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On the gap symmetry in KFe_2As_2 and $\cos 4\theta$ gap component in LiFeAs

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We revisit the issue of the gap symmetry in KFe_2As_2 , which is an Fe-pnictide superconductor with only hole pockets. Previous theoretical studies mostly argued for a d -wave gap in KFe_2As_2 since transport and thermodynamic measurements point to the presence of the gap nodes. However, a d -wave gap is inconsistent with recent laser-based angle-resolved photoemission measurements. We propose the scenario for a nodal s -wave superconductivity induced by a non-magnetic intra-band and inter-band interactions between fermions near hole pockets. The superconducting gap changes sign between the hole pockets and has $\cos 4\theta$ angular dependence and accidental nodes on one or several hole pockets. We argue that strong angle dependence is the consequence of near-degeneracy between inter-pocket and intra-pocket interaction on the hole pockets. We also analyze $\cos 4\theta$ angular dependence of the gap in other Fe-pnictides and compare theoretical results with the photoemission experiments of LiFeAs .

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I. INTRODUCTION

One of the most interesting features in the rapidly growing family of the Fe-based superconductors (FeSCs) is the manifestation of different gap structures in the superconducting (SC) state which may potentially indicate different gap symmetries in different materials¹. An important step towards identifying the gap symmetry is to establish whether or not the system shows nodal behavior and whether or not the nodes are symmetry-related. In the weakly and moderately doped FeSCs, which have electron-like and hole-like pockets, there is a strong experimental evidence¹ and general agreement amongst theoretical approaches²⁻⁶ that the gap symmetry is of s^\pm type with opposite sign of the gap on the electron and hole pockets. Angle-Resolved Photo-Emission Spectroscopy (ARPES) on optimally doped $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$ ^{7,8}, $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ ⁹ and undoped LiFeAs ^{10,11} has identified nodeless gaps on the hole pockets ruling out non- s -wave gap symmetry, up to certain exceptions¹². Thermodynamic measurements on these materials¹³⁻¹⁵ show nodeless behavior consistent with s -wave gap symmetry. In some other compounds (such as $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$) electronic transport and thermodynamic measurements¹⁶ reveal the presence of nodes and at the same time ARPES¹⁷ clearly rules out nodes on hole pockets. This is still consistent with s^\pm symmetry provided that the gap nodes are accidental and reside on the electron pockets. The reasoning behind the existence of no-nodal and nodal s^\pm gap structures is specific to the Fermi surface (FS) geometry in FeSCs and is related to the interplay between inter-pocket and intra-pocket electron(e)-hole(h) couplings (u_{eh} and u_{ee} , u_{hh} , respectively). When the interactions are even slightly anisotropic, a larger inter-pocket coupling ($u_{eh}^2 > u_{ee}u_{hh}$) leads to a nodeless structure while a smaller inter-pocket coupling ($u_{eh}^2 < u_{ee}u_{hh}$) leads to acciden-

tal nodes on electron pockets^{6,18}.

This reasoning, however, does not apply to FeSCs with only one kind of carriers, either holes or electrons. In this article we focus on systems with only hole pockets. The primary example here is KFe_2As_2 which is at the end point of the family of hole-doped $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$. Synchrotron-based ARPES measurements on this material¹⁹⁻²¹ show two distinct hole pockets centered at Γ point ($\mathbf{k} = (0, 0)$) and small hole blades near (π, π) point, but no electron pockets. Recent laser-based ARPES measurement²² resolved three hole pockets near Γ , of which, the inner and the middle ones, two have orbital content d_{xz}/d_{yz} and the third, outer pocket is d_{xy} . The electronic structure with 3 hole pockets at Γ and hole blades at the corners of the Brillouin zone (BZ) is consistent with DFT band structure calculations for this material²³ and with the trends observed in ARPES studies of $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$ with increasing x (Ref. 24).

Penetration depth and transport measurements of KFe_2As_2 ²⁵ show linear in T behavior, similar to that in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$. There are two existing theoretical scenarios for this behavior. One is that the gap has $d_{x^2-y^2}$ symmetry, induced primarily by $2k_F$ intra-pocket interaction within the largest hole pocket. In this case, the gap has nodes along $k_x = k_y$ which naturally explains the observed linear in T behavior. Another scenario is that the magnetically enhanced electron-hole interaction still gives rise to s^\pm superconductivity²⁶, despite the electron states being gapped. Within this scenario, the observed linear in T dependencies are either due to the smallness of the gap on one of hole pockets or, potentially, due to the presence of horizontal line nodes at some k_z on the other hole pocket. Functional renormalization group (fRG) study²⁷ found d -wave as a clear winner, while FS-restricted RPA-type spin-fluctuation (SF) analysis²⁶ and the analytical study in which the interactions are approximated by their lowest angular harmonics (LAH)¹⁸

have found that s -wave and d -wave pairing amplitudes have near-equal strength, primarily because $2k_F$ for the largest hole FS is not far from the distance between hole and the would-be electron pockets.

Because d -wave gap naturally explains the linear in T behavior it had been generally considered as the most plausible gap structure. This further raised speculations about potential time-reversal symmetry breaking $s + id$ pairing state in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ at $x \leq 1^{28}$. However, the neutron scattering analysis of the vortex lattice in KFe_2As_2 ²⁹ and, particularly, the laser-based ARPES measurements of the gaps along the three hole FSs at Γ point²² cast strong doubts that the gap is d -wave. The ARPES data show that: (i) the measured gap is definitely the smallest at the outer pocket, while all theoretical calculations point out^{18,26,27} that it should be the largest, if the gap is d -wave; (ii) the gap along the smallest (inner) hole pocket has angular dependence but no nodes, and (iii) the gap along the middle hole pocket has accidental nodes. All three results are inconsistent with the d -wave gap. The data are partly consistent with the theoretical prediction for s -wave gap^{18,26} in that it is the smallest on the outer pocket. However, the substantial angular variation of the gaps and the nodal behavior of the gap on the middle hole FSs is inconsistent with the angle-independent s -wave gap obtained in the LAH approximation¹⁸ and also inconsistent with the SF analysis according to which s -wave gap has no nodes except at a particular k_z where the gap on the middle hole pocket just vanishes. Experimentally, laser-based ARPES measures the gap averaged over some range of k_z ²², which should wipe out such horizontal nodes.

In this article we argue that the superconducting state with an s -wave gap symmetry *and* nodes appears quite naturally when only hole pockets are present if the interaction between fermions is the largest at a small momentum transfer. This is the case when spin and charge fluctuations are not strong, and the effective pairing interaction is well approximated by the first-order term, which is the combination of Hubbard and Hund intra- and inter-orbital interactions, dressed up by ‘coherence factors’ which hybridize electron orbitals and produce bands and consequently hole pockets. We consider only direct $Fe - Fe$ interaction and neglect the induced interaction via a pnictide. In this situation, to treat interactions adequately one should move to the unfolded BZ, in which the hole blades are at $(\pi, 0)$ and symmetry-related points, and the outer d_{xy} hole pocket is at (π, π) .

When the interaction in the unfolded zone is peaked at a small momentum transfer, the (π, π) hole pocket and $(\pi, 0)$ hole blades are not overly relevant, and the physics is determined by intra-pocket and inter-pocket interactions for the two hole pockets centered at Γ point. For strictly angle-independent interactions, superconductivity is only possible when the inter-pocket coupling exceeds the intra-pocket one. Then the system develops an s^\pm gap which changes sign between the two hole pockets. We show, however, that, once we allow the interaction to

have some angular dependence, superconductivity develops even when intra-pocket coupling is larger. Moreover, when intra-pocket and inter-pocket interactions are of near-equal strength, which is the case for KFe_2As_2 because both hole FSs are small and centered at the same point, the angular component of intra-pocket interaction is enhanced in a resonance-type fashion, and the SC gap acquires strong variations along the hole FSs and accidental nodes, even if this angular component is small. Such resonant enhancement of the angular-dependent component of the gap has been previously found³⁰ for the case when both hole and electron pockets are present and the dominant inter-pocket interaction is between hole and electron pockets. Here we apply the same reasoning to the case when inter-pocket interaction is between the two hole pockets at the Γ point.

For completeness, we also consider in some detail $\cos 4\theta$ gap components on hole pockets in other FeSCs, which have both hole and electron FSs, and discuss the interplay between $\cos 4\theta$ and $\cos 2\theta$ gap variations along electron pockets. In this context we compare theoretical results with recent ARPES measurements of gap variations in LiFeAs along both hole and electron FSs^{31,32}. We argue, in particular, that the data unambiguously show the presence of $\cos 4\theta$ and $\cos 2\theta$ oscillations on electron FSs. We argue that the sign of $\cos 2\theta$ term is consistent with the theoretical prediction for the case when the pairing interaction is predominantly between electron and hole pockets.

II. THE APPROACH

We consider intra-pocket and inter-pocket pairing interactions between low-energy hole-like fermions which we label as h_i where i specifies the pocket. The physics we consider is not overly sensitive to k_z variations of the electronic dispersion, and we restrict ourselves to a pure 2D model. The interactions $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$, generally depend on the angles along hole FSs. By general reasons¹⁸ the angle dependencies of the interactions $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ can be expanded in powers of $\cos 4n\theta_i$, $\cos 4n\theta_j$, where $\theta_{i,j}$ are the angles along the corresponding FS^{6,18}. The first term in the series is a constant U_{h_i, h_j} for s -wave pairing and $\cos 2\theta_i \cos 2\theta_j$ for d -wave pairing. The d -wave pairing has been analyzed in detail in Ref. 18, here we consider s -wave pairing.

In Ref. 18 only the constant s -wave terms had been kept. Accordingly, s -wave gaps Δ_i were angle-independent. Here we go a step further and include into consideration the sub-leading $\cos 4\theta_{i,j}$ and, later, also $\cos 8\theta_{i,j}$ terms in $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$. This gives rise to $\cos 4\theta_i$ and $\cos 8\theta_i$ angle dependent terms in the gaps Δ_i . We do not consider higher-order harmonics as measured gaps are well fitted by the $\cos 4\theta_i$ and $\cos 8\theta_i$ forms²².

The magnitude of angle-dependent terms in the interactions $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ depends on the structure of the hopping integrals in the orbital basis³³ and

can be material-dependent. Still, ARPES data on weakly/moderately doped $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$ show almost no angle variation on the hole gaps which most likely indicates that the angle-dependent terms in $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ in K-doped 122 systems are weak¹⁷. Naively, one could then expect little angle dependence of s -wave gaps in KFe_2As_2 as well. We show, however, that this is not the case if the pairing interaction in KFe_2As_2 involves the two hole pockets centered at Γ . Then the angular dependent $\cos 4\theta$ term in the gap is enhanced in a resonance-like fashion and may give rise to accidental nodes.

That an s -wave gap on the hole pocket can have nodes due to strong 4θ variations that has been found before³⁴ in the study of a 3D band structure of $\text{Ba}_{1-x}\text{K}_x(\text{FeAs})_2$ where electron pockets were still present and the pairing was driven by large momentum scattering enhanced by spin fluctuations. In that work, the nodes were only present for a particular k_z . In our case, the gap has vertical line nodes, present at any k_z .

To make the presentation more transparent and physically insightful, we first consider analytically in the next section the case of just two hole pockets h_1 and h_2 at $(0, 0)$, include the $\cos 4\theta$ dependence of the intra-pocket $h_1 - h_2$ interaction and show how accidental nodes appear on either both or one of these pockets already for weakly angle-dependent interaction. We then consider in Sec. IV the full model with 3 hole pockets, use as inputs the interactions $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ obtained from the underlying 5-orbital model, fit all interactions by the first three angular harmonics (a constant, $\cos 4\theta_i$, and $\cos 8\theta_i$ terms) and solve 9×9 matrix gap equation. We show that intra-pocket and inter-pocket interactions involving h_1 and h_2 pockets are almost identical, and the angular dependent components of the interactions are rather weak. Nevertheless, the solution of 9×9 matrix gap equation shows that the s -wave gap has accidental nodes on at least one hole pocket. This analysis also confirms that the gap at (π, π) pocket is rather small, i.e., the pairing is predominantly determined by the interactions between fermions near the Γ point.

In Sec. V we consider relative phases of $\cos 4\theta$ terms on different hole FSs and argue that the sign of the $\cos 4\theta$ component of the gap on a given FS is at least partly determined by its shape. In this section we also discuss the situation in another Fe-pnictide, LiFeAs , in which $\cos 4\theta$ variations have been observed on both hole and electron FSs^{31,32,35}. We argue that the data also show the presence of $\cos 2\theta$ variations along electron FSs, predicted by the theory.

III. THE MODEL WITH TWO HOLE POCKETS AT $(0, 0)$

Like we said above, we keep $\cos 4\theta$ angular dependence in the inter-pocket interaction $U_{h_1 h_2}$ and approximate the

intra-pocket $U_{h_1 h_1}$ and $U_{h_2 h_2}$ by constants, i.e., set

$$\begin{aligned} U_{h_1 h_1}(k, p) &= U_{11}; \quad U_{h_2 h_2}(k, p) = U_{22} \\ U_{h_1 h_2}(k, p) &= U_{12} (1 + \alpha_{12} \cos 4\theta_k + \alpha_{21} \cos 4\theta_p) \end{aligned} \quad (1)$$

where θ are measured from the x axis.

The linearized BCS gap equation that one needs to solve is

$$\begin{aligned} \Delta_{h_1}(p) &= -LN_{F_1} \int_0^{2\pi} \frac{d\theta_k}{2\pi} U_{h_1 h_1}(p, k) \Delta_{h_1}(k) - \\ &\quad LN_{F_2} \int_0^{2\pi} \frac{d\theta_k}{2\pi} U_{h_1 h_2}(p, k) \Delta_{h_2}(k) \\ \Delta_{h_2}(p) &= -LN_{F_1} \int_0^{2\pi} \frac{d\theta_k}{2\pi} U_{h_2 h_1}(p, k) \Delta_{h_1}(k) - \\ &\quad LN_{F_2} \int_0^{2\pi} \frac{d\theta_k}{2\pi} U_{h_2 h_2}(p, k) \Delta_{h_2}(k) \end{aligned} \quad (2)$$

where $L = \log \frac{\Lambda}{T_c}$ and $N_{F_{1,2}}$ are the densities of states. For the interaction of Eq. (1), the gap structure is

$$\begin{aligned} \Delta_{h_1}(p) &= \Delta_1 (1 + r_1 \cos 4\theta_p) \\ \Delta_{h_2}(p) &= \Delta_2 (1 + r_2 \cos 4\theta_p) \end{aligned} \quad (3)$$

A. Equivalent hole pockets

We first consider the case when the densities of states on the two hole pockets are the same, $N_{F_1} = N_{F_2} \equiv N_F$, and then extend the consideration to $N_{F_1} \neq N_{F_2}$. For the first case, it is natural to take $U_{11} = U_{22} = U$ and $\alpha_{12} = \alpha_{21} = \alpha$, and introduce dimensionless couplings $u_{12} = N_F U_{12}$ and $u = N_F U$. For positive u_{ab} , which we consider, the solution of the gap equation is $\Delta_{h_1} = -\Delta_{h_2}$ with $r_1 = r_2 = u_{12} \alpha L$ and it develops at

$$L = \frac{-(u - u_{12}) + \sqrt{(u - u_{12})^2 + 2(u_{12} \alpha)^2}}{(u_{12} \alpha)^2} \quad (4)$$

Observe that, for any $\alpha \neq 0$, $L > 0$ (i.e., $T_c > 0$) no matter what the signs of $u_{12} - u$ and α are (c.f. Ref.30). Observe also that this s^\pm gap structure with opposite signs of the gaps on different hole pockets is different from that proposed in Ref.26 where the gaps on hole pockets have the same sign and that on the would-be electron pockets have opposite sign.

One can further discuss the characteristics of the solution by looking into different parameter regimes. For small α and $u > u_{12}$, we have $r_1 = \frac{2(u - u_{12})}{|u_{12} \alpha|}$ and $L = \frac{2(u - u_{12})}{(u_{12} \alpha)^2}$. For small α this yields the solution with nodes ($r_1 > 1$), although T_c is quite small. For $u < u_{12}$, we have $r_1 = \frac{|u_{12} \alpha|}{|u - u_{12}|} < 1$ and $L = \frac{1}{|u - u_{12}|}$. For small α , the gap is nodeless, and T_c is larger than in the previous case. The most interesting case, relevant to KFe_2As_2 , is

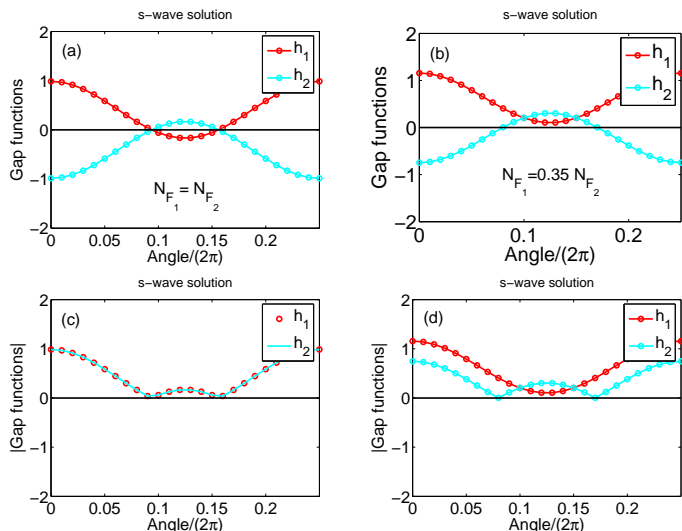


FIG. 1: (a) The gap structure obtained for equal density of states ($N_{F_1} = N_{F_2}$) on the two hole pockets at Γ . We used $U_{11} = U_{22} = U_{12}$ and $\alpha = 0.1$. The gap satisfies $\Delta_{h_1} = -\Delta_{h_2} = \Delta(1 + \sqrt{2} \cos 4\theta)$ and has nodes on both FSs. (b) The same as (a), but with $N_{F_1} = 0.35 N_{F_2}$. Now the two gaps are non-equivalent and the gap on the inner hole FS has angle variation but no nodes. For comparison with ARPES, in panels (c) and (d) we plot the absolute values of the gaps from panels (a) and (b), respectively.

the one with $u = u_{12}$ (because the two FSs are centered at the same Γ point, intra-pocket and inter-pocket interactions are undistinguishable). In this case we get $r_1 = \sqrt{2}$ independent of α , indicating that nodes arise even for a very weak angular dependence of the interaction³⁰. This is what we mean by a resonant enhancement of the angular dependence of the interactions. Fig. 1(a) shows the gap structure obtained for this case.

B. Non-equivalent hole pockets

We next consider the case of non-equivalent hole pockets, when $N_{F_1} \neq N_{F_2}$ and, generally, $U_{11} \neq U_{22}$. Both lead to $u_{11} = N_{F_1} U_{11}$ being different from $u_{22} = N_{F_2} U_{22}$. In principle, α_{12} is also different from α_{21} , but since we keep α small, an inequality of $\alpha_{12,21}$ is not relevant and we continue to treat them equal ($\alpha_{12} = \alpha_{21} = \alpha$).

There are two issues that one needs to consider for non-equivalent pockets – whether the solution exists for all parameters, and what is the structure of the two gaps. From Eq. (2) one obtains the fourth-order equation for L

$$\frac{(u_{12}\alpha)^4}{4} L^4 - \frac{(u_{12}\alpha)^2(u_{11} + u_{22})}{2} L^3 + (u_{11}u_{22} - u_{12}u'_{12} - (u_{12}\alpha)^2) L^2 + (u_{11} + u_{22})L + 1 = 0 \quad (5)$$

where $u_{12} = N_{F_1} U_{12}$ and $u'_{12} = N_{F_2} U_{12}$. T_c exists if this equation has a solution at $L > 0$. The full analysis

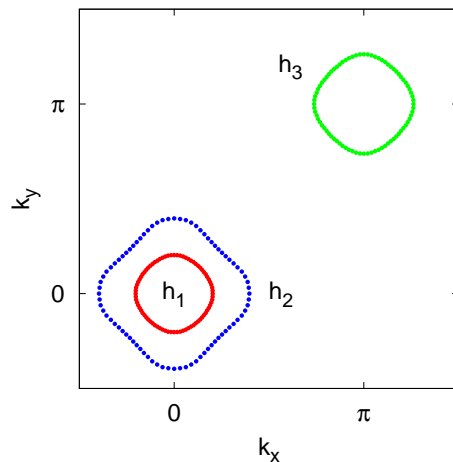


FIG. 2: The FS for our 5-orbital model in the unfolded BZ. Only hole FSs are present; the case corresponding to KFe_2As_2 . Two hole FSs, h_1 and h_2 , are centered at the Γ point, and one hole the FS, h_3 , is centered at (π, π) . The electronic structure was obtained in a band structure calculation for the 5-orbital model¹⁸. The energy of the $d_{3z^2-r^2}$ orbital was slightly modified to remove an additional hole pocket at (π, π) .

of (5) is elementary but cumbersome⁶ and it shows that for arbitrary U_{11} , U_{22} , and U_{12} , the solution exists when the parameters satisfy a certain inequality. However, for the case relevant to KFe_2As_2 , when $U_{11} = U_{22} = U_{12}$, i.e., $u_{11}u_{22} = u_{12}u'_{12}$ the solution exists for arbitrary N_{F_1}/N_{F_2} , and L is of order $1/(\sqrt{u_{12}u'_{12}}\alpha)$. We analyzed the gap structure for this particular case and found that, predictably, the gaps on the two pockets no longer satisfy $\Delta_{h_1} = -\Delta_{h_2}$ and also $r_1 \neq r_2$. As a result, in some range of N_{F_1}/N_{F_2} , one gap remains nodal while in the other the nodes are lifted. We illustrate this in Fig. 1(b).

We see therefore that nodal s^\pm solutions are generally favorable when $U_{11} \approx U_{22} \approx U_{12}$, which by all accounts is the case for KFe_2As_2 , and already infinitesimal α gives rise to the nodes. The T_c for a nodal solution is lower than for a non-nodal solution (for which T_c is independent of α at small α), what is also consistent with the smaller T_c in KFe_2As_2 compared to optimally doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$.

IV. 5-ORBITAL MODEL WITH 3 HOLE POCKETS

We now turn to a more microscopic description and solve the pairing problem using as input the bare interactions $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ obtained from the underlying 5-orbital model by converting Hubbard and Hund intra-orbital and inter-orbital interactions into the band basis, i.e., dressing up the interactions by angle-dependent coherence factors associated with the transformation from orbital to band basis for electron states^{18,33}. We used

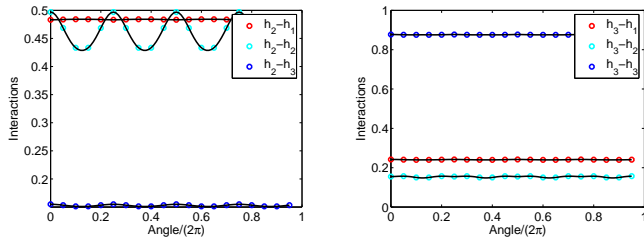


FIG. 3: The fits of s-wave components of the interactions obtained from 5-orbital model by $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$. We set $\mu = -0.2$ (in the notations of Ref. 18), when electron pockets just disappear. We fix \mathbf{k}_{F_i} to be along x direction on the h_2 pocket (left) and h_3 pocket (right) and vary \mathbf{k}_{F_j} on all three hole FSs. The interactions are almost perfectly reproduced by keeping angular harmonics up to 8θ .

band structure from Ref.18 for the hole doping, when electron pockets disappear leaving only two hole pockets at Γ point and one at (π, π) . The FS for this case is shown in Fig. 2. We fit s-wave components of *all* interactions by the first three angular harmonics: a constant, a $\cos 4\theta_i$ term and a $\cos 8\theta_i$ term, i.e, approximate $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ by

$$U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j}) = U_{ij} (1 + \alpha_{ij} \cos 4\theta_k + \alpha_{ji} \cos 4\theta_p + \beta_{ij} \cos 8\theta_k + \beta_{ji} \cos 8\theta_p) \quad (6)$$

We show the fit in Fig. 3. The agreement is nearly perfect, which makes us believe that higher harmonics can be safely neglected. The values of U_{ij} , α_{ij} , and β_{ij} are shown in the Table I. Observe that U_{11} , U_{22} and U_{12} are comparable, and the angle-dependent parts of the interactions are rather small. These are precisely the conditions we considered in the analytical analysis above.

For the interactions given by Eq. (6) each gap Δ_{h_i} has the form

$$\Delta_{h_i} = \Delta_i (1 + r_i \cos 4\theta + \bar{r}_i \cos 8\theta) \quad (7)$$

We obtain Δ_i by solving 9×9 matrix gap equation and choosing the solution with the largest attractive eigenvalue. For simplicity, we set all N_{F_i} to be equal. The result is presented in Fig. 4a.

The key observation in Fig. 4a is that s -wave gap has nodes, despite that angle-dependent terms in the interaction potentials are quite small (see Table I). We see that the gap on the outer hole FS is the smallest, as we anticipated, i.e., the dominant interaction leading to s^\pm superconductivity is between h_1 and h_2 pockets. For the particular set of interaction parameters used in 5-orbital model, the interplay between the interactions is such that the gap on the h_2 FS is the largest and has accidental nodes. This is the consequence of the fact that intra-pocket repulsion is larger on h_1 FS than on h_2 FS. We verified, however, that the interplay between the gap

on h_1 and h_2 FSs depends on tiny details of the interactions, and the two gaps become of comparable magnitude once we change input parameters by a small amount. To illustrate this, we show in Fig. 4b,c the gap structure for the cases when intra-pocket repulsion U_{11} is changed by a tiny bit – to $0.97U_{11}$ and $0.95U_{11}$, respectively. We see that such a minor modification of the coupling strength substantially affects the gap structure, making the magnitudes of the gaps on h_1 and h_2 pockets comparable, and also lifting the nodes on the h_2 pocket. This is fully consistent with our argument that the angular dependencies of the gap on the h_1 and h_2 pockets and the interplay between the magnitudes of these two gaps is the resonance phenomenon, which for small α_{ij} crucially depends on the interplay between U_{12}^2 and $U_{11}U_{22}$.

V. THE RELATIVE PHASE OF THE $\cos 4\theta$ COMPONENTS OF THE GAPS ON DIFFERENT FERMI SURFACES

In this section we consider in some detail the issue about what determines relative phases of $\cos 4\theta$ oscillations of the s-wave gaps along different hole FSs not only in KFe_2As_2 but also in other FeSCs, which contain both hole and electron pockets. For the latter, we also consider the interplay between $\cos 4\theta$ and $\cos 2\theta$ gap variations along electron pockets. These issues are relevant to experiments as angular variations of the gaps have been detected not only in KFe_2As_2 (Ref. 22) but also in LiFeAs (Refs. 31,32,35) in which both hole and electron pockets are present. To make comparisons with experiments more direct, we consider in this section the folded BZ and measure θ for both hole and electron FSs as deviations from the zone diagonal (the axis connecting hole and electron pockets).

We found from our analytical analysis in Sec. III that the sign of the $\cos 4\theta$ variation of the gap on h_1 and h_2 FSs is the same as the sign of the corresponding component of inter-pocket interaction [i.e., the sign of $r_{1,2}$ in Eq. (3)] is the same as the sign of $\alpha_{12,21}$ in Eq. (1). We assumed that the signs of α_{12} and α_{21} are positive and obtained in-phase, $\cos 4\theta$ oscillations on h_1 and h_2 FSs, with gap maxima along the direction towards the would-be electron pockets (see Fig. 1). For the 5-orbital model, $\alpha_{21} > 0$ and α_{12} is essentially zero. One should then expect $\cos 4\theta$ component of Δ_{h_1} to be small and $\cos 4\theta$ component of Δ_{h_2} to be positive, i.e., Δ_{h_2} to be the largest in the direction towards would be electron pockets. This agrees with the actual solution in Fig. 4. This form of Δ_{h_2} is consistent with the laser-ARPES results for KFe_2As_2 (Ref. 22), although the data show two additional features not captured in our analysis: (i) Δ_{h_1} also has a substantial angular dependence, and (ii) $\cos 8\theta$ gap modulations are substantial for both Δ_{h_1} and Δ_{h_2} .

The issue we address now is what determines the sign of α_{ij} . We argue that two effects contribute, one is the shape of the FS, another is the type of s-wave function

TABLE I: s -wave interaction parameters obtained from fitting by Eq. (6) the interactions between hole pockets obtained from 5-orbital model at strong hole doping (the case corresponding to KFe_2As_2 with $\mu = -0.20$, $U = 1$, $J = 0.25$, and $V = 0.69$ in the notations of Ref. 18). The numbers in bold are the magnitude of the interactions involving fermions from h_1 and h_2 pockets.

U_{11}	α_{11}	β_{11}	U_{22}	α_{22}	β_{22}	U_{12}	α_{12}	α_{21}	β_{12}	β_{21}	U_{33}	U_{13}	U_{23}
0.48	0.00	0.00	0.42	0.08	0.00	0.44	0.00	0.08	0.00	0.00	0.87	0.24	0.15

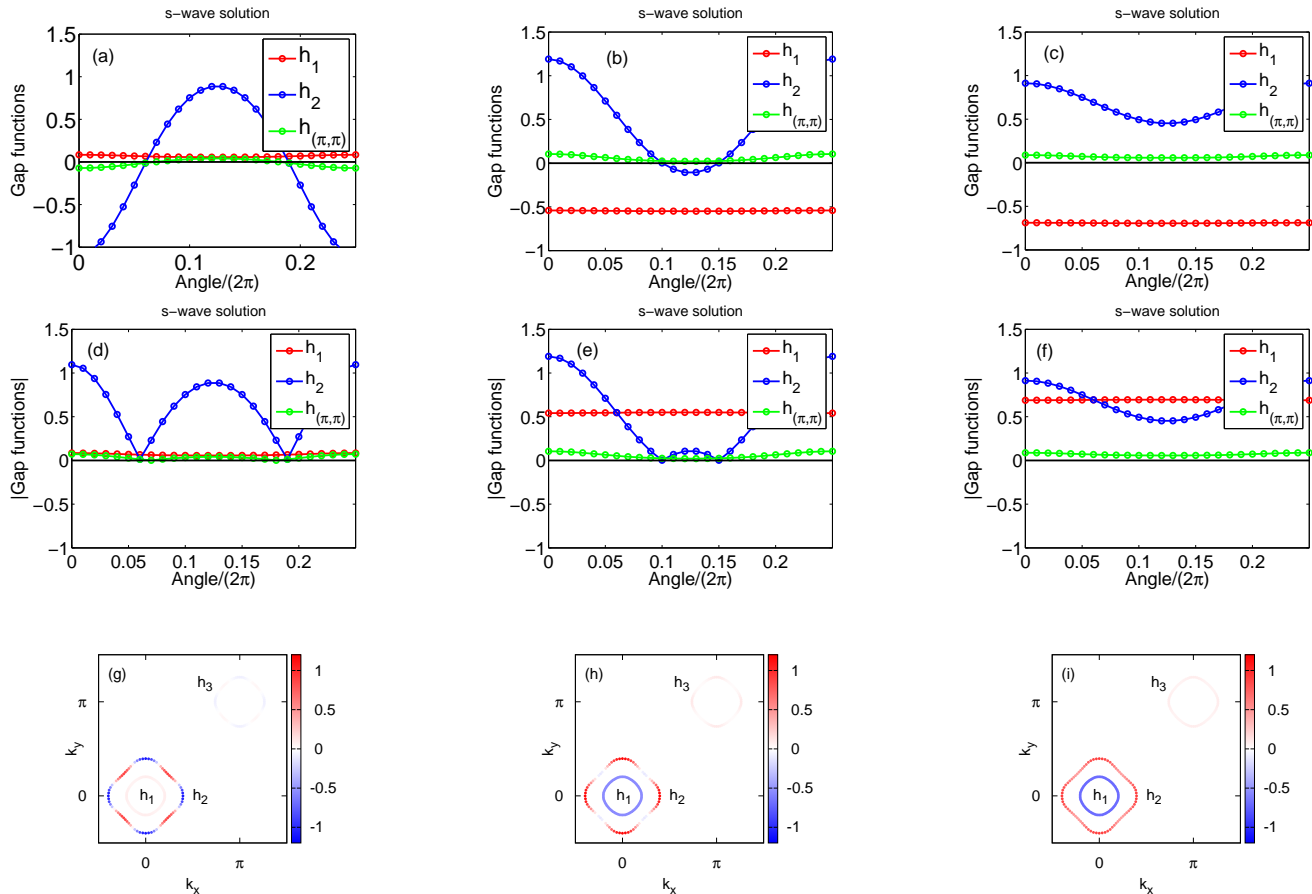


FIG. 4: (a) s -wave gap structure obtained by solving 9×9 gap equation for a 5-orbital model. The parameters are listed in Table I. (b) and (c) s -wave gap structure obtained by changing $U_{11} \rightarrow 0.97U_{11}$ and $0.95U_{11}$, respectively. We see that the gap structure is very sensitive to small changes in U_{11} . Panels (d), (e), and (f) – the absolute values of the gaps from panels (a), (b), and (c), respectively. Panels (g), (h) and (i) are the color-coded gap structures shown on the entire FS which correspond to panels (a), (b), (c) respectively. The gap on h_3 FS is small and is barely visible on the color plot.

which gives the largest contribution to the pairing interaction.

The reasoning goes as follows. Consider the pairing interaction $U(k_1, k_2)$ between two fermions located on the either h_1 or h_2 FSs. The s -wave component of the interaction is a combination of products of the A_{1g} eigenfunctions $\phi_i(k_1)\phi_j(k_2)$, where (in the folded zone) $\phi_j(k) = 1, \cos k_x + \cos k_y, \cos k_x \cos k_y$, etc. We consider interactions between particles on the FS, hence $\mathbf{k}_1 = \mathbf{k}_{F,i}$. Because k_1 and k_2 are small, $\phi_i(k)$ can be expanded in k . To the order k^4 , the dependence is $(1 - b_2\mathbf{k}^2 + b_4\mathbf{k}^4 \cos 4\theta) + \dots$, where ‘...’ stand for subleading terms. For all eigenfunc-

tions, $b_2 > 0$. And b_4 is zero if $\phi_j(k) = 1$, it is negative if $\phi_j(k) = \cos k_x + \cos k_y, \cos 2k_x + \cos 2k_y$, etc, and it is positive if $\phi_j(k) = \cos k_x \cos k_y, \cos 2k_x \cos 2k_y$, etc. For a circular FS, \mathbf{k}_F^2 is just a constant and $\cos 4\theta$ dependence comes exclusively from b_4 term. If a FS at Γ point is elongated (such that the deformation still respects C_4 symmetry of the lattice), k_F^2 along this FS can be modeled as $\mathbf{k}_F^2 = \mathbf{k}_{F_0}^2 + \varepsilon_k \cos 4\theta$, where $\mathbf{k}_{F_0}^2$ is a constant and $\varepsilon_k > 0$ if the FS is elongated along x and y directions, and $\varepsilon_k < 0$ if the FS is elongated along $x = \pm y$. This gives rise to an additional $\cos 4\theta$ dependence of the interaction potential, with the prefactor $-b_2\varepsilon_k$. The combined prefactor of the

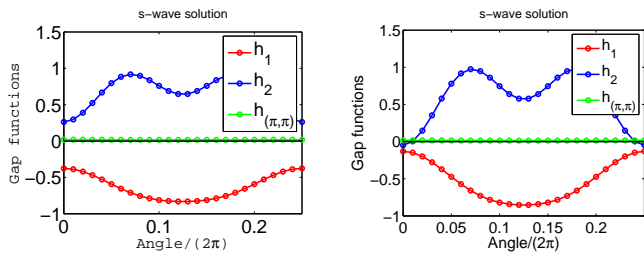


FIG. 5: *Left* – s -wave gaps along the two FSs h_1 and h_2 centered at Γ point obtained by solving 9×9 gap equations with $U_{h_i, h_j}(\mathbf{k}_{F_i}, \mathbf{k}_{F_j})$ obtained from the same 5-orbital model as before, but with RPA-renormalization of the interactions. The primary effect of RPA renormalization on hole-hole interaction is the increase of the overall magnitude of U_{ij} . The increase is somewhat larger for U_{12} than for U_{11} and U_{22} simply because the renormalized interaction is still larger for larger momentum transfers. *Right* – the same but with slightly larger intra-pocket $U_{11,22} \rightarrow 1.23U_{11,22}$ and slightly smaller inter-pocket $U_{12} \rightarrow 0.85U_{12}$, in which case the gap on h_2 FS contains nodes. The main difference between this figure and Fig. 4 is 45° rotation of the direction of the gap maxima.

$\cos 4\theta_k$ term in $U_{ij}(k, p)$ is then $\alpha_{ij} \propto -b_2\varepsilon_k + b_4$. The signs of α_{12} and α_{21} then generally depend on the interplay between the elongation of the FS and the type of the key s -wave eigenfunction. The same reasoning can be also applied to h_3 hole pocket.

The generic implication is that there is no simple way to relate the sign of $\cos 4\theta$ component of the gap to a FS geometry. And the analysis based on 5-orbital model reflects the non-universality: the maxima of the gaps on the FS h_2 are along the direction of elongation of the FS (see Figs. 2 and 4) if we use bare interactions, as we did in the previous section, but the maxima rotate by 45° if we use RPA-renormalized interactions. We show the results for the latter case in Fig. 5. In previous studies of 5-orbital model for smaller hole dopings, when both hole and electron pockets are present^{5,33}, s -wave gaps on the FSs h_1 and h_2 have maxima along the direction of elongation of each of the two FSs, but how sensitive the result is to the variation of parameters is unclear.

The situation is more transparent in the case when b_4 is small (e.g., when the leading eigenfunction is $\phi_j(k) = 1$). Then the sign of a $\cos 4\theta$ component of the gap $\Delta(k)$ *anti-correlates* with the elongation of the corresponding FS, i.e., if a FS is elongated along x and y , the gap on this FS has maxima along $x = \pm y$ directions, and if a FS is elongated along $x = \pm y$, the gap has maxima along x and y directions.

This simple reasoning works amazingly well for the experimental data. Indeed, according to laser-ARPES data²², the measured FSs h_1 and h_2 are elongated along x and y directions, while Δ_{h_1} and Δ_{h_2} extracted from ARPES have $\cos 4\theta$ terms with negative prefactors (the behavior is the same as in Fig. 5). It also works for another Fe-pnictide superconductor, LiFeAs, in which the $\cos 4\theta$ variation of the gaps on the hole FSs have been

measured in ARPES experiments^{31,32} and extracted from the STM data³⁵. The hole pockets around Γ point in LiFeAs have been identified in ARPES measurements¹⁰ and extracted from de Haas-van Alphen oscillations³⁶. The two groups agree that the inner hole pocket is either very small or doesn't even exist and that outer hole pocket is elongated along $x = \pm y$. If the $\cos 4\theta$ dependence is predominantly due to a FS elongation, the gap maxima on the h_3 pocket should then be at 45° with respect to the direction towards electron pockets. This agrees with both ARPES and STM results^{31,35}. There is a discrepancy between ARPES and dHvA results concerning the size of the middle hole pocket³⁷ (it is larger in the extraction from dHvA). Still, according to ARPES and STM measurements^{10,35}, the middle pocket is elongated along x and y , hence the gap maxima on this FS should be in the direction towards electron pockets (i.e., along $x = \pm y$). The $\cos 4\theta$ variation along h_2 FS has not been directly measured in ARPES, but it was extracted from the analysis of the STM data (Ref. 35) and found to be along the direction towards electron pockets, again in agreement with our simple reasoning. Whether the anti-correlation between the direction of the elongation of a FS and the direction along which s -wave gap is specific to KFe₂As₂ and LiFeAs or is more “universal” remains to be seen.

ARPES measurements on LiFeAs^{31,32} also detected variations of the gaps along the two electron FSs, which in the folded zone are inner and outer electron pockets centered at (π, π) . These pockets are intersecting ellipses splitted due to small hybridization. The hybridization vanishes (in the absence of spin-orbit terms) at the crossing points, and, as the consequence, inner and outer pockets touch each other^{31,32} along $k_x = \pi$ and $k_y = \pi$ lines (i.e., at 45° with respect to the direction towards Γ point).

According to theory, s -wave gaps on electron FSs should have both $\cos 4\theta$ and $\cos 2\theta$ variations. $\cos 4\theta$ variations originate by the same reasons as on hole FSs, i.e., from the expansion to forth order in $\pi - k$ of the s -wave gap functions which do not vanish at (π, π) , like $\cos k_x + \cos k_y$ or $\cos k_x \cos k_y$. By obvious reasons, $\cos 4\theta$ terms have the same signs on both electron FSs. $\cos 2\theta$ gap variations have different signs on the two electron FSs (before hybridization) and originate by two reasons: (i) electron pockets are ellipses, and (ii) s -wave gap function generally contains components in the form $\cos(2n+1)k_x/2 \cos(2n+1)k_y/2$ which vanish at (π, π) and yield $\cos 2\theta$ dependencies in the expansion near (π, π) (see e.g., Ref. 30). When hybridization is rather weak, the $\pm \cos 2\theta$ terms on the non-hybridized FSs become $\pm |\cos 2\theta|$ after hybridization, and the gaps on the inner and outer FSs have angular dependence in the form

$$\begin{aligned} \Delta_{inner}(\theta) &= \Delta_0 (1 + r_2 |\cos 2\theta| + r_4 \cos 4\theta) \\ \Delta_{outer}(\theta) &= \Delta_0 (1 - r_2 |\cos 2\theta| + r_4 \cos 4\theta) \end{aligned} \quad (8)$$

For strongly elliptical FSs, like in Ba(Fe_{1-x}Co_x)₂As₂,

$\cos 2\theta$ terms should be dominant, and RPA calculations for the band structure of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ do show that the angular dependence of a gap along an electron FS is predominantly $\cos 2\theta$ ^{5,18,33,38}. However, electron FSs in LiFeAs are almost circular, in which case it is likely that $\cos 2\theta$ terms are comparable to $\cos 4\theta$ terms.

ARPES experiments detect both r_2 and r_4 terms. In Fig. 6 we show a fit to the experimental data on the electron gaps from Ref. 32 (the data from Ref. 31 are very similar). We see that the angular dependence of each of the two gaps is quite accurately described by Eq. 8, and the difference between the gaps in the inner and outer pockets scales as $\cos 2\theta$, as it should according to Eq. 8. The parameters r_2 and r_4 extracted from the fit are $r_2 = 0.16$ and $r_4 = 0.11$.

Some useful information about underlying interaction can be also obtained from the fact that both r_2 and r_4 are positive. For near-circular electron pockets, the primary reason for $\cos 2\theta$ variation is the dependence of the pairing interaction on θ along the electron FS, which is generally in the form $U(\theta) = U_0(1 + \beta \cos 2\theta + \dots)$. One can easily make sure that the sign of r_2 is the same as the sign of β . The latter, in turn depends on the orbital character of FSs involved in the pairing interaction. If this interaction is predominantly between hole and electron pockets, then it is maximized in the direction towards the Γ point ($\theta = 0$)³⁹ resulting in positive β . Then r_2 should be positive as well, which is consistent with the sign of r_2 extracted from the fit. This agreement suggests that the electron-hole interaction, which is believed to determine pairing properties of 1111 and 122 materials, may also be the key pairing interaction in LiFeAs.

The sign of r_4 is less universal feature. As we said, one can obtain $\cos 4\theta$ terms in the gaps on electron FSs by expanding in $\pi - k_{x,y}$ s -wave eigenfunctions which do not vanish at (π, π) . A simple exercise in trigonometry shows that the sign of r_4 depends on the type of eigenfunction – the eigenfunction $\cos k_x + \cos k_y$ gives $r_4 < 0$, while the eigenfunction $\cos k_x \cos k_y$ gives $r_4 > 0$. The data show that $r_4 > 0$ [the gap maxima are along the direction towards Γ point], and from this perspective $\cos k_x \cos k_y$ is more likely candidate. However, to address the issue why this function and not $\cos k_x + \cos k_y$ is the primary gap component one has to perform full microscopic analysis.

VI. CONCLUSIONS

We argued in this paper that superconductivity in KFe_2As_2 , which has only hole pockets, can be s -wave with the nodes in the gap. We have demonstrated that such a state appears quite naturally if the dominant interaction between fermions is the one at small momentum transfer. This is the case when the system is far from a spin or a charge density-wave instability, and the

interactions can be well approximated by their bare values. We argued that in this situation the pairing chiefly comes from interactions between the two hole pockets

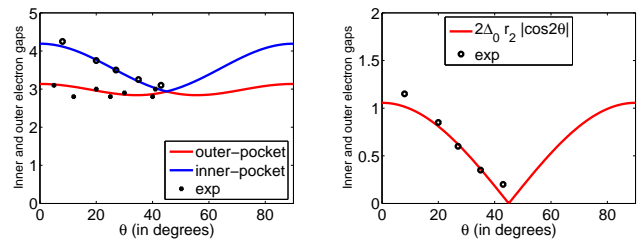


FIG. 6: *Left* – Fit, using Eq. 8, to the gap structure on electron pockets measured in Ref. 32. The symbols are the experimental data, the lines are theoretical curves. The parameters extracted from the fit are $\Delta_0 = 3.3\text{meV}$, $r_2 = 0.16$, $r_4 = 0.11$. *Right* – Plot of $\Delta_{inner} - \Delta_{outer} = 2\Delta_0 r_2 |\cos 2\theta|$. The experimental data nicely fall onto $\cos 2\theta$ dependence.

centered at Γ point in the unfolded BZ. When inter-pocket and intra-pocket interactions between these two hole pockets are of near-equal strength, s -wave solution exists, but the gap changes sign between the hole pockets and has nodes on at least one of them due to the resonant enhancement of the contribution to the s -wave gap from $\cos 4\theta$ and $\cos 8\theta$ components of the interaction. The nodes are not symmetry-related and are located at accidental θ . This s^\pm -wave state with nodes is consistent with thermodynamic, transport, and laser-based ARPES measurements of KFe_2As_2 and is in our view a viable candidate for the pairing state in this material.

We also provided a simple explanation for the relative phases of the 4θ components of the gaps along hole FS by relating the signs of the $\cos 4\theta$ terms to the shapes of the hole FSs and argued that this simple explanation is consistent with the data for KFe_2As_2 and also for LiFeAs. We argued that in LiFeAs ARPES experiments also detected both $\cos 2\theta$ and $\cos 4\theta$ gap variations along the inner and outer electron FSs.

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