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# $\pi$-phase shift at the interface of two pnictide superconductors with antiphase $s$-wave pairing

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We examine the nature of Josephson junction between two identical Fe-pnictides with antiphase $s$-wave pairing. $\pi$-phase shift is found if the junction barrier is thick and the two Fe-pnictides are oriented in certain directions relative to the interface. Our theory provides a possible explanation for the observed half integer flux quantum transitions in a niobium/polycrystal NdFeAsO loop, and attributes the $\pi$-phase shift to intergrain junctions of Fe-pnictides.

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Since the discovery of a class of unconventional superconductors based on Fe compounds, their pairing symmetry has been one of the most interesting issues. Different from the high $T_c$ cuprates, where the pairing symmetry is universally d-wave, there are experimental evidences that pairing symmetry in the iron pnictides may not be universal. The superconductors with higher transition temperature, $T_c$, are supported by spin singlet $s$-wave,[1–4] while LaFePO with lower $T_c$ seems to have nodal in its gap function.[5] It is interesting to note that the iron pnictide has both hole and electron Fermi pockets, and the predicted $s$-wave pairing state has superconducting order parameters with opposite signs on the electron and hole pockets, often called antiphase $s$-wave or $s_\pm$-wave state.[6–12] Among the experiments in support of the $s_\pm$-pairing state, the phase sensitive experiment reported by Chen *et al.*[4] provides the most convincing evidence, where they observed integer and half integer flux quantum transitions in a niobium/polycrystal NdFeAsO loop. The observed half integer flux quantum demonstrates the existence of $\pi$-junctions in the loop of niobium and polycrystal pnictides, hence a direct evidence for the opposite signs of the superconducting order parameters in different Fermi pockets. In passing, we recall that phase sensitive experiments provided a direct evidence for the $d_{x^2-y^2}$ pairing in superconducting cuprates.[13,14]

Because of the polycrystal nature in the sample of the NdFeAsO, a phase shift of $\pi$ in the composite loop in tunneling could occur at the Nb-Nd-1111 interface, or at the junction between two Nd-1111 grains.[4] Theoretically, there have been several studies to examine the possible $\pi$-phase shift involving an interface between a conventional superconductor and a Fe-pnictide with $s_\pm$ pairing under certain conditions,[15–19] which may help understand the possible $\pi$-junction at the Nb-Nd-1111 interface. The possibility of a $\pi$-phase shift in the interface of two Fe-pnictide intergrains of the same doping has not been carefully examined, although intuitively one may consider it unlikely. In this paper, we study a Josephson junction between the two iron pnictides. We find that when the junction barrier is thick and the two Fe-pnictide grains are oriented in certain directions relative to the interface, the junction gives a $\pi$-phase shift.

We start with a brief review on the charge current $I_J$ passing through a Josephson junction of two superconductors. $I_J = I_c \sin\delta\phi$,[20] with $I_c$ the critical current and $\delta\phi$ the phase difference between the two superconductors. The $\pi$-junction is a Josephson junction with negative critical current. The critical current for a junction between two conventional superconductors is defined as

$$I_c \propto \int d\mathbf{k}d\mathbf{q}\frac{|T_{\mathbf{kq}}|^2\Delta_1(\mathbf{k})\Delta_2(\mathbf{q})}{E_1(\mathbf{k})E_2(\mathbf{q})[E_1(\mathbf{k})+E_2(\mathbf{q})]}, \tag{1}$$

where $T_{\mathbf{kq}}$ is the tunneling matrix, $E_i(\mathbf{k}) = \sqrt{\epsilon_i(\mathbf{k})^2 + \Delta_i(\mathbf{k})^2}$ is the quasiparticle energy of the superconductor $i = 1,2$, respectively, $\epsilon_i(\mathbf{k})$ is the single electron energy measured relative to the chemical potential, and $\Delta_{1(2)}$ are superconducting gap functions, which we shall assume to be real here. The coefficient of the integral in Eq. (1) will always be taken positive throughout this paper. Equation (1) can be easily generalized to the iron pnictide superconductors, where electronic structure near the Fermi level is described by multibands. The critical current in this case is given by

$$I_c \propto \sum_{\alpha\beta}\int d\mathbf{k}d\mathbf{q}\frac{\left|T^{\alpha\beta}_{\mathbf{kq}}\right|^2\Delta^\alpha_1(\mathbf{k})\Delta^\beta_2(\mathbf{q})}{E^\alpha_1(\mathbf{k})E^\beta_2(\mathbf{q})\left[E^\alpha_1(\mathbf{k})+E^\beta_2(\mathbf{q})\right]}, \tag{2}$$

where all the notations are the same as in the single band case except for the additional band indices $\alpha$ and $\beta$. As pointed out by Sigrist and Rice,[21,22] though the critical current is not gauge invariant, the parity of the number of the $\pi$-junctions in a loop is gauge invariant. For the purpose of studying the possible $\pi$-phase shift in a closed loop involving Fe-pnictide superconductors, we choose a convenient gauge where the gap functions of the hole pockets are positive and the gap functions of the electron pockets are negative.

In the usual case, the junction between two identical superconductors is a 0-junction where $I_c$ is positive. Let us consider a point junction of two identical pnictide superconductors. In this case, $T^{\alpha\beta}_{\mathbf{kq}} = t_0$ is independent of crystal momentum and the band indices. The critical current is found to be

$$I_c \propto \sum_{\alpha\beta}\int d\mathbf{k}d\mathbf{q}\frac{\Delta^\alpha_1(\mathbf{k})\Delta^\beta_2(\mathbf{q})}{E^\alpha_1(\mathbf{k})E^\beta_2(\mathbf{q})\left[E^\alpha_1(\mathbf{k})+E^\beta_2(\mathbf{q})\right]}. \tag{3}$$

According to Ambegaokar and Baratoff, the above formula can be further written as

$$I_c \propto \sum_{\alpha\beta}\mathrm{sgn}(\Delta_\alpha\Delta_\beta)N_\alpha N_\beta\Delta_m K\left(\sqrt{1-\frac{\Delta^2_m}{\Delta^2_M}}\right), \tag{4}$$

where $N_\alpha$ is the density of states of the Fermi pocket $\alpha$, $\Delta_m = \min(|\Delta^\alpha|,|\Delta^\beta|)$, and $\Delta_M = \max(|\Delta^\alpha|,|\Delta^\beta|)$ are the smaller and larger gaps on the two Fermi pockets, respectively. $K$ is

 

the elliptical integral. In the special case, all the gap functions have the same amplitude, the elliptical function $K(0) = \pi/2$, so that $I_c \propto (\sum_\alpha \mathrm{sgn}(\Delta_\alpha) N_\alpha)^2 > 0$. This positive definiteness appears to remain valid when the gap amplitudes are different. To illustrate this point further, we consider below iron-based superconductor in the two-dimensional $\Delta$. We shall work in the extended Brillouin zone for convenience and set the Fe-Fe distance to be the length unit. There are two electron Fermi pockets with one around $(\pi,0)$ and one around $(0,\pi)$, and two hole Fermi pockets around $(0,0)$ point. We consider the case, where the superconducting gaps on one of the hole pockets and on the electron pockets are about the same while the gap on another hole pocket is smaller, as reported in ARPES for $BaFe_2As_2$.[22] By using the properties of the elliptical function, $\sqrt{1-k^2}K(k) \leqslant K(0) = \frac{\pi}{2}$, the critical current $I_c$ is found to be always positive. This illustrates that the different signs of the $s$-wave gap functions is a necessary but not a sufficient condition for a $\pi$-junction. Below, we shall examine a thick barrier junction between two pnictide superconductors of certain orientation and show that such a junction may give a $\pi$-phase shift.

We consider two half-infinite iron pnictide samples separated by a vacuum barrier with height $U$ and width $d$ as shown in Fig. 1. The interface is along $yz$ plane so that the momentum components along $y$ and $z$ directions are conserved in the tunneling process. For a thick barrier, the usual assumption that the tunneling matrix element $T$ is independent of momentum or crystal momentum is no longer valid. This can be illustrated by examining the free electron tunneling process in quasi one dimension, where $|T|^2$ is the transmission coefficient of the scattering problem. For a potential barrier normal to $x$ direction with height $U$ and length $d$, the transmission coefficient reads

$$|T|^2 = \frac{4\kappa^2 k_x q_x}{\kappa^2(k_x+q_x)^2 + \left(\kappa^2+k_x^2\right)\left(\kappa^2+q_x^2\right)\sinh^2(\kappa d)}, \tag{5}$$

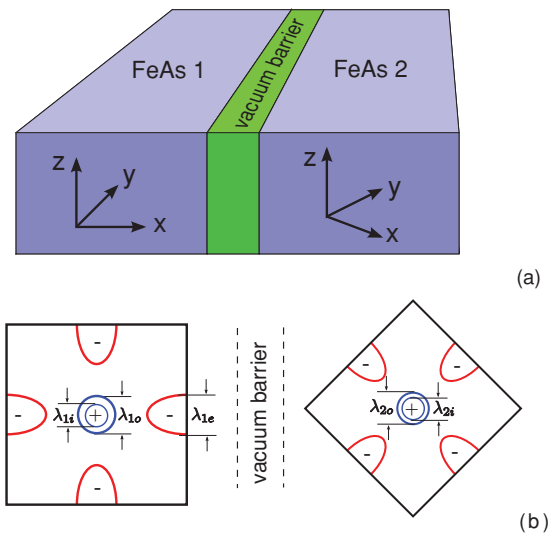


FIG. 1. (Color online) (a) Schematic diagram of a Josephson junction of two iron pnictides separated by a thick vacuum barrier. (b) The corresponding Fermi surfaces in the Brillouin zone for the two materials.

where $k_x$ and $q_x$ are the $x$-direction wavevector of the incoming and outgoing plane waves, respectively, $\kappa$ is the imaginary wavevector inside the barrier with $\kappa = \frac{1}{\hbar}\sqrt{2m(U-E)+\hbar^2 k_\parallel^2}$, $m$ is the mass of the electron, and $k_\parallel$ is the wavevector parallel to the barrier interface, which is conserved in the scattering process. In the thick barrier limit, i.e., $\kappa d \gg 1$, one have

$$|T|^2 \simeq \frac{16\kappa^2 k_x q_x}{\left(\kappa^2+k_x^2\right)\left(\kappa^2+q_x^2\right)} e^{-2\kappa d}. \tag{6}$$

If we assume that $p \equiv \frac{1}{\hbar}\sqrt{2m(U-E)} \gg k_\parallel$, Eq. (6) can be further simplified,

$$|T|^2 \propto \frac{\kappa^2 k_x q_x}{\left(\kappa^2+k_x^2\right)\left(\kappa^2+q_x^2\right)} e^{-\frac{k_\parallel^2}{p}d}, \tag{7}$$

so the transmission coefficient decays exponentially with the increment of planar wavevector $k_\parallel$. The above formula can be extended to the electron tunneling process in a lattice with the following modifications as pointed out by Mazin.[23] All the wavevectors in the above equation are replaced by the corresponding group velocities except $k_\parallel$ in the exponential factors which tracks the oscillation of the wavefunction parallel to the interface direction. The second modification is to replace the plane wavefunction in the free electron case by a Bloch wave $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\omega_{n\mathbf{k}}(\mathbf{r})$. The periodical function $\omega_{n\mathbf{k}}$ can be further Fourier transformed to $\omega_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{K}} F_{n\mathbf{k},\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}}$, where $\mathbf{K}$ is reciprocal lattice vector. If $\omega_{n\mathbf{k}}(\mathbf{r})$ is localized, one can approximate $F_{n\mathbf{k},\mathbf{K}} \sim$ constant for not very large $\mathbf{K}$. The wavefunction can finally be written as

$$\psi_{n\mathbf{k}}(\mathbf{r}) = F_{n\mathbf{k}} \sum_{\mathbf{K}} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}. \tag{8}$$

As shown in Fig. 2, the tunneling matrix reduces very fast with increasing $(\mathbf{k}+\mathbf{K})_\parallel$. This indicates that the contribution is mainly from the component with $K_\parallel = 0$, so the tunneling

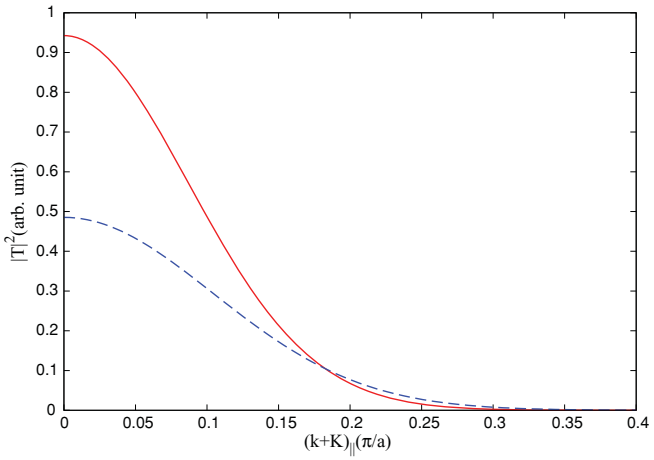


FIG. 2. (Color online) $|T|^2$ for various $(\mathbf{k}+\mathbf{K})_\parallel$ with $U-E=1$ eV (red solid line) and $U-E=2$ eV (blue dashed line), respectively. Here we assume $v_{\alpha\mathbf{k}x} = v_{\beta\mathbf{q}x} \approx 10^5$ m/s, $m = m_e$, $d = 10a$.

matrix reads

$$\left|T_{\mathbf{kq}}^{\alpha\beta}\right|^2 \propto A_{\alpha\mathbf{k},\beta\mathbf{q}} \sum_{\mathbf{K},\mathbf{Q}} 4m^2\hbar^2\kappa^2\delta_{(\mathbf{k}+\mathbf{K})_\parallel,(\mathbf{q}+\mathbf{Q})_\parallel} \times \frac{v_{\alpha\mathbf{k}x}v_{\beta\mathbf{q}x}}{\left(\hbar^2\kappa^2+m^2v_{\alpha\mathbf{k}x}^2\right)\left(\hbar^2\kappa^2+m^2v_{\beta\mathbf{q}x}^2\right)} e^{-\frac{(\mathbf{k}+\mathbf{K})_\parallel^2}{p}d}, \quad (9)$$

where $\mathbf{K}$ and $\mathbf{Q}$ are the reciprocal lattice vectors of FeAs samples 1 and 2, respectively, $\kappa = \frac{1}{\hbar}\sqrt{2m(U-E)+\hbar^2(\mathbf{k}+\mathbf{K})_\parallel^2}$, the delta function tracks the planar momentum conservation, $A$ is a factor related to the detail information of the electron wavefunction and can usually be approximated as constant, and $v_{\alpha\mathbf{k}x}$ is the group velocity along $x$ direction of the electron in band $\alpha$ with lattice wavevector $\mathbf{k}$.

The exponential factor in Eq. (9) can be rewritten as $e^{-\frac{\mathbf{k}_\parallel^2}{p}d}e^{-\frac{(2\mathbf{k}+\mathbf{K})_\parallel\cdot\mathbf{K}_\parallel}{p}d}$, where the first term is the contribution of the Brillouin zones with $K_\parallel = 0$. In the following, we neglect the z-axis dispersion, which is very weak in 1111 compound, and only consider the physics of FeAs plane. We find that only the contribution from the Brillouin zone with $K_\parallel = 0$ is important,[24] and therefore Eq. (7) becomes

$$\left|T_{\mathbf{kq}}^{\alpha\beta}\right|^2 \propto \delta_{k_y,q_y} v_{\alpha\mathbf{k}x}v_{\beta\mathbf{q}x}e^{-\frac{k_\parallel^2}{p}d}. \quad (10)$$

Because of the fast drop of the coherence factor $\frac{\Delta}{2E}$ in the critical current when the state is away from the Fermi surface, the planar momentum conservation parallel to the interface, and the exponential factor in tunneling matrix in Eq. (10), only the electron pockets around $X$ and the hole pockets of iron-pnictide sample 1 and the hole pockets of sample 2 are important in the configuration shown in Fig. 1. Because $\mathbf{k}_\parallel \sim 0$, the exponential factor in Eq. (10) becomes a constant. For simplicity, we assume that the gap $\Delta$ is momentum independent which is consistent with the ARPES result.[2] By substituting Eq. (10) into Eq. (2) and noticing that velocity $v_x \propto \frac{\partial\epsilon}{\partial k_x}$, the critical current reads

$$I_c \propto \sum_{\alpha\beta}\int dk_y \int_{\epsilon_m^\alpha(k_y)}^{\epsilon_M^\alpha(k_y)} d\epsilon_1 \int_{\epsilon_m^\beta(k_y)}^{\epsilon_M^\beta(k_y)} d\epsilon_2 \frac{\Delta_1^\alpha\Delta_2^\beta}{E_1^\alpha E_2^\beta\left[E_1^\alpha+E_2^\beta\right]}, \quad (11)$$

where $\epsilon_m^\alpha(k_y)$ and $\epsilon_M^\alpha(k_y)$ are the minimum and maximum energies, respectively, of the electron in band $\alpha$ with given $k_y$ and any $k_x$. If $\epsilon_m^{\alpha(\beta)}(k_y) - E_f \ll -\Delta_{\alpha(\beta)}$ and $\epsilon_M^{\alpha(\beta)}(k_y) - E_f \gg \Delta_{\alpha(\beta)}$, the last two integrals can be approximated by $\mathrm{sgn}(\Delta_\alpha\Delta_\beta)\Delta_m K(\sqrt{1-\Delta_m^2/\Delta_M^2})$, where $\Delta_m$ and $\Delta_M$ are the smaller and larger amplitudes of the two gaps $\Delta_\alpha$ and $\Delta_\beta$, respectively. Then Eq. (11) becomes

$$I_c \propto \sum_{\alpha\beta}\mathrm{sgn}(\Delta_\alpha\Delta_\beta)\Delta_m K\left(\sqrt{1-\frac{\Delta_m^2}{\Delta_M^2}}\right)\min(\lambda_{1\alpha},\lambda_{2\beta}), \quad (12)$$

where $\lambda_{l\gamma}$ is the length of the Fermi pocket $\gamma$ of FeAs sample $l$ in the direction parallel to the interface as indicated in Fig. 1(b). Equation (12) is the main result of the present work on $\pi$- or 0-Josephson junction of two pnictide superconductors shown in Fig. 1 with a thick barrier.

In the iron pnictides case, we consider three Fermi pockets, the electron pocket, the inner hole pocket, and the outer hole pocket, which are denoted by "e", "i", and "o", respectively. Note that the other electron pocket does not come into play in the thick barrier of our interest, and will not be considered. According to the ARPES result,[2] we assume that $\Delta_e = \Delta_o = 2\Delta_i$. With $K(\sqrt{3}/2) \approx 2.44$ and $K(0) = \pi/2 \approx 1.57$, we have

$$I_c \propto 1.57[\min(\lambda_{1o},\lambda_{2o}) + \min(\lambda_{1i},\lambda_{2i}) - \min(\lambda_{1e},\lambda_{2o})] + 1.22[\min(\lambda_{1o},\lambda_{2i}) + \min(\lambda_{1i},\lambda_{2o}) - \min(\lambda_{1e},\lambda_{2i})]. \quad (13)$$

From the above equations, we can see that $I_c$ is usually positive and is negative only if the conditions below are fulfilled: an anisotropic outer hole pocket ($\lambda_{2o} > \lambda_{1o}$), a large electron pocket ($\lambda_e > \lambda_o$), and a rather small inner pocket ($\lambda_i < \lambda_o$). In a hole-doped pnictide superconductor, the inner hole pocket is not small, and our theory predicts a 0-junction between two identical hole-doped pnictides. In the electron-doped material, these conditions may be fulfilled. In that case, Eq. (13) becomes

$$I_c \propto -1.57\delta\lambda_o + 2.79\lambda_i, \quad (14)$$

where $\delta\lambda_o = (\lambda_{2o} - \lambda_{1o})$ is the anisotropy of outer hole Fermi pocket. The anisotropy of the inner pocket is neglected because the pocket is very small, and the parameter regime for $\pi$-junction is shown in Fig. 3.

To be more specific, we consider the material used in the experiment by Chen *et al.*[4] which is a polycrystal Nd-1111 crystal with electron concentration $x \sim 0.12$. The experimental study of Fermi surface topology of doped 1111 material is still absent because there is no such single crystal. But according to the ARPES experiment on electron-doped 122 material $Ba(Fe_{1-x}Co_x)_2As_2$, the inner hole pocket vanishes while the width of electron pocket is comparable with the width of the outer hole pocket, i.e., $\lambda_i \approx 0$ and $\lambda_e \approx \lambda_o$, in the case of a smaller electron doping $x = 0.075$. With further doping of

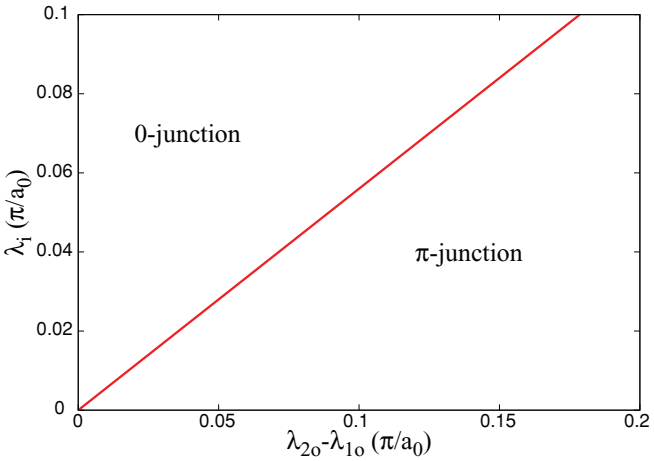


FIG. 3. (Color online) Parameter space for $\pi$-phase of a thick barrier Josephson junction between two identical pnictide superconductors shown in Fig. 1. $\lambda_i$ is the inner hole pocket length, and $\lambda_{2o} - \lambda_{1o}$ describes the anisotropy of the outer hole pocket, as indicated in Fig. 1 The red solid line is $\lambda_i = 0.56(\lambda_{2o} - \lambda_{1o})$, which separate the parameter space for 0 and $\pi$ junctions. The junctions in the hole-doped pnictides are expected to have 0-phase. The junction in electron-doped 1111 compound reported in Ref. 4 is likely to be at low corner of $\pi$-phase parameter space. (See text for discussions.)

the electrons, we have $\lambda_e > \lambda_o$. On the other hand, the density functional theory suggested that LaFeAsO, the hole pocket, has a small anisotropy and the Fermi wavevector along (110) direction is slightly larger than the one along (100) direction,[25] i.e., $\lambda_{2o} > \lambda_{1o}$. Therefore, we may conclude that the material used in Chen *et al.*'s experiment fulfills the requirement of Eq. (14). And according to Eq. (14), the junction depicted in Fig. 1 can be a $\pi$-junction in this case. In the extreme case, with $\lambda_i = 0$, one should get a $\pi$-junction in the thick barrier case. This result is consistent with the analysis on the Josephson junction between a $s_\pm$-pnictide superconductor and a single band $s$-wave superconductor in Ref. 26, where a $\pi$-junction may appear in an appropriate parameter regime.

In summary, we have examined the Josephson junctions between two Fe-pnictides with the same electron concentration assuming $s_\pm$-phase pairing. We found that it is impossible for the two Fe-pnictides to form a $\pi$-junction if the junction has a narrow vacuum barrier, where the tunneling matrix element is momentum independent. On the other hand, a $\pi$-junction can be formed in the thick barrier case for electron-doped pnictides with vanishing or small inner hole pockets. Such $\pi$-junctions may be the origin of the $\pi$-flux jump in Chen *et al.*'s experiment.

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