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Designing phase-sensitive tests for Fe-based superconductors

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We suggest experimental designs suitable to test pairing symmetry in multiband Fe-based superconductors. These designs are based on combinations of tunnel junctions and point contacts and should be accessible by existing sample fabrication techniques. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4788720]

Four years after the discovery of the family of high-T_c Fe-based superconductors (FeBS),[1] their pairing symmetry is still under dispute.[2] While most researchers favor the so-called $s_\pm$ pairing, whereupon the sign of the order parameters changes between the hole and the electron bands,[3] some advocate[4] the more conventional anisotropic s, and for the extreme cases, such as KFe_2As_2 and $K_xFe_2Se_2$, other alternatives have been suggested (d-wave, or other types of sign-changing s). This reminds us of the controversy in the high-T_c cuprates, when proponents and deniers of the d-wave pairing were clinched in dead heat for several years, until the first phase-sensitive tunneling experiments had been performed,[5–8] and showed unambigously that the Josephson current flowing from a cuprate sample along the y direction is shifted by $\phi = \pi$ with respect to the corresponding current flowing in the x direction.

Despite recent progress in junction fabrication,[9,10] no such (or similar) phase-sensitive experiments have been performed so far in FeBS-based Josephson junctions, designed and produced in a controllable way. Only indirect evidence that Josephson loops with a π phase shift can be formed in these materials was reported in Ref. 11, where samples with a large number of randomly formed contact pairs were measured.

Apart from problems with sample preparations, and other technical obstacles, a serious barrier preventing similar decisive experiments in FeBS is the fact that the two main contenders for the pairing state in the "mainstream" FeBS are $s_\pm$ and s_{++}, two states that have the same orbital symmetry. Therefore, one needs to design the experimental geometry in a particular clever way so that the current in one contact would be dominated by the carriers having one sign of the order parameter, and in the other by carriers with the opposite sign. Note that designing the Josephson contacts so that current would be flowing in different Cartesian directions is not necessary, and in fact not helpful at all, because an s-wave superconductor is invariant under the x-y rotation.

Several designs aimed at exploiting particular Fermi surface topology of FeBS have been suggested, such as placing contacts at an angle different from 90° or below and above a sandwich of two different superconductors.[12,13] All these suggestions have proven to be too complicated to be realized in practice. In this letter, we suggest three experimental designs, all of them much simpler than all proposed previously. All these designs should be accessible by available experimental techniques and existing sample manufacturing is already at a level sufficient for exploiting the ideas suggested in this work.

Before describing our suggestions in detail, we would like to make a general observation that in fact allowed us to come up with the designs so much simpler than those discussed previously. There is a powerful tool in our hands, namely, a choice between planar tunnel junctions, where the current is dominated by the electrons with the momentum normal to the interface, and point contacts that collect the current indiscriminately from all electrons.

Let us elaborate more on the first point.

For planar tunnel junctions with a thick specular barrier electrons tunneling normal to the interface have an exponentially big advantage over those with a finite momentum parallel to the interface, $k_\parallel \neq 0$. For instance, the tunneling probability $T_\mathbf{k}$ for a simple vacuum barrier can be expressed as[14]

$$T_\mathbf{k} = \frac{4m_0^2\hbar^2K^2 v_L v_R}{\hbar^2 m_0^2 K^2 (v_L + v_R)^2 + (\hbar^2K^2 + m_0^2 v_L^2)(\hbar^2K^2 + m_0^2 v_R^2)\sinh^2(dK)}. \quad (1)$$

Here, m_0 is the electron mass, $v_{L,R}$ are the Fermi velocity projections on the tunneling directions, d is the width of the barrier, and the quasimomentum of the evanescent wavefunction in the barrier, iK, is from the energy conservation,

$$K = \sqrt{k_\parallel^2 + 2(U - E_F)m_0}, \quad (2)$$

where U is the barrier height. If $dK \gg 1$, in other words, if the barrier is sufficiently thick, this expression reduces to $4m_0^2 v_L v_R/\hbar^2K^2\sinh^2(dK) \approx 16 m_0^2 v_L v_R \exp(-2dK)/\hbar^2K^2 \approx T_{\mathbf{k}=0}\exp[-\ k_\parallel^2/4m_0(U - E_F)]$. Thus, the conductance is exponentially suppressed except when $k_\parallel^2/2m_0 \lesssim 2(U - E_F)$. Since $U - E_F \ll E_F$, this is usually a rather narrow cone, provided that $k_\parallel$ is conserved.

The Josephson current in such tunnel junction between a single- and multi-band superconductor is determined by a standard Ambegaokar-Baratoff formula

$$I_S = \frac{\pi T}{eR_0} \sum_{n,i=1,2} \frac{\Delta_L \Delta_R \sin\phi}{\sqrt{\omega_n^2 + \Delta_L^2}\sqrt{\omega_n^2 + \Delta_R^2}}, \tag{3}$$

where Δ_L is the gap in a single-band superconductor, Δ_R is the gap in a multi-band superconductor corresponding to a Fermi surface sheet in the center of the Brillouin zone, and R_0 is the corresponding tunneling resistance, controlled by small values of $k_\parallel$.

As mentioned, special precautions need to be taken to ensure the $k_\parallel$ conservation. On the other hand, point contacts (PC) that are usually forced mechanically into a sample have no lateral translational invariancy and thus no conservation of $k_\parallel$. In real life, a point contact is a complex system containing multiple microcontacts, some of them are diffusive and some ballistic. The only important issue for us is that electrons with all values of $k_\parallel$ contribute roughly equally to the total current (no tunneling cone effect). This situation can be modeled by a diffusive contact that does not respect momentum conservation (we do not imply that *all* point contacts are diffusive, but we use a diffusive contact as an illustration of the effects of the loss of the $k_\parallel$ conservation).[15] Then, the relative contribution to supercurrent from band "i" is determined by the partial resistance $R_{Ni}^{-1} = (2Se^2/L)N_i D_i$,[16] where N_i, D_i are densities of states and diffusion coefficients in the corresponding band, L and S are the length and cross-section area of a contact. This amounts to adding all conductivity channels for each direction independently, resulting in the DOS-weighted average of the corresponding squared Fermi velocity, e.g., $\langle N(E_F)v_F^2\rangle$. In the practically relevant case when $\Delta_L \ll \Delta_{Ri}$, the Josepshon current in a diffusive ScS contact between a single- and a two-band superconductors is is given by the following simple expression:

$$I_S = \frac{\Delta_L}{e} \sum_{i=1,2} \left[\ln \frac{\Delta_{Ri}\cos\phi/2}{\Delta_L(1+\cos\phi)}\right] \frac{\sin\phi}{R_{Ni}}, \tag{4}$$

which is a multiband generalization of the well known formula (see, e.g., Refs. 16–18). From this formula, it follows, with logarithmic accuracy, that current-phase relation is sinusoidal with critical current controlled by the corresponding resistance R_{Ni} only.

Based on the theoretical consideration above, we want to suggest three experimental designs to test pairing symmetry in FeBS.

1. *Epitaxial sandwich.* Here, we propose to grow an electron-doped film (for instance, Co-doped $BaFe_2As_2$), and on top of this film, as shown in Fig. 1, to grow epitaxially a hole-doped film (K-doped $BaFe_2As_2$). Epitaxially grown films (there is hardly any lattice mismatch[19] between the optimally doped $K_xBa_{1-x}Fe_2As_2$ and optimally doped $BaCo_xFe_{2-x}As_2$) conserves the lateral translational symmetry, and therefore the electron momentum parallel to the interface is also conserved. This means that the conductance between the sandwich buns is dominated by the electron-electron and hole-hole currents,

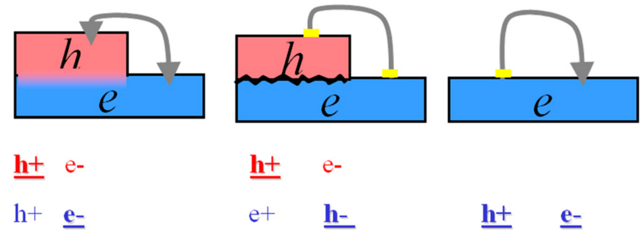

FIG. 1. Suggested experimental designs of Josephson π-loops: epitaxial sandwich (left); rough sandwich (middle); single sample (right).

while the electron-hole and hole-electron conversion, requiring a lateral momentum transfer of the order of $\hbar\pi/a$, will be suppressed (Table I).

Maximizing the Josephson energy at this epitaxial interface, we have to assign the same phases to the electron Fermi surfaces in both films, and the opposite phase to the hole Fermi surfaces. We now close the loop by attaching to the two films, as shown in Fig. 1, point contacts made out of a conventional superconductor. As discussed above, the current through a point contact is averaged over all electrons. Now, the current from the electron doped film into the point contact will be dominated by the electron Fermi surfaces, simply because these carriers dominate the bulk, and the current from the hole-doped film will be dominated by holes (we will give a quantitative justification of this assertion later in the paper). These two currents will thus have the opposite signs, or the phase shift of π.

2. *Rough sandwich.* Here, we suggest to physically combine two single crystals, or two films, without creating epitaxial contact between the two. Now our goal is to create a rough interface where the lateral momentum is not conserved at all, and any state in the electron-doped part of the sample can tunnel into any state of the hole part. In fact, a rough interface can be substituted by a thin layer of a conventional superconductor with no lattice matching to the FeBS, if that is more feasible experimentally. But, as long as we have created a contact between the two FeBS without momentum conservation, the current in this contact will be controlled by the majority carriers in each electrode, so that the hole in the hole-doped part will be in phase coherence with the electron

TABLE I. Three suggested designs for probing the relative phases of the order parameter in Fe-based superconductors. A tunneling barrier here is assumed to be thick enough to filter through the "tunneling cone" effect only the states near the zone center (holes), while a point contact is supposed to collect current in all directions and thus be dominated by the majority carriers. The sign of the order parameter is selected in such a way that the current through the left (upper) contact is always considered positive.

	Design		
Fig. 1 panel	Left	Middle	Right
Upper/left contact	Point	Tunnel	Tunnel
Lower/right contact	Point	Tunnel	Point
Upper Δ_{hole}	$-$	$+$	$+$
Upper Δ_{elec}	$+$	$-$	$-$
Interface	Epitaxial	Rough	n/a
Lower Δ_{hole}	$-$	$-$	n/a
Lower Δ_{elec}	$+$	$+$	n/a
Upper contact current dominated by	Electrons	Holes	Holes
Lower contact current dominated by	Holes	Holes	Electrons

one in the electron-doped part (to minimize the Josephson energy).

Now, we need to attach contacts to a conventional superconductor in such a way that the current in both will be dominated by holes, even in the part that is electron-doped, since now holes in the two electrodes have superconducting order parameters of the opposite signs. This can be achieved by using a planar junction with a sufficiently thick tunneling barrier in both contacts. As discussed above, a conventional planar tunneling barrier filters exponentially electrons with the momentum $\hbar\mathbf{k}$ such that $k_\parallel \sim 0$, where $k_\parallel \sim 0$ is the projection on the interface plane. This condition filters out electron states near the corner of the Brillouin zone and lets through only the hole states. Since, in this design, the phase coherence between the hole and the electron doped electrodes is between the carriers of the opposite character, we achieve a Josephson loop with a π shift between the contacts.

3. *Single sample*. The previous two designs relied on manufacturing a composite sample where the two contacts will be attached to two parts with different properties. In our last design, the job of creating a phase shift between the contacts is relegated to the difference in contacts themselves. Here, we propose a single sample (which can be a single crystal or a thin film), to which two contacts of different nature are attached. Importantly, the sample must be electron-doped, so that the normal current (and, by implication, the current through a point contact) would be dominated by electrons. We use one point contact, and one planar thick-barrier tunnel junction with the current direction along z. As discussed above, the former will be dominated by electrons and the latter by holes, which have small $k_\parallel$, thus again creating a π shift.

In all three designs discussed above, a π shift can be detected by combining the contacts into a two-junction interferometer with critical current $I_c = \sqrt{I_{c1}^2 + I_{c2}^2 \pm 2I_{c1}I_{c2}\cos 2\pi\Phi/\Phi_0}$. Here, $I_{c1,2}$ are critical currents of individual junctions, Φ is magnetic flux through the interferometer, Φ_0 is flux quantum, and sign $+$ $(-)$ corresponds to zero (π) shift between the contacts. In such interferometer, a π-shift shows up as a minimum of I_c at $\Phi = 0$ (the so-called π-SQUID behavior). It is important to note that to observe significant $I_c(\Phi)$ modulation, the critical currents $I_{c1,2}$ (and thus junctions resistances) should be of similar order of magnitude. Tunnel junctions have much higher specific barrier resistance R_0S than that in PC's; therefore, in our last design (3), tunnel contact should have large enough area to fulfill the above condition. Note that the ratio of the junction resistances, I_{c1}/I_{c2}, easily translates into the ratio of the I_c minima and maxima: $I_{\max}/I_{\min} = (I_{c1} + I_{c2})/|I_{c1} - I_{c2}| \approx 1 + 2\min(I_{ci}/I_{cj})$ (for a large current disparity). For instance, if $I_{c1} \ll I_{c2}$, this ratio is $2I_{c1}/I_{c2}$. This suggests that even an order of magnitude difference in contact resistances should not prevent the effect from being observed.

Finally, one may ask a question: our proposals are based on the assumption that the normal (diffusive) transport in electron and hole doped FeBS is dominated by the carriers of the corresponding sign; to what extent this assumption is justified in actual material? To answer this question, we have performed the standard linear augmented plane wave (LAPW) band structure calculations[20] and have computed the relevant quantity,[21] $\langle N(E_F)v_F^2\rangle$, as a function of doping (in the rigid band approximation, which is enough for our qualitative purpose). The results are shown in Fig. 2. As one can see, the condition that the diffusive current for electron-doped Ba122 material is dominated by electrons is well satisfied for both in-plane (x) and out-of-plane (y) directions, particularly well for overdoped ($\gtrsim$10%) samples (which are therefore preferable). The condition that for the hole doping the current be dominated by holes is less well fulfilled. Indeed, for optimal (0.2 hole/Fe) and even overdoped samples, the current in the z direction is still dominated by electrons, because the electron Fermi surfaces are more warped. However, the in-plane current is firmly dominated by holes for all composition with higher than 20% K content. Thus, the recommendation in this case is to manufacture a point contact that probes preferentially the in-plane conductivity. One possible way to pursue this goal is to use a needle that penetrates into the sample deep enough, so that the contacts form predominantly at its sides. In that case, the dominance of the hole current will be assured.

To conclude, we have suggested three experimental designs in order to test pairing symmetry in FeBS. These

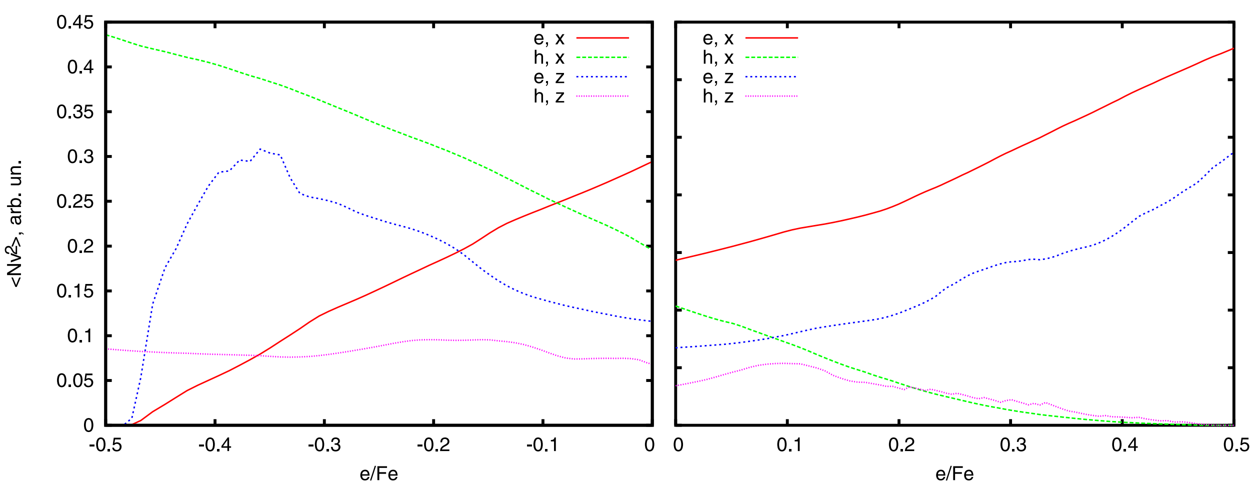

FIG. 2. Calculated transport function, $\langle N(E_F)v_F^2\rangle$, for the hole-doped (left panel) and electron-doped (right panel) $BaFe_2As_2$. Calculation for the electron-doped case was self-consistent in the virtual crystal approximation for the 10% Co doping and the rigid band approximation used around this composition. Similarly, the hole-doped composition was self-consistent for the 40% K doping and the rigid bands used thereafter.

designs involve Josephson two-junction interferometers where current in different contacts is dominated by different type of carriers, electrons, or holes. If pairing symmetry is of the $s_{\pm}$-type, a Josephson π-loop is realized (π-SQUID), while in the s_{++} case the standard SQUID behavior is expected. The suggested designs should be accessible by available fabrication techniques and should allow to probe pairing symmetry in FeBS.

It is worth noting that our predictions rely upon conservation of $k_{\|}$ at the epitaxial interface (in our design #1) or in the planar junctions (designs #2 and #3). For well controlled semiconducting interfaces, this is not a problem. On the other hand, for such materials as FeBS, it is hard to determine the degree of the momentum conservation. The corollary is that a failure to observe π-shifts in any of these experiments does not prove that superconductivity in FeBS is a constant-sign s-wave, although a success undoubtedly proves that it is $s_{\pm}$.

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