Plaquette-centered rotation symmetry and octet-nodal superconductivity in KFe$_2$As$_2$

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A plaquette-centered rotation symmetry $C_4^d$ is identified to play a significant role in determining and stabilizing the Fermi-surface structure of Fe-based superconductors. Together with the $S_4$ symmetry previously found, we are able to sort out the tangling orbitals and solve the puzzle of pairing symmetry of superconductivity in KFe$_2$As$_2$ in a simple but comprehensive way. By modeling the material with a strong coupling $t - J_1 - J_2$ model, we find phase transitions of pairing symmetry driven by the competition between the local spin antiferromagnetic couplings from nodal $d_{x^2-y^2} \times s_{x^2+y^2}$-wave to nodeless $s_{x^2+y^2}$-wave through the intermediate $s + id \times s$ mixed pairing phase, which is consistent with the observation of pressure experiments. The emergent $d$-wave form factor inevitably arises from the projection of inter-orbital Cooper pairing onto the Fermi surface and is inherited from the electronic structure in the representation of $C_4^d$ symmetry. Moreover, the $S_4$ symmetry dictates 2 copies of $d$-wave pairing condensates, counting 8 nodes in total. We further show that weakly breaking $C_4^d$ naturally leads to the octet nodal gap as precisely observed in laser angle resolved photoemission spectroscopy. The octet nodes reflect the collaboration of the $C_4^d$ and $S_4$ symmetries, which sheds new light on the enigma of the pairing symmetry in KFe$_2$As$_2$.

As the first family of high temperature superconductivity (SC), the cuprates have been under elaborate studies for nearly thirty years$^{[1-4]}$, and a consensus has been reached by the majority of condensed matter physicists that the intriguing superconducting phase of cuprates are rooted in the electronic strong antiferromagnetic (AF) correlation. The SC in optimally doped compounds is rooted in the electronic structure of Fe-based SCs. However, the presence of weakly breaking $C_4^d$ naturally leads to the octet nodal gap as precisely observed in laser angle resolved photoemission spectroscopy. The octet nodes reflect the collaboration of the $C_4^d$ and $S_4$ symmetries, which sheds new light on the enigma of the pairing symmetry in KFe$_2$As$_2$.

The phase diagrams of Fe-based superconductors show significant similarity with those of the cuprates, suggesting deep connection of the essential physics between them. However, distinct from the cuprates, the family of Fe-based superconductors has a seemingly less unified picture as to their Fermi surface (FS) structure, pairing symmetries and pairing phases$^{[11-10]}$. From the perspective of band structure, they owe their complexity to the multi-orbital character. Some Fermi pockets could vanish under doping or pressure and are less robust than the others$^{[17-18]}$. Regarding the pairing symmetry, the $s_{\pm}$-wave pairing symmetry has been established for many iron-pnictides from different approaches$^{[19-21]}$, but it fails to account for all the materials observed experimentally. When it comes to the interactions responsible for pairing, there are weak coupling theories that count on the antiferromagnetic spin fluctuation$^{[19]}$, but they are less satisfying when FS nesting is absent, nor when there exists strong correlation between local magnetic moments$^{[11-10]}$. After all these considerations, a simple but unifying theoretical recipe for the Fe-based superconductors is still elusive, and we still need deep reflection upon the electronic structure and interactions of Fe-based superconductors.

To model the Fe-based SCs, we have to firstly understand the electronic structure. There have been many theoretical treatments by taking all five or even ten 3$d$-orbitals of Fe into consideration, but the necessity for such a huge parameter space is hardly conceivable, because the pairing symmetries are so robust. From this point of view, we especially appreciate the $S_4$ symmetry found by Hu and Hao$^{[22]}$, which provides a rational way to sort out the tangling multi-orbitals of Fe-based SCs and reduce the parameters of the electronic structure. In the presence of $S_4$, the band structure of multi-orbitals is then reduced to a minimal two-band model. Based on this $S_4$ symmetry, the model with a few parameters is capable of accommodating most FS structures of both iron-pnictides and iron-chalcogenides$^{[22]}$, potentially unifying the electronic structure of Fe-based SCs. However, the heavily hole doped limit of iron-pnictides KFe$_2$As$_2$ is left behind.

The representative of heavily hole doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$ family - KFe$_2$As$_2$ is a particular intriguing case among the Fe-based superconductors, regarding its pairing symmetry and interaction. Angle resolved photoemission spectroscopy (ARPES) experiments$^{[17-18]}$ report the absence of electron pockets and leave only three hole Fermi pockets around the Brillouin zone (BZ) center (Γ point). Usually the nodeless $s$-wave pairing symmetry is favorable. But it turns out that nodal gap structure was observed by thermal conductivity measurement$^{[23]}$, penetration depth measurement$^{[24]}$, and NMR probe$^{[25-27]}$. The $d$-wave pairing symmetry was then proposed after functional renormalization group calculation$^{[28]}$, which seems...
consistent with the measurement of heat conduction\[29\]. Later on Okazaki et. al. utilized the ultra-high energy resolution of laser ARPES to map the gap structure much more explicitly\[30\]. Quite dramatically, their report showed octet nodal gap on the middle hole pocket while nodeless gap on the inner hole pocket, in striking contrast to the theoretical expectation. Then there were attempts to resort to accidental nodes to account for the octet nodes. But as far as we are concerned, the nodes robustly observed in various experiments deserve far more convincing explanation. If the octet nodes was given by an effective g-wave pairing condensate phenomenologically, it is a natural question how the Cooper pair obtains angular momentum as high as $l = 4$ microscopically. Although the so-called concealed d-wave scenario was proposed to explain the formation of the effective g-wave Cooper pair, such a theory starts from an orbital selective pairing form, and their orbital triplet pairing vector field is required to be locked with the orbital Rashba vector field and to rotate oppositely\[31\].

In this paper, we will provide a mechanism based on a microscopic minimal model, which is much simpler but more transparent. Our idea is inspired by another experiment. Taillefer’s group reported their pressure study on KFe$_2$As$_2$, in which they witnessed a non-monotonic V-shaped tendency of the superconducting transition temperature with increasing pressure\[32\]. Their results clearly indicated a phase transition near the point of the sudden change of $T_c$. The possibility of FS transition was ruled out by their Hall coefficient measurement, pointing towards a phase transition of pairing symmetry. It should be emphasized that the KFe$_2$As$_2$ is regarded as a strongly correlated system with strong AF fluctuation evidenced by the remarkable mass enhancement\[17\] and high incoherent spectral weight\[33\]. Since the two ingredients determining the pairing symmetry are the FS structure and the electronic interactions responsible for pairing, it can be concluded that the phase transitions are essentially driven by the competition between the local spin AF exchanges, because the FS remains almost the same.

First of all, we identify a plaquette-centered rotation symmetry $C_4^p$ which is complementary to the $S_4$ symmetry, providing a simple and potentially universal organizing principle for the tangling orbitals of Fe-based superconductors. We explicitly show that, while $S_4$ plays the role of organizing two groups of orbitals, $C_4^p$ is responsible for determining and stabilizing the FS structure of iron-pnictides, including the heavily hole doped limit where the electron Fermi pockets are absent. The joint cooperation of the $S_4$ and $C_4^p$ symmetries manifest its power particularly in settling the controversy of pairing symmetry and nodeness in KFe$_2$As$_2$.

To study the pairing symmetry of SC in KFe$_2$As$_2$, we take the strong coupling approach by modeling this material with the $t - J_1 - J_2$ model subjected to the particle occupancy constraint, in contrast to the models with the on-site Coulomb repulsion and Hund’s coupling\[35\]. Since we are mainly concerned with the pairing symmetry of superconductivity, we can neglect the quantum fluctuation for the moment and adopt the slave-boson mean-field approximation. We find that, by decreasing the ratio of $J_1/J_2$, the KFe$_2$As$_2$ samples could experience phase transitions of pairing symmetry from the $d_{x^2-y^2} \times s_{2z^2+y^2}$-wave SC to $s_{2z^2+y^2}$-wave SC through a narrow intermediate $s+id \times s$ mixed pairing phase. Although the $d$-wave pairing symmetry is indeed energetically unfavorable compared with the $s$-wave pairing, the electronic structure imposes an indispensable $d$-wave form factor on the Cooper pairs glued by the local spin AF coupling $J_1$. This $d$-wave form factor is inherited from the orbital hybridization in the representation of $C_4^p$ and becomes the characteristic nature of multi-orbital iron-pnictide superconductors. Moreover, together with the $S_4$ symmetry, we are in fact bestowed with 2 copies of $d$-wave gap structure, counting 8 nodes in total. By weakly breaking $C_4^p$ we are naturally led to the so-called "octet-noded monster" observed by laser ARPES. We thus propose a symbolic equation "8 = 4 + 4" that captures the essential physics ruled by $S_4$ and $C_4^p$ symmetries, exhibiting the origin of nodes in a rather simple and comprehensive way.

Moreover, we find that a different representation of this plaquette-centered rotation symmetry $C_4^p$ can stabilize the FS structure of iron-chalcogenides, including the monolayer FeSe on SrTiO$_3$ substrate where a tiny hole Fermi pocket around $\Gamma$ vanishes\[36, 37\]. So both families of Fe-based superconductors share the plaquette-centered rotation symmetry, and the importance of this symmetry lies in its capability to understand the band topology and robustness of FSs, and to reconcile some seemingly contradictory experimental observations in a rather simple, inevitable, and comprehensive manner.

**RESULTS**

$C_4^p$ symmetry and band topology

Due to the weak out-of-plane coupling (along c-axis), the electronic properties of Fe-based SCs are mainly contained in the FeAs plane, where the Fe atoms form a square lattice and the As atoms alternate above or below the Fe plaquette center (Fig.1). Because of the checkerboard pattern of As lattice, the FeAs plane does not respect the site-centered $C_4^s$ symmetry, but is invariant under the site-centered $C_4^s$ rotation followed by a mirror reflection with respect to the plane\[22\]: $S_4 \equiv C_4^s \times R_z$. We further discover that the plaquette-centered rotation symmetry $C_4^p$ is preserved.

Among the five $d$-orbitals, the low-energy physics near the FS is mainly contributed by the $d_{xz}, d_{yz}, d_{xy}$ orbitals. Instead of a direct tunneling via the wave function over-
lap, the hopping between \(d_{xz}\)- and \(d_{yz}\)-orbitals is primarily contributed by their hybridization with the \(p\)-orbitals on the As atoms, whereas the \(d_{xy}\) orbitals do not have this privilege and are not included in our minimal model.

The As atoms on plaquette centers polarize the \(d_{xz}\)- and \(d_{yz}\)-orbitals into \(d'_{xz}\)- and \(d'_{yz}\)-orbitals to maximize energy gain from hopping (Fig.1a and Fig.1b). Therefore the square lattice with \(d_{xz}\) and \(d_{yz}\) orbitals on each site is effectively factorized into the top and bottom layers where each site has one orbital but the unit cell has to be doubled. As shown in Fig.1a, the top layer has \(d_{xz}\) living on the odd lattice sites (denoted as A) and \(d_{yz}\) on the even lattice sites (denoted as B). Likewise, the bottom layer has \(d_{yz}\) living on the odd lattice sites (denoted as C) and \(d_{xz}\) on the even lattice sites (denoted as D). For convenience we will denote the top layer as "AB layer" while the bottom layer as "CD layer". Although weakly coupled by inter-layer tunneling, the two layers are related by the \(S_4\) symmetry, while the sublattice degrees of freedom inside each layer are rotated by \(C_4^p\).

To demonstrate the symmetries, we introduce the notion \(\tau_{\mu\nu} \equiv I_{\mu} \otimes I_{\nu}\), \(\mu, \nu = 0, 1, 2, 3\), where the first Pauli matrix \(I_{\mu}\) acts on the \(S_4\) spinor space spanned by those states living on either layer, and the latter Pauli matrix \(I_{\nu}\) acts on the \(C_4^p\) spinor space composed of states living on each sublattice. By choosing the simple gauge as shown in Fig.1b, the representation of \(S_4\) and \(C_4^p\) symmetries can be explicitly expressed as

\[
S_4 : \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \\ C_{k,\sigma} \\ D_{k,\sigma} \end{pmatrix} \rightarrow \begin{pmatrix} C_{k',\sigma} \\ D_{k',\sigma} \\ -A_{k',\sigma} \\ -B_{k',\sigma} \end{pmatrix} = i\tau_{23} \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \\ C_{k,\sigma} \\ D_{k,\sigma} \end{pmatrix},
\]

\[
C_4^p : \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \\ C_{k,\sigma} \\ D_{k,\sigma} \end{pmatrix} \rightarrow \begin{pmatrix} B_{k,\sigma} \\ A_{k,\sigma} \\ D_{k,\sigma} \\ -C_{k,\sigma} \end{pmatrix} = i\tau_{32} \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \\ C_{k,\sigma} \\ D_{k,\sigma} \end{pmatrix},
\]

where \(k' = C_4 k\). Since the spin-orbit coupling is not concerned, the spin degeneracy is always present. The rotation factor contributed by the spin rotation \((1+i\sigma_z)/\sqrt{2}\) does not affect the physics and can be absorbed by a basis transformation. Moreover, we would like to point out that these two symmetries commute with each other.

Formally, the \(C_4^p\) symmetry operation is indeed diagonal in the \(S_4\) spinor space and mainly rotates the intralayer sublattices, while the \(S_4\) operation is diagonal in each sublattice but primarily rotates the layers. It is worth noticing that the \(S_4\) spinor and \(C_4^p\) spinor look like dual to each other. But the inter-sublattice hopping is much stronger than the inter-layer tunneling, which makes the \(S_4\) doublet weakly coupled but \(C_4^p\) doublet strongly hybridized. The power of the \(S_4\) symmetry lies in that, once the dynamics of one layer is obtained, it is straightforward to derive the other. Therefore, in the presence of \(S_4\) symmetry, we are bestowed with a minimal

\[
\Psi_{k,\sigma} = (A_{k,\sigma}, B_{k,\sigma})^T, \quad \text{it is then expressed as}
\]

\[
H_{\text{AB}} = \frac{1}{2} \sum_{k,\sigma} \left[ \epsilon_0(k) + \epsilon_z(k) I_1 + \epsilon_2(k) I_3 \right] \Psi_{k,\sigma}, \quad (1)
\]

where \(k\) ranges in the unfolded BZ and

\[
\epsilon_0(k) = 4t_{2s} \cos k_x \cos k_y - \mu, \\
\epsilon_z(k) = -4t_{2d} \sin k_x \sin k_y, \\
\epsilon_2(k) = 2t_{1d} (\cos k_x - \cos k_y) + 2t_{1s} (\cos k_x + \cos k_y) \equiv \epsilon_{xz}(k) + \epsilon_{xx}(k).
\]
Note that $\epsilon_s(k)$ denotes the sublattice energy difference and $\epsilon_x(k)$ is the energy gain from the NN hopping process. A vector can be defined by $h(k) \equiv (\epsilon_x, 0, \epsilon_s)$, which acts as a "magnetic field" in the momentum space and pinning the $C^\varphi_4$ spinor (Fig.1c). It should be noted that the sublattice degree of freedom in AB layer is locked with the atomic internal angular momentum i.e. the odd sites carry $d'_{x'z}$ orbitals while the even sites carry $d_{y'z}$ orbitals, so that the $C^\varphi_4$ spinor is actually a composite of the sublattice degree of freedom and the internal atomic angular momentum. For instance, when $t_{1s} = 0$, $t_{1d} < 0$, $t_{2s} > 0$, and $t_{2d} > 0$, the spinor along $k_x$ with the lowest energy is composed of the equal superposition of $d'_{x'z}$-orbitals on odd sites and $d_{y'z}$-orbitals on even sites (Fig.1c), equivalent to $d_{xz}$-orbitals. But along the BZ diagonal, the spinor with the lowest energy consists of the $d'_{x'z}$-orbitals on odd sites or $d_{y'z}$-orbitals on even sites.

Before diagonalization, there are several remarks about the symmetries in this kinetic part. The $d$-wave and $s$-wave NN hopping correspond to two distinctive symmetry representations of the plaquette-centered rotation symmetry, respectively. Based on the sketch of a snapshot of the wave function distribution in Fig.1, we naturally expect $|t_{1d}| \gg |t_{1s}| \approx 0$. Indeed, adding a nonzero $t_{1s}$ would break the symmetry $C^\varphi_4$. So the ideal case of $t_{1s} = 0$ and $t_{1d} \neq 0$ respects the symmetry $C^\varphi_4$, which can faithfully characterize the FS structure of iron-pnictides.

In the helicity basis, $H^\text{AB}_t$ can be directly diagonalized

$$H^\text{AB}_t = \frac{1}{2} \sum_{k, \sigma} \left[ \xi_e(k) \alpha^\dagger_{k, \sigma} \alpha_{k, \sigma} + \xi_h(k) \beta^\dagger_{k, \sigma} \beta_{k, \sigma} \right],$$

where $\xi_e(h)(k) = \epsilon_0 \pm \sqrt{\epsilon_x^2 + \epsilon_s^2}$ represents the electron (hole) band with ± helicity, respectively:

$$\alpha^\dagger_{k, \sigma} = \left( \begin{array}{c} \cos \theta_k/2 \alpha^\dagger_{k, \sigma} + \text{sgn} (\epsilon_s) \left( \sin \theta_k/2 \beta^\dagger_{k, \sigma} \right) A^\dagger_{k, \sigma}, \\ \sin \theta_k/2 \beta^\dagger_{k, \sigma} - \text{sgn} (\epsilon_x) \left( \cos \theta_k/2 \alpha^\dagger_{k, \sigma} \right) B^\dagger_{k, \sigma} \end{array} \right),$$

$$\beta^\dagger_{k, \sigma} = \left( \begin{array}{c} \cos \theta_k/2 \beta^\dagger_{k, \sigma} + \text{sgn} (\epsilon_s) \left( \sin \theta_k/2 \alpha^\dagger_{k, \sigma} \right) B^\dagger_{k, \sigma}, \\ \sin \theta_k/2 \alpha^\dagger_{k, \sigma} - \text{sgn} (\epsilon_x) \left( \cos \theta_k/2 \beta^\dagger_{k, \sigma} \right) A^\dagger_{k, \sigma} \end{array} \right),$$

and the hybridization angle is given by $\theta_k = \tan^{-1} |\epsilon_s/\epsilon_x| \in [0, \pi]$. The band dispersion and the corresponding FS structures can be easily obtained. Fig.2 exhibits the coexistence of a hole pocket around $\Gamma$ and an electron pocket around $X$ point in the presence of the $s$-wave NN hopping, a characteristic FS structure of most iron-pnictides. As the $d$-wave NN hopping is growing, the electron band is gradually pushed upwards, shrinking the electron pocket. It finally leads to the FS structure of KFe$_2$As$_2$ (Fig.2a), where the electron pocket completely vanishes. This evolution is also related to the doping process of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ iron-pnictides [39].

Note that the shape of the hole pocket has the $C_4$ rotational symmetry thanks to the symmetry $C^\varphi_4$, and the two bands touch each other quadratically at zone center $\Gamma$ point, which is not accidental but rather due to the topological nature. Namely, the helical spinor is pinned by the vector field $h(k)$ to wind around the $\Gamma$ point twice, yielding a topological number $w = 2\text{sgn}(t_{1d}t_{2d})$ (Ref.40). It is this topological number that forces the electron and hole bands to touch quadratically at the vortex core of $h(k)$, which becomes the source of the Berry flux experienced by the helical spinor (see Fig.1b). Consequently, the hole pocket surrounding the vortex core is protected by topology, whereas the electron pocket is less robust. As long as the time reversal (TR) symmetry is present, the occurrence of $I_2$ is forbidden and this vortex core is robust. However, the TR symmetry cannot prevent the double Dirac point at $\Gamma$ from splitting apart into
two separated Dirac nodes, which could be driven by a weak $C^p_d$-breaking perturbation. This is indeed the case when the s-wave hoping comes in mixing the d-wave NN hopping (Fig.2), where the hole pocket experiences a "nematic force" and is simultaneously elongated. When the $C^p_d$ symmetry breaking term is large enough, the hole pocket around $\Gamma$ is going to be torn apart, resulting in two pockets surrounding the Dirac nodes, which is not seen in the real materials. So the iron-pnictides with hole pockets around $\Gamma$ robustly observed in experiments must preserve the $C^p_d$ symmetry, at least approximately.

In other words, the FS structure of iron-pnictides is stabilized by the $C^p_d$ symmetry which helps the TR symmetry protect and confine the double Dirac point to the hole pocket center. In this sense, the $C^p_d$ symmetry is one of the key relevant features of iron-pnictides, which can tolerate only tiny amount of s-wave hoping. In the next section, we will focus on the ideal case of d-wave NN hopping limit by setting $t_{1d}=0$ for KFe$_2$As$_2$. Specifically, we choose the realistic hopping parameters as $t_{1d} = -1.2$, $t_{2s} = 0.5$, and $t_{2d} = 1$, whose corresponding band structure is shown by Fig.2b. When things are clear in the ideal case, we will introduce a weak s-wave NN hoping to model the more realistic material later on.

**$C^p_d$ protected d-wave renormalized pairing SC**

Provided the electronic structure of KFe$_2$As$_2$, we need to include the electronic interactions. The strong correlation evidenced by experiments [17, 33, 34] requires to include the electronic interactions. The strong correlation evidenced by experiments [17, 33, 34] requires a strong coupling approach. Particularly, the optical measurement [34] had showed the incoherent spectral weight of KFe$_2$As$_2$ as high as 10% hole-doped La$_{2-x}$Sr$_x$CuO$_4$, revealing the strong local AF correlation similar to the cuprates. Therefore, we would like to model this system with AF super-exchanges containing the NN and NNN interactions as shown in Fig.1. Distinct from the $t-J_1-J_2$ model in the previous form [20], our model Hamiltonian is subjected to a constraint that projects out double-occupancy. Thus, the model Hamiltonian for AB layer is described by $H^{AB} = \mathcal{P}H^{AB}_{\mathcal{P}} + H^{AB}_{\mathcal{P}}$ with interaction terms:

$$H^{AB}_{\mathcal{P}} = J_1 \sum_{r,\delta} S^A_r \cdot S^B_{r+\delta} + J_2 \sum_{r} \left( S^A_r \cdot S^A_{r+(\tilde{x}+\tilde{y})} + S^B_r \cdot S^B_{r+(\tilde{x}-\tilde{y})} \right) + J_2' \sum_{r} \left( S^A_r \cdot S^B_{r+(\tilde{x}-\tilde{y})} + S^B_r \cdot S^B_{r+(\tilde{x}+\tilde{y})} \right), (4)$$

where $\delta = \pm \tilde{x}, \tilde{y}$ is the NN vector. As the low-energy descendant of the on-site Hubbard interaction, the AF super-exchange $J$-terms rely on the corresponding hopping integrals. Like cuprates, the parameters can be chosen as $J_2 = 0.5$ and $J_2' = 0.2$ as roughly one third of the corresponding hopping integrals and the dopant concentration is fixed at 0.05. Note that although $J_2'$ differs from $J_2$, only the combination $J_{2s} = 2J_2J_2'/ (J_2 + J_2')$ contributes to pairing. So that the physics is essentially captured by the competition between $J_1$ and $J_{2s}$. The parameter $J_1$ is chosen as the tuning parameter that mimics the inverse pressure when compared with the pressure experiments [32].

The projector $\mathcal{P}$ declares the particle occupancy constraint: $\sum_{\sigma} a^\dagger_{r,\sigma} a_{r,\sigma} \leq 1$ and $\sum_{\sigma} b^\dagger_{r,\sigma} b_{r,\sigma} + h^\dagger_r h_r = 1$, which lead to emergent spin-charge separation physics. To tackle the constraint, we adopt the well-established slave-boson decomposition to factorize electron into fermionic spinon and bosonic holon:

$$A_{r,\sigma} = h^\dagger_r a_{r,\sigma}, B_{r,\sigma} = h^\dagger_r b_{r,\sigma}, (5)$$

in which way the constraint becomes equalities: $\sum_{\sigma} a^\dagger_{r,\sigma} a_{r,\sigma} + h^\dagger_r h_r = 1$ and $\sum_{\sigma} b^\dagger_{r,\sigma} b_{r,\sigma} + h^\dagger_r h_r = 1$, and can be enforced via a Lagrangian multiplier. After the bosonic holons are condensed $\langle h^\dagger_r \rangle = \langle h_r \rangle = \sqrt{\tau}$, we introduce the uniform valence bond and singlet pairing order parameters

$$\kappa_{ij} = -\frac{J}{4} \left( \sum_{\sigma} a^\dagger_{i,\sigma} a_{j,\sigma} \right), \Delta_{ij} = \frac{J}{4} \left( a_{i,\uparrow} a_{j,\downarrow} - a_{i,\downarrow} a_{j,\uparrow} \right),$$

to decouple the local AF interactions. Moreover, the NN and NNN valence bond and singlet pairing order parameters in real space can be rearranged into the s-wave and d-wave representations: $\kappa_i$ is automatically of d-wave symmetry required by $C^p_d$ symmetry and other valence bond orders are

$$\kappa_{2s} = (\kappa_2 + \kappa'_2)/2, \kappa_{2d} = (\kappa_2 - \kappa'_2)/2, \Delta_{1s} = (\Delta_{1x} + \Delta_{1y})/2, \Delta_{1d} = (\Delta_{1x} - \Delta_{1y})/2, \Delta_{2s} = (\Delta_2 + \Delta'_2)/2, \Delta_{2d} = (\Delta_2 - \Delta'_2)/2. (6)$$

Finally, a mean-field Hamiltonian can be obtained

$$H^{ab}_{\text{MF}} = H^{ab} + H^{ab}_\Delta, (7)$$

which describes the superconducting quasiparticles on the AB layer. The kinetic part $H^{ab}$ has the same band structure as we discussed in the last section. $H^{AB} \rightarrow H^{ab}$ requires replacing the electrons with the corresponding quasiparticles $\Psi_{k,\sigma} = (A_{k,\sigma}, B_{k,\sigma})^T \rightarrow \psi_{k,\sigma} = (a_{k,\sigma}, b_{k,\sigma})^T$, while renormalizing the hopping integrals and the chemical potential as

$$t_{1d} \rightarrow \tilde{t}_{1d} = (t_{1d}x + \kappa_1), \quad t_{1s} \rightarrow \tilde{t}_{1s} = t_{1s}x, \quad t_{2s} \rightarrow \tilde{t}_{2s} = (t_{2s}x + \kappa_2), \quad t_{2d} \rightarrow \tilde{t}_{2d} = (t_{2d}x + \kappa_2), \quad \mu_0 \rightarrow \mu = \mu_0 - \lambda - (J_2 + J_3)/4. (8)$$

The hybridization relation Eq. (3) also holds by replacing A(B) with a(b), and the mean-field pairing terms can be compactly expressed in terms of the $C^p_d$ spinor:

$$H^{ab}_\Delta = \frac{1}{2} \sum_k \left[ \psi^\dagger_{k,\uparrow} (\Delta_0 + i \Delta_x I_x + i \Delta_z I_z) (\psi^\dagger_{k,\downarrow})^T + h.c. \right] (9)$$
with
\[
\Delta_0(k) = 4\Delta_{2s}\cos k_x \cos k_y, \quad \Delta_\Delta(k) = 4\Delta_{2d}\sin k_x \sin k_y,
\]
\[
\Delta_\Delta(k) = 2\Delta_{1d}\cos(k_x + k_y) + i2\Delta_{1d}\cos(k_x - k_y).
\]

Provided with all the form factors available from the interactions, we can eliminate some of them which are apparently unfavorable energetically.

In this minimal model for KFe$_2$As$_2$, within the AB layer there is only a small hole pocket around $\Gamma$ point. The Cooper pair formed on the FS is more likely to be scattered onto the same FS with small momentum transfer. And the pairing interactions $J_1(q) \propto -2J_1(q, z)$ and $J_2(q) \propto -4J_2(q, z)$ are attractive when $q \approx 0$, while $J_{2d}(q) \propto 4J_{2d}(q, z)$ tends to vanish. Therefore, the pairing components $\Delta_{1d}$ and $\Delta_{2d}$ are energetically unfavorable compared to $\Delta_{1s}$ and $\Delta_{2s}$, which endow the FS with largest possible energy gain. In fact, we did some self-consistent calculation numerically to verify the results $\Delta_{1d} = \Delta_{2d} = 0$. Thus we are left with two $s$-wave pairing components $\Delta_{1s}$ and $\Delta_{2s}$ to be determined self-consistently by minimizing the ground state energy.

As there is only single hole pocket FS in the low energy excitations, we can project the effective Hamiltonian onto the hole band and especially focus on the vicinity of FS. Turned to the band basis $\Gamma_{k,\sigma} \equiv (\alpha_{k,\sigma}, \beta_{k,\sigma})^T$, the mean-field Hamiltonian can be straightforwardly obtained
\[
H_{\text{eff}}^{\text{MF}} = \frac{1}{2} \sum_{k,\sigma} \left( \xi_h(k) + \frac{i\epsilon_{xd}(k)\Delta_x(k)}{\sqrt{\epsilon_{zd}^2 + \epsilon_z^2}} \right) \beta_{k,\sigma}^\dagger \beta_{k,\sigma}^\dagger + \text{h.c.}
\]

Here we can see that the $s$-wave pairing component $\Delta_x$ arising from the NN spin exchange interaction is renormalized by a $d$-wave form factor $\epsilon_{xd} \propto (\cos k_x - \cos k_y)$, which is inherited from the NN hopping integral in the $C_4$ symmetry representation. Actually it should be no surprise, since we can physically understand this renormalization factor in the following way. The NN pairing interaction glues the inter-sublattice particles, which coexist in the hole band with probability proportional to the hybridization energy gain. As a result, the effective intra-band pairing condensate is supposed to be renormalized by $\epsilon_{xd}$. As shown in Fig[4], along the zero lines of hybridization energy $\epsilon_{xd}$, there is no coexistence of the sublattice degrees of freedom so that there are no inter-orbital Cooper pairs, regardless of their internal pairing symmetry. Such a mechanism is parallel to the effective intra-band $p$-wave pairing induced on the helical electrons in proximity to the $s$-wave superconductors[38].

Then the Bogoliubov quasi-particle spectrum can be derived
\[
E(k) = \pm \sqrt{\xi_h^2(k) + \Delta_0^2(k) + \Delta_x^2(k)},
\]
where $\Delta_x(k) = \frac{\epsilon_{xd}(k)}{\sqrt{\epsilon_{zd}^2 + \epsilon_z^2}}\Delta_x(k)$ and $E(k)$ exhibits the nodal excitations when $\Delta_0(k) = 0$. Note that the inter-band pairing between hole band and high energy electron band only contributes second order perturbation corrections to the gap structure, but is unable to alter its symmetry. The $d$-wave gap nodes carrying one unit of vorticity in the Nambu space are topologically protected[32,33]. Within the AB layer, there are only two ways to destroy these nodes. The first one is to generate a mass upon the massless Bogoliubov quasi-particles[41] which is forbidden by the TR symmetry in pairing sector. The mass term is an additional pairing component with phase difference that cannot be gauged away. The other way is to move the nodes with opposite vorticity to annihilate each other, which is prevented by the $C_4^p$ symmetry that confines the nodes to the unfolded BZ diagonal.

Now we have two competing pairing components: the NNN Cooper pair condensate $\Delta_0(k)$ with the $s_{x'y'}$-wave form factor and the NN Cooper pair condensate $\Delta_x(k)$ carrying the $d_{x'y'-y}$-wave form factor. They can be varied by the NN interaction $J_1$ for a fixed NNN interaction $J_{2s} \approx 0.3$. The detailed self-consistency calculation explicitly shows phase transitions of pairing symmetry displayed in Fig[3]. When $J_1 \ll J_{2s}$, the NNN interaction overwhelms the NN interaction, leading to the $s_{x'y'}$-wave pairing, whereas $J_1 \gg J_{2s}$ results in the $d_{x'y'-y}$-wave pairing. In between, the SC with a mixed pairing $s + id \times s$ is energetically more favorable, which spontaneously breaks the TR symmetry. To compare with the pressure experiments[32], we notice that, upon increasing pressure, both $t_2$ and $J_2$ are expected to grow faster than $t_1$ and $J_1$. Since the dopant concentration is fixed and the small hole pocket FS does not change qualitatively, we expect that decreasing the ratio of $J_1/J_{2s}$ is adequate to capture the essential physics during the period of increasing pressure. When the superfluid density does not vary drastically, the superconducting critical temperature would be roughly proportional to the maximum gap on the FS, and it turns out the tendency of maximum gap on the FS along $J_1$ shown by the black solid line in Fig[3] concurs qualitatively well with the $T_c$ trend under decreasing pressure in experiments[32]. Moreover, the phase transition from the $d \times s$-wave nodal SC to the $s + id \times s$ nodeless SC belongs to the TR breaking mass generation scenario of destroying the pairing gap nodes.

For the CD layer, we can simply apply the $S_4$ symmetry to obtain its low-energy effective Hamiltonian:
\[
H_{\text{eff}}^{\text{CD}} = \frac{1}{2} \sum_{k,\sigma} \xi_h(k) \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma}^\dagger + \frac{\eta}{2} \sum_k \left( \Delta_0(k) + \frac{\epsilon_{xd}(k)}{\sqrt{\epsilon_{zd}^2 + \epsilon_z^2}}\Delta_x(k) \right) \gamma_{k,\uparrow}^\dagger \gamma_{-k,\downarrow}^\dagger + \text{h.c.}
\]
where $\gamma_{k,\sigma}^\dagger = (\cos \frac{\eta k}{2} c_{k,\sigma}^\dagger - \text{sgn} (\epsilon_{xx}) (\sin \frac{\eta k}{2})^\prime a_{k,\sigma}^\dagger)$. $\eta$ embodies the global phase difference between the pairing condensates of the two layers, and is restricted to be either $\pm 1$ or $\pm i$ as the one-dimensional representations of the $S_4$ point group [22]. The relative phase difference can be pinned down by inter-layer couplings for the benefit of energetics.

**Octet nodal SC from distorting $d$-wave pairing**

We are now in a good position to focus on the nodal phase at ambient pressure, which appears like a sphinx in a variety of experiments. Based on what we obtained, we have two $S_4$-related $C_4^d$ symmetric hole pockets which are absolutely degenerate. They can form $d$-wave pairing condensates with degenerate quartet nodes residing on the unfolded BZ diagonal (Fig.4a and 4b). Such degeneracy is highly unstable against any arbitrary perturbation, so we are obliged to return to the more realistic materials by involving the weak $C_4^d$-breaking hopping $t_{1s}$ and inter-layer tunneling $t_{2d}$. As for the inter-layer tunneling, the $s$-wave NN tunneling would be the dominant term, from the estimate of orbitals overlap and symmetry analysis (see Fig.4b). Note that the on-site tunneling is suppressed because of the orbital orthogonality. Surprisingly, the $S_4$ symmetry survives this tunneling process. When $t_{2d} < t_{1s} < t_{1d}$, the effective Hamiltonians for the AB and CD layers are modified by $t_{1s}$ in their respective ways:

$$H_{\text{eff}}^{1s} \rightarrow \frac{1}{2} \sum_{k,\sigma} \Delta_{1s}^\dagger (k) \beta_{k,\sigma}^\dagger \beta_{k,\sigma} + \frac{1}{2} \sum_{k} J_2 \Delta_x (k) \beta_{k,\uparrow} \beta_{k,\downarrow}^\dagger + h.c. \quad (13)$$

$$H_{\text{eff}}^{2s} \rightarrow \frac{1}{2} \sum_{k,\sigma} \Delta_{2s}^\dagger (k) \gamma_{k,\sigma}^\dagger \gamma_{k,\sigma} + \frac{1}{2} \sum_{k} J_2 \Delta_x (k) \gamma_{k,\uparrow} \gamma_{k,\downarrow}^\dagger + h.c. \quad (14)$$

where the global phase of $\Delta_{1s}$ has been gauged to absorb the phase factor $-i$. Meanwhile, the normal state dispersion and the hybridization angle for AB/CD layer are given by

$$\xi_{1s}^\dagger (k) = \xi_{0} (k) - \sqrt{\epsilon_{sd}^2 + \epsilon_{ss}^2} \quad (15)$$

and $\theta^{\pm} = \tan^{-1} \frac{\epsilon_{sd} + \epsilon_{sx}}{\epsilon_{sd} - \epsilon_{sx}},$ so that the quasiparticles, $\beta_{k,\sigma}^\dagger$ and $\gamma_{k,\sigma}^\dagger$ are adapted (see Supplementary Material for detail). As a result, the $d$-wave nodal lines that used to lie across the unfolded BZ diagonal are now twisted and dragged away from the $\Gamma$ point by a “nematic force”, resulting in a simultaneous movement of nodes along the elongating direction of the hole Fermi pockets (Fig.4a and 4b). Since the nodes with opposite vorticity need to travel a finite path along the FS before annihilation, they can survive a finite weak $C_4^d$-breaking term depending on the size of the FS.

The hole pockets from the AB and CD layers are required by $S_4$ symmetry to intersect at the unfolded BZ diagonal (Fig.4a). Degeneracy at this point is unstable against any arbitrarily weak perturbation of inter-layer tunneling:

$$H_{c} = \frac{1}{2} \sum_{k,\sigma} \xi_{c} (k) \left( a_{k,\sigma}^\dagger d_{k,\sigma} + b_{k,\sigma}^\dagger c_{k,\sigma} \right) + h.c. \quad (16)$$

So the degenerate Fermi-points at the unfolded BZ diagonal are split by $\xi_{c} (k)$ into two Fermi-points, whose corresponding quasi-particles are given by the bonding and anti-bonding states of the two layers. The split Fermi points smoothly join the Fermi sheets far away from the unfolded BZ diagonal, where $\xi_{c} (k)$ amounts only up to second order perturbation corrections (Fig.4c). Next let’s consider how the pairing matrix changes with the inter-layer tunneling. It is expected that $\eta = 1$ to avoid the destructive interference along the BZ diagonal where two layers strongly hybridize. Therefore, the pairing condensates on the unfolded BZ diagonal were identical for hole pockets from both layers, guaranteed by the $S_4$ symmetry.

**FIG. 3**: Phase diagram of the superconducting phases for KBFe$_2$As$_2$ under pressure (decreasing $J_1$ mimics the trend of increasing pressure). The parameters are $x = 0.05$, $t_{1d} = -1.2$, $t_{2s} = 0.5$, $J_2 = 0.5$, $J_2 = 0.2$ in unit of $t_{2d} = 1$. Red line is for the NN Cooper pair $|1s\rangle$ that obtains $s_{1s}$ form factor in momentum space, while blue line is for the NNN Cooper pair condensate $|2s\rangle$ that is endowed with $d_{2s}\times s_{2s}$-wave form factor. The $d_{2s}\times s_{2s}$-wave SC comes to replace the $s_{1s}$-wave SC when $J_1$ overcomes $J_{2s}$. The grey color region marks the intermediate phase region with $s_{2s}$+$td_{2s}\times s_{2s}$-wave mixed pairing SC. Black solid line shows the maximal gap along the FS, which is roughly proportional to the critical temperature when superfluid density does not vary drastically. Insets show the pairing gap structure on the FS, characteristic of the three pairing phases, respectively.
FIG. 4: Distorted $d$-wave nodes on the Fermi surfaces. The white diamond emphasizes the folded BZ; the orange dashed lines denote the nodal lines of the effective $d_{x^2-y^2}$-wave pairing condensate on the FS distorted by $s_{x^2+y^2}$-wave factor (the effect of weak $s$-wave is moderately exaggerated for illustration); The FS is separated by pairing nodal lines into the segments with positive (negative) pairing condensate marked by red (blue) color, respectively. (a) In the AB layer, the mixing weak $s$-wave NN hopping acts like a ”nematic force” that elongates the FS and distorts the $d$-wave nodal lines, leading to shifted quartet nodes. (b) As the CD layer is related to AB layer by the $S_4$ symmetry, the distortion occurs in the perpendicular direction. (c) Near unfolded BZ diagonal the quasi-particles from the AB and CD layers are strongly hybridized with each other by any infinitesimal inter-layer tunneling. The intersecting elliptic hole pockets are therefore reconstructed into inner and outer pockets. The inner one has nodeless pairing gap whereas the outer one shows octet nodal gap structure. The origin of nodes can be attributed to a rather simple symbolic equation ”$8=4+4$”.

Inspired by this organizing principle governed by $C^p_4$ and $S_4$ symmetries, we can gain some insight into the electronic structure and pairing symmetry of iron-selenide (FeSe). While the $d$-wave representation $C^p_4$ of plaquette-centered rotation symmetry stabilizes the FS structure of iron-pnictides, the $s$-wave representation $C^s_4$ captures the key feature of FSs in FeSe as shown in Fig.4, where the NN $s$-wave hopping dominates. In Fig.5, it can be shown that, when the $d$-wave NN hopping is completely replaced by the $s$-wave hopping followed by a particle-hole transform, we can obtain the FS with a robust electron pocket around $X$ point without hole pocket around $\Gamma$ point, which is characteristic of FeSe\cite{31}. In this case, the electron pocket and its central double Dirac point are protected by the TR symmetry together with the $s$-wave representation of the plaquette-centered rotation symmetry $C^p_4 \equiv \tau_{31}$. Thus, the band structure of FeSe is related to that of iron-pnictides by a gauge transform combined with a particle-hole transform.

FIG. 5: (a) Gauge choice characteristic of FeSe, followed by a particle-hole transform. (b) Band dispersion typical of iron-chalcogenides, where the electron pocket around $(\pi,0)$ is robust while hole pocket around $(0,0)$ is dispensable. The parameters for the demonstration are chosen to be $t_{1d} = 0$, $t_{1s} = 0.45$, $t_{2s} = 0.5$ in unit of $t_{2d} = 1$. 
When the pairing symmetry is considered, we can just focus on the monolayer FeSe with only electron Fermi pockets around X point \[\Gamma\]. Parallel to the above discussion for KFe\(_2\)As\(_2\), there are two possible pairing symmetries for the monolayer FeSe: one is the \(s_\pm y^2\)-wave Cooper pair glued by the dominant NNN AF coupling \(J_2\) and the other one is the effective \(s_\pm x^2+y^2 \times d_{x^2-y^2}\)-wave Cooper pair on the electron pockets around the X point for a relatively large NN AF coupling \(J_1\). Although the inter-orbital Cooper pairs glued by \(J_1\) has \(d_{x^2-y^2}\)-wave symmetry, whose nodal line avoids the FS to maximize the energy gain, the projection of the inter-orbital Cooper pairs onto the FS yields an additional \(s_\pm x^2+y^2\) form factor inherited from the electronic structure. However, when \(J_2\) overwhemls \(J_1\), the pairing symmetry is the \(s_\pm y^2\)-wave. Without more interactions, the two layers tolerating weak inter-layer tunneling tend to lock their respective phases of Cooper pairs to be identical, otherwise there would be destructive interference. This supports the plain s-wave pairing symmetry as observed by the STM measurement\[15\]. But when \(J_1\) dominates over \(J_2\), the effective \(s_\pm x^2+y^2 \times d_{x^2-y^2}\)-wave pairing condensate would show a gap minimum near the folded BZ boundary and a gap maximum along the unfolded BZ boundary, which seems to concur with the superconducting gap anisotropy measured by ARPES\[11\].

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