Ambegaokar-Baratoff relations of Josephson critical current in heterojunctions with multi-gap superconductors

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I. INTRODUCTION

Since the discovery of iron-based superconductors1–7, their pairing symmetry has been intensively debated. According to the spin fluctuation mechanism associated with the Fermi surface nesting, ±s-wave symmetry was proposed as a pairing scenario8–14. However, the debate has not been settled down. The ±s-wave symmetry is expected to be fragile against non-magnetic impurities15. Some experiment16 supported this idea, while the others17–21 presented controversial results. Hence, a direct and unambiguous evidence like the phase sensitive measurement in High-Tc cuprate superconductors22 is now in great demand. In fact, a large number of the methods to seek a definite signature have been examined, e.g., tunneling spectroscopy23–27, corner junctions26,21, observation of half-integer flux-quantum jump32, scanning tunnel microscopy33, and so on.

Josephson junctions are sensitive devices reflecting superconducting states of each electrode. Very recently, various types of Josephson junctions with iron-pnictide superconductors were successfully fabricated and typical Josephson effects were confirmed24–26. Among them, a Josephson junction between an iron-based and a conventional s-wave single-gap superconductors has been regarded as a possible candidate to directly detect the pairing symmetry of iron-based superconductors. The heterojunction system is theoretically described by multiple tunneling channels, some of which are π channels and the others are 0 ones38,39. Authors suggested anomalous critical current reduction39, Riedel anomaly cancellation40, and enlargement of the Josephson vortex core41.

In this paper, we derive Ambegaokar-Baratoff relation42 in the heterojunctions with multiple tunneling channels and clarify that a theoretical bound of \( I_s R_n \) products distinguishes ±s-wave from s-wave without any sign changes, which is simply denoted as s-wave throughout this paper. We examine two kinds of materials, \((\text{Ba,K})\text{Fe}_2\text{As}_2\) (122 compound) and \(\text{LaFeAs}(\text{O,F})\) (1111 compound) as the iron-based superconducting electrode in the heterojunction. Employing the density of states (DOS) ratios and the superconducting gap ratios given by five-band quasi-classical theory with the first-principlies calculation43, the theoretical bounds are evaluated. The temperature dependences of \( I_s R_n \) are also demonstrated in both ±s-wave and s-wave.

The paper is organized as follows. Section II is the derivation of the Ambegaokar-Baratoff relation in the junction with multiple tunneling channels. Based on the result, we propose a criterion for identifying the pairing symmetry of iron-based superconductors. The key criterion is an upper bound of the Josephson critical current for the ±s-wave, which corresponds to a lower bound for the s-wave. In Sec. III we apply this criterion to typical iron-pnictide superconducting materials and theoretically confirm its effectiveness. Section IV is devoted to the summary.

II. THEORETICAL BOUNDS OF JOSEPHSON CRITICAL CURRENTS

We examine a superconductor-insulator-superconductor (SIS) Josephson junction, as shown in Fig. 1. The electrode 1 (2), whose length is \( s^\prime (s) \) in the direction of the z axis, is a single-band (five-band) superconductor. The insulator, whose length is \( d \) in the direction of the z axis and the dielectric constant is \( \varepsilon \), is sandwiched between
density is given by phase fluctuations to Josephson effects elsewhere. Un-
are fully pinned. We will discuss corrections of relative
We remark that such a rigid parallel circuit modeling is a
is no relative superconducting phase fluctuation in multi-
la case. Throughout this paper, we assume that there
ences
the two different superconducting electrodes.
One of the fundamental quantities characterizing Josephson junctions is the Josephson critical current
density. One can find various discussion for the cases
including two-band superconductors in several refer-
cences. However, there is no work on arbitrary
N-band superconductors. This paper treats such a gen-
eral case. Throughout this paper, we assume that there
is no relative superconducting phase fluctuation in multi-
band superconducting electrodes. In this case, the sys-
tem is described by an electric circuit as shown in Fig. 2.
We remark that such a rigid parallel circuit modeling is a
good description as far as the relative phase fluctuations
are fully pinned. We will discuss corrections of relative
phase fluctuations to Josephson effects elsewhere.
Under this assumption, the total Josephson critical current
density is given by
\[ j_c = \sum_i j_i \cos \chi_0^{(i)} \]  
(1)
\( \chi_0^{(i)} \) is a constant phase between the \( i \)th and the \( j \)th
superconducting gaps, which reflects the symmetry of a
static gap solution. Equation (1) includes \( \pi \) channels
when sign changes occur between the superconducting
gaps. The basic formalism to derive Eq. (1) is shown
in Appendix A. For the \( s \)-wave case, \( \chi_0^{(1)} = 0 \) for any \( i \).
On the other hand, a part of \( \{\chi_0^{(i)}\} \) should be \( \pi \)
for the \( \pm s \)-wave symmetry. As an example for the \( \pm s \-
wave case in the electrode 2, we take \( \chi_0^{(21)} = \chi_0^{(31)} = \chi_0^{(32)} = 0 \)
and \( \chi_0^{(41)} = \chi_0^{(51)} = \pi \) as schematically shown
in Fig. 2. Equation (1) indicates that \( j_c \) for the \( \pm s \)-wave
symmetry is always smaller than that for the \( s \)-wave, i.e.,
\( j_c(\pm s\text{-wave}) > j_c(s\text{-wave}) \).

Let us turn to a microscopic formula for \( j_i \) in Eq. (1). First,
we give notations. As for the electrode 1, we denote
the DOS on the Fermi surface and the superconduct-
ing gap amplitude as, respectively, \( N_s \) and \( \Delta^{(s)}(>0) \)
are the \( i \)th DOS and the \( i \)th gap amplitude, respectively.
In addition, we define “smaller” and “larger” gaps as
\( \Delta_{S,i} = \min \{ \Delta^{(i)}, \Delta^{(s)} \} \) and \( \Delta_{L,i} = \max \{ \Delta^{(i)}, \Delta^{(s)} \} \),
respectively. Thus, assuming the full gap solutions in both
superconducting electrodes, we microscopically calculate
\( j_i \) using a standard second order perturbation theory
with respect to a tunneling channel. Then, we have
\[ j_i = \frac{1}{W} \frac{1}{r_{n,i}} \frac{\pi \Delta_{\text{eff},i}}{2e} \]
where
\[ \frac{1}{r_{n,i}} = \frac{4\pi e^2}{\hbar} [T^{(i)}]^2 N_s N_i, \quad \Delta_{\text{eff},i} = \frac{2}{\pi} K(k_i; \beta \Delta_{L,i}) \Delta_{S,i}, \]
and \( W \) is the area of the junction interface. In the defi-
nition of \( r_{n,i}^{-1} \), the tunneling constant associated with the
\( i \)th tunneling channel is denoted as \( T^{(i)} \). The quantity \( k_i \)
corresponds to the ratio of the smaller gap to the larger
one, \( k_i = [1 - (\Delta_{S,i}/\Delta_{L,i})^2]^{1/2} \). The function \( K(k; \nu) \) is
given by
\[ K(k; \nu) = \int_0^1 \frac{\tanh(\nu \sqrt{1-k^2 x^2}/2)}{\sqrt{(1-k^2 x^2)(1-x^2)}} \ dx. \]
Combining the above arguments with Eq. (1), we obtain
\[ I_c R_n = \sum_i \frac{R_n}{r_{n,i}} \frac{\pi \Delta_{\text{eff},i}}{2e} \cos \chi_0^{(i)}, \]
where \( I_c = j_c W \). The combined resistance \( R_n = 1/\sum_i r_{n,i}^{-1} \)
can be experimentally measured when a bias current is greater than \( I_c \), while the individual measure-
ment of \( r_{n,i}^{-1} \) is practically impossible. Equation (2) is a
generalized formula of the Ambegaokar-Baratoff relation
for multi-channel heterojunctions. Brinkman et al.,
Agterberg et al., obtained similar results in the context
of MgB\( _2 \), i.e., two-band superconductor.

Here, we derive a simple relation from Eq. (2) when
the electrode 2 has the \( s \)-wave symmetry. The resultant
TABLE I: DOS ratios on the Fermi surfaces of iron-based materials evaluated by a first-principles calculation. The first three DOS’s \((N_1, N_2, N_3)\) corresponds to the hole bands, while the remaining DOS’s \((N_4 \text{ and } N_5)\) to the electric bands.

| \((T = 0 \text{ K})\) | \(\Delta^{(1)}/\Delta_{\text{max}}\) | \(\Delta^{(2)}/\Delta_{\text{max}}\) | \(\Delta^{(3)}/\Delta_{\text{max}}\) | \(\Delta^{(4)}/\Delta_{\text{max}}\) | \(\Delta^{(5)}/\Delta_{\text{max}}\) | \(2\Delta_{\text{max}}/k_B T^\text{iron}\) | \(\Delta^{(0)}/\Delta_{\text{max}}\) |
|-----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| \((\text{Ba, K})\text{Fe}_2\text{As}_2\) | 0.9395 | 1 | 0.5189 | 0.9415 | 0.9691 | 3.785 | 0.192 |
| \(\text{LaFeAs(O, F)}\) & 0.5052 & 1 | 0.2677 | 0.5084 | 0.5300 | 4.426 | 0.232 |

TABLE II: Superconducting gap amplitude ratios of iron-pnictide materials at zero temperature estimated by a five-band quasi-classical theory.

expression can give useful information about the pairing symmetry. The right hand side of Eq. \((2)\) is a summation of positive quantities in this case (i.e., \(\chi^{(i)}_{0} = 0\) for any \(i\)). Accordingly, we find that

\[
I_c(s\text{-wave})R_n \geq \frac{\pi \Delta_s}{2e}, \quad \Delta_s = \min \Delta_{\text{eff},i}, \quad (3)
\]

which gives a theoretical lower bound of \(I_cR_n\) for the \(s\)-wave. From the above argument, we find that if the symmetry of the electrode 2 is \(s\)-wave then Eq. \((6)\) must be fulfilled. Namely, if a measured value of \(I_cR_n\) satisfies

\[
I_cR_n < \frac{\pi \Delta_s}{2e}, \quad (4)
\]

then one can exclude the possibility of the \(s\)-wave. This method does not give more detailed information about the symmetry but clarify whether \(\pi\) channels exist in the multiple tunneling junctions with iron-pnictides. The present scheme, “lower-bound criterion” is a simple and convenient classification of iron-based superconducting materials.

Let us discuss experimental applicability of the criterion. The direct experimental data for bulk superconducting samples, e.g., angle resolved photoemission spectroscopy, provides the gap amplitudes in the 1-gap expression.

FIG. 3: (color online) Temperature dependence of iron-pnictide and single-band superconductor gap amplitudes. As for the iron-pnictide materials, we employ the previous results. The gap amplitudes are normalized by \(eV_0 = e[\Delta^{(i)}(0) + \Delta_{\text{max}}(0)]\). The solid lines (\(\Delta^{(1)}, \Delta^{(2)}, \text{and } \Delta^{(3)}\)) correspond to the hole band, while the dashed lines (\(\Delta^{(4)}\) and \(\Delta^{(5)}\)) the electric band. In the case of the \(\pm s\)-wave symmetry, the gaps corresponding to the dashed lines have the relative minus signs (i.e., \(\chi^{(4)}_{0} = \chi^{(5)}_{0} = \pi\)). (a) \((\text{Ba, K})\text{Fe}_2\text{As}_2\) \((T_{\text{c}122} = 38 \text{ K})\) and (b) \(\text{LaFeAs(O, F)}\) \((T_{\text{c}1111} = 27 \text{ K})\).

FIG. 4: (color online) \(I_cR_n\) products normalized by Eq. \((5)\). The red squares are for the \(s\)-wave, while the green crosses are for the \(\pm s\)-wave symmetry (i.e., \(\chi^{(21)}_{0} = \chi^{(31)}_{0} = 0\) and \(\chi^{(41)}_{0} = \chi^{(51)}_{0} = \pi\)). We also show the theoretical lower bounds for the \(s\)-wave symmetry at zero temperature (\(\pi \Delta_s(0)/2eV_0\)), depicted as the blue solid lines. We find that \(I_cR_n/V_0\) for \(\pm s\)-wave is much smaller than the theoretical lower bound for the \(s\)-wave at zero temperature. (a) \((\text{Ba, K})\text{Fe}_2\text{As}_2\) \((T_{\text{c}122} = 38 \text{ K})\) and (b) \(\text{LaFeAs(O, F)}\) \((T_{\text{c}1111} = 27 \text{ K})\).
which is much smaller than in the present figure.

One finds that a difference between the two functions exists around $T_c / T_c^{122} = 0.4 - 0.8$. We can find a similar discrepancy for $\Delta^{(1)}$, which is much smaller than in the present figure.

Therefore, in principle, one can input $\Delta_\ast$ in Eq. (3). However, superconducting gap amplitudes relevant to Josephson junctions is generally smaller than the ones in the bulk superconductors due to the damage piled up in interface fabrication. It indicates that direct comparison of a measured $I, R_n$ product to $\Delta_\ast$ based on the bulk data may give no practical information. Therefore, we focus on a transition voltage of the all tunneling channels into running state at zero temperature.$^{49}$

$V_0 = \frac{1}{e} [\Delta^{(s)}(T = 0) + \Delta_{\text{max}}(T = 0)]$, \hspace{1cm} (5)

in which $\Delta_{\text{max}} = \max_i \Delta^{(i)}$. One can measure the suppressed $V_0$ experimentally if the junction shows hysteretic $I-V$ characteristics.$^{22}$ We emphasize that a scaled quantity $\Delta_\ast / e V_0$ is given by only the gap amplitude ratios since the bulk gap ratios are expected to be kept as long as the damage is not too severe. Therefore, the scaled lower bound $\Delta_\ast / e V_0$ is experimentally evaluated by the gap amplitude ratios for the bulk samples, and this quantity should be compared to measured $I_c R_n / V_0$.

Consequently, we conclude that the inequality (4) is an effective formula to examine the pairing symmetry.

III. APPLICATION OF LOWER-BOUND CRITERION TO IRON-PNICTIDE SUPERCONDUCTORS

Let us evaluate the right hand side of Eq. (2) in real iron-pnictide materials and check how the criterion based on the inequality (4) works. For the sake of simplicity, we employ a simple model for the tunneling constants. Namely, we assume that $T^{(i)}$'s take channel-independent constants. It means that $R_{n_i} / r_{n_i}$ is equal to $N_i / N_{\text{tot}}$, where $N_{\text{tot}} = \sum_i N_i$. Then, we find that $I_c R_n / V_0$ is simply a function of the superconducting gap ratios (i.e., $\Delta^{(s)} / \Delta_{\text{max}}$ and $\Delta^{(i)} / \Delta_{\text{max}}$) and the DOS ratios (i.e., $N_i / N_{\text{tot}}$).

We concentrate on two iron-pnictide superconducting materials, (Ba,K)Fe$_2$As$_2$ ($T_c^{122} = 38$ K) and LaFeAs(O,F) ($T_c^{111} = 27$ K). Here, we denote each superconducting transition temperature as $T_c^{122}$ or $T_c^{111}$.
As for the single-gap superconducting electrode material, we choose an alloy of Pb, i.e., Pb-In-Au. The superconducting transition temperature $T_c^s = 7$ K and $\Delta^{(s)}(0)/k_BT_c = 1.98$, respectively. The gap amplitude ratios and their temperature dependence of (Ba, K)Fe$_2$As$_2$ and LaFeAs(O, F) were evaluated by five-band quasi-classical theory combined with the DOS’s via the first-principles calculations and several kinds of experimental data for the bulk properties. We label three hole bands as 1 to 3 and two electron ones as 4 to 5. The sign changes are assumed to occur between the hole and the electron bands. The DOS and the gap ratios are summarized in Tables I and II respectively. As for the temperature dependence of the single-band superconducting gap, we utilize the BCS type gap formula.

$$\Delta^{(s)}(T) = \Delta^{(s)}(0) \tanh \left\{ A \left[ B \left( \frac{T_c^s}{T} - 1 \right) \right] \right\},$$

where $A = 1.82$, $B = 1.018$, and $C = 0.51$.

Figure 3 displays the temperature dependence of the superconducting gap amplitudes. Figure 4 shows the temperature dependence of $I_cR_n$ normalized by $V_0$. The lower bound at $T = 0$ given by the right hand side of the inequality (3) is also depicted by the (blue) horizontal line. Due to $j_c(s$-wave) $> j_c(\pm s$-wave), $I_cR_n$ for the $\pm s$-wave becomes smaller than the one for the $s$-wave over all temperature regions. Here, let us focus on the zero temperature. $I_cR_n/V_0$ for the $\pm s$-wave is smaller than the lower bound ($\pi\Delta_c(0)/2eV_0$) while that for $s$-wave is larger for both of the iron-pnictide superconducting materials. Hence, the comparison of a measured value of $I_cR_n$ to the theoretical bound gives a useful criterion for the symmetry in the iron-based superconductors.

Next, we investigate specific cases in which a part of or all iron-based superconducting gaps are smaller than the single-band BCS gap, as shown in Fig. 5(a) and 5(b). In such a study, we keep the gap ratios to be the val-
ues for (Ba,K)Fe$_2$As$_2$ shown in Tables I and II except for $\Delta^{(s)}/\Delta_{max}$. Figures 5(c) and 5(d) show the $I_cR_n$'s for $T_c^s = 10$ K and 6 K, respectively. We find again that the inequality (4) is fulfilled at zero temperature. It means that the present criterion works in every case. On the other hand, we notice that the temperature dependences of $I_cR_n$ are relatively anomalous. We find a convex behavior in the middle temperature range (i.e., $T/T_c^s$ $\sim$ 0.2-0.8) contrary to our naive expectation. Such peculiarity comes from a discrepancy between the gap functions calculated by the five-band quasi-classical theory and the BCS type gap formula (6), as shown in Fig. 6. In the previous case as Fig. 4 the single-band BCS gap solely provides the contributions to the temperature dependence of $I_cR_n$. However, the present case reflects all the gap temperature dependences. Thus, the temperature dependence of $I_cR_n$ is found to be quite sensitive to the difference of the gap functions from the single-band BCS type gap formula.

IV. SUMMARY

We derived the Ambegaokar-Baratoff relation in the SIS Josephson junction with multiple (more than two) tunneling channels and proposed a criterion to identify the pairing symmetry of the iron-based superconductors. If a measured value of $I_cR_n$ product is smaller than the lower bound for the $s$-wave, then one concludes that the symmetry of the superconducting electrode is the $\pm s$-wave. We actually revealed that the criterion well works in the typical iron-pnictide superconductors by employing the DOS and the gap ratios calculated by the five-band quasi-classical theory and the first-principles calculation. In addition, the theory predicted that the temperature dependence of $I_cR_n$ is sensitive to the deviation of the temperature dependence of the gap from the single-band BCS formula. The method is simple and convenient in contrast to the phase sensitive measurement like $\pi$ junctions which require much more elaborate setups.

The Ambegaokar-Baratoff relation is one of the fundamental identity in the SIS Josephson junction. The present analysis suggested that this type of the relation provides more fruitful information when the junction has multiple tunneling channels.

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Appendix A: Formalism for gauge-invariant phase differences

A basic formalism for the hetero Josephson junction dealt in this paper is presented. Assuming uniformity along $y$ axis, the effective Lagrangian density on the $zx$ plane is given by

$$\mathcal{L}_{eff} = \frac{s'}{8\pi\mu'_{T_r}^2}(q^0)^2 + \sum_{i=1}^5 \frac{s}{8\pi\mu_i^2}(q^0_i)^2 + \frac{5}{6} \frac{\hbar j_i}{e^*} \cos \theta(i)$$

$$+ \sum_{i < j} \frac{\hbar j_{ij}}{e^*} \cos \chi(i'j') + \frac{d}{8\pi}(E_{21}^z)^2, \quad (A1)$$

where $\theta(i) = \varphi(i) - \varphi(0)(e^*d/hc)A_{21}^z$ and $\chi(i'j') = \varphi(i') - \varphi(i) = \theta(i') - \theta(i)$. $\chi(i'j')$ is the relative phase difference between the different superconducting gaps. The first and the second terms in Eq. (A1) represent charge compressibility in the electrode 1 and 2, respectively,
where \( q^0 = (h/e^*)p^0 \), \( \phi^0 = (h/e^*)\phi^0 \) \( \phi^0 \), and \( e^* = 2e \). The electric scalar potential in the electrode \( \ell = 1, 2 \) is denoted as \( \phi^0 \), and the charge screening length in the electrode 1 (2) is written as \( \mu^0 \) (\( \mu^0 \)).

The third term in Eq. (A1) is the Josephson coupling, in which \( hj_i/e^* \) is the coupling constant associated with the \( \text{th} \) tunneling channel. The forth term in Eq. (A1) is the inter-band Josephson coupling energy \( 53 \), whose origin is the inter-band interaction between different bands in the electrode 2.

In the gauge-invariant \( \theta^0 \), the vector potential in the insulator \( \alpha \), the vector potential in the electrode 1 (2) is written as \( \mu^0 \).

As the Euler-Lagrangian equation with respect to \( \theta^0 \), we have the Maxwell equation

\[
0 = \frac{e^* d}{c^2} \frac{\hbar}{\Lambda} E_{21}^2 + \sum_i \frac{4\pi e^* d}{\hbar} j_i \sin \theta^0.
\]

Combining Eq. (A3) with Eq. (A2) leads to the equation

\[
\frac{e^* d}{c^2} \frac{\hbar}{\Lambda} \sum_i \frac{\alpha_i}{\alpha_0} \partial^2_i \theta^0 + \sum_i j_i \sin \theta^0 = 0.
\]

If one adds a dissipation and an external bias current terms to Eq. (A1), one has the resistively and capacitively shunted junction model with multi-tunneling channels.

Let us turn to a formula for the Josephson critical current density. Generally, the system has a relative superconducting phase fluctuation originating from the inter-band Josephson coupling \( \sum_{i<i'} J_{ii'} \cos \chi^{(ii')} \), which generates Josephson-Leggett collective excitation modes \( 22, 23 \). The equations of motion for \( \chi^{(ii')} \) can be obtained as the Euler-Lagrangian equations with respect to \( \phi^0 \) and \( \phi^{(ii')} \) \( 29 \). In this paper, we simply assume that each \( \chi^{(ii')} \) is fixed as a constant \( \chi_0^{(ii')} \) reflecting the symmetry of a static gap solution. Such an assumption can be validated when \( |J_{ii'}| \gg j_1, j_2 \). In this case, we have \( \theta^0(t) = \theta^1(t) + \chi_0^{(ii)} \), where \( \chi_0^{(ii)} = 0 \) or \( \pi \). Equation (A1) is then rewritten by

\[
\frac{e}{4\pi \Lambda d} \frac{\hbar}{e^*} \partial^2 \theta^0 + \sum_i j_i \cos \theta^0 \sin \theta^0 = j_{\text{bias}}.
\]

Here, we add a bias current density \( j_{\text{bias}} \) to the right hand side. Equation (A5) indicates that a static solution exists as long as \( j_{\text{bias}} < \sum_i j_i \cos \theta^0 \).

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