Scattering theory of the Josephson effect in iron based superconductors

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Abstract. We study the Josephson effect in $S_\pm IS_\pm$ junctions made by a two band superconductor with $s_\pm$ wave symmetry. We derive the Andreev coefficients for the scattering problem at the junction interface and the temperature dependence of the critical current. We predict various features of the Josephson current for certain values of the second band strengths and tunnel barrier amplitude among which a high temperature $\pi$ state coupling, and a $\pi$ to 0 transition as the temperature lowers.

1. Introduction
The Fermi surface of recently discovered iron-based superconductors is composed of several electron and hole sheets. Theory suggests that the superconducting order parameter has opposite signs in the electronlike and holelike bands in these materials ($s_\pm$ state or reversed sign $s$ state). Several theoretical models have already analyzed the consequences of such an extended $s$-wave symmetry on interface tunneling and also on Josephson junctions [1]. Most of these studies have been focused on junctions between a conventional superconductor and an iron-pnictide with $s_\pm$ pairing. Different methods have been proposed to include interband scattering into the microscopic theory of tunneling spectroscopy, which remains still a puzzling issue [2, 3, 4, 5, 6]. Recently, we have studied the Josephson effect in an all-pnictide superconducting junctions ($S_\pm IS_\pm/S_\pm NS_\pm$ junctions) [7] by adopting the method used in Ref. [4] for a two-band NS point contact interface. Focusing on the possibility of $\pi$-phase shifts formation in the interface of two iron-pnictide intergrains, we obtained results relevant to possible experiments in submicron iron based Josephson junctions and also to possible further theoretical developments. The possibility that the symmetry in these materials be $s_{++}$, instead of $s_\pm$, has not been completely ruled out, at moment. To this end in the present work besides providing details of the calculation method we briefly compare the model predictions for $s_{++}$ and $s_\pm$ symmetry material based junctions.

2. A two-band superconductor junction model
We model the $S_\pm IS_\pm$ (or the $S_{++} IS_{++}$ ) junction by assuming the following space dependent pair potential for the two bands $j = 1, 2$ along the x coordinate, normal to the junction interface

$$\Delta_j(x) = \Delta_j e^{i\varphi} \Theta(-x) + \Delta_j e^{i(\varphi_j + \varphi)} \Theta(x), \quad j = 1, 2$$

(1)
Here $\Theta(x)$ is the Heaviside function, $\varphi$ is the global phase difference between the two superconductive regions and $\varphi_1$ and $\varphi_2$ are the ‘internal’ pair potential phases. In the case of $s_\pm$ wave gap model, $\varphi_2 - \varphi_1 = \pi$, while in the standard two band model, with gaps of the same sign ($s_{++}$ wave, like in $MgB_2$), $\varphi_2 - \varphi_1 = 0$. We neglect the self-consistency condition for $\Delta_1(x)$, $\Delta_2(x)$, which is equivalent to neglecting the proximity effect. The quasiparticle wave functions, $u_j(x)$ and $v_j(x)$, satisfy the following Bogoliubov de Gennes equations [8]:

\[
\begin{align*}
\left[-\left(\frac{\hbar^2}{2m}\right)\left(\frac{d^2}{dx^2}\right) + U(x) - E_F\right]u_j(x) &+ \Delta_j(x)v_j(x) = Eu_j(x) \\
\left(\frac{\hbar^2}{2m}\right)\left(\frac{d^2}{dx^2}\right) - U(x) + E_F\right]v_j(x) &+ \Delta_j^*(x)u_j(x) = Ev_j(x), \quad j = 1, 2
\end{align*}
\]

where $E$ is the energy of the quasiparticles relative to the Fermi energy $E_F$. The potentials $U(x) = U_0\delta(x)$ and $\Delta_j(x)$ are responsible for the normal scattering and the scattering of electrons into holes (Andreev scattering), respectively.

3. Wave functions and boundary conditions in the presence of a second band

The two gaps are felt by the quasiparticles as potential wells. To solve the resulting quasiparticle scattering problem, $E > \Delta_1$ (we assume $\Delta_1 < \Delta_2$), in a $S_{+-}$/$S_{+-}$ or a $S_{+-}$/$S_{++}$ junction, one should write four independent eigenfunctions, one for each elementary scattering process [9], and include the presence of the second band. For instance, for the scattering of electronlike excitations incoming from the left (passage of Cooper pairs to the right), we have [4]

\[
\Psi_{SL}^a(x) = \left(\begin{array}{c}
u_1 e^{-i\varphi_1} \\ u_1 e^{-i\varphi_2}
\end{array}\right) \phi_{p_1}(x) + \alpha_0 \left(\begin{array}{c}
u_2 e^{-i\varphi_2} \\ u_2 e^{-i\varphi_1}
\end{array}\right) \phi_{q_1}(x) + \\
\Psi_{SR}^b(x) = \left(\begin{array}{c}
u_1 e^{-i\varphi_1} \\ u_1 e^{-i\varphi_2}
\end{array}\right) \phi_{p_1}(x) + \alpha_0 \left(\begin{array}{c}
u_2 e^{-i\varphi_2} \\ u_2 e^{-i\varphi_1}
\end{array}\right) \phi_{q_1}(x) + \\
\Psi_{SR}^c(x) = \left(\begin{array}{c}
u_1 e^{-i(\varphi_1+\varphi)} \\ u_1 e^{-i\varphi_2}
\end{array}\right) \phi_{p_1}(x) + \alpha_0 \left(\begin{array}{c}
u_2 e^{-i(\varphi_2+\varphi)} \\ u_2 e^{-i\varphi_1}
\end{array}\right) \phi_{q_1}(x) + \\
\Psi_{SL}^d(x) = \left(\begin{array}{c}
u_1 e^{-i\varphi_1} \\ u_1 e^{-i\varphi_2}
\end{array}\right) \phi_{p_1}(x) + \alpha_0 \left(\begin{array}{c}
u_2 e^{-i\varphi_2} \\ u_2 e^{-i\varphi_1}
\end{array}\right) \phi_{q_1}(x)
\]

where $a_e$ is the Andreev coefficient, $b_e$ accounts for the normal (specular) reflection of the incoming electronlike excitation, $c_e$ and $d_e$ represent the normal transmission and the anomalous transmission of the excitation in the right electrode as an electronlike excitation or a hololeke excitation, respectively. The coefficient $\alpha_0$ defines the ratio of the probability amplitudes for the incoming electronlike excitation that these four processes occur in the second band $q$ rather than in the first $p$, with $p \neq q$. The functions $\phi_{p,q}(x)$ represent Bloch waves in the two-band superconductor. The use of Bloch waves, instead of simple plane waves, here, is imposed by the obvious circumstance that two plane waves of the same energy would necessarily share the same momentum [4, 7]. $u_1$ and $v_1$ and $u_2$ and $v_2$ are the standard Bogoliubov coefficients $u_{1,2}^2 = 1/2 + \sqrt{E^2 - \Delta_{1,2}^2}/2E$ and $v_{1,2}^2 = 1/2 - \sqrt{E^2 - \Delta_{1,2}^2}/2E$ while $p_{e,h}$ and $d_{e,h}$ are the Fermi vectors of the two bands (taken up to a reciprocal lattice constant), $p_{e,h}^2 = k_F^2 - k_0^2 \pm 2m\sqrt{E^2 - \Delta_0^2}/h^2$ and $q_{e,h}^2 = k_F^2 - k_0^2 \pm 2m\sqrt{E^2 - \Delta_0^2}/h^2$ respectively. The total wave function $\Psi_1 + \alpha \Psi_2$ has to satisfy the following boundary conditions at the interfaces $x = 0$.

\[
\Psi_{SL}^a(0^-) = \Psi_{SR}^a(0^+), \quad \frac{d\Psi_{SR}^a(0^+)}{dx} - \frac{d\Psi_{SL}^a(0^-)}{dx} = \frac{2mU_0}{h^2} \Psi_{SL}^a(0^-)
\]
Assuming $E > \Delta_1$ [10] and equal band interface velocities, i.e. $v_q = -(ih/m)\phi_q'(0)/\phi_q(0) = v_p = -(ih/m)\phi_p'(0)/\phi_p(0) = v$, [4, 7], plugging (3) in (4) gives the Andreev coefficient $a_e$ (and the coefficients $b_e, c_e, d_e$). In the same way, consideration of scattering of holelike excitations incoming from the left (passage of Cooper pairs to the left), provides the Andreev coefficient $a_h$.

4. Josephson current from the scattering coefficients

The total Josephson current, i.e. the Cooper pair flow, is given by [9]

$$ I = \frac{e\Delta_1 k_B T}{\hbar} \sum_{\omega_n} \frac{1}{\Omega_{1n}} \left[ a_e(\varphi, i\omega_n, \alpha) - a_h(\varphi, i\omega_n, \alpha) \right] $$  \hspace{1cm} (5)

Here, $\Omega_{1n} = \sqrt{\omega_n^2 + \Delta_1^2}$, $\omega_n = \pi k_B T(2n + 1)$ are the Matsubara frequencies and the detailed balance requires $a_h(\varphi) = a_e(-\varphi)$.

![Figure 1. Maximum Josephson current as a function of the temperature for a high transparency ($Z = 0.0001$) $S_{++}IS_{++}$ junction. The red line is the clean limit of Kulik-Omelyanchuk.](image1.png)

$$4.1. \ s_{++} - symmetry$$

For a $S_{++}IS_{++}$ junction, i.e. $\varphi_2 - \varphi_1 = \pi$, Eqs. (3) and (4) provides for $a_e$ the expression

$$ a_e(\varphi, E) = \frac{1}{M} \left[ A_1 \sin(\varphi/2) \left( A_2 \sin(\varphi/2) - A_3 \cos(\varphi/2) \right) \right] $$ \hspace{1cm} (6)

where

- $M = M_1 - M_2 + M_3 \cos \varphi; \quad M_1 = \left( 1 + 2Z^2 \right) \left( 1 + 2\alpha^2 \sqrt{(E^2 - 1)(E^2 - r^2)} + r^2\alpha^4 \right) ;$
- $M_2 = 2E^2 \left[ 1 - \alpha^2 + \alpha^4 + Z^2(1 + \alpha^4) \right]; \quad M_3 = 1 + \alpha^2 \left( -2E^2 + 2\sqrt{(E^2 - 1)(E^2 - r^2)} + r^2\alpha^2 \right) ;$
- $A_1 = 2\alpha \left[ \sqrt{(E - 1)(E + r)} - \sqrt{(E + 1)(E - r)} \right] + 2(\alpha^2 r - 1);$
- $A_2 = E(\alpha^2 - 1); \quad A_3 = i \left( \sqrt{E^2 - 1} - \alpha^2 \sqrt{E^2 - r^2} \right);$

![Figure 2. Maximum Josephson current as a function of the temperature for a low transparency ($Z = 3$) $S_{++}IS_{++}$ junction. The red line is the Ambegaokar-Baratoff limit (tunnel limit).](image2.png)
We have introduced here the barrier strength \( Z = U_0/\hbar v \) and the second band weight parameter \( \alpha = \alpha_0 \phi_{p_0}(0)/\phi_{p_0}(0) \) \([4],[7]\). For values of \( \alpha \) such that \( 0 < \alpha < \sqrt{\Delta_1/\Delta_2} \), \( \alpha_e \) has poles which correspond to discrete Andreev states. In this case the supercurrent is essentially determined by the the Andreev discrete spectrum \([7]\). Figs.(1) and (2) show the maximum Josephson current, in the clean and tunnel limit, respectively, as a function of the reduced temperature \( T/T_c \) calculated for different \( \alpha \) values in a \( S_{++}IS_{++} \) junction. The current is in units of \( I_0 = e\Delta_1(0)/\hbar \). The gap ratio has been set to \( \Delta_2/\Delta_1 = 2.5 \). Noteworthy, independent from the barrier transparency, negative critical currents appear for sufficiently high values of the \( \alpha \) parameter, i.e. when the contribution of the second band has a stronger influence. Negative critical currents indicate the formation of \( \pi \)-state coupling junctions \([12, 13, 14]\).

4.2. \( s_{++} \)-symmetry

Figs.(3) and (4) show the model predictions for a \( S_{++}IS_{++} \) junction, i.e. \( \varphi_2 - \varphi_1 = 0 \). In this case too we have assumed the gap ratio \( \Delta_2/\Delta_1 = 2.5 \). The expression of \( \alpha_e \) is more involved and is not reported. Notably, no discrete spectrum exists and only the continuous spectrum contributes to the supercurrent. No negative critical current are predicted for any \( \alpha \) value, neither in the clean limit (Fig.(3)) nor in the tunnel limit (Fig.(4)); the inter-band interference effect however makes the current exceed the usual values obtained in a \( s \)-wave junction (\( \alpha = 0 \)).

4.3. Conclusions

We have presented a model theory describing the temperature dependence of the Josephson critical current in \( S_{+-}IS_{+-}/S_{+-}NS_{+-} \) junctions. Starting from the Bogoliubov - de Gennes equations, the Josephson-like current is derived in the presence of double-band superconductor electrodes. Depending on the barrier strength and the range of the second band weight parameter \( \alpha \), a \( \pi \) to 0 crossover is predicted. On the contrary the same analysis for a \( S_{++}IS_{++} \) junction points out the total absence of \( \pi \)-state in such structures and no anomalous dependence of the critical Josephson current on the temperature.
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