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Displacement and annihilation of Dirac gap-nodes in d-wave iron-based superconductors

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Several experimental and theoretical arguments have been made in favor of a $d-$wave symmetry for the superconducting state in some Fe-based materials. It is a common belief that a $d-$wave gap in the Fe-based superconductors must have nodes on the Fermi surfaces centered at the Γ point of the Brillouin zone. Here we show that, while this is the case for a single Fermi surface made out of a single orbital, the situation is more complex if there is an even number of Fermi surfaces made out of different orbitals. In particular, we show that for the two Γ-centered hole Fermi surfaces made out of d_{xz} and d_{yz} orbitals, the nodal points still exist near T_c along the symmetry-imposed directions, but are are displaced to momenta between the two Fermi surfaces. If the two hole pockets are close enough, pairs of nodal points can merge and annihilate at some $T < T_c$, making the $d-$wave state completely nodeless. These results imply that photoemission evidence for a nodeless gap on the d_{xz}/d_{yz} Fermi surfaces of KFe_2As_2 does not rule out $d-$wave gap symmetry in this material, while a nodeless gap observed on the d_{xy} pocket in $K_xFe_{2-y}Se_2$ is truly inconsistent with the $d-$wave gap symmetry.

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I. INTRODUCTION

One of the most interesting features of Fe-based superconductors (FeSC) is the observation of different structures of the superconducting (SC) gap in different materials, which may indicate that the gap symmetry in FeSC is material dependent. [1] Weakly or moderately doped FeSC have both hole and electron pockets, and the gap symmetry there is very likely $s-$wave, with a π phase shift between hole pockets and electron pockets – the so-called s^{+-}-wave state [2]. The situation is less clear in materials with only one type of Fermi pocket, such as strongly hole doped KFe_2As_2, which contain only hole pockets [3], and $K_xFe_{2-y}Se_2$ or monolayer FeSe, which have only electron pockets [5]. Thermal conductivity and Raman scattering measurements in KFe_2As_2 [6–8], as well as the observation of a neutron resonance peak in the superconducting state of $K_xFe_{2-y}Se_2$ [9], were interpreted as evidence for a $d-$wave gap symmetry in these materials. Theoretical studies also found a strong enhancement of the $d-$wave superconducting susceptibility [11, 13], and at least one study of KFe_2As_2 have found [12] a much stronger attraction in the $d-$wave channel than in the s^{+-} channel.

The arguments in favor of a $d-$wave gap symmetry, however, have been questioned by angle-resolved photoemission (ARPES) measurements [4, 14]. For hole-doped KFe_2As_2, these measurements have found [14] that the gap on the inner hole pocket centered at the Γ point ($\mathbf{k} = 0$) displays some angle variation but has no nodes [15]. The conventional wisdom is that a $d-$wave gap must vanish on all Fermi surfaces (FSs) centered at $\mathbf{k} = 0$ along symmetry-imposed directions in momentum space – specifically, a $d_{x^2-y^2}$ gap, which we consider hereafter, must vanish on the FS points along the diagonals $k_x = \pm k_y$ in the 1-Fe Brillouin zone (1Fe BZ). The non-vanishing of the gap on the inner FS along these direction in ARPES measurements was interpreted [14] as the smoking-gun evidence ruling out a $d-$wave gap in KFe_2As_2. Similarly, in $K_xFe_{2-y}Se_2$, the gap has been measured on the electron pocket centered at the Z-point ($k_x = k_y = 0$ and $k_z = \pi$), and was found to be almost angle-independent [10]. Again, the conventional wisdom is that this result is fundamentally inconsistent with a $d-$wave gap symmetry.

It was argued in Ref. [16] that the $d-$wave order parameter in FeSCs necessarily contains both intra-pocket and inter-pocket components, and by this reason a $d-$wave gap has no nodes along the Fermi surfaces. A similar effect was previously shown to impact the behavior of accidental nodes in an s^{+-} superconductor [17, 18]. In this paper, we revisit this issue and investigate the fate of the $d-$wave nodes in FeSCs on the FSs centered at the high symmetry Γ and Z points. We argue that one has to distinguish between the cases when a FS centered at $k_x = k_y = 0$ is made out of a single orbital, like the Z-centered electron pocket of certain compounds, and the cases when the FSs centered at these points are made out of even number of orbitals, like the Γ-centered hole pockets present in most compounds, which are made out of d_{xz}/d_{yz} orbitals. In the first case, the symmetry-imposed $d-$wave nodes remain on the FS. In the second case, the $d-$wave gap *does not have nodes* on the normal state FSs (see Fig. 1a.) We demonstrate, however, that *this does not imply that the electronic spectrum is gapped.* We show that the nodes remain along the high-symmetry directions, but get displaced from the original FSs, at least near T_c, when the gaps are small. If the difference

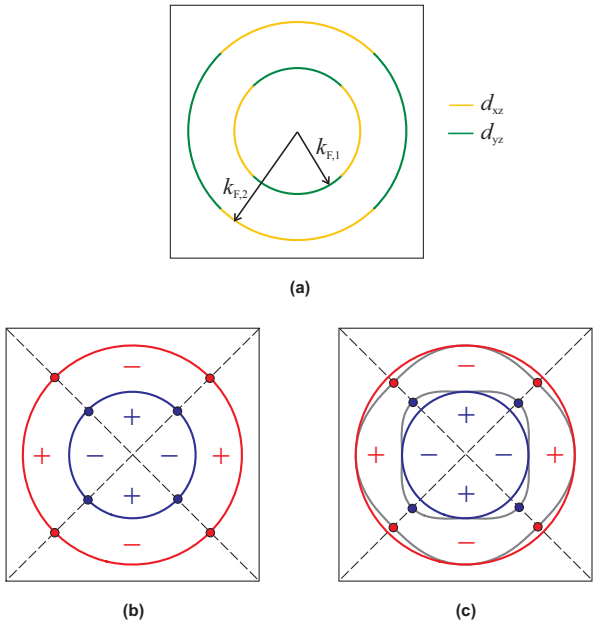

FIG. 1: The Fermi surfaces (FS) and the location of the nodal points near the two Γ-centered d_{xz}/d_{yz} pockets. Panel (a) shows the two FS in the normal state, highlighting the orbital that gives the largest spectral weight at each point along the FS (yellow for d_{xz} and green for d_{yz}). Panel (b) illustrates the location of the $d-$wave nodes on the two FS (blue and red lines) if the band off-diagonal gap term was absent. Panel (c) presents the actual location of the nodal points (red and blue dots) for the case $\Delta = 0.8\Delta_{\rm cr}$. The dispersions are given by $E_{a,b} = \sqrt{\Delta^2 \cos^2 2\theta + \epsilon_{a,b}^2}$ and the terms $\epsilon_{a,b}$ vanish along the two gray lines adjacent to the FS.

between the Fermi momenta of the two pockets is substantial, the nodes persist down to $T = 0$. If, however, the pockets are close to each other, pairs of nodes with opposite winding numbers can annihilate at $T_{\rm cr} < T_c$, rendering the spectrum gapped.

The displacement of the nodes from the FSs is related to how intra-orbital pairing in the orbital basis is displayed in the band basis [16, 19]. Namely, in the absence of spin-orbit interaction, tetragonal symmetry requires that the $d-$wave gap on these pockets must be diagonal in the orbital basis, i.e. $\langle d_{xz,-\mathbf{k}\downarrow} d_{xz,\mathbf{k}\uparrow}\rangle = \Delta$, $\langle d_{yz,-\mathbf{k}\downarrow} d_{yz,\mathbf{k}\uparrow}\rangle = -\Delta$. However, to analyze the gap structure near the FS, one needs to change basis from orbital space to band space. The latter is characterized by the band operators $c_{1,\mathbf{k}\sigma}$ and $c_{2,\mathbf{k}\sigma}$, which describe excitations near the two hole FS. As a result, in band basis, the same $d-$wave gap acquires both diagonal and off-diagonal components: $\langle c_{1,-\mathbf{k}\downarrow} c_{1,\mathbf{k}\uparrow}\rangle = -\langle c_{2,-\mathbf{k}\downarrow} c_{2,\mathbf{k}\uparrow}\rangle = \Delta\cos 2\theta$ and $\langle c_{2,-\mathbf{k}\downarrow} c_{1,\mathbf{k}\uparrow}\rangle = \langle c_{1,-\mathbf{k}\downarrow} c_{2,\mathbf{k}\uparrow}\rangle = \Delta \sin 2\theta$, respectively. For circular and small hole FS, θ coincides with the angle along the FS.

Because the off-diagonal gap term mixes the two FS, the $d-$wave gap varies as function of θ but does not have nodes. The strength of the variation depends on the interplay between Δ and the splitting between the two hole FS, as we discuss below. Such an effect does not happen for an s-wave gap, since the orbital and band representations are identical in this case, implying that off-diagonal terms do not emerge, unless there is hybridization between the pockets. The orbital and the band representations are also identical, for any gap symmetry, on a pocket made out of a single orbital, such as the d_{xy} Z-pocket in $K_xFe_{2-y}Se_2$.

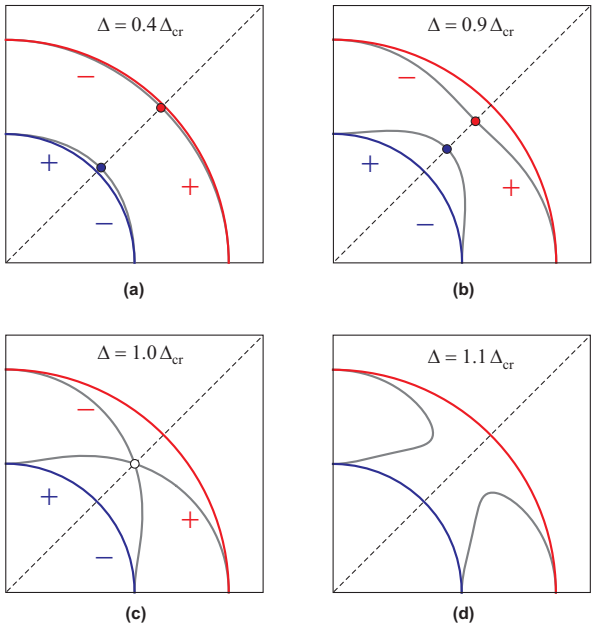

FIG. 2: The evolution of the $d-$wave nodes as Δ increases beyond the critical value $\Delta_{\rm cr}$. The blue and red lines are the normal state FS. The gray lines denote the locations of $\epsilon_{a,b} = 0$, and the dispersions are given by $E_{a,b} = \sqrt{\Delta^2 \cos^2 2\theta + \epsilon_{a,b}^2}$. The nodal points are marked by the red and blue dots. Four pairs of nodal points are present for $\Delta < \Delta_{\rm cr}$ and disappear for $\Delta > \Delta_{\rm cr}$. In this figure, we used circular band dispersions with $m_2 = 3m_1$.

However, by extending the analysis to momenta away from the normal state FS, we found that the nodes in the $d-$wave excitation spectrum near the d_{xz}/d_{yz} hole pockets do survive, and are just displaced from the normal state hole FSs. Specifically, the excitation spectrum has the form [16]

$$E_{a,b}^2 = \Delta^2 \cos^2 2\theta + \epsilon_{a,b}^2 \tag{1}$$

with

$$\epsilon_{a,b} = \mathrm{sgn}\left(\epsilon_{1,\mathbf{k}} + \epsilon_{2,\mathbf{k}}\right) \sqrt{\left(\frac{\epsilon_{1,\mathbf{k}} + \epsilon_{2,\mathbf{k}}}{2}\right)^2 + \Delta^2 \sin^2 2\theta} \pm \left(\frac{\epsilon_{1,\mathbf{k}} - \epsilon_{2,\mathbf{k}}}{2}\right) \tag{2}$$

where $\epsilon_{1,\mathbf{k}}$ and $\epsilon_{2,\mathbf{k}}$ are the normal state dispersions of bands 1 and 2, respectively. If the off-diagonal term

$\Delta \sin 2\theta$ was absent, $\epsilon_a = \epsilon_{1,\mathbf{k}}$, $\epsilon_b = \epsilon_{2,\mathbf{k}}$, and the dispersions would be the conventional ones for a $d-$wave SC, namely, $E^2_{a,b} = \Delta^2 \cos^2 2\theta + \epsilon^2_{1,2}$. In this case, each dispersion would have nodal points on the FS at $\theta = \theta_n \equiv (2n+1)\,\pi/4$, with $n = 0, 1, 2, 3$ (see Fig. 1b). Because of the off-diagonal term, however, ϵ_a does not vanish when $\epsilon_1 = 0$ and ϵ_b does not vanish when $\epsilon_2 = 0$. However ϵ_a (ϵ_b) does vanish along the lines specified by $\epsilon_{1,\mathbf{k}}\epsilon_{2,\mathbf{k}} = -\Delta^2 \sin^2 2\theta$, which are displaced from the actual FS, see Fig. 1c.

When the magnitude of the $d-$wave gap is small, the two lines are well separated and cross the direction $\theta = \theta_n$ at the momenta $k_a > k_{F,1}$ and $k_b < k_{F,2}$. At these crossing points, the full quasiparticle energy E_a (E_b) vanishes. These are new $d-$wave nodal points, shifted from their corresponding FS by the mixing term. For small Δ, this shift is small, of order Δ^2. However, as temperature decreases, Δ becomes larger and the nodal points become closer. If the gap reaches the critical value $\Delta_{\rm cr}$, which depends on the radii of the two pockets, the two nodal points merge and annihilate each other. In particular, at the Lifshitz transition taking place for $\Delta = \Delta_{\rm cr}$, the $\epsilon_a = 0$ and $\epsilon_b = 0$ lines mix and split in the orthogonal direction, see Fig. 2. For $\Delta > \Delta_{\rm cr}$, these lines no longer cross the directions $\theta = \theta_n$, i.e. $\epsilon_{a,b}$ and $\Delta \cos 2\theta$ do not vanish simultaneously. In this situation, $E_{a,b}$ do not have nodal points, implying that the excitations of the $d-$wave superconductor are fully gapped.

When nodal points are present, the excitations near $E_{a,b} = 0$ are Dirac-cones, $E_{a,b} = \sqrt{\tilde{k}_x^2 + \tilde{k}_y^2}$, where $\tilde{x}$ and $\tilde{y}$ are directions along and transverse to the lines $\epsilon_a = \epsilon_b = 0$, defined by $\tilde{k}_x = 2\Delta(\theta - \theta_n)$ and $\tilde{k}_y = (\frac{d\epsilon_{a,b}}{dk})\ (k - k_{a,b})$, where the derivative is taken at $\theta = \theta_n$. At the critical gap value $\Delta = \Delta_{\rm cr}$, because $d\epsilon_{a,b}/dk$ vanishes we find $\tilde{k}_y \propto (k - k_{a,b})^2$. This dispersion has the same form as the dispersion of fermions at the critical point between a semi-metal and an insulator [20–22]. It was argued [21] that for such a dispersion the system with dynamically screened Coulomb interaction should display a highly non-trivial quantum-critical behavior in both fermionic and bosonic sectors. Our study shows that a $d-$wave FeSC provides an interesting realization of such behavior.

The displacement of the nodes to momenta away from the normal state FSs has been previously discussed for accidental nodes on electron pockets in an s^{+-} superconductor. In this case, the displacement is due to hybridization between these pockets [17, 23]. The authors of Ref. [17] argued that, as the hybridization parameter gets larger, pairs of accidental nodes come close, and at some critical hybridization merge and annihilate. The same effect occurs [18] when one increases the pnictogen/chalcogen-induced interaction between fermions on Fe sites (i.e. interaction with momentum non-conservation by (π, π) in the 1Fe BZ). For a $d-$wave superconductor, the lifting of the nodes on the normal state FSs was first discussed in Ref. [16]. These authors concluded that, for arbitrary Δ, the nodes are lifted not only on the normal state FSs, but that the whole electronic spectrum is generally gapped, except for possible accidental nodes. We, on the contrary, argue that, at least for small Δ, the symmetry-imposed nodes do survive and just shift from the original FSs to momenta located between the original FSs. This is similar to what happens with the accidental nodes in an s^{+-} superconductor in the presence of hybridization. From a generic perspective, the persistence of the nodal points is associated with the fact that each Dirac node has a nonzero winding number. Only when the two nodal points with opposite winding numbers come close to each other under the variation of some parameter (the magnitude of the gap in the $d-$wave case), they can merge and annihilate. We discuss the comparison with earlier works in more detail later in the paper.

We also emphasize that the nodal points in the $d-$wave case are true symmetry-imposed $d-$wave nodes, and the damping near each nodal point is the same as near a $d-$wave node on the FS in a conventional case. Therefore, all thermodynamic properties of the system are also the same as in a conventional $d-$wave superconductor. Only in ARPES one can distinguish between a conventional d-wave case with nodes on the original FS and the case when the nodes are shifted away from the normal state FS due to the presence of the inter-pocket pairing component.

The paper is organized as follows: in Section II, we introduce the model, in Section III we derive the excitation spectrum, in Section IV we compare our results with the case of a semi-metal to insulator transition. In Sec. V we compare our results with earlier studies and in Section VI we present comparisons with experiments. We present our conclusions in Section VII.

II. MODEL FOR d-WAVE SUPERCONDUCTIVITY

To focus on the main message of this paper, we consider a simplified model of an FeSC with two Γ-centered hole pockets made out of the d_{xz} and d_{yz} orbitals (Fig. 1a), and assume that 4-fermion interactions give rise to $d-$wave superconductivity with $d_{x^2-y^2}$ gap symmetry (for a d_{xy} gap symmetry, the results are analogous to the ones that we obtain below). The attraction in the $d-$wave channel may be due to the interactions within the d_{xz}/d_{yz} subset, as we assume for simplicity, or it can be induced by the coupling to other orbitals. In the $d_{x^2-y^2}$ ordered state, which belongs to the B_{1g} irreducible representation of the D_{4h} group, the gap function in the orbital basis is given by $\langle d_{xz,-\mathbf{k}\downarrow} d_{xz,\mathbf{k}\uparrow}\rangle = \Delta$, $\langle d_{yz,-\mathbf{k}\downarrow} d_{yz,\mathbf{k}\uparrow}\rangle = -\Delta$. There are no inter-orbital terms $\langle d_{yz,-\mathbf{k}\downarrow} d_{xz,\mathbf{k}\uparrow} \pm d_{xz,-\mathbf{k}\downarrow} d_{yz,\mathbf{k}\uparrow}\rangle$ as they belong to the different irreducible representations B_{2g} (plus sign) and A_{2g} (minus sign).

Although the anomalous terms $\langle d_{i,-\mathbf{k}\downarrow} d_{j,\mathbf{k}\uparrow}\rangle$ are diag-

onal, the kinetic energy near the Γ point does contain terms describing hoping from one orbital to the other. The kinetic energy is diagonalized by converting from the orbital to the band basis, yielding:

$$\mathcal{H}_0 = \sum_{\mathbf{k},\alpha} \left(\epsilon_{1,\mathbf{k}} c^\dagger_{1,\mathbf{k}\alpha} c_{1,\mathbf{k}\alpha} + \epsilon_{2,\mathbf{k}} c^\dagger_{2,\mathbf{k}\alpha} c_{2,\mathbf{k}\alpha} \right). \quad (3)$$

The dispersions $\epsilon_{1,k}$ and $\epsilon_{2,k}$ are C_4-symmetric. We assume for simplicity that the system parameters are such that the hole pockets can be approximated as circular [24], i.e. $\epsilon_{1,\mathbf{k}} = \mu - k^2/(2m_1)$ and $\epsilon_{2,\mathbf{k}} = \mu - k^2/(2m_2)$. The two dispersions are not identical when $m_1 \neq m_2$, but are degenerate by symmetry at $\mathbf{k} = 0$ in the absence of spin-orbit coupling [25, 26].

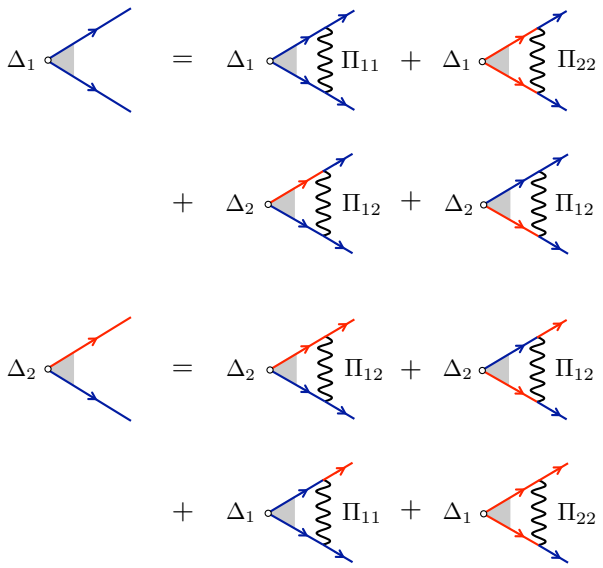

FIG. 3: The diagrammatic representation of the linearized gap equations, Eqs. 8. Blue and red lines denote fermions from bands c_1 and c_2.

The transformation from the orbital operators d_{xz}/d_{yz} to the band operators c_1 and c_2 is a $U(1)$ rotation:

$$\begin{aligned} d_{xz,\mathbf{k}\alpha} &= \cos\theta_{\mathbf{k}} c_{1,\mathbf{k}\alpha} + \sin\theta_{\mathbf{k}} c_{2,\mathbf{k}\alpha}, \\ d_{yz,\mathbf{k}\alpha} &= \cos\theta_{\mathbf{k}} c_{2,\mathbf{k}\alpha} - \sin\theta_{\mathbf{k}} c_{1,\mathbf{k}\alpha}, \end{aligned} \quad (4)$$

For circular Fermi pockets the rotation angle $\theta_{\mathbf{k}}$ coincides with the polar angle θ along the FS [24]. Using Eq. (4) we also re-express the anomalous term $\mathcal{H}_\Delta = \Delta \sum_{\mathbf{k}} \left(d^\dagger_{xz,\mathbf{k}\uparrow} d^\dagger_{xz,-\mathbf{k}\downarrow} - d^\dagger_{yz,\mathbf{k}\uparrow} d^\dagger_{yz,-\mathbf{k}\downarrow} \right)$ in the band basis. We obtain a combination of inter-band and intra-band terms:

$$\begin{aligned} \mathcal{H}_\Delta = \Delta_a \sum_{\mathbf{k}} \left(i\sigma^y_{\alpha\beta} \right) \left(c^\dagger_{1,\mathbf{k}\alpha} c^\dagger_{1,-\mathbf{k}\beta} - c^\dagger_{2,\mathbf{k}\alpha} c^\dagger_{2,-\mathbf{k}\beta} \right) + \\ \Delta_b \sum_{\mathbf{k}} \left(i\sigma^y_{\alpha\beta} \right) \left(c^\dagger_{1,\mathbf{k}\alpha} c^\dagger_{2,-\mathbf{k}\beta} + c^\dagger_{2,\mathbf{k}\alpha} c^\dagger_{1,-\mathbf{k}\beta} \right) + h.c \end{aligned} \quad (5)$$

where σ are Pauli matrices and in the $d-$wave case $\Delta_a = \Delta \cos 2\theta$ and $\Delta_b = \Delta \sin 2\theta$. Without loss of degeneracy, one can set Δ_a to be real. Δ_b is, in general, a complex variable.

Note that in the $d-$wave case, the inter-band anomalous terms are of the same order Δ as intra-band terms and differ only by their angular dependence. This may seem counterintuitive, as the pairing kernel involving fermions from different bands is much smaller than the kernel involving fermions from the same band. To see why inter-band and intra-band pairing terms are nevertheless comparable, one can explicitly solve for the intra-band and inter-band pairing vertices by using a microscopic interaction that favors $d-$wave. For concreteness, consider a toy model with pair-hopping interaction:

$$H_{\text{int}} = \frac{g}{2} \sum \left[d^\dagger_{xz\alpha} d_{yz\alpha} d^\dagger_{xz\beta} d_{yz\beta} + d^\dagger_{yz\alpha} d_{xz\alpha} d^\dagger_{yz\beta} d_{xz\beta} \right] \quad (6)$$

where the summation over momenta and spin indices is left implicit. A positive g favors B_{1g} pairing as one can verify in a straightforward way by solving the gap equation in the orbital basis. Converting this Hamiltonian into band basis and projecting onto the B_{1g} channel, we obtain

$$H_{\text{int}} = -\frac{g}{4} \sum \left[\eta^\dagger_{1,\mathbf{k}} \eta_{1,\mathbf{p}} \cos 2\theta_{\mathbf{k}} \cos 2\theta_{\mathbf{p}} + \eta^\dagger_{2,\mathbf{k}} \eta_{2,\mathbf{p}} \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{p}} + \left(\eta^\dagger_{1,\mathbf{k}} \eta_{2,\mathbf{p}} + \eta^\dagger_{2,\mathbf{k}} \eta_{1,\mathbf{p}} \right) \sin 2\theta_{\mathbf{p}} \cos 2\theta_{\mathbf{k}} \right] \quad (7)$$

where $\eta^\dagger_{1,\mathbf{k}} = c^\dagger_{1,\mathbf{k}\alpha} c^\dagger_{1,-\mathbf{k}\beta} - c^\dagger_{2,\mathbf{k}\alpha} c^\dagger_{2,-\mathbf{k}\beta}$, $\eta^\dagger_{2,\mathbf{k}} = c^\dagger_{1,\mathbf{k}\alpha} c^\dagger_{2,-\mathbf{k}\beta} + c^\dagger_{2,\mathbf{k}\alpha} c^\dagger_{1,-\mathbf{k}\beta}$, and the summation is over momentum and spin indices. Introducing the two anomalous vertices $\Delta_1 \left(i\sigma^y_{\alpha\beta} \right) \eta^\dagger_{1,\mathbf{k}} \cos 2\theta_{\mathbf{k}}$ and $\Delta_2 \left(i\sigma^y_{\alpha\beta} \right) \eta^\dagger_{2,\mathbf{k}} \sin 2\theta_{\mathbf{k}}$, and solving the BCS-like gap

equations shown graphically in Fig. 3, we obtain

$$\Delta_1 = \frac{g}{4}\left(\frac{\Pi_{11}+\Pi_{22}}{2}\right)\Delta_1 + \frac{g}{4}\Pi_{12}\Delta_2$$
$$\Delta_2 = \frac{g}{4}\Pi_{12}\Delta_2 + \frac{g}{4}\left(\frac{\Pi_{11}+\Pi_{22}}{2}\right)\Delta_1 \qquad (8)$$

where Π_{11}, Π_{22}, and Π_{12} (all positive) are particle-particle polarization bubbles made out of c_1 and c_2 fermions in the superconducting state. Near T_c, we obtain

$$\Pi_{11} = \frac{1}{2}\int d^2\mathbf{k}\,\frac{\tanh\left(\frac{\epsilon_{1,\mathbf{k}}}{2T}\right)}{|\epsilon_{1,\mathbf{k}}|},\ \Pi_{22} = \frac{1}{2}\int d^2\mathbf{k}\,\frac{\tanh\left(\frac{\epsilon_{2,k}}{2T}\right)}{|\epsilon_{2,\mathbf{k}}|},$$
$$\Pi_{12} = \frac{1}{2}\int d^2\mathbf{k}\,\frac{\tanh\left(\frac{\epsilon_{1,\mathbf{k}}}{2T}\right)+\tanh\left(\frac{\epsilon_{2,\mathbf{k}}}{2T}\right)}{|\epsilon_{1,\mathbf{k}}+\epsilon_{2,\mathbf{k}}|}. \qquad (9)$$

Comparing the two expressions in Eq. (8), we see that $\Delta_1 = \Delta_2 = \Delta$, no matter what is the ratio of the inter-pocket and intra-pocket polarization operators. This holds as long as the interaction g is momentum-independent. If momentum dependence is included, the intra-pocket and inter-pocket interaction terms in (7) differ more than by their distinct angular dependences. In this situation, the r.h.s. of the two equations in (8) are no longer identical, and generally $\Delta_1 > \Delta_2$. In the limiting case $\Delta_2 \to 0$ one recovers the conventional case with only intra-band pairing condensate.

III. EXCITATION SPECTRUM

We now return to Eqs. (3) and (5). The quadratic Hamiltonian $\mathcal{H}_0 + \mathcal{H}_\Delta$ can be straightforwardly diagonalized and yields

$$\mathcal{H} = \sum_{\mathbf{k},\alpha} E_a(\mathbf{k}) a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\alpha} + \sum_{\mathbf{k},\alpha} E_b(\mathbf{k}) b^\dagger_{\mathbf{k}\alpha} b_{\mathbf{k}\alpha} \qquad (10)$$

where

$$E^2_{a,b}(\mathbf{k}) = \frac{\epsilon^2_{1,\mathbf{k}}+\epsilon^2_{2,\mathbf{k}}}{2} + \Delta_a^2 + |\Delta_b^2| \pm \sqrt{\left(\frac{\epsilon^2_{1,\mathbf{k}}-\epsilon^2_{2,\mathbf{k}}}{2}\right)^2 + (\epsilon_{1,\mathbf{k}}-\epsilon_{2,\mathbf{k}})^2|\Delta_b|^2 + 4\Delta_a^2(\mathrm{Re}\Delta_b)^2} \qquad (11)$$

In the $d-$wave case ($\Delta_a = \Delta\cos 2\theta$ and $\Delta_b = \Delta \sin 2\theta$), Eq. (11) can be simplified to

$$E_{a,b}(\mathbf{k}) = \sqrt{\Delta^2\cos^2 2\theta + \epsilon^2_{a,b}(\mathbf{k})}, \qquad (12)$$

where

$$\epsilon_{a,b}(\mathbf{k}) = \mathrm{sgn}\,(\epsilon_{1,\mathbf{k}}+\epsilon_{2,\mathbf{k}})\sqrt{\left(\frac{\epsilon_{1,\mathbf{k}}+\epsilon_{2,\mathbf{k}}}{2}\right)^2 + \Delta^2\sin^2 2\theta} \pm \left(\frac{\epsilon_{1,\mathbf{k}}-\epsilon_{2,\mathbf{k}}}{2}\right) \qquad (13)$$

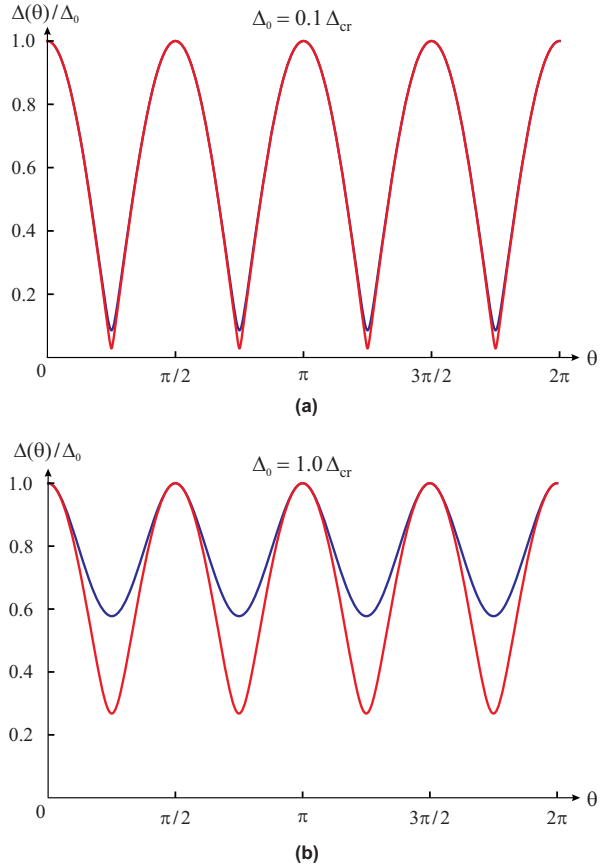

FIG. 4: The dispersion of the $d-$wave gap along the two FS, Eq. 14, for two values of Δ. Blue (red) lines denote band c_1 (c_2). There is substantial angular variation but no nodes. Note also that the minimum value of the gap is different in both bands.

Eq. (11) was first obtained in Ref. [17] for an s^{+-} superconductor with accidental nodes ($\Delta_a = \Delta$, $\Delta_b = i\Delta\alpha\cos 2\theta$, $\alpha > 1$). For a $d-$wave superconductor, Eqs. (12), (13) were first derived in Ref. [16].

The dispersions $E_{a,b}$ in Eqs. (12), (13) have the same forms as in a conventional d-wave superconductor, but are actually more complex because $\epsilon_{a,b}$ themselves depend on Δ. For a vanishing Δ, ϵ_a and ϵ_b coincide with the normal state dispersions, $\epsilon_a = \epsilon_{1,\mathbf{k}}$ and $\epsilon_b = \epsilon_{2,\mathbf{k}}$, as they indeed should. At a finite but small Δ (i.e., near T_c), $\epsilon_a = \epsilon_{1,\mathbf{k}} + \frac{\Delta^2\sin^2 2\theta}{\epsilon_{1,\mathbf{k}}+\epsilon_{2,\mathbf{k}}}$ and $\epsilon_b = \epsilon_{2,\mathbf{k}} + \frac{\Delta^2\sin^2 2\theta}{\epsilon_{1,\mathbf{k}}+\epsilon_{2,\mathbf{k}}}$. We see that ϵ_a (ϵ_b) *does not* vanish on the FS, where $\epsilon_1 = 0$ ($\epsilon_2 = 0$), except along the particular directions $\sin 2\theta = 0$. For such values of θ, however, $\Delta^2\cos 2\theta$ has a maximum value Δ^2. As a result, there are no zeroes of $E_{a,b}$ along each of the two FSs, despite the fact that the gap is $d-$wave. At arbitrary $T < T_c$ we have at $\epsilon_{1,\mathbf{k}} = 0$

(and $\epsilon_{2,\mathbf{k}} > 0$)

$$E_a = \sqrt{\Delta^2 \cos^2 2\theta + \left(\sqrt{\frac{\epsilon_{2,k}^2}{4} + \Delta^2 \sin^2 2\theta} - \frac{\epsilon_{2,k}}{2} \right)^2} \tag{14}$$

We plot the excitation energies E_a and E_b as a function of θ along both FS in Fig. 4 for two values of Δ. We see that there is substantial angular variation of $E_{a,b}(\theta)$, but no nodes.

We now analyze the excitation energies $E_{a,b}$ away from the FS. A straightforward analysis of Eq. (13) shows that $\epsilon_{a,b}$ vanish along the lines where

$$\epsilon_{1,\mathbf{k}}\ \epsilon_{2,\mathbf{k}} = -\Delta^2 \sin^2 2\theta \tag{15}$$

For small Δ (i.e, near T_c), Eq. (15) is satisfied along two separate lines, one adjacent to the inner FS, ($\epsilon_{1,\mathbf{k}} = 0$) and another adjacent to the outer FS ($\epsilon_{2,\mathbf{k}} = 0$). We show the lines $\epsilon_a = 0$ and $\epsilon_b = 0$ in Fig 2 for different values of Δ. Because these lines cross the directions along which $\cos 2\theta = 0$, E_a or E_b vanish at the crossing points, i.e. *the full excitation energy vanishes*. This implies that the nodal points of the $d-$wave superconductor still exist near T_c, but get shifted away from the normal state FS by the inter-band component of the $d-$wave gap. The nodal points are located along $\cos 2\theta = 0$, at $k = k_{a,b}$ given by

$$k_{a,b}^2 = \left(\frac{k_{F,1}^2 + k_{F,2}^2}{2} \right) \pm \sqrt{\left(\frac{k_{F,1}^2 - k_{F,2}^2}{2} \right)^2 - 4 m_1 m_2 \Delta^2}, \tag{16}$$

where $k_{F,i}^2 = 2 m_i \mu$.

The behavior of $E_{a,b}$ at smaller temperatures depends on the interplay between the gap value and the difference between m_2 and m_1, or specifically, between $\Delta(T)$ and

$$\Delta_{\rm cr} = \mu \left(\frac{m_2 - m_1}{2\sqrt{m_1 m_2}} \right) \tag{17}$$

If $\Delta_{\rm cr}$ is large enough, the nodes survive down to $T = 0$. However, if $m_2 - m_1$ is small enough (i.e., the inner and the outer hole pockets are close), $\Delta(T)$ reaches $\Delta_{\rm cr}$ at some $T = T_{\rm cr}$ below T_c. At this temperature, a Lifshitz transition occurs when the two nodal points merge at $k = k_{\rm cr}$ and then split in orthogonal directions, see Fig. 2c.

On a technical side, we found that, when Δ is slightly below $\Delta_{\rm cr}$, the two nodal points of the dispersion are the nodes of ϵ_b (and E_b), while the dispersion ϵ_a has no nodes. The change of the behavior from the nodes in both ϵ_a and ϵ_b to two nodes in ϵ_b occurs when Δ reaches the value $\Delta^* = \mu \left(\frac{m_2 - m_1}{m_1 + m_2} \right)$, which is comparable but smaller than $\Delta_{\rm cr}$. The ratio $\Delta^*/\Delta_{\rm cr} = 2\sqrt{m_1 m_2}/(m_1 + m_2) < 1$. This change does not affect the location of the zeros of $\epsilon_{a,b}$ in momentum space (gray lines in Fig. Fig. 2), just the identification of these lines with ϵ_a or ϵ_b becomes more complex.

At $\Delta > \Delta_{\rm cr}$, the lines where $\epsilon_{a,b} = 0$ form four disconnected closed loops (see Fig. 2d). Along these loops the excitation energy becomes $E = \Delta |\cos 2\theta|$. However, because the closed loops do not cross the directions $\cos 2\theta = 0$, the nodes disappear, i.e. the excitation spectrum of a $d-$wave superconductor becomes *fully gapped*.

IV. ANALOGY WITH SEMI-METAL TO INSULATOR TRANSITION

There is a close analogy between the Lifshitz transition at $T = T_{\rm cr}$ in our problem and the transition from a 2D massless Dirac semi-metal to an insulator. In the latter case, the semi-metal phase has two separate Dirac nodal points with the winding numbers ± 1 [27]. Upon variation of some system parameter (e.g., strain in graphene), the distance between the two nodal points decreases until they merge and annihilate at a critical value of such parameter. At the critical point, the system is described by fermions with linear dispersion in one spatial direction and quadratic in the other. [20–22] Similarly, in our case, near T_c, the dispersion along one of the four directions specified by $\cos 2\theta = 0$ has two nodal points with Dirac-like dispersions. Just as in the semi-metal to insulator transition, the winding numbers near the two Dirac points are ± 1. At $T = T_{\rm cr}$ (if it exists), the Dirac points merge. At this temperature the excitation spectrum around the single nodal point is quadratic along the direction in which $\cos 2\theta = 0$ and linear in the transverse direction. At a smaller temperature, the excitation spectrum is fully gapped, like in an insulator. Recent studies of the semi-metal to insulator transition have shown [21] that at the critical point the dynamically screened Coulomb interaction gives rise to a highly nontrivial quantum-critical behavior in both fermionic and bosonic sectors. A $d-$wave state in the FeSC will provide a realization of such behavior if $T_{\rm cr}$ can be tuned to zero by changing some external parameter, such as pressure. An s^{+-} superconductor, in which accidental nodes can be lifted by varying an external parameter [17, 18], is another realization of such semi-metal to insulator transition [28–30].

V. COMPARISON WITH EARLIER WORKS

Several earlier studies of the pairing involving fermions from two different bands have already pointed out that an intra-pocket pairing condensate generates an inter-band pairing condensate, generally of the same order as the intra-band one [16, 31]. Ref. [31] focused on the system with only electron pockets. When inter-pocket repulsion is dominant, the analysis within 1Fe BZ shows that the system develops d-wave superconductivity with sign change of the gap on the two electron pockets [32].

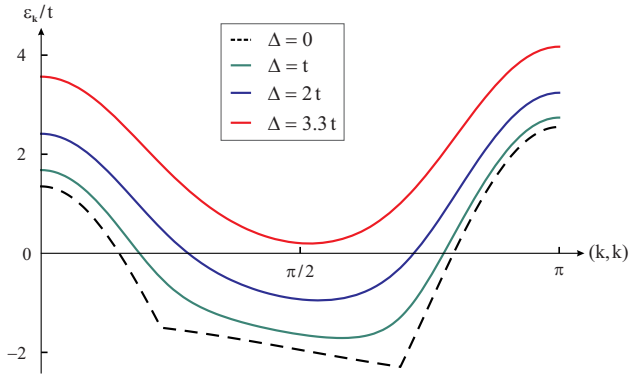

FIG. 5: The quasiparticle dispersion in the $d-$wave superconducting state for the two-orbital model of Raghu *et al.* [35]. The dispersion has the form $E_{\mathbf{k}}^2 = \epsilon_{\mathbf{k}}^2 + \Delta^2 \cos^2 2\theta_{\mathbf{k}}$, where $\epsilon_{\mathbf{k}} = (\xi_+^2 + \Delta^2 \sin^2 2\theta_{\mathbf{k}})^{1/2} \pm |\vec{B}|$ (see Eqs. (12), (13) and Ref. [16]). Ref. [16] used the parameters from Ref. [35]: $\xi_+ = -0.3t(\cos k_x + \cos k_y) + 3.4t \cos k_x \cos k_y - 1.45t$, $|\vec{B}| = t\left[2.3^2(\cos k_x - \cos k_y)^2 + 3.4^2 \sin^2 k_x \sin^2 k_y\right]^{1/2}$, and $\sin 2\theta_{\mathbf{k}} = 3.4t \sin k_x \sin k_y/|\vec{B}|$, where t sets the overall energy scale. Nodal points of the dispersion are the ones for which $\cos 2\theta_{\mathbf{k}} = 0$ and $\epsilon_{\mathbf{k}} = 0$. We plot $\epsilon_{\mathbf{k}}$ as a function of momentum $\mathbf{k}$ along the direction $k = k_x = k_y$ (for which $\cos 2\theta_{\mathbf{k}} = 0$) for different gap values Δ. A pair of nodal points is observed unless Δ exceeds the critical value $\Delta_c \approx 3.08t$, which is about a quarter of the bandwidth.

However, the result holds only as long as one neglects the coupling between electron pockets, i.e., the processes with momentum non-conservation by (π, π) in the 1Fe BZ. Hybridization, which is the combined effect of glide plane symmetry and of spin-orbit interaction, triggers the appearance of a inter-pocket pairing condensate in terms of the band fermions, in analogy to what happens in our case. This effect does not affect substantially the $d-$wave gap on the electron pockets, which in 2D has no nodes anyway, but it gives rise to a novel s^{+-} pairing between inner and outer hybridized electron pockets [31, 33], when the coupling associated with the hybridization exceeds a certain critical value.

A shift of the nodal points to momenta away from the FS and their subsequent merging and annihilation (a Lifshitz transition) has been analyzed in several publications [17, 18, 23] in the context of the behavior of accidental nodes under a change of system parameters such as hybridization [17], interaction with momentum non-conservation by (π, π) in the 1Fe BZ [18], or application of strain [34]. The key features in the s^{+-} case are the same as in the $d-$wave case, namely, under a change of some parameter, which induces inter-pocket pairing term in the band basis, nodal points initially survive, but shift away from the FS, into the region between the pockets (electron pockets in s^{+-} case). As the strength of the inter-pocket pairing term increases, neighboring nodal points come closer to each other and eventually merge and annihilate. There is one distinction to our case, however – the merging of accidental nodes in $s-$wave superconductor involves neighboring nodal points which were originally on the same FS, i.e., nodal points have to travel in the direction along the FS.

The non-trivial interplay between the $d-$wave order parameter in the orbital and the band basis has been first analyzed in Ref. [16]. The authors of [16] correctly pointed out that the inter-band pairing component makes the excitations along the FS nodeless despite that the gap has a d-wave symmetry. In Ref. [16] the $d-$wave order parameter in the orbital basis was assumed to have the form $\Delta(\mathbf{k}) = g_{\mathbf{k}} \left\langle d^\dagger_{xz,\mathbf{k}\uparrow} d^\dagger_{xz,-\mathbf{k}\downarrow} - d^\dagger_{yz,\mathbf{k}\uparrow} d^\dagger_{yz,-\mathbf{k}\downarrow} \right\rangle$, with $g_{\mathbf{k}}$ changing sign between hole and electron pockets (such an order parameter has been listed previously among other singlet pairing order parameters in Eq. D1 of Ref. [25]). For the purposes of comparison with our paper, where only hole pockets are studied, it is sufficient to consider $g_{\mathbf{k}}$ near hole pockets, where it can be approximated by a constant.

Our result for the electronic dispersion, Eqs. (12) and (13), reproduces Eq. (5) of Ref. [16], yet the conclusions are somewhat different. The authors of Ref.[16] concluded that the presence of inter-pocket pairing component makes the electronic spectrum generically gapped, except for possible accidental nodes. We, on the contrary, argue that the true symmetry-imposed $d-$wave nodal points survive, at least near T_c, and just shift away from the normal state FS. We further argue that a $d-$wave superconductor can be fully nodeless, but this happens only when pairs of nodal points with opposite winding numbers come close, merge, and annihilate. The presence of two nearly-located hole FSs is crucial for this last effect, otherwise the critical $\Delta_{\rm cr}$, above which the spectrum becomes nodeless, is comparable to the bandwidth, and the gap Δ necessary remains smaller than $\Delta_{\rm cr}$ down to $T = 0$.

As one illustration of their analysis, the authors of Ref. [16] considered the two-orbital lattice model with tight-binding parametrization of Ref. [35]. This model is different from two-orbital low-energy model and has one hole pocket at the center of the 1Fe BZ and another hole pocket at the corner of the 1Fe BZ. We argue that in this model, $\Delta_{\rm cr}$ is large – a fraction of the bandwidth. To demonstrate this, in Fig. 5 we plot the dispersion along the $k_x = k_y$ direction, showing that the symmetry-imposed $d-$wave nodes are indeed present at Δ smaller than the hopping integral t, only their position shifts from the normal state FS. The nodes annihilate and fully gapless spectrum appears only for $\Delta > \Delta_{\rm cr} = 3.08t$. The large value of $\Delta_{\rm cr}$ is due to the fact that the two hole pockets are centered at different points of the 1Fe BZ. When both hole pockets are centered at Γ, $\Delta_{\rm cr}$ is much smaller.

We emphasize that at $\Delta < \Delta_{\rm cr}$ the nodal points are not accidental – they are true symmetry-imposed $d-$wave nodal points, protected by the fact that each is a Dirac point with a non-zero winding number. Accordingly, because the damping near these new nodal points is the same as near $d-$wave nodes on the FS in a conventional

case, all thermodynamic properties are the same as in a conventional $d-$wave superconductor. Only in ARPES one can distinguish between a conventional d-wave case with the nodes on the original FS and the case when the nodes move away from the original FS due to the presence of the inter-pocket pairing component. Still, this is a non-trivial effect as the shift in $\epsilon_{\mathbf{k}}$ in Eqs. (12) and (13) vanishes along the directions $\sin 2\theta = 0$ and in this respect is qualitatively different from the overall shift of the FS due to a change of the chemical potential.

The authors of Ref. [16] also argued that the presence of inter-pocket pairing component eliminates the nodes on the electron FS near Z point in $K_xFe_{2-y}Se_2$ ($Z = (0, 0, \pi)$). We, on the contrary, argue that this is not so, because the Z-pocket is made out of single d_{xy} orbital, with negligibly small admixture of d_{xz} and d_{yz} orbitals, which at Z point are located far way from the chemical potential. In this situation, the nodes should remain, if the pairing symmetry is $d-$wave. Moreover, the displacement of the nodes from the FS is negligibly small, even if the pocket itself is tiny, because the displacement is determined by the ratio of the small Δ and the large distance between the energies of d_{xy} and other orbitals at Z.

VI. RELATION TO EXPERIMENTS

Our results have important consequences for the experimental identification of d-wave states in FeSC, particularly for strongly hole doped systems, like KFe_2As_2, which contain only hole pockets [3], and $K_xFe_{2-y}Se_2$ or monolayer FeSe, which have only electron pockets [5].

Like we said earlier, thermal conductivity and Raman scattering measurements in KFe_2As_2 [6, 8], were interpreted as evidence for a $d-$wave gap symmetry in this material. On the other hand, ARPES measurements on KFe_2As_2 have found [14] that the gap on the inner hole pocket centered at the Γ point ($\mathbf{k} = 0$) displays some angle variation but has no nodes [15].

The results of Ref. [16] and of this work show that the fact that ARPES does not see nodes at the momenta corresponding to the inner d_{xz}/d_{yz} Fermi surface of KFe_2As_2 is, in principle, not inconsistent with a $d-$wave state because a $d-$wave superconducting gap has no nodes at these momenta. We argue, however, that the $d-$wave nodes are still present, if the gap is small enough, but are located away from the normal state Fermi surfaces. If the gap value exceeds a certain threshold, the nodes disappear, and the $d-$wave superconducting state become fully nodeless.

The values of the gap and of the radii of the d_{xz}/d_{yz} hole pockets can be extracted from ARPES data from Ref. [37]. Based on this data, we found that $k_{F,1} \approx 0.22/A$ and $k_{F,2} \sim 0.3/A$ on the two d_{xz}/d_{yz} pockets, and the Fermi velocity is, roughly $v_F \sim (50-100) meV A$. Then $v_F(k_{F,2} - k_{F,1}) \sim 4 - 8\ meV$. The superconducting gap $\Delta \sim 1 - 2\ meV$, hence $v_F(k_{F,2} - k_{F,1}) > \Delta$. In this situation the nodes must still be present along the diagonal directions at momenta in between the normal state Fermi momenta of d_{xz}/d_{yz} pockets, if the pairing symmetry in KFe_2As_2 is $d-$wave. We call for ARPES measurements on KFe_2As_2 at momenta away from the normal state Fermi surfaces. These measurements should truly distinguish between $d-$wave and $s-$wave gap symmetries.

We also argued that a $d-$wave gap should retain nodes along a pocket made predominantly out of a single orbital. This result has consequences for $K_xFe_{2-y}Se_2$. ARPES measurements on this material [10] have found a pocket centered at Z pocket ($k_x - k_y = 0, k_z = \pi$). According to calculations [36], this pocket is predominantly made out of a single d_{xy} orbital. If the pairing state in $K_xFe_{2-y}Se_2$ was $d-$wave, the gap on this pocket should have nodes along the diagonal direction. ARPES measurements [10], however, found a nodeless gap along the Z-pocket. According to our calculations, this result is inconsistent with $d-$wave gap symmetry in $K_xFe_{2-y}Se_2$.

VII. CONCLUSIONS

In this work we analyzed the $d-$wave gap structure of multi-orbital FeSC, as several experimental and theoretical studies suggested that such a state may be realized in materials with only hole-like or only electron-like Fermi pockets. We showed that the common belief that a $d-$wave gap must have nodes right on the Fermi surfaces located at the center of the BZ is correct only if this Fermi surface is made out of a single orbital, but it is not true if there is an even number of pockets made out of different orbitals. In FeSCs, there are two pockets made out of d_{xz} and d_{yz} orbitals. We argued that symmetry-imposed $d-$wave nodal points near Γ-point remain, at least near T_c, but are shifted away from the normal state FSs into the momentum region between the pockets. Depending on the magnitude of the gap, as compared to the relative radii of the two Fermi surfaces, the $d_{x^2-y^2}$-wave nodal points either persist down to $T = 0$, or come closer with decreasing T and merge and annihilate at a finite $T < T_c$ via a Lifshitz transition. This transition, in which the Dirac gap nodes annihilate, is analogous to a transition from a 2D massless Dirac semi-metal to an insulator. Because the electron pockets are small and centered at $(\pi, 0)$ and $(0, \pi)$, they do not cross the diagonals of the Brillouin zone, i.e. there are no $d-$wave gap nodes on these pockets as well. Thus, a $d-$wave FeSC with two d_{xz}/d_{yz} hole pockets and two electron pockets may display a completely nodeless $d-$wave superconductivity.

With regard to experiments, we argued that the fact that ARPES does not see nodes right on the inner d_{xz}/d_{yz} Fermi surface of KFe_2As_2 is, in principle, not inconsistent with a $d-$wave gap symmetry. However, based on the values of the gap and of the radii of the d_{xz}/d_{yz} hole pockets extracted from ARPES, it is likely that in KFe_2As_2 the nodes are still present, but are located away

from the normal state Fermi surfaces. We call for ARPES measurements at momenta in between the two d_{xz}/d_{yz} Fermi surfaces in KFe_2As_2. We also argued that the observation of a nodeless gap in $K_xFe_{2-y}Se_2$ on a Z-pocket, consisting of a single orbital, provides strong evidence against a $d-$wave gap symmetry in this material.

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