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Metastable π-junction between an $s_{\pm}$-wave and an s-wave superconductor

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We examine a contact between a superconductor whose order parameter changes sign across the Brillioun zone, and an ordinary, uniform-sign superconductor. Within a Ginzburg-Landau type model, we find that if the the barrier between the two superconductors is not too high, the frustration of the Josephson coupling between different portions of the Fermi surface across the contact can lead to surprising consequences. These include time-reversal symmetry breaking at the interface and unusual energy-phase relations with multiple local minima. We propose this mechanism as a possible explanation for the half-integer flux quantum transitions in composite niobium-iron pnictide superconducting loops, which were discovered in a recent experiment[1].

Introduction– Understanding the structure of the order parameter of the iron-based pnictide superconductors[2] is the key to unveil their pairing mechanism. A conventional, phonon-mediated mechanism is usually associated with an order parameter of a uniform sign, while sign changes in the order parameter are typical of unconventional mechanisms, in which pairing is driven by purely repulsive Coulomb interactions.

In the cuprates, the unambiguous identification of the d-wave symmetry of the order parameter came primarily from phase-sensitive experiments[3, 4]. These experiments exploit the fact that due to the d-wave symmetry, specific geometries (such as a corner junction with an s-wave superconductor, or a tri-junction between three d-wave superconductors) are guaranteed to produce a π phase shift in the phase of the superconducting order parameter. In the iron arsenides, similar experiments[5, 6] have found no evidence for d-wave symmetry.

From the theory side, it has been proposed that the pnictides have an extended s-wave ("$s_{\pm}$ wave") order parameter[7, 8], which can be chosen to be real but changes sign between the electron and hole pockets, and is invariant under the overall tetragonal symmetry (A_{1g}). Such a pairing state has been found from solving both weakly [9–12] and strongly [13–15] interacting models. Although there exist several experimental indications that this is indeed the correct pairing state in certain pnictide superconductors[16–19], more direct experimental evidence is highly desirable. Designing a Josephson interferometry device which could detect the $s_{\pm}$ state poses a significant challenge, since symmetry alone does not guarantee a π phase shift in *any* geometry. Several ideas have been proposed to overcome this difficulty[20–24], but none were realized to date.

Progress has been made recently, in the work of Chen *et al.*[1]. In this experiment, the flux through a composite Niobium(Nb)-$NdFeAsO_{0.88}F_{0.12}$(FeAs) superconducting loop was measured. By using an external electromagnetic pulse, is was shown that both integer and half-integer flux jumps can be induced in the loop, in units of the superconducting flux quantum $\Phi_0 = hc/2e$. While providing a strong indication for a sign change in the order parameter, these results are surprising, because neither a π-junction nor a 0-junction between the Nb and the FeAs superconductors would lead to the possibility of half-integer flux quantum jumps.

Motivated by these experiments, we study a model of a junction between a sign-changing and a conventional (s-wave) superconductor. The model allows us to interpolate between the tunneling (weak coupling) and the metallic contact (strong coupling) regime. We find that above a certain critical coupling strength, the frustration of the Josephson coupling across the barrier can lead to unusual energy-phase relations in the junction. If the phase stiffness of the superconductors is small enough, the energy-phase relation has two minima which break time-reversal symmetry; if the phase stiffness is large, the global minimum of the energy is at a phase difference of $\Delta\varphi = 0$, but an additional meta-stable minimum at $\Delta\varphi = \pi$ appears. The latter situation can explain the Chen *et al.* experiment, since it allows allows the junction to switch from $\Delta\varphi = 0$ to π, causing a half-flux quantum jump in the loop. The fact that the half-integer jumps appear only beyond a certain value of the critical current in the loop, as well as the relatively small probability of half-integer jumps[1], can both be understood within our model.

The model– We consider a planar Josephson junction between an s-wave and a sign-changing s-wave, shown in Fig. 1. Since we are interested in the crossover from a tunneling barrier to a metallic contact, in which the order parameters of both superconductors are modified significantly at distances of the order of a few coherence lengths from the junction [25], the problem needs to be treated self-consistently. Rather than solving the full Bugoliubov-de Gennes equations, we use an effective Ginzburg-Landau type free energy functional which depends on the superconducting order parameter near the junction [26]. Although the Ginzburg-Landau description is strictly valid only close to the critical temperature

(T_c) of both superconductors, we expect it to capture the qualitative behavior of the system even at lower temperatures.

In order to capture the multi-band nature of the system, we introduce two superconducting order parameters, Δ_i where $i = 1, 2$. Microscopically, these can be viewed as belonging to regions of different momenta parallel to the junction:

$$\Delta_i(x) = \frac{1}{A} \sum_{k_\parallel \in \Omega_i} V_{k_\parallel, k'_\parallel} \left\langle \psi_{k'_\parallel \uparrow} \psi_{-k'_\parallel \downarrow} \right\rangle, \tag{1}$$

where $\psi^\dagger_{k_\parallel \sigma}(x)$ is the electron creation operator at position x, momentum $k_\parallel$ parallel to the junction, and spin σ, $V_{k_\parallel, k'_\parallel}$ is the pairing interaction in the Cooper channel, x is the coordinate perpendicular to the junction, A is the area of the junction, and the two momentum regions Ω_i are defined by $\Omega_1 = \left\{ k_\parallel \middle| k_0 > |k_\parallel| \right\}$ and $\Omega_2 = \left\{ k_\parallel \middle| k_0 \leq |k_\parallel| \right\}$, where k_0 is an arbitrary momentum chosen such that in the $s_\pm$ side, $\Delta_1 > 0$ and $\Delta_2 < 0$. There, Δ_1 and Δ_2 can be thought of as the order parameters on different bands. Note that such as a decomposition is possible irrespective of the relative orientation of the two crystals, as long as in the sign-changing s-wave side, the region Ω_1 (Ω_2) is dominated by the positive (negative) part of the order parameter.

We describe the junction using the following phenomenological Ginzburg-Landau free energy:

$$F[\Delta_1, \Delta_2] = F_L + F_R + F_c. \tag{2}$$

Here,

$$\begin{aligned} F_\nu[\Delta_1, \Delta_2] \; = \; & \int_\nu dx \Bigg\{ \sum_{i=1,2} \left[\frac{1}{2} \kappa_i^\nu \left| \partial_x \Delta_i \right|^2 - \frac{1}{2} r_i^\nu \left| \Delta_i \right|^2 \right. \\ & \left. + \frac{1}{4} u_i^\nu \left| \Delta_i \right|^4 + \frac{1}{4} \alpha_i^\nu \left(\Delta_i^* \partial_x \Delta_i - \Delta_i \partial_x \Delta_i^* \right)^2 \right] \\ & - v^\nu (\Delta_1^* \Delta_2 + c.c.) \Bigg\}, \end{aligned} \tag{3}$$

where $F_{\nu=L,R}$ are the free energies of the left (Nb) and right (FeAs) sides, with $\int_L \equiv \int_{-\ell}^0$ and $\int_R \equiv \int_0^\ell$ (2ℓ is the system length), and

$$F_c[\Delta_1, \Delta_2] = \sum_{i=1,2} \left[T_i \left| \Delta_i(0^+) - \Delta_i(0^-) \right|^2 \right] \tag{4}$$

describes the contact between the two superconductors. In some cases, we will consider a "ring" geometry in which we add to F_c another term, $\sum_{i=1,2} \left[T_i \left| \Delta_i(\ell) - \Delta_i(-\ell) \right|^2 \right]$.

κ_i^ν,r_i^ν,u_i^ν in Eq. 3 are the standard Ginzburg-Landau parameters of band $i = 1, 2$ on the left/right ($\nu = L, R$ respectively) of the junction[27]. The α_i^ν terms represent an additional energy cost of creating supercurrents. These terms turn out to be necessary to describe the transition from a single-minimum to a double-minimum junction (see below). Close to the critical temperature, the α term becomes negligible compared to the other terms in Eq. 3, since it is of higher order in the Δ_i's and their derivatives. At lower temperatures, however, it can become important.

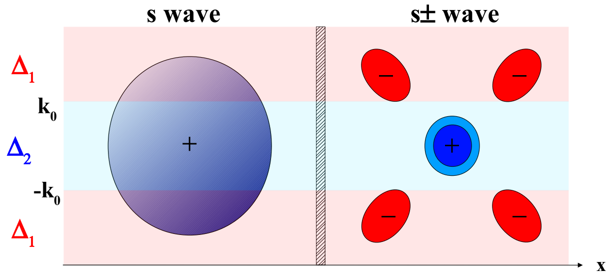

FIG. 1: (Color online.) Junction between an s-wave and an $s_\pm$ wave superconductor. We define two order parameters, $\Delta_{i=1,2}$ (see Eq. 1), which belong to different regions in momentum space. In the $s_\pm$ side, $\Delta_{1,2}$ have an opposite sign.

The parameter v^ν describes the inter-band coupling, and encodes the tendency towards s or $s_\pm$ pairing: positive (negative) $v^{L,R}$ corresponds to an s– ($s_\pm$–) wave superconductor, respectively.

T_i (Eq. 4) represent the strengths of the couplings of the two order parameters across the barrier. These parameters allow us to interpolate between the tunneling regime ($T_i \to 0$) to the metallic contact regime ($T_i \to \infty$). Note that in the latter regime, $\Delta_{1,2}$ become continuous at the junction. This is the boundary condition of a metallic contact between two superconductors, assuming for simplicity that the density of states at the Fermi energy times the pairing interaction is continuous at the contact [25]. Our results do not depend qualitatively on this assumption.

Results– We minimize the free energy (Eq. 2) numerically. The minimization is done on a discrete lattice, with a small enough lattice spacing such that the results are independent of its size. In order to map the energy-phase relation of the s-$s_\pm$ junction, we use the following boundary conditions at $x = \pm\ell$: $\arg \Delta_1(-\ell) = 0$, $\arg \Delta_1(\ell) = \Delta\varphi$, where φ is varied between 0 and π. The results (in particular, the qualitative behavior of the junction) do not depend on the choice of ℓ.

Depending on the contact strength and on various material parameters, we find three qualitatively different regimes: 1. A "single minimum" regime, which is realized for small T_i, in which the free energy is minimal at $\Delta\varphi = 2n\pi$ (where n is an integer); 2. A "time reversal breaking" (TRB) regime[28] at intermediate T_i and small α, where the free energy exhibits degenerate minima at $\Delta\varphi = 2n\pi \pm \varphi_0$; 3. A "double minimum" regime,

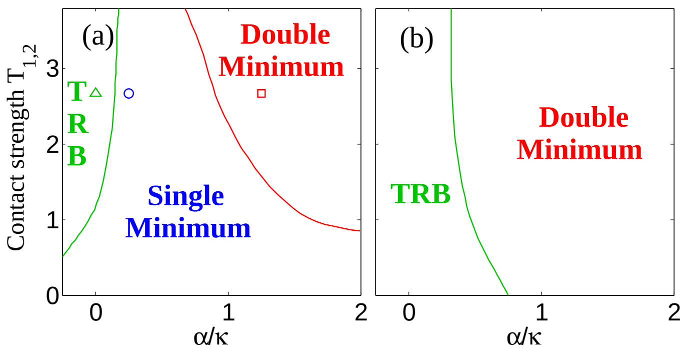

FIG. 2: (Color online.) (a) Phase diagram of an $s - s_\pm$ junction, using $r_i^\nu = 1$, $\kappa_i^\nu = 4$, $u_1^\nu = 1$, $u_2^\nu = 2$, $v^L = -v^R = 1$, $\alpha_i^\nu = \alpha$, $\ell = 3$ and $T_1 = T_2$. The different states correspond to different qualitative behaviors of the energy-phase relation in the junction: a "single minimum" state in which the minima of the free energy occur at a phase difference of $2n\pi$, a "time-reversal breaking" (TRB) phase in which the minima occur at $2n\pi \pm \Delta\varphi_0$, and a "double minimum" phase in which there are minima at $n\pi$. The triangle, the circle and the square correspond to the three parameter sets which are used in Fig. 3. (b) Same as (a), for a case where the parameters are tuned such that $\Delta_{1,2}$ are equivalent (by setting $u_1^\nu = u_2^\nu = 1$). In this case, the single minimum phase does not occur.

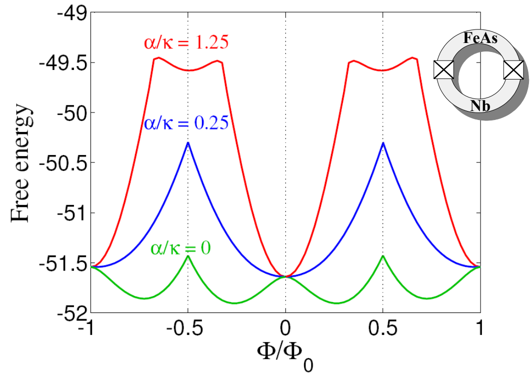

FIG. 3: (Color online.) Free energy as a function of flux in a composite s–s$_\pm$ loop (inset) of length $2\ell = 20$, for $T_{1,2} = 2.67$ and $\alpha/\kappa = 0, 0.25, 1.25$. These correspond to the "time-reversal breaking", "single minimum" and "double minimum" states, respectively. The self-inductance of the loop was chosen such that $\Phi_0^2/2L = 0.1$.

in which there are global minima at $\Delta\varphi = 2n\pi$ and local minima at $\Delta\varphi = (2n+1)\pi$. This regime is realized for sufficiently large α and T_i.

The phase diagram as a function of α and T_i, showing the three phases described above, is shown in Fig. 2a. The parameters used are listed in the figure caption.

In order to understand these results, we consider an artificial situation in which the parameters of the free energy are tuned such that the two order parameters $\Delta_{1,2}$ are exactly equivalent. In this case, the free energy of the junction $F(\Delta\varphi)$ (after minimization over $\Delta_{1,2}$) is invariant under a shift of $\Delta\varphi$ by π. Together with time-reversal symmetry, $F(\Delta\varphi) = F(-\Delta\varphi)$, this dictates that there are two generic situations: $F(\Delta\varphi)$ is minimal for either $\Delta\varphi = n\pi$ or $\Delta\varphi = (n+1/2)\pi$. This can be understood as follows: due to the sign change of the order parameter in the FeAs side, the Josephson coupling is frustrated. In order to relieve this frustration, the system can either twist the relative phase of $\Delta_{1,2}$ close to the interface, or deform the amplitudes of $\Delta_{1,2}$ such that $|\Delta_1| \neq |\Delta_2|$. The first effect favors $\Delta\varphi = (n+1/2)\pi$, and the second favors $\Delta\varphi = n\pi$. Which effect dominates depends on the energy cost of a non-uniform phase relative to that of a non-uniform amplitude of the order parameter. Increasing α/κ increases the phase stiffness, and hence drives a transition between the two regimes. The phase diagram for the case of equivalent $\Delta_{1,2}$ is shown in Fig. 2b.

Upon making $\Delta_{1,2}$ inequivalent, the period of $F(\Delta\varphi)$ becomes 2π. However, the local minima of $F(\Delta\varphi)$ remain stable over a finite region in parameter space. Therefore, the two phases described above survive. Between them, a third phase with minima at $\Delta\varphi = 2n\pi$ appears.

A composite s-s$_\pm$ superconducting loop (shown schematically in Fig. 3) is also described by three qualitatively different regimes, corresponding to the three phases of a single junction. The free energy of the loop as a function of the flux through the loop is given by[29]

$$F_{\rm loop} = F(\Phi) + \frac{\Phi^2}{2L}, \qquad (5)$$

where $F(\Phi)$ is the free energy of Eq. 2 with $\partial_x \to \partial_x - 2eA/h$ ($A = \Phi/2\ell$ is the vector potential), supplemented with an additional contact term (of the form of Eq. 4 with $x = \ell$), and L is the self-inductance of the loop. Fig. 3 shows the free energy of the loop as a function of Φ, with parameters (α, T) which place the system in one of the three distinct regimes described above. For intermediate values of α/κ, the free energy of the loop has minima at approximately $\Phi = n\Phi_0$ where n is an integer ("single minimum" regime). For smaller α/κ, each minimum splits into two degenerate minima at $\Phi = n\Phi_0 \pm \Delta\Phi$ where $\Delta\Phi$ depends continuously on the various parameters of the junction (TRB regime). Finally, for α/κ larger than a critical value, minima appear both at $\Phi = n\Phi_0$ and $\Phi = (n+1/2)\Phi_0$ ("double minimum" regime).

Comparison to the Chen et al. experiment– The experiment of Chen *et al.*[1] can be interpreted in terms of our model as follows. As the critical current in the composite Nb–FeAs loop is increased, the Nb–FeAs junction undergoes a transition from a single minimum to a double minimum phase. Upon entry to the double minimum phase, both $n\Phi_0$ and $(n+1/2)\Phi_0$ flux jumps are observed, and the probability for $(n+1/2)\Phi_0$ jumps increases with increasing critical current (which corresponds to increasing $T_{1,2}$ in Fig. 2).

Whenever the composite loop is excited electromagnetically, the flux through the loop acquires a random "kick", and the system can jump from one local minimum to another. The probability of ending at a metastable local minimum, $\Phi = (n+1/2)\Phi_0$, is smaller than the probability of ending in a global minimum, $\Phi = n\Phi_0$. Therefore, if the system jumps from $n_1\Phi_0$ to $(n_2+1/2)\Phi_0$, the next jump is likely to be to $n_3\Phi_0$ (with integer n_1, n_2, n_3). This implies that the half flux quantum jumps are correlated, and tend to appear in pairs. Such a trend is clearly visible in the experimental results [1, 30]. We conclude that the experimental results of Ref. [1] can be naturally explained by the appearance of a metastable local minimum in the energy-phase relation of the Nb-FeAs junction at $\Delta\varphi = (n+1/2)\pi$, corresponding to the "double minimum" phase in our model.

Conclusions– We have presented a model for a Josephson junction between a simple s–wave and a sign-changing $s_\pm$ wave superconductor. Due to the sign change in the $s_\pm$ side, the Josephson coupling across the junction is partially frustrated. If the barrier between the two superconductors is low enough, corresponding to a metallic contact, the system can relieve this frustration by either breaking time-reversal symmetry, or developing additional local minima at a phase difference of $(2n+1)\pi$. The half-flux quantum jumps in the experiment of Chen *et al.* can be explained by the second scenario. (Note that a time-reversal breaking junction would correspond to fractional flux jumps which are neither $n\Phi_0$ nor $(n+1/2)\Phi_0$, which were not observed.)

It is important to note that this behavior is *unique* to a junction between an s–wave and a sign changing superconductor. In a junction between two s–wave superconductors, only the single minimum phase is realized, for *any* strength of the coupling $T_{1,2}$. To verify this, we considered a case in which $v^L = v^R > 0$, *i.e.* both sides of the junction are s-wave superconductors, and found only a single-minimum phase. In this respect, the observation of half-flux quantum jumps is a strong indication of a sign-changing order parameter. Together with the lack of observation of spontaneous flux in a polycrystalline sample[5], which essentially rules out a d-wave order parameter, we conclude that the $s_\pm$ is the most likely candidate for the order parameter of F-doped NdFeAsO.

We note also that according to our model, the multigrain nature of the NdFeAsO is, in fact, not essential for the observation of half-flux jumps. Similar phenomena should occur even in a loop made of a *single crystal* of NdFeAsO and a conventional superconductor.

The presence local minima in the energy-phase relation of a contact between a conventional and an iron-based superconductor can be looked for in experiments. The AC Josephson effect should reveal pronounced high harmonics of the AC current as a function of the bias voltage. In a composite loop, of the same kind as the one studied by Chen *et al.*, half-flux quantum entries should be observed as a function of an external field.

On the theoretical side, it will be interesting to examine a strongly-coupled s–$s_\pm$ junction in a microscopic model. Within our phenomenological model, we found that the fate of the junction in the strong coupling limit is determined by the ratio of the phase and amplitude stiffnesses. In a Bardeen-Cooper-Schrieffer superconductor at low temperatures, these stiffnesses both scale in the same way – their magnitude is proportional to the Fermi energy. Therefore, the relative magnitude of the two stiffnesses is sensitive to microscopic details. It will be particularly interesting to look for parameter regimes in which the broken time-reversal junction can arise.

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[1] Chen et al., Nature Physics **6**, 260 (2010).
[2] Y. Kamihara et al., J. Am. Chem. Soc. **130**, 3296 (2008).
[3] D. Wollman et al., Phys. Rev. Lett. **71**, 2134 (1993).
[4] C. Tsuei et al., Phys. Rev. Lett. **73**, 593 (1994).
[5] C. W. Hicks et al., J. Phys. Soc. Jap. **78**, 013708 (2008).
[6] X. Zhang et al., Phys. Rev. Lett. **102**, 147002 (2009).
[7] I. I. Mazin et al., Phys. Rev. Lett. **101**, 057003 (2008).
[8] V. Cvetkovic and Z. Tesanovic, EPL (Europhysics Letters) **85**, 37002 (2009).
[9] K. Kuroki et al., Phys. Rev. Lett. **101**, 087004 (2008).
[10] A. Chubukov, D. Efremov, and I. Eremin, Phys. Rev. B. **78**, 134512 (2008).
[11] S. Graser et al., New J. Phys. **11**, 025016 (2009).
[12] F. Wang et al., Phys. Rev. Lett. **102**, 047005 (2009).
[13] K. Seo, B. A. Bernevig, and J.-P. Hu, Phys. Rev. Lett. **101**, 206404 (2008).
[14] E. Berg, S. A. Kivelson, and D. J. Scalapino, Phys. Rev. B **81**, 172504 (2010).
[15] F. Yang et al., arXiv:1007.2643v2 (2010).
[16] A. D. Christianson et al., Nature **456**, 930 (2008).
[17] S. Chi et al., Phys. Rev. Lett. **102**, 107006 (2009).
[18] T. Hanaguri et al., Science **328**, 474 (2010).
[19] M. Teague et al., arXiv:1007.5086 (2010).
[20] D. Parker and I. Mazin, Phys. Rev. Lett. **102**, 227007 (2009).
[21] J. Linder, I. Sperstad, and A. Sudbø, Phys. Rev. B **80**, 020503 (2009).
[22] W.-Q. Chen et al., Phys. Rev. Lett. **103**, 207001 (2009).
[23] W.-F. Tsai et al., Phys. Rev. B **80**, 012511 (2009).
[24] W.-Q. Chen and F.-C. Zhang, arXiv:1009.4756v1 (2010).
[25] P. G. de Gennes, Rev. Mod. Phys. **36**, 225 (1964).
[26] F. Sols and J. Ferrer, Phys. Rev. B **49**, 15913 (1994).
[27] In Eq. 3, we have not included all the possible quartic

terms which are allowed by symmetry. These terms are not expected to lead to any qualitatively new effects.
[28] Time reversal symmetry breaking at an s-$s_\pm$ junction was proposed in: T. Ng et al., Europhys. Lett. **87**, 17003 (2009); V. Stanev et al., Phys. Rev. B **81**, 134522 (2010).
[29] C. C. Tsuei and J. R. Kirtley, Rev. Mod. Phys. **72**, 969 (2000).
[30] For experimental data demonstrating the pairing of half flux quantum events, see Supplementary Material.