Gap symmetry in KFe_2As_2 and the cos 4θ 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 a scenario for a nodal s-wave superconductivity induced by a nonmagnetic intraband and interband interactions between fermions near hole pockets. The superconducting gap changes sign between the hole pockets and has cos 4θ angular dependence and accidental nodes on one or several hole pockets. We argue that strong angle dependence is the consequence of near-degeneracy between interpocket and intrapocket interaction on the hole pockets. We also analyze the cos 4θ 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 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 materials.[1] 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 strong experimental evidence[1] and general agreement among theoretical approaches[2–6] 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 $Ba_{1-x}K_x(FeAs)_2$,[7,8] $Ba(Fe_{1-x}Co_x)_2As_2$,[9] and undoped LiFeAs[10,11] has identified nodeless gaps on the hole pockets, ruling out non-s-wave gap symmetry, with certain exceptions.[12] Thermodynamic measurements on these materials[13–15] show nodeless behavior consistent with s-wave gap symmetry. In some other compounds [such as $BaFe_2(As_{1-x}P_x)_2$] electronic transport and thermodynamic measurements[16] reveal the presence of nodes and at the same time ARPES[17] 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 intrapocket and interpocket electron-hole (e-h) couplings (u_{ee}, u_{hh} and u_{eh} respectively). When the interactions are even slightly anisotropic, a larger interpocket coupling ($u_{eh}^2 > u_{ee}u_{hh}$) leads to a nodeless structure while a smaller interpocket coupling ($u_{eh}^2 < u_{ee}u_{hh}$) leads to accidental nodes on electron pockets.[6,18]

This reasoning, however, does not apply to FeSCs with only one kind of carrier, either holes or electrons. In this paper 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 $Ba_{1-x}K_x(FeAs)_2$. Synchrotron-based ARPES measurements on this material[19–21] show two distinct hole pockets centered at Γ point [$\mathbf{k} = (0,0)$] and small hole blades near the (π,π) point, but no electron pockets. Recent laser-based ARPES measurements[22] resolved three hole pockets near Γ, of which two (the inner and the middle) have orbital content d_{xz}/d_{yz} and the third, outer pocket is d_{xy}. The electronic structure with three hole pockets at Γ and hole blades at the corners of the Brillouin zone (BZ) is consistent with density functional theory band structure calculations for this material[23] and with the trends observed in ARPES studies of $Ba_{1-x}K_x(FeAs)_2$ with increasing x (Ref. 24).

Penetration depth and transport measurements of KFe_2As_2[25] show a behavior that is linear in T, similar to that in $BaFe_2(As_{1-x}P_x)_2$. There are two existing theoretical scenarios for this behavior. One is that the gap has $d_{x^2-y^2}$ symmetry, induced primarily by $2k_F$ intrapocket 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 $s^{\pm}$ superconductivity,[26] 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. A functional renormalization group (fRG) study[27] showed the d-wave to be a clear winner, while FS-restricted random-phase-approximation-type spin-fluctuation (SF) analysis[26] and an analytical study in which the interactions are approximated by their lowest angular harmonics (LAH)[18] have revealed 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 the hole and the would-be electron pockets.

Because the 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 a potential time-reversal-symmetry-breaking $s + id$ pairing

state in $Ba_{1-x}K_xFe_2As_2$ at $x \leqslant 1$.[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 the Γ point[22] cast strong doubts that the gap is a d-wave one. 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 from a 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 a d-wave gap. The data are partly consistent with the theoretical prediction for an 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 approximation[18] and also inconsistent with the SF analysis according to which the 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 paper 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 interorbital 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 the $(\pi,0)$ hole blades are not overly relevant, and the physics is determined by intrapocket and interpocket interactions for the two hole pockets centered at the Γ point. For strictly angle-independent interactions, superconductivity is only possible when the interpocket coupling exceeds the intrapocket 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 intrapocket coupling is larger. Moreover, when intrapocket and interpocket 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 effect of the angular component of intrapocket 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 found[30] for the case when both hole and electron pockets are present and the dominant interpocket interaction is between hole and electron pockets. Here we apply the same reasoning to the case when the interpocket 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 the $\cos 2\theta$ term is consistent with the theoretical prediction for the case when the pairing interaction is predominantly between electron and hole pockets.

II. APPROACH

We consider intrapocket and interpocket pairing interactions between low-energy holelike 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 two-dimensional model. The interactions $U_{h_i,h_j}(\mathbf{k}_{F_i},\mathbf{k}_{F_j})$ generally depend on the angles along hole FSs. In general[18] 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 subleading $\cos 4\theta_{i,j}$ 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 $\cos 8\theta_i$ forms.[22]

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 basis[33] and can be material dependent. Still, ARPES data on weakly and moderately doped $Ba_{1-x}K_x(FeAs)_2$ 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 weak.[17] 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 has been found before[34] in the study of a three-dimensional band structure of $Ba_{1-x}K_x(FeAs)_2$, 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 intrapocket h_1-h_2 interaction, and show how accidental nodes appear on either both or one of these pockets already for a weakly angle dependent interaction. We then consider in Sec. IV the full model with three hole pockets, use as inputs the interactions $U_{h_i,h_j}(\mathbf{k}_{F_i},\mathbf{k}_{F_j})$ obtained from the underlying five-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 a 9×9 matrix gap equation. We show that intrapocket and interpocket interactions involving h_1 and h_2 pockets are almost identical and that the angular-dependent components of the interactions are rather weak. Nevertheless, the solution of the 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. In Sec. VI we present our conclusions.

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

Like we said above, we keep the $\cos 4\theta$ angular dependence in the interpocket interaction $U_{h_1h_2}$ and approximate the intrapocket $U_{h_1h_1}$ and $U_{h_2h_2}$ by constants; i.e., we set

$$\begin{aligned} &U_{h_1h_1}(k,p)=U_{11};U_{h_2h_2}(k,p)=U_{22},\\ &U_{h_1h_2}(k,p)=U_{12}(1+\alpha_{12}\cos 4\theta_k+\alpha_{21}\cos 4\theta_p), \end{aligned} \quad (1)$$

where θ is measured from the x axis.

The linearized BCS gap equation that one needs to solve is

$$\begin{aligned} \Delta_{h_1}(p)=&-LN_{F_1}\int_0^{2\pi}\frac{d\theta_k}{2\pi}U_{h_1h_1}(p,k)\Delta_{h_1}(k)\\ &-LN_{F_2}\int_0^{2\pi}\frac{d\theta_k}{2\pi}U_{h_1h_2}(p,k)\Delta_{h_2}(k),\\ \Delta_{h_2}(p)=&-LN_{F_1}\int_0^{2\pi}\frac{d\theta_k}{2\pi}U_{h_2h_1}(p,k)\Delta_{h_1}(k)\\ &-LN_{F_2}\int_0^{2\pi}\frac{d\theta_k}{2\pi}U_{h_2h_2}(p,k)\Delta_{h_2}(k), \end{aligned} \quad (2)$$

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 $u_{12}=N_FU_{12}$ and $u=N_FU$. 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 (cf. Ref. 30). Observe also that this $s^{\pm}$ gap structure with opposite signs of the gaps on different hole pockets is different form 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 $L=\frac{2(u-u_{12})}{(u_{12}\alpha)^2}$. 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 the one with $u=u_{12}$ (because the two FSs are centered at the same Γ point, intrapocket and interpocket interactions are undistinguishable). In this case we get $r_1=\sqrt{2}$ independent of α, indicating that nodes will arise even for a very weak angular dependence of the interaction.[30] This is what we mean by a resonant enhancement of the angular dependence of the interactions. Figure 1(a) shows the gap structure obtained for this case.

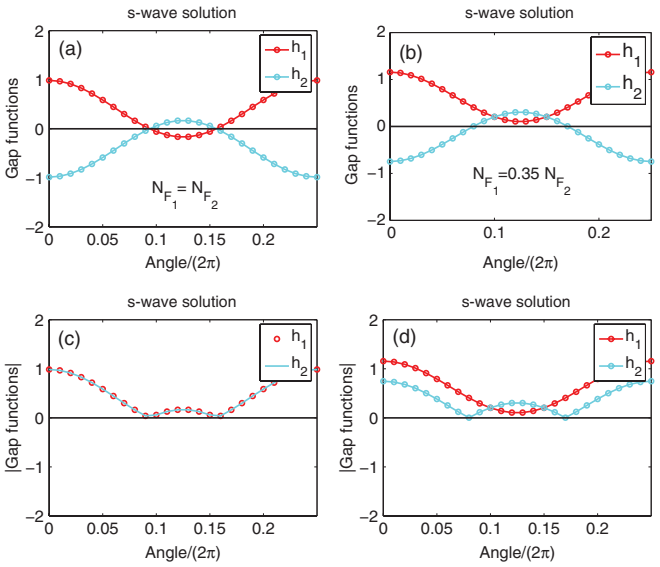

FIG. 1. (Color online) (a) The gap structure obtained for equal density of states ($N_{F_1}=N_{F_2}$) on the two hole pockets at Γ. We used $U_{11}=U_{22}=U_{12}$ and $\alpha=0.1$. The gap satisfies $\Delta_{h_1}=-\Delta_{h_2}=\Delta(1+\sqrt{2}\cos 4\theta)$ and has nodes on both FSs. (b) The same as (a), but with $N_{F_1}=0.35N_{F_2}$. Now the two gaps are nonequivalent 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.

B. Nonequivalent hole pockets

We next consider the case of nonequivalent 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 as equal ($\alpha_{12} = \alpha_{21} = \alpha$).

There are two issues that one needs to consider for nonequivalent pockets—whether the solution exists for all parameters and what the structure of the two gaps are. 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 of (5) is elementary but cumbersome[6] 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 value for a nodal solution is lower than that for a no-nodal solution (for which T_c is independent of α at small α), which is also consistent with the smaller T_c in KFe_2As_2 compared to optimally doped $Ba_{1-x}K_xFe_2As_2$.

IV. A FIVE-ORBITAL MODEL WITH THREE 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 five-orbital model by converting Hubbard and Hund intraorbital and interorbital 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 the band structure from Ref. 18 for the hole doping, when electron pockets disappear leaving only two hole pockets at the 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., we approximate $U_{h_i,h_j}(\mathbf{k}_{F_i},\mathbf{k}_{F_j})$ by

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

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 Table I.

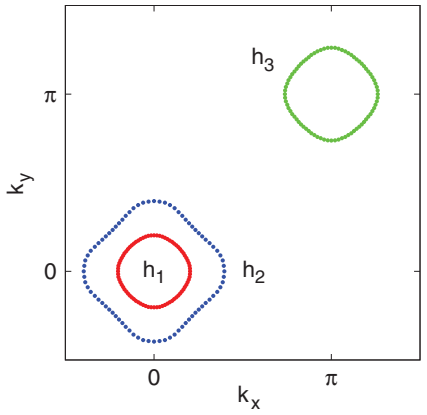

FIG. 2. (Color online) The FS in the unfolded BZ for our 5-orbital model for KFe_2As_2. Only hole FSs are present. Two hole FSs, h_1 and h_2, are centered at the Γ point, and one hole FS, h_3, is centered at (π,π). The electronic structure was obtained in a band structure calculation for the five-orbital model.[18] The energy of the $d_{3z^2-r^2}$ orbital was slightly modified to remove an additional hole pocket at (π,π).

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 a 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. 4(a).

The key observation in Fig. 4(a) is that s-wave gap has nodes, despite the fact that the 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 the five-orbital model, the interplay between the interactions is such that the

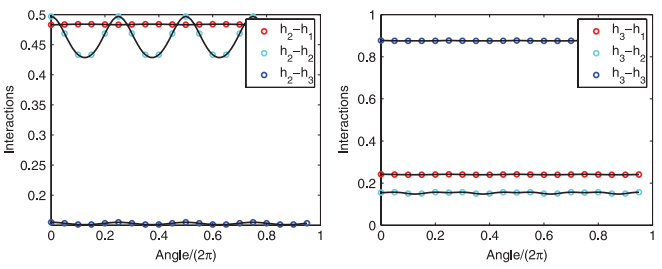

FIG. 3. (Color online) The fits of s-wave components of the interactions obtained from the five-orbital model by $U_{h_i,h_j}(\mathbf{k}_{F_i},\mathbf{k}_{F_j})$. We set $\mu = -0.2$ (in the notation of Ref. 18), when electron pockets just disappear. We fix $\mathbf{k}_{F_i}$ to be along the x direction 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.

TABLE I. s-wave interaction parameters obtained from fitting by Eq. (6) the interactions between hole pockets obtained from the five-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 notation 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

gap on the h_2 FS is the largest and has accidental nodes. This is a consequence of the fact that intrapocket 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 Figs. 4(b) and 4(c) the gap structure for the cases when intrapocket 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 about the angular dependencies of the gap on the h_1 and h_2 pockets and the interplay between the magnitudes of these two gaps being the resonance phenomenon, which for small α_{ij} crucially depends on the interplay between U_{12}^2 and $U_{11}U_{22}$.

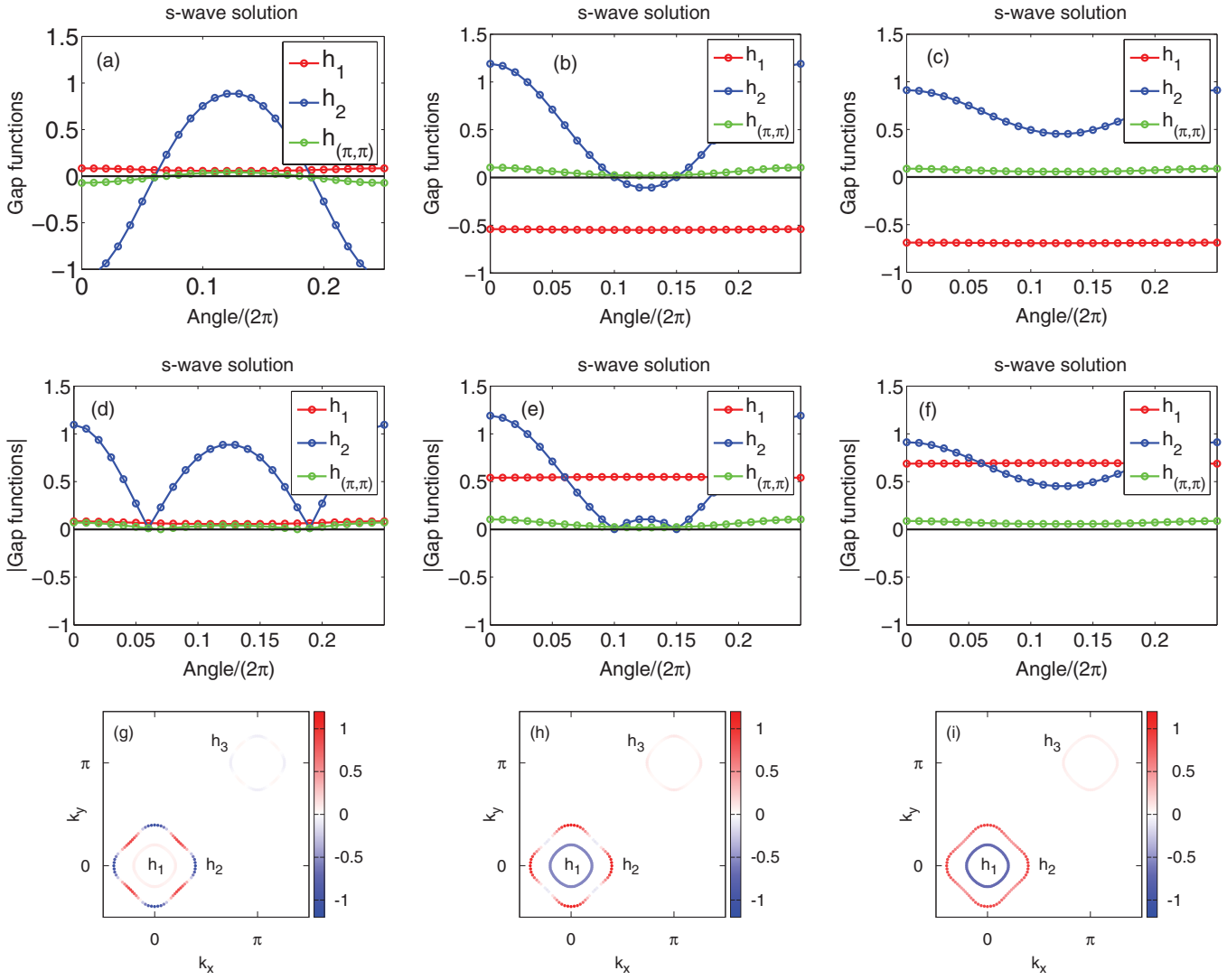

FIG. 4. (Color online) (a) s-wave gap structure obtained by solving a 9×9 gap equation for a five-orbital model. The parameters are listed in Table I. (b) and (c) s-wave gap structure obtained by changing U_{11} to $0.97U_{11}$ and $0.95U_{11}$, respectively. We see that the gap structure is very sensitive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

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 of 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, and 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 interpocket 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 toward the would-be electron pockets (see Fig. 1). For the five-orbital model, $\alpha_{21} > 0$ and α_{12} is essentially zero. One should then expect the $\cos 4\theta$ component of Δ_{h_1} to be small and the $\cos 4\theta$ component of Δ_{h_2} to be positive, i.e., Δ_{h_2} to be the largest in the direction toward 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: the shape of the FS and the type of s-wave function 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, and hence $\mathbf{k_i} = \mathbf{k}_{F,i}$. Because k_1 and k_2 are small, $\phi_i(k)$ can be expanded in k. To the order k^4, the dependence is $(1 - b_2\mathbf{k}^2 + b_4\mathbf{k}^4 \cos 4\theta) + \ldots$, where "..." stand for subleading terms. For all eigenfunctions, $b_2 > 0$. 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 the $\cos 4\theta$ dependence comes exclusively from the b_4 term. If a FS at the 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 $\cos 4\theta_k$ 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 the h_3 hole pocket.

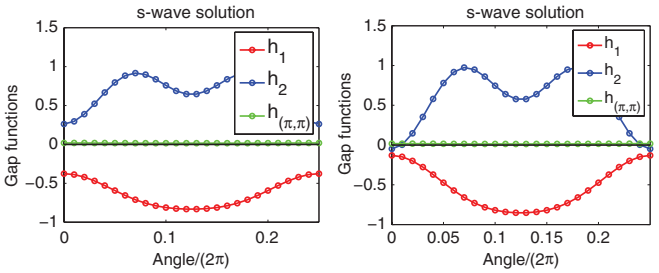

FIG. 5. (Color online) Left: s-wave gaps along the hole FSs obtained by solving a 9×9 gap equation with $U_{h_i,h_j}(\mathbf{k}_{F_i},\mathbf{k}_{F_j})$ obtained from the same five-orbital model as before, but with RPA renormalization of the interactions. The primary effect of RPA renormalization on 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 intrapocket $U_{11,22} \to 1.23U_{11,22}$ and slightly smaller interpocket $U_{12} \to 0.85U_{12}$, in which case the gap on h_2 FS contains nodes. The main difference between this figure and Fig. 4 is a 45° rotation of the direction of the gap maxima.

The generic implication is that there is no simple way to relate the sign of the $\cos 4\theta$ component of the gap to a FS geometry. And the analysis based on the five-orbital model reflects the nonuniversality: 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 random-phase-approximation-renormalized (RPA-renormalized) interactions. We show the results for the latter case in Fig. 5. In previous studies of five-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 the $\cos 4\theta$ component of the gap $\Delta(k)$ *anticorrelates* 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 data,[22] the measured FSs h_1 and h_2 are elongated along x and y directions, while Δ_{h1} and Δ_{h2} extracted from ARPES have $\cos 4\theta$ terms with negative prefactors (the same behavior as in Fig. 5). It also works for another Fe pnictide superconductor, LiFeAs, in which the $\cos 4\theta$ variations of the gaps on the hole FSs have been measured in ARPES experiments[31,32] and extracted from the scanning tunneling microscopy (STM) data.[35] The hole pockets around the Γ point in LiFeAs have been identified in ARPES measurements[10] and extracted from

de Haas–van Alphen (dHvA) oscillations.[36] The two groups agree that the inner hole pocket is either very small or does not even exist and that the 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 toward the 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 pocket[37] (it being larger in the extraction from dHvA). Still, according to ARPES and STM measurements,[10,35] the middle pocket is elongated along x and y, and hence the gap maxima on this FS should be in the direction toward the 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 toward the electron pockets, again in agreement with our simple reasoning. Whether the anticorrelation between the direction of the elongation of a FS and the direction along which s-wave gap is specific to KFe_2As_2 and LiFeAs or is more universal remains to be seen.

ARPES measurements on LiFeAs[31,32] also revealed 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 that are split 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 toward the Γ point).

According to theory, s-wave gaps on electron FSs should have both $\cos 4\theta$ and $\cos 2\theta$ variations. The $\cos 4\theta$ variations originate as on hole FSs, i.e., from the expansion to fourth 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 $\cos k_x \cos k_y$. For obvious reasons, the $\cos 4\theta$ terms have the same signs on both electron FSs. The $\cos 2\theta$ gap variations have different signs on the two electron FSs (before hybridization) and originate because (i) electron pockets are ellipses and (ii) the 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 unhybridized FSs become $\pm|\cos 2\theta|$ after hybridization, and the gaps on the inner and outer FSs have angular dependence of the form

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

For strongly elliptical FSs, as in $Ba(Fe_{1-x}Co_x)_2As_2$, $\cos 2\theta$ terms should be dominant, and RPA calculations for the band structure of $Ba(Fe_{1-x}Co_x)_2As_2$ 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 the $\cos 2\theta$ terms are comparable to the $\cos 4\theta$ 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 (with the data from Ref. 31 being very similar). We see

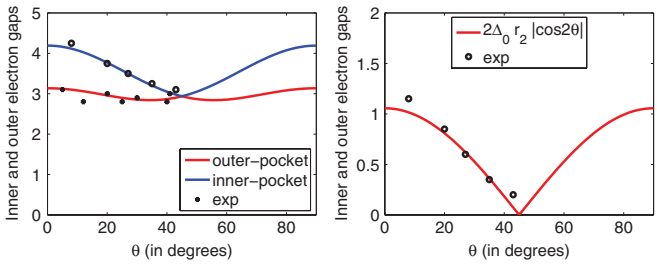

FIG. 6. (Color online) Left: Fit, using Eq. (8), to the gap structure on electron pockets measured in Ref. 32. The symbols are the experimental data; the lines are theoretical curves. The parameters extracted from the fit are $\Delta_0 = 3.3$ meV, $r_2 = 0.16$, and $r_4 = 0.11$. Right: Plot of $\Delta_{\text{inner}}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

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 the 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 the $\cos 2\theta$ variation is the dependence of the pairing interaction on θ along the electron FS, which is generally in the form $U(\theta) = U_0(1 + \beta \cos 2\theta + \ldots)$. 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 toward 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 a 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 toward the Γ point], and from this perspective $\cos k_x \cos k_y$ is a more likely candidate. However, to address the issue of why this function and not $\cos k_x + \cos k_y$ is the primary gap component one has to perform a full microscopic analysis.

VI. CONCLUSIONS

We argued in this paper that superconductivity in KFe_2As_2, which has only hole pockets, can be of s-wave type 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 centered at the Γ point in the unfolded BZ. When interpocket and intrapocket interactions between these two hole pockets are of near-equal strength, an 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 the 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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