\(\pi\)-States in all-pnictide Josephson Junctions

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We study the Josephson effect in \(s_s\)/I/\(s_s\) junctions made by two bands reversed sign \(s\)-wave \((s_s)\) superconductive materials. We derive an equation providing the bound Andreev energy states parameterized by the band ratio \(\alpha\), a parameter accounting for the weight of the second band with respect to the first one at the interface. For selected values of the band ratio and tunnel barrier amplitude, we predict various features of the Josephson current, among which a possible high temperature \(\pi\) state of the junction (a doubly degenerate junction ground state) and a \(\pi \to 0\) crossover with decreasing temperature.

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The importance of the Josephson effect as a tool to probe the properties of new discovered superconductive materials can hardly be underestimated. This has been true in the past in investigating the \(d\)-wave cuprate materials and is nowadays the case for the multi-gap iron based superconductors \(^1\) whose complex behavior, beyond the BCS theory, is presently a focus in condensed matter theory \(^2,3\) and material science \(^4\).

There is a rather solid indication now, supported by experiments, that the pair potential symmetry in these compounds is \(s\)-wave with sign-reversing order parameter \((s^\pm)\). Several theoretical models have already discussed the experimental consequences of an extended \(s\)-wave \((s_s^\pm\) wave) order parameter symmetry on the Andreev conductance of an \(NS\) interface and on the Josephson effect in the iron-based superconductor junctions \(^5-19\). In particular the Josephson effect has been studied in hybrid devices i.e. \(sIs_s\) junctions, as summarized by Seidel in his review \(^{20}\) and reference therein.

In this Letter we study an all-pnictide symmetric \(s_s\)/\(s_s\) Josephson junction and we discuss a number nontrivial physical consequences on the Josephson effect due to the presence of a second conduction band. We show that, depending on the band ratio parameter \(\alpha\), which accounts for the weight the second band, a \(\pi\)-state \(^{21}\) can develop for a wide range of junction transparencies and temperatures. This \(\pi\)-state can persist in the full range of temperatures or can undergo a \(\pi \to 0\) (inverse \(0 \to \pi\) crossover as the temperature decreases, depending on the band ratio parameter. This crossover is analogous to the \(0 \to \pi\) crossover \(^{22,23}\), found in mesoscopic \(d\)-wave superconductor Josephson junction \(^{24}\).

We adopt the simplest model of a Josephson junction that shows the essential features of the Josephson effect in the presence of two gaps, namely we consider a superconductor(S)-insulator(I)-superconductor(S) contact. The iron based junction is modeled by considering a one-dimensional conductor, whose left \((x < 0)\) and right \((x > 0)\) halves are both two band metals (two different states at the Fermi level, one with the wave vector \(p\) and the other with \(q\)). We assume that the motion of quasiparticles is described by the Bogoliubov de Gennes (BdG) equation \(^{25}\) and that the order parameter has already been obtained self-consistently from the gap equation. Therefore we choose a one dimensional model for the gap, such that the left and right two band superconductors have pair potentials given by

\[
\Delta_j(x) = \Delta_j e^{i\varphi_q} \theta(-x) + \Delta_j e^{i(\varphi_p + \varphi)} \theta(x), \quad j = 1, 2 \quad (1)
\]

The normal region, where \(\Delta_j = 0\), has an infinitesimal width and we also introduce a scattering potential \(U(x) = U_0 \delta(x)\). The possibility of nodes in the gap function is not considered. In the case of the two-gap model with unequal \(s\)-wave gaps, we write a wave function of the same type introduced in the Blonder Tinkham Klapwijk model \(^{26}\) as solution of the BdG equations and treat the presence of the second band through the introduction of Bloch wave functions \(^8\). The bound state (B) eigenfunction with energy \(|E| < \Delta_1\) (we assume \(\Delta_1 < \Delta_2\)) can be written as
where \( \varphi \) is a global phase difference between the two superconductive regions and \( \varphi_1, \varphi_2 \) are the phases of the gaps \( \Delta_1, \Delta_2 \) in both \( p \) and \( q \) bands respectively. In the case of \( s^\pm \) gap model, \( \varphi_2 - \varphi_1 = \pi \). In the considered energy range the wave function has to decay exponentially for \( |x| \to \infty \). The coefficients \( a_B, b_B, c_B, d_B \) are the probability amplitudes transmission with branch crossing or without branch crossing. Essential above is the introduction of \( \alpha_0 \), a mixing coefficient defining the ratio of probability amplitudes for a quasiparticle to be transmitted to the first, \( (p) \), or second, \( (q) \), band \( \Psi \); the functions \( \phi \)'s are the Bloch waves in the two-band superconductor; \( p \) and \( q \) are the Fermi vectors for the two bands corresponding to the same energy \( E \) \( \Psi \):

\[
\Psi^S_\xi (x) = \left( \begin{array}{c} u_B(x) \\ v_B(x) \end{array} \right) = a_B \left[ \begin{array}{c} u_1 \phi_{p_1} (x) + \alpha_0 \phi_{q_1} (x) \\ v_1 \phi_{p_1} (x) + \alpha_0 \phi_{q_1} (x) \end{array} \right] x < 0
\]

\[
\Psi^S_R (x) = \left( \begin{array}{c} u_B(x) \\ v_B(x) \end{array} \right) = c_B \left[ \begin{array}{c} u_2 \phi_{p_2} (x) + \alpha_0 \phi_{q_2} (x) \\ v_2 \phi_{p_2} (x) + \alpha_0 \phi_{q_2} (x) \end{array} \right] x > 0
\]

\[
(2)
\]

The global wave function \( \Psi \) must satisfy the following boundary conditions at the interfaces \( x = 0 \)

\[
\Psi^S_L (0^-) = \Psi^S_R (0^+)
\]

\[
\Psi^S_R (0^+) - \Psi^S_L (0^-) = \frac{2mU_0}{\hbar^2} \Psi^{S_R} (0^+)
\]

condition requirements. In fact, the assumed wave function \( \Psi \) is of the form \( \Psi = \Psi_1 + \alpha_0 \Psi_2 \) where, separately, \( \Psi_1 \) and \( \Psi_2 \) solve BdG equations for excitations of energy \( E \) for the gap \( \Delta_1 \) and \( \Delta_2 \), respectively. The boundary conditions, Eqs. (4), are requested to be a constrain for the whole function \( \Psi \).

The above matching procedure, with the requirement of non-triviality of the solution for the coefficients \( a_B, b_B, c_B, d_B \) provides for the \( s^\pm /1/s^\pm \) junction, the spectral equation

\[
\left( -1 + 2\sqrt{1 - E^2}\sqrt{r^2 - E^2\alpha^2 - r^2\alpha^4} \right) (2Z^2 + 1) + 2E^2 \left[ Z^2 (1 + \alpha^4) + (1 - \alpha^2 + \alpha^4) \right] + \left[ -1 + \alpha^2 \left( 2E^2 + 2\sqrt{1 - E^2}\sqrt{r^2 - E^2 - r^2\alpha^2} \right) \right] \times \cos(\varphi) = 0
\]

where we have introduced the gap ratio \( r = \Delta_2/\Delta_1 \), the band ratio parameter \( \alpha = \alpha_0 \phi_1 (0)/\phi_2 (0) \) and the barrier strength \( Z = U_0/\hbar v \). The energy is given in units of \( \Delta_1 (T) \), and the two gaps will be assumed to obey the same BCS-like temperature law. Boundary conditions on the wave function derivatives are usually discussed in terms of Fermi velocities in the case of plane waves. For Bloch waves we have to introduce "interface velocities"

\[
v_\lambda = - \frac{i \hbar \phi'_\lambda (0)}{m \phi_\lambda (0)}
\]

In deriving the spectral equation we have assumed, for the sake of simplicity, equal band interface velocities \( v_\lambda = v \).

An analysis of the spectral equation shows that for \( \alpha \neq 0 \) there are, in general, four energy levels, \( E_1 = \pm \epsilon_1 (\varphi, \alpha) \) and \( E_2 = \pm \epsilon_2 (\varphi, \alpha) \) (see Fig. 1). In a single-band case \( (\alpha = 0) \) Eq (4) provides the well known result for a conventional SIS junction [27, 28], namely \( E_1 = \pm \epsilon_1 (\varphi, 0) = \pm \Delta_1 (T) \left[ 1 - D \sin^2 (\varphi/2) \right]^{1/2} \), where \( D = \)
1/(1 + Z^2) is the transmission probability through the δ-function barrier, i.e. the junction transparency.

As \( \alpha \) increases, the energy levels \( E_2 = \pm \varepsilon_2(\varphi, \alpha) \) start to branch off the levels \( E_1 = \pm \varepsilon_1(\varphi, \alpha) \), while these latter gradually approach the zero energy state. As an example, Fig. 1 (a) and (b) show the modifications of the Andreev levels for increasing values of the band ratio, for two values of the barrier parameter, \( Z = 0.7 \) and \( Z = 2 \) and for the band gap ratio \( r = 2 \), respectively.

The condition for the existence of a zero energy level can easily be obtained from the spectral equation. It is given by \( (1 - r^2)^2(1 + 2Z^2 + \cos(\varphi)) = 0 \). Accordingly, a zero energy state \( E_1 = \pm \varepsilon(\varphi, \alpha_c) = 0 \), is obtained for the critical value of the band ratio \( \alpha_c = \sqrt{\frac{1}{r}} \), for any \( Z \) value. The energy level \( E_2 = \pm \varepsilon_2(\varphi, \alpha_c) \) corresponding to the critical value of the band ratio is given by \[ E_2 = \pm \varepsilon_2(\varphi, \alpha_c) = \pm \frac{2Dr^2(2 - D + D \cos \varphi) \sin^2(\varphi/2)}{1 + r(2 - 2D + r) + 2Dr \cos \varphi} \] (8)

and it is shown as a blue line in Fig. 1 for the indicated values of \( D \) and \( r \). For low transparencies (\( D \ll 1 \)), Eq. 8 reduces to \( E_2 = \pm \varepsilon_2(\varphi, \alpha_c) = \pm \Delta_1(T)2r/(1 + r)\sqrt{D} \sin(\varphi/2) \), a result closely resembling the midgap states of d-wave superconductor Josephson junctions. For \( \alpha > \alpha_c \), there are no surface bound states with real energy eigenvalues.

For \( 0 < \alpha < \alpha_c \), the two emerging levels \( E_2 = \pm \varepsilon_2(\varphi, \alpha) \) and the levels \( E_1 = \pm \varepsilon_1(\varphi, \alpha) \) have, in general, opposite dispersions, i.e. \( dE_2/d\varphi > 0 , dE_1/d\varphi < 0 \) as can be seen in Fig. 1 (a) and (b). The sign difference of the dispersions is the key point in determining the Josephson current-phase relation, as it will be discussed below.

The Josephson current \( I_d \) carried by the discrete Andreev levels \( E_k \) through the contact can be found from the free energy, according to the following relation \[ I_d(\varphi, \alpha) = \frac{2e}{\hbar} \sum_{k=1,2} \frac{\partial E_k}{\partial \varphi} f(E_k) = \frac{-2e}{\hbar} \sum_{k=1,2} \left( \frac{\varepsilon_k}{\partial \varphi} \tanh \frac{\varepsilon_k}{2kBT} \right) \] (10)

where \( f(E_k) \) is the Fermi distribution function and \( k \) labels the Andreev level with energy \( E_k = \pm \varepsilon_k(\varphi, \alpha) \).

In the nearly insulating limit (\( Z \rightarrow \infty \)), the system decouples and we obtain information on the two separate electrodes. More precisely, in this limit, the spectral equation (8) describes surface bound states of energy \[ E_B = \pm \sqrt{\frac{1 - r^2\alpha^4}{1 - \alpha^4}} \]

already discussed in ref. 8 for a junction \( N/I/s^\pm \).

For \( Z = 0.7 \), (black line, \( \alpha = 0.01 \), red line, \( \alpha = 0.5 \), green line, \( \alpha = 0.7 \)). (b) \( Z = 2 \). (black line, \( \alpha = 0.01 \), red line, \( \alpha = 0.4 \), green line, \( \alpha = 0.7 \)).

Fig. 2 (a) and (b) show the current-phase relations \( I_d(\varphi, \alpha) \), at low temperature, corresponding to the discrete spectrum of Andreev levels represented in Fig. 1 (a) and (b) respectively and calculated through Eq. 10. The current in this figure is normalized with respect to \( I_0 = e\Delta_1(0)/\hbar \), which is the zero temperature maximum Josephson current through a one dimensional s-wave junction in the clean limit. The three curves correspond to values of the band ratio approaching the critical value \( \alpha_c = 0.7071 \). The current-phase relation represented by the green lines (\( \alpha = 0.7 \)) in both Figs 2 (a) and (b) shows a clear \( \pi \) phase-shift (the maximum Josephson current for \( 0 < \varphi < \pi \) has a negative value). For the considered \( \alpha \) value this \( \pi \) state persists in the whole temperature range (see Fig. 3 (a) and (b)). The mechanism of formation of this state is the following. As the band ratio increases an upper \( +\varepsilon_2(\varphi, \alpha) \) and a lower \( -\varepsilon_2(\varphi, \alpha) \) extra Andreev bands gradually emerge. These two bands have different character compared to the low energy bands \( \pm \varepsilon_1(\varphi, \alpha) \); they transport supercurrents in the opposite directions. As the temperature
decreases, only low energy level are populated while those at higher energy are empty. In the competition between these opposite carrying current energy levels \(\pm \varepsilon_0(\varphi, \alpha)\) and \(\pm \varepsilon_1(\varphi, \alpha)\), which coexist for any value of the band ratio, it is the temperature that determines the direction of the total current and the possible existence of a \(\pi \to 0\) crossover in the considered two gap superconductor one-dimensional junction.

The situation is similar, although not identical, to that found in a two-dimensional d-wave \(\pi\) junction. In this case \([24]\), two kinds of bands, conventional and midgap, alternate, without coexisting and compete each other in determining the supercurrent, depending on the angle of incidence of the Andreev quasiclassical trajectories with the interface. Therefore it is the two-dimensionality here that plays the key role.

In Fig. 3, (a) and (b), we report, for increasing values of \(\alpha\), the dependencies of the normalized Josephson critical current \(I_c/I_0\) \((I_c = \max_x I_c(\varphi))\) from the reduced temperature \(T/T_c\), derived by the discrete Andreev spectra for a nearly clean junction \((Z = 0.001)\) and a low transparency junction \((Z = 3)\), respectively.

The negative sign of \(I_c\) (blue lines, Fig. 3 a) and b) indicates that the junction free energy, i.e. the quantity \(F(\varphi) = \Phi_0/2\pi \int_0^{\varphi} d\varphi I(\varphi)\), has a minimum at \(\varphi = \pi\) such that the ground state of the junction is \(\pi\) shifted. As discussed above, the \(\pi \to 0\) crossover occurring with decreasing temperature for \(\alpha = 0.065\) in figure 3(a) and for \(\alpha = 0.6\) (green line) in figure 3(b)(see inset) is due to the competition between the contribution to the current from the high energy band \(E_2\) and that low energy band \(E_1\).

So far, by using Eq. (10), we have included the contribution to the Josephson current from the discrete energy spectrum only. However the continuous-spectrum states make their own contribution to the current which has to be accounted for properly. Following the approach developed by Furusaki Tsukada \([32]\) the total Josephson current, including contributions from both the Andreev bound states and the continuous spectrum is given by

\[
I = \frac{e \Delta_0 k_B T}{\hbar} \sum_{\omega_n} \left| \frac{1}{\Omega_1} \left[ a(\varphi, i\omega_n, \alpha) - a(-\varphi, i\omega_n, \alpha) \right] \right| (11)
\]

Here we have defined \(\Omega_1 = \sqrt{\omega_n^2 + \Delta_1^2}\) and introduced the Matsubara frequencies \(\omega_n = \pi k_B T(2n + 1)\), with \(n\) ranging from \(-\infty\) to \(+\infty\). \(a(\varphi, i\omega_n, \alpha)\) is a scattering amplitude coefficient for the process in which an electron-like quasiparticle traveling from the left of the junction is reflected back as a hole-like quasiparticle in the presence of two bands. This coefficient is derived by solving the BdG equations under the assumption \(E > \Delta_1\) and dropping the requirement of exponentially decay of the solutions for \(|x| \to \infty\). The details of this procedure will be given elsewhere \([33]\). The results of the calculated total critical current \(I_c\) as a function of the reduced temperature, are shown in Fig. 4 (a) and (b), for different values of the band ratio \(\alpha\) and already considered in Fig. 3.

![FIG. 3: Critical current as a function of temperature for a s± superconductor S/I/S junction with \(r = 2\), \(T/T_c = 0.01\) (a) \(Z = 0.001\); black line, \(\alpha = 0.001\), red line \(\alpha = 0.5\), green line, \(\alpha = 0.65\), blue line, \(\alpha = 0.7\). (b) \(Z = 3\); black line, \(\alpha = 0.001\), red line, \(\alpha = 0.5\), green line, \(\alpha = 0.6\), blue line, \(\alpha = 0.7\). The negative sign of \(I_c\) indicates that the junction minimum is at \(\varphi = \pi\) (\(\pi\)-junction). The inset in panel (b) shows, on a larger scale, the transition \(\pi \to 0\) for \(\alpha = 0.6\)](image)

![FIG. 4: Critical current as a function of temperature. The contribution of the continuous energy spectrum states has been added. (a) \(Z = 0.001\); (b) \(Z = 3\); in both figures, (a) and (b), the black, red, green, brown, blue lines correspond to the curves with \(\alpha = 0.001, 0.5, 0.6, 0.65, 0.7\), respectively.](image)
Most notably they confirm the $\pi - 0$ junction crossover. However some noticeable differences may be pointed out. For instance, the $\pi - 0$ step-like crossover, calculated for $\alpha = 0.65$ and shown in Fig. 3, is smoothed out when considering the continuous spectrum contribution, as can be seen by comparing with the corresponding curve in Fig. 4.

In conclusion the model investigated in this paper for a multiband superconductor symmetric $s^\pm Is^\pm$ junction, predicts a number of non trivial details related to the Josephson effect in these systems. These results are of relevant interest for the case of all-pnictide Josephson micro-junctions. The spectral equation provides the Andreev bound levels as a function of the band ratio parameter $\alpha$. The main effect of the presence of the second band is the building up of two extra Andreev levels which drive Cooper pairs in a direction opposite to that observed in the presence of a single band.

The phase-current relations predicted on the basis of the Andreev levels (without consideration for the continuous energy spectrum) shows the formation of a noteworthy $\pi$-state in the junction coupling. For selected values of the band ratio, a $\pi \to 0$ crossover may occur as the temperature decreases. In this case the $\pi$-state is observed at high temperature whereas the $0$-state is observed below the crossover temperature. In this region the junction recovers the behavior of a conventional "0" junction. These results are confirmed by means of a more exhaustive evaluation of the Josephson current englobing the contribution of the continuous spectrum energy states.

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