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π Junction to Probe Antiphase s-Wave Pairing in Iron Pnictide Superconductors

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Josephson junctions between a FeAs-based superconductor with antiphase s-wave pairing and a conventional s-wave superconductor are studied. The translational invariance in a planar junction between a single crystal pnictide and an aluminum metal greatly enhances the relative weight of electron pockets in the pnictide to the critical current. In a wide doping region of the pnictide, a planar and a point contact junction have opposite phases, which can be used to design a trijunction ring with π phase to probe the antiphase pairing.

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One of important issues for the newly discovered iron pnictide superconductors (SCs) [1–9] is their pairing symmetries. A number of experiments [10–13] have suggested a spin singlet s-wave pairing. The iron pnictide has hole and electron Fermi pockets (Fig. 1). Theories have predicted an antiphase s wave or $s_{\pm}$ state, where the pairing has an s-wave symmetry, but the order parameters on the electron and hole pockets have opposite signs [14–19]. It will be important to confirm the $s_{\pm}$ state for pnictides, especially using more decisive phase sensitive experiments, which provided a direct evidence for the $d_{x^2-y^2}$ pairing for cuprates [20,21]. Since $s_{\pm}$ phase is related to the $\vec{k}$-space location instead of the orientation, different types of phase sensitive experiments are needed to probe the signs of the gap functions [22–26]. Very recently, Chen *et al.* [13] have carried out a new phase sensitive experiment on polycrystal NdFeAsO compound, and observed integer and half-integer flux quantum transitions in a niobium/Fe pnictide loop, which clearly demonstrates the sign changes of the order parameters in Fe pnictides.

In this Letter, we study Josephson junctions between a FeAs-based SC of $s_{\pm}$ pairing and a conventional s-wave SC. The translational invariance in a planar junction between a single crystal pnictide and an aluminum metal greatly enhances relative weight of electron pockets to the critical current. In a wide doping region for both $BaFe_2As_2$ (122 hereafter) and LaFeAsO (1111 hereafter) compounds, a planar and a point-contact junction have opposite phases. This property can be used to design a trijunction ring with π phase to probe the antiphase s-wave pairing.

We start with a brief review on the charge current I_J passing through a Josephson junction of two conventional SCs. $I_J = I_c \sin\delta\phi$, with I_c the critical current and $\delta\phi$ the phase difference between the two SCs. In the absence of magnetic fields or magnetic impurities, we may focus on I_c, which is of the form

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

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 SC $i = 1, 2$, $\epsilon_i(\mathbf{k})$ is the single electron energy measured relative to the chemical potential, and $\Delta_{1(2)}$ are superconducting gap functions (assumed to be real). The proportional coefficient in I_c are always positive throughout this Letter. The junction is a 0 junction if $I_c > 0$, and a π junction if $I_c < 0$. If both SCs are simple s wave, $\Delta_i(\mathbf{k})$ are independent of $\mathbf{k}$, and the sign of I_c is determined by the relative signs of Δ_1 and Δ_2. Though Δ is not gauge invariant, Sigrist and Rice [27] have pointed out that the π junctions cannot be gauged away if there are odd numbers of π junctions in a loop.

Equation (1) can be extended to study Josephson junctions between a pnictide and a conventional SC. Let Δ_2 be the superconducting gap and $E_2(\mathbf{q})$ the quasiparticle energy of a conventional s-wave SC, and γ the band index of the pnictide. We shall neglect the interband pairing amplitude in the pnictide, whose effect is small due to the energy splitting of the bands [19]. Denoting $\Delta_1^{\gamma}(\mathbf{k})$ the supercon-

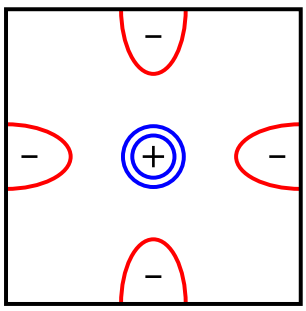

FIG. 1 (color online). Schematic plot of Fermi surface of pnictide in an extended Brillouin zone where each unit cell contains one Fe ion. Signs represent phase of the superconducting gap.

ducting gap of the band γ and $E_1^\gamma(\mathbf{k})$ the corresponding quasiparticle energy, we have

$$I_c \propto \Delta_2 \sum_\gamma \int d\mathbf{k} d\mathbf{q} \frac{|T_{\mathbf{kq}}|^2 \Delta_1^\gamma(\mathbf{k})}{E_1^\gamma(\mathbf{k}) E_2(\mathbf{q})[E_1^\gamma(\mathbf{k}) + E_2(\mathbf{q})]}. \quad (2)$$

Because of small value in Δ/E for states far from the Fermi surface, the integral in Eq. (2) is of appreciable value only for $\mathbf{k}$ and $\mathbf{q}$ near their Fermi surfaces. The Fermi pockets in Fe pnictide are well separated, so we may replace $\sum_\gamma \int d\mathbf{k}$ in Eq. (2) by integrals over $\mathbf{k}$ within a small cutoff around each Fermi pocket α. Assuming Δ_1^α to be isotropic near each Fermi pocket α, we have

$$I_c \propto \Delta_2 \sum_\alpha \Delta_1^\alpha \int d\mathbf{k} d\mathbf{q} \frac{|T_{\mathbf{kq}}|^2}{E_1^\alpha(\mathbf{k}) E_2(\mathbf{q})[E_1^\alpha(\mathbf{k}) + E_2(\mathbf{q})]}, \quad (3)$$

where the sum of α is over all the Fermi pockets within the Brillouin zone (BZ), and the integral of $\mathbf{k}$ is over the Fermi pocket α within a small cutoff.

We choose a convenient gauge where the gap function of the conventional s-wave SC is positive and the gap function of the hole (electron) pockets in the Fe pnictide SC is positive (negative). To simplify the calculations, we shall neglect the dispersion of the Fermi surface in the direction perpendicular to the Fe plane in the pnictide [11]. In what follows we will use Eq. (3) to study point and planar junctions. While our formalisms may be applied to all the iron-based SC, we will primarily discuss 122-based SC for its availability of good single crystals. The junctions for 1111-based SC will be briefly discussed.

Point junction between $s_\pm$ and s-wave SC.—For point junction, there is no momentum conservation in the tunneling. The tunneling direction relative to the FeAs plane is also random, so that the tunneling matrix is insensitive to the d orbitals and, hence, to the bands in the Fermi pockets. We may then set $T_{\mathbf{kq}} = T_0$ to be a constant, and Eq. (3) becomes

$$I_c \propto |T_0|^2 \sum_\alpha \Delta_1^\alpha \Delta_2 N_{1F}^\alpha N_{2F} \int d\epsilon_1 d\epsilon_2 \frac{1}{E_1^\alpha E_2[E_1^\alpha + E_2]},$$

where N_{1F}^α and N_{2F} are the density of states (DOS) on the Fermi pocket α of the pnictide and of the s-wave SC at the Fermi level, respectively. Following Ambegaokar and Baratoff [28], assuming $\Delta_2 \ll |\Delta_1^\alpha|$, we have

$$I_c \propto N_{2F} \Delta_2 \sum_\alpha \mathrm{sgn}(\Delta_1^\alpha) N_{1F}^\alpha K\left[\sqrt{1 - \frac{\Delta_2^2}{(\Delta_1^\alpha)^2}}\right], \quad (4)$$

where $K(x)$ is the first kind complete elliptic integral. The amplitude of Δ_1^α of the Fe pnictide are of the same order [11]. In the limit of $|4\Delta_1^\alpha/\Delta_2| \gg 1$, I_c is given by

$$I_c \propto \sum_{\alpha \in BZ} \mathrm{sgn}(\Delta_1^\alpha) N_{1F}^\alpha, \quad (5)$$

where the sum is over pockets α within the BZ. Therefore, $I_c > 0$ if the hole DOS N_h is larger than the electron DOS N_e, and $I_c < 0$ if $N_h < N_e$. We have carried out density functional theory (DFT) calculations and the results for 122 compounds are shown in Fig. 2(a). From the figure, the point-contact junctions are 0 junctions except at very large electron doping.

Planar junction.—We now consider a junction between a 122 single crystal and a nearly free electron Al with a spherical Fermi surface, as shown in Fig. 3. The thin insulator plane in the junction is parallel to the FeAs plane (x-y plane) of the pnictide. In a nearly free electron metal, the lattice potential of the material is very weak, so that we may neglect the lattice effect, and the junction has a translational symmetry in the x-y plane. Otherwise, we assume the tunneling matrix element to be independent of the Fermi pockets, $T_{\mathbf{kq}} = T_0 \delta_{k_{xy}, q_{xy}}$, where k_{xy} and q_{xy} are the planar wave vectors. This assumption is valid if there are only two orbitals d_{xz} and d_{yz} involved, for they are related by a 90° rotational symmetry. In Fe pnictide, there are five $d-$ orbitals with more weight on d_{xz} and d_{yz}, but finite weight on others [29]. We expect that our approximation is reasonably good, and will return to discuss the correction to this approximation.

It is convenient to work on the repeated zone scheme, where the BZ of the wave vector $\mathbf{k}$ of the pnictide is expanded into an infinite plane. Because of the planar momentum conservation, noting that the integral in Eq. (2) is

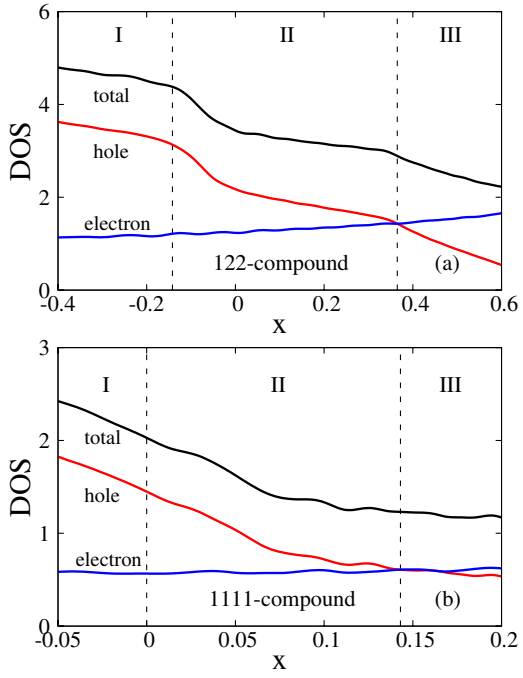

FIG. 2 (color online). Hole DOS N_h (red curve) and electron DOS N_e (blue curve), and total DOS versus doping x for 122 compound (a) and 1111 compound (b), where $x > 0$ for electron and $x < 0$ for hole dopings. The point junction is a 0 junction in regions I and II, and a π junction in region III. The planar junction is a 0 junction in region I, and a π junction in regions II and III. So the trijunction loop in Fig. 4 has a π phase in region II.

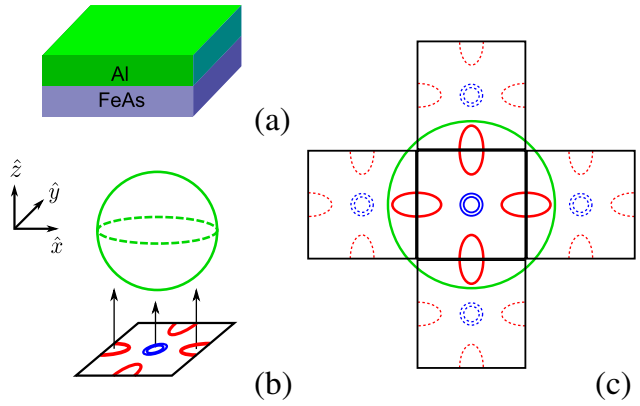

FIG. 3 (color online). (a) Proposed planar junction, whose interface is parallel to the x-y plane. (b) Illustration of electron tunneling (black arrows) with planar momentum conservation. Top sphere (green): Fermi surface of Al metal; bottom: Fermi surface of Fe pnictide. (c) Fermi surface of Al (green circle) and Fe pnictide (blue lines near the center of the circle for hole and red lines near the circles for electron pockets) at $q_z = 0$. Black lines are the BZ boundary. The Fermi pockets outside the green circle have no contribution to the Josephson current.

only of appreciable value near the Fermi surfaces or pockets, Eq. (3) becomes

$$I_c \propto |T_0|^2 \Delta_2 \int_{|k_{xy}|<q_F} dk_{xy} dq_z \sum_\alpha \frac{\Delta_1^\alpha}{E_1^\alpha(k_{xy}) E_2(k_{xy}, q_z)} \times \frac{1}{E_1^\alpha(k_{xy}) + E_2(k_{xy}, q_z)}, \quad (6)$$

where q_F is the Fermi wave vector and q_z the z-component wave vector of the conventional SC. The sum of k_{xy} is within the circle of a radius q_F in the x-y plane, and $\sum_\alpha$ stands for the summation over all the Fermi pockets within the circle of radius q_F as illustrated in Fig. 3. The tunneling process for the wave vector outside the BZ is due to the umklapp process.

For a free electron metal, we have $\int dq_z \approx (C/\sqrt{q_F^2 - k_{xy}^2}) \int d\epsilon_2$, with C a constant. To further calculate I_c, we approximate k_{xy} in the term of $1/\sqrt{q_F^2 - k_{xy}^2}$ by a mean squared average of the wave vector Q_α within the Fermi pocket α, and obtain

$$I_c \propto T_0^2 \Delta_2 \sum_{\alpha \in q_F} \frac{\mathrm{sgn}(\Delta_1^\alpha) N_{1F}^\alpha}{\sqrt{q_F^2 - Q_\alpha^2}} K\left(\sqrt{1 - \frac{\Delta_2^2}{(\Delta_1^\alpha)^2}}\right) \sim \Delta_2 \sum_\alpha \frac{\mathrm{sgn}(\Delta_1^\alpha) N_{1F}^\alpha}{\sqrt{q_F^2 - Q_\alpha^2}}. \quad (7)$$

For Al, the Fermi surface is a sphere [see Fig. 3(b)] of a radius of the Fermi wave vector $q_F = 1.75$ Å$^{-1} = 1.56\pi/a$, with $a = 2.8$ Å the distance of two nearest neighbor irons in 122 compound. As we can see from Fig. 3(c), the area, hence, the DOS of the electron pockets enclosed within a circle of q_F, is twice the area or the DOS within the BZ of the Fe pnictide. By using Eq. (7) and the results of N_e and N_h from DFT, approximating $Q_\alpha = \pi/a$ for the electron pockets, and $Q_\alpha = k_F^h(k_z = 0)$, the Fermi momentum for the hole pockets, we find $I_c < 0$ when $N_h/N_e < 2.58$ which corresponds to regions II and III in Fig. 2(a). In our calculations, we have assumed the tunneling matrix to be independent of the momentum or the Fermi pockets. In 122 compounds, in addition to d_{xz} and d_{yz} orbitals, the electron configuration on the hole pockets contains d_{3z^2-1} orbital, and also contains more $d_{x^2-y^2}$ or d_{xy} orbitals than on the electron pockets. Because of their orbital orientations, the d_{3z^2-1} orbital enhances the tunneling matrix, and the $d_{x^2-y^2}$ and d_{xy} orbitals do the opposite. Therefore, their overall effect to the condition of the π junction is partially canceled. We expect the results obtained by this approximation to be qualitative or semiqualitatively correct.

We have also combined DFT results and angle-resolved photoemission spectroscopy (ARPES) data to calculate I_c and obtained similar results. In the calculation, we use Eq. (3) directly by taking into account the planar momentum conservation. We apply a rigid band approximation for the normal state electron state in DFT and take the gap functions of the hole doped 122 compound from ARPES data of Ding *et al.* [11]. The dispersion in Al is modeled by $\epsilon_{\mathbf{q}} = q^2\hbar^2/2m^*$, with the effective mass of the electron $m^* = 1.16 m_e$, and m_e the free electron mass. We assume a BCS gap function for Al SC at $T = 0$ based on the value of $T_c = 1.175$ K. We have found the planar junction is of π phase at hole doping up to 0.4, which gives a wider region for the π junction.

Trijunction to probe $s_\pm$ symmetry.—We now discuss Josephson trijunction to probe the $s_\pm$ pairing in Fe pnictide SC. The experimental setup is illustrated in Fig. 4, similar to that in Ref. [13]. Fe pnictide is chosen so that its planar junction with Al is a π junction, and its point junction with

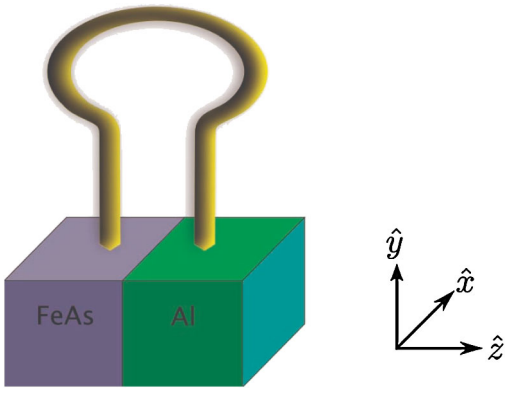

FIG. 4 (color online). A Trijunction setup, consisting of a planar junction between Al and Fe pnictide SC, and a point junction between a conventional SC (say, niobium) and Al and a point junction between the niobium and the pnicitide.

niobium is a 0 junction. The trijunction configuration is then a π loop characterized by half-integer flux quantization. The condition for the such a π junction of the planar and 0 junction of the point junctions is illustrated in Fig. 2(a) for a 122 compound. As we can see, there is a large region of the material space to satisfy the π trijunction condition.

Let us briefly discuss the electron doped 1111 compound, which will be important when its single crystal becomes available. Our DFT calculations show that $N_h/N_e > 1$ at the doping $x < 0.15$, and $N_h/N_e < 1$ at $x > 0.15$. Therefore, its point junction with a conventional SC will be a 0 junction at $x < 0.15$ and a π junction at $x > 0.15$, as shown in Fig. 2(b). A planar junction between 1111 compound and Al SC is found to have π phase for all the electron doped region studied. Hence a setup in Fig. 4 for 1111 with $x < 0.15$ is expected to be a π-junction loop.

We remark on the implication of the experimental observation of the π-junction loop in the setup of Fig. 4. A π junction indicates the opposite phases in the point and planar junctions in which the FeAs SC are involved. This would rule out a conventional s-wave pairing or a d-wave pairing such as $d_{x^2-y^2}$ or d_{xy}. The latter will result in a vanishing critical current in a junction with an s-wave SC. Thus the observation of the π-junction loop should be a clear indication of the $s_{\pm}$ pairing state for the FeAs SC.

Trijunction with two-pnictide SCs.—We now turn to a discussion of a Josephson trijunction ring, consisting of two single crystal Fe pnictides and one conventional SC, say, niobium. The junctions between each of the Fe pnictide and the niobium are both point contact, and the junction between the two pnictides is a planar one with the junction plane parallel to the FeAs planes in both the pnictides. We request $N_h > N_e$ in the first Fe pnictide, and $N_h < N_e$ in the second Fe pnictide. Therefore, one of the point junctions is 0 junction, and the other is π junction. The pnictide-pnictide planar junction is a 0 junction because of the x-y plane crystal momentum conservation in the tunneling process, where the tunnelings only occur between hole pockets or between electron pockets in the two SCs. The trijunction ring thus designed should have a π junction in nature. The experimental challenge to design this trijunction is related to the sample quality and the selection of the second Fe pnictide where the electron DOS is larger. The DFT calculations suggest that the 1111 compound is a good candidate for this type of trijunctions when the single crystals become available.

In summary, we have examined the phase of the Josephson junctions between Fe pnictide and conventional s-wave superconductors. The sign of a point-contact junction is positive if the hole DOS is larger than the electron DOS in Fe-pnictide and is negative otherwise. In the planar junction between a single crystal Fe pnictide and Al, planar translational invariance in the tunneling enhances the contribution of electron pockets to the critical current. We have proposed a Josephson trijunction to probe the $s_{\pm}$ symmetry in Fe pnictide, which appears to be accessible in experiments.

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