$0-\pi$ phase shifts in Josephson junctions as a signature for the s₊-wave pairing state

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We investigate Josephson junctions with superconducting ferropnictides, both in the diffusive and ballistic limit. We focus on the proposed s_{\pm} -wave state and find that the relative phase shift intrinsic to the s_{\pm} -wave state may provide 0- π oscillations in the Josephson current. This feature can be used to discriminate this pairing state from the conventional s-wave symmetry. The 0- π oscillations appear both as a function of the ratio of the interface resistances for each band and, more importantly, as a function of temperature, which greatly aids in their detection.

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The discovery of high- T_c superconductivity in the ferropnictides¹ has triggered an avalanche of investigations (see the reviews² and references therein) from a broad range of communities in condensed-matter physics. A crucial issue which remains unresolved is the nature of the superconducting order-parameter (OP) symmetry in ferropnictide superconductors. This topic is particularly intriguing since the ferropnictides feature a multiband Fermi surface where the Cooper pairs may reside.

In order to identify the symmetry of the superconducting OP, several recent experimental studies^{3,4} utilized the method of point-contact spectroscopy in order to study the symmetry of the superconducting OP in the ferropnictides. The findings were, however, not easily reconcilable. Using an extended Blonder-Tinkham-Klapwijk (BTK) theory⁵ to fit their data, some groups³ found a zero-bias conductance peak, indicative of a nodal order parameter such as *d*-wave. However, other groups⁴ interpreted their data in terms of one or more nodeless OPs, such as *s*-wave.

One of the leading candidates for the pairing symmetry is the so-called s_{\pm} -wave state proposed in Refs. 6 and 7. This pairing symmetry consists of two s-wave order parameters for the electronlike and holelike Fermi surfaces that differ in sign. Some progress has been made in mapping out the ramifications of the s_{\pm} -wave symmetry to quantum transport properties of the ferropnictides. $^{8-10}$ For instance, it has been predicted that subgap surface states should appear in the presence of interband scattering. 10 Unfortunately, such subgap surface states are not unique for the s_{\pm} -wave state and do not provide unambiguous evidence for this pairing symmetry.

To shed more light on the pairing symmetry in the ferropnictide superconductors, we present results for both the proximity effect and the Josephson current in hybrid structures involving normal-metal elements and superconducting ferropnictides. The motivation for this is that both of these phenomena are expected to produce valuable information about the pairing state in the superconductor. We take into account the intrinsic multiband nature of this material class and include results for the diffusive limit of transport, in contrast to previous theoretical works on these systems.

For Josephson junctions with conventional superconductors (*s*-wave), it is well known that the supercurrent decays in a monotonous fashion as a function of both temperature and interlayer width, when the material separating the supercon-

ductors is nonmagnetic. If the interlayer is ferromagnetic, the current oscillates and goes to zero at certain critical widths and temperatures. This phenomenon is known as $0-\pi$ oscillations¹¹ and serves as a signature of either ferromagnetic correlations or nodal OPs, such as d-wave, present in the Josephson junction.

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In this Rapid Communication, we show that the aforementioned prerequisites for $0-\pi$ oscillations are rendered unnecessary in the presence of an s_{\pm} -wave pairing state. We find that $0-\pi$ oscillations may occur in a Josephson junction consisting of a conventional s-wave superconductor and a s_{\pm} -wave superconductor separated by a normal (nonmagnetic) interlayer and thus in the complete absence of any ferromagnetic elements or nodal superconducting OPs. This effect is explained in terms of the relative phase shift between the bands in the s_{\pm} -wave superconductor and constitutes a signature of the s_+ -wave state, which can be probed in experiments. In fact, using such an observation in conjunction with other experiments that report a nodeless OP, ruling out d-wave pairing, would strongly support the realization of a s_{\pm} -wave state. Our results are qualitatively independent of the interband scattering strength and are induced solely by the s_+ -wave symmetry. This renders our prediction more robust than recent proposals regarding subgap bound states as probes for the s_+ -wave state, which rely heavily on substantial interband scattering.

We will employ the quasiclassical theory of superconductivity in form of the Usadel¹² equation and the accompanying Kupriyanov-Lukichev boundary conditions¹³ modified for a multiband situation. 14 The quasiclassical approach is justified under the condition that the Fermi energy is much larger than the superconducting gap and the impurity scattering selfenergy, which should be a safe assumption for the ferropnictides. The notation and conventions of Ref. 15 will be used in what follows. For equilibrium situations, it suffices to consider the retarded part of the matrix Green's function, \hat{g} , which is parametrized conveniently by the quantity θ_{σ}^{N} , σ $=\uparrow$, \downarrow . The Green's function satisfies $\hat{g}^2=\hat{1}$ and consists of entries with $c_{\sigma}^{N} = \cosh(\theta_{\sigma}^{N})$ and $s_{\sigma}^{N} = \sinh(\theta_{\sigma}^{N})$ as measures of the proximity effect induced by the multiband superconductor. In this parametrization, the Usadel equation¹² is obtained as $D_N \partial_x^2 \theta_\sigma^N + 2i\varepsilon s_\sigma^N = 0$, where D_N is the diffusion coefficient in the normal metal and ε is the quasiparticle energy. In the superconducting region, we use the bulk Green's functions \hat{g}_{λ} (Refs. 11 and 15) for each band as denoted by the

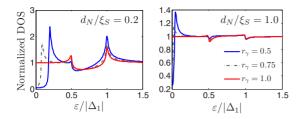


FIG. 1. (Color online) Plot of the DOS at x=0 (at the N|I interface) for thin $(d_N/\xi_S=0.2)$ and thick $(d_N/\xi_S=1.0)$ normal-metal regions. We have set $r_\Delta=0.5$ and considered several values of r_γ .

index $\lambda = (1,2)$, with belonging gaps $\Delta_{\lambda} = |\Delta_{\lambda}| e^{i\varphi_{\lambda}}$. The unique feature of the s_{\pm} -wave state is that the relative phase between the bands is π , i.e., $\varphi_1 = \varphi$ and $\varphi_2 = \varphi + \pi$, where φ is the superconducting phase associated with the broken U(1) gauge symmetry.

The Usadel equation must be supplemented with boundary conditions at the interface of the superconducting region. Under the assumption of a low interface transparency, we may employ generalized Kupriyanov-Lukichev boundary conditions that for an $N|s_\pm$ -wave interface at $x=d_N$ take the form $d_N\hat{g}_N\partial_x\hat{g}_N|_{x=d_N}=\sum_\lambda\frac{1}{\gamma_\lambda}[\hat{g}_N,\hat{g}_\lambda]|_{x=d_N}$ where d_N is the thickness of the normal-metal layer while $\gamma_\lambda=R_B^\lambda/R_N$. Here, R_N is the resistance of the normal-metal region, while R_B^λ is the effective barrier resistance for band λ . At x=0, we have $\partial_x\theta_0^N=0$, corresponding to zero outgoing current at the insulating/vacuum interface.

Let us first briefly investigate the full proximity-effect regime in a $N|s_{\pm}$ junction by solving the Usadel equation numerically with its boundary conditions. The normalized density of states (DOS) reads as $N(\varepsilon)/N_0 = \frac{1}{2} \sum_{\sigma} \text{Re}\{c_{\sigma}^N\}$. There are three parameters that are free to vary in our theory. One is the thickness of the normal-metal layer d_N/ξ_S , where ξ_S $=\sqrt{D_N/|\Delta_1|}$. The two others are the ratio between the gaps and the ratio between the barrier parameters, defined respectively as $r_{\Delta} = |\Delta_2/\Delta_1|$ and $r_{\gamma} = \gamma_2/\gamma_1$. In Fig. 1, we contrast the thin junction case $d_N/\xi_S \ll 1$ with a thick junction d_N/ξ_S =1 for a representative choice of parameters. We fix r_{Δ} =0.5 and plot the DOS in the N region at x=0 for several values of r_{γ} , with $\gamma_1 = 5$ corresponding to a low barrier transparency. There are in general three peaks in the energyresolved DOS. Two of these peaks pertain to the bulk gaps of the s_+ superconductor, while the third demarcates the opening of a minigap in the spectrum. This is qualitatively the same as what would be expected for a multiband superconductor with a conventional s-wave symmetry, such as MgB_{2} . 14

Therefore, the proximity effect and its impact on the DOS do not appear to provide a unique diagnostic tool in order to distinguish s_{\pm} -wave symmetry from ordinary s-wave symmetry. We thus turn our attention to the Josephson coupling for s_{\pm} -wave superconductors as a possible mean to reveal this symmetry. To this end, we will consider a s-wave $|N|s_{\pm}$ -wave junction, where the s-wave gap is given by $\Delta_s = |\Delta_s|e^{i\varphi_s}$, and assume a weak proximity effect that allows us to linearize the Usadel equation and proceed analytically, facilitating the interpretation of the obtained results. Also, the linearized approach is expected to yield excellent

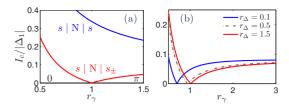


FIG. 2. (Color online) (a) Plot of the critical current for an s-wave |N|s-wave and s-wave $|N|s_{\pm}$ -wave junction, using $r_{\Delta}=1.0$ and $|\Delta_s/\Delta_1|=1.0$. (b) Plot of the critical current in the s-wave $|N|s_{\pm}$ -wave case, using $|\Delta_s/\Delta_1|=0.5$. In both (a) and (b), we have set $d_N/\xi_S=1.0$.

results in the experimentally relevant low-transparency case. The supercurrent is given by $I_J \sim \int_{-\infty}^{\infty} d\varepsilon \operatorname{Tr}\{\hat{\rho}_3(\hat{g}\,\partial_x\hat{g})^K\}$, where $\hat{\rho}_3 = \operatorname{diag}(1,1,-1,-1)$ and 'K' denotes the Keldysh component of the Green's function.¹¹ After solving the Usadel equation, one may insert \hat{g} into the above equation for the supercurrent. We find the following expression for the normalized zero-temperature Josephson current:

$$I_J = I_0 \sin \Delta \varphi, \quad I_0 = \int_0^\infty d\varepsilon \operatorname{Re} \{ \mathcal{RL} / [ikd \sin(kd)] \}, \quad (1)$$

where $\mathcal{L} = \Sigma_{\lambda} \delta_{\lambda}^{L} \mathcal{F}_{\lambda}^{L} / \gamma_{\lambda}$ and $\mathcal{R} = \Sigma_{\lambda} \delta_{\lambda}^{R} \mathcal{F}_{\lambda}^{R} / \gamma_{\lambda}$. Here, $\Delta \varphi = \varphi$ $-\varphi_s$ is defined as the phase difference between band $\lambda=1$ in the right superconductor and the left superconductor, k = $\sqrt{2i\varepsilon/D_N}$, while $\mathcal{F}_{\lambda}^{L,R}$ describe the anomalous Green's functions on the left/right side of the junction. These are proportional to the off-diagonal entries in the bulk Green's functions for the superconductors, which have the form $\mathcal{F}^{L,R}_{\lambda}$ $\propto s_{\lambda}^{L,R}$. We defined $\delta_{\lambda=1}=1$ and $\delta_{\lambda=2}=-1$. Note that the above expressions are valid for both a s-wave and s_{\pm} -wave superconductor on either side of the diffusive normal metal, which is why we have included the band index also on the left side. In the s-wave case, we have $\mathcal{F}_{\lambda} = \delta_{\lambda} \sinh[\arctan(|\Delta_s|/\varepsilon)]$, s_+ -wave case we while in the $=\sinh[\arctan(|\Delta_{\lambda}|/\varepsilon)].$

We now solve Eq. (1) numerically to obtain the Josephson critical current, corresponding to $I_c = |I_0|$, which is the relevant quantity measured experimentally. In Fig. 2(a), we plot the critical current as a function of the ratio between the barriers for each band, r_{γ} s-wave |N|s-wave and s-wave |N|s_±-wave junctions. In the former case, the current decays monotonously as is well known. However, the situation is very different when we replace, say, the right s-wave superconductor with an s_+ -wave state. The current now displays $0-\pi$ oscillations, even in the complete absence of any ferromagnetic elements. This is very different from the conventional s-wave case, where a ferromagnetic element is required in order to induce the 0- π oscillations. Thus, experimental observation of such 0- π oscillations in a Josephson junction with ferropnictides would provide a strong indication of the presence of an s_+ -wave state. In Fig. 2(b), we give results up to large r_{ν} for the s-wave $|N|s_{\pm}$ -wave case. As seen, the current saturates after the 0- π oscillation since $r_{\gamma} \gg 1$ means that one of the band interface transparencies tends to zero and does not contribute to transport.

The appearance of the $0-\pi$ oscillations in the current may be understood as follows. The transport of charge in an s-wave $|N|s_+$ -wave junction takes place both through interand intraband channels, as may be inferred directly by observing that the product LR in Eq. (1) produces precisely such terms. Due to the relative phase shift of π between the two bands in the s_+ -wave state, these contributions to the critical current have opposite signs. For simplicity, consider the case where all gap magnitudes are equal in the Josephson junction, $|\Delta_{\lambda}| = |\Delta_{s}|$, which leads to equal anomalous Green's functions \mathcal{F} on both sides of the junction. We then have $\mathcal{LR} = \mathcal{F}^2(1/\gamma_1^2 - 1/\gamma_2^2)$ in Eq. (1), which is clearly seen to change sign at $r_{\nu}=1$. This does not occur in a conventional s-wave superconductor, where there is no relative phase shift. The basic mechanism behind the $0-\pi$ oscillations is thus that variations in the barrier parameters γ_{λ} for the bands will lead to either a dominant contribution between bands with no phase shift relative each other or bands with order parameters that differ in sign.

Let us also consider the ballistic limit to show that the mechanism for the $0-\pi$ oscillations persists in clean samples. The only other change in the physical system under consideration is that we replace the normal interlayer with a thin insulating barrier (I), which in the BTK approach introduces the dimensionless barrier strengths Z_{λ} . In this manner, we can parametrize the relative barrier resistance in an analogous manner as with r_{γ} in the diffusive case by introducing $r_z = Z_2/Z_1$. We construct and solve the full 4×4 Bogoliubov-de Gennes equation for the two-band system, where we for generality also include coupling between the two bands parameterized by the interband coupling strength α . This yields in general four current-carrying Andreev bound states (ABSs) $E_{\lambda}^{\pm}(\Delta\varphi)$. The Josephson current for this s-wave $|I|s_{\pm}$ -wave Josephson junction is then found in the ordinary way from $I_J = 2e\sum_{i=1}^4 \frac{\partial E_i}{\partial \varphi} f(E_i)$, where E_i denotes the four ABS and f(E) is the Fermi-Dirac distribution function.

To present an explicit illustration of the mechanism of $0-\pi$ oscillations in a s_+ system in the ballistic limit, we proceed analytically for the special case of α =0. Here, we have for simplicity assumed that $|\Delta_{\lambda}| = |\Delta_{s}| \equiv |\Delta|$. This gives solutions for the ABS on the well known¹⁶ $E_1^{\pm} = \pm |\Delta| \sqrt{1 - D_1 \sin^2(\Delta \varphi/2)}$ $=\pm |\Delta| \sqrt{1-D_2 \cos^2(\Delta \varphi/2)}$, with $D_{\lambda} = 4/(4+Z_{\lambda}^2)$. At T=0, the above expression for the Josephson current yields in the tunneling limit $I_J = I_1 \sin \varphi$, with $I_1 = (D_1 - D_2)I_0/4$ and $I_0 = 2e|\Delta|$. It is obvious that for $Z_2 < Z_1$ one will have $I_1 < 0$, i.e., the system being in the π state, as explained for the diffusive case. As shown in Fig. 3, the crossover point above which the $\lambda=1$ contribution dominates instead is $r_z=1$. Notice however that the current does not vanish entirely at the crossover point due to a second-harmonic component in the current-phase relation (as shown in the inset of Fig. 3), which dominates close to the transition point. This is demonstrated explicitly by taking the approximation to the next order in the limit $Z_2 = Z_1$, which yields $I_J = I_2 \sin(2\Delta\varphi)$, with $I_2 = -I_0 D_{\lambda}^2 / 16$. We note that this nonsinusoidality of the current-phase relation was absent in the diffusive case since the linearized Usadel equation corresponds to a first-order approximation in the interface resistance. We also emphasize

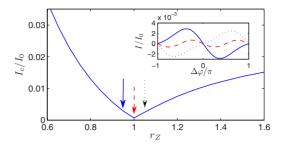


FIG. 3. (Color online) Critical current for a ballistic s-wave $|I|s_{\pm}$ -wave Josephson junction as a function of the relative barrier strength r_Z . Interband coupling is neglected, and we have set Z_1 =6, T=0, and $|\Delta_{\lambda}|=|\Delta_{s}|$. *Inset:* current-phase relation for selected values of r_Z , as indicated by the arrows in the main figure.

that in this treatment, interband coupling is not essential for the occurrence of the 0- π -transition. However, we have verified numerically that the results of Fig. 3 are qualitatively valid also for $\alpha > 0$ so that the predicted experimental signature should be equally distinct for strong interband coupling.

From the analysis above, it is seen that the crucial ingredient for the observation of the $0-\pi$ oscillations is having different barrier parameters for each band λ , or alternatively different probabilities for Cooper-pair tunneling. As suggested in Ref. 9, these probabilities may be artificially altered by selecting materials with appropriate Fermi surfaces. Different Fermi-vector mismatches would then lead to different tunneling probabilities. In our case, the size of the Fermi surface of the diffusive normal-metal region could be modified by doping. Thus, whereas $0-\pi$ oscillations in S|F|S junctions can be seen as a function of the width d_F of the ferromagnetic layer,17 necessitating the fabrication of several samples with different widths, the present scenario requires fabrication of several samples with the doping level in the normal metal varying in a systematic way. We note that it was also observed in Ref. 9, although in the context of a superconducting s-wave|s-wave|s-wave trilayer, that a π junction could be fabricated in a similar manner.

Although the above procedure is in principle feasible, it is very challenging to quantitatively relate the Fermi-vector mismatch directly to the parameter r_{γ} . However, we find that the $0-\pi$ oscillations also occur as a function of temperature in the diffusive limit, thus constituting an alternative, and simpler, approach to the recipe sketched above for altering r_{γ} . Assuming a Bardeen-Cooper-Schrieffer (BCS) temperature dependence for the gaps, with a critical temperature $T_{c,\lambda} = T_c$ for the s_{\pm} -wave superconductor and $T_{c,s}$ for the s-wave superconductor,²⁰ we plot the results in Fig. 4. As seen, $0-\pi$ oscillations appear as a function of temperature for a wide range of interface parameters r_{γ} . For large values of r_{Λ} , a normal monotonous decay of the critical current is seen. Although the exact relation between r_{γ} and r_{Δ} which renders possible the $0-\pi$ oscillations is difficult to extract analytically from Eq. (1), the basic mechanism is nevertheless the same as the one explained previously. From Fig. 4, we see that the absence of $0-\pi$ oscillations not necessarily rules out that s_+ state, whereas the presence of them rules out the s-wave state.

Finally, we point out that very strong impurity interband

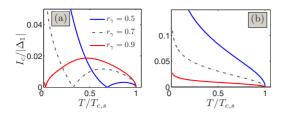


FIG. 4. (Color online) Plot of the critical current as a function of temperature for an s-wave $|N|s_{\pm}$ -wave junction, using $d_N/\xi_S=1.0$ and $|\Delta_s/\Delta_1|=0.5$. In (a), we have $r_{\Delta}=0.3$ while in (b) $r_{\Delta}=1.3$.

scattering Γ would eventually suppress the critical temperature for the s_{\pm} ground state. ¹⁸ The difference between the DOS on the hole and electron Fermi pockets would determine how fast the suppression rate increases with Γ as compared to, e.g., a d-wave scenario. For intraband scattering, however, the s_{\pm} state is protected by Anderson's theorem. In our model, we have incorporated interband scattering only near the interface. A further extension of the model considered here could be to incorporate magnetic correlations in the s_{\pm} state and also investigate strong interband scattering in the bulk of the superconductor to see how it affects the transport properties, ¹⁹ although we expect that they would remain

qualitatively the same as reported here since the basic mechanism for the $0-\pi$ oscillations would remain intact.

In summary, we have investigated the Josephson coupling properties of junctions with s_{\pm} -wave superconductors. In contrast to previous literature, we have here included results for both the ballistic and diffusive regimes. The relative phase shift of the bands intrinsic for the s_{+} -wave state leads to $0-\pi$ oscillations in an s-wave $|N|s_{\pm}$ -wave Josephson junction, even in the absence of any ferromagnetic elements. The mechanism behind these oscillations is a competition between the sign-dependent contribution of transport from different bands in the s_+ -wave superconductor to the s-wave superconductor. The $0-\pi$ oscillations are seen as a function of temperature, thus vastly facilitating the experimental testing of our predictions compared to methods that involve changing the parameters of the model system. Our results may aid in identifying the possible existence of an s_+ -wave pairing state in the superconducting ferropnictides.

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²⁰Note that at $T \neq 0$, an additional term $\tanh(\beta \varepsilon/2)$ appears in the integrand of Eq. (1), where $\beta = 1/T$.