B 25, 4515
[13] Kashiwaya S, Tanaka Y, Koyanagi M and Kajimura K, 1996 Phys. Rev B 53, 2667
[14] Araujo M A N and Sacramento P D 2009 Preprint 0901.0398
[15] Cvetkovic V and Tesanovic Z, Europhys. Lett. 2009 85, 37002.
[16] Raghu S, Qi X L, Liu C X, Scalapino D J and Zhang S C 2008 Phys. Rev B 77, 220503(R)