Consistent picture of the octet-nodal gap and its evolution with doping in heavily overdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

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Abstract
We investigate the pairing symmetry in heavily overdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ based on the spin-fluctuation mechanism. We propose a Fermi-patch mechanism that is different from the conventional Fermi-surface-nesting picture. The exotic octet nodes of the superconducting gap and the unusual evolution of the gap with doping observed by the recent experiments are well explained in a unified manner. We demonstrate that the scattering of electrons on the Fermi patches is mainly responsible for the incommensurate spin fluctuations and consequently the Fermi-surface-dependent multi-gap structure, since the Fermi level is close to the flat band. In addition, we find that a $d$-wave pairing state will prevail over the $s$-wave pairing state around the Lifshitz transition point.

Keywords: KFe$_2$As$_2$, spin fluctuation, pairing symmetry

I. Introduction
Since the discovery of iron-based superconductors (FeSCs) in 2008 [1, 2], the mechanism underlying the superconductivity has been one of the most challenging problems. Despite great efforts, the pairing mechanism and the pairing symmetries are still under debate. The prevailing theoretical suggestion is that the electron pairing is mediated by the collinear antiferromagnetic spin-fluctuations and the superconducting (SC) gap changes sign between the hole and electron Fermi surfaces (FSs) (the so-called $s_\pm$ state) in the underdoped and optimally doped regimes [3–7], though there are other proposals [8–10].

Recently, the over-hole-doped compounds $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (BaK122) have attracted much attention, as they exhibit many anomalies deviating from the known FeSC trends [11–26]. Thus, the understanding of the gap symmetries in these superconducting materials will provide more insights into the microscopic pairing mechanism in the FeSC.

$\text{KFe}_2\text{As}_2$ is the end member of the BaK122 series with $x = 1$. Unlike the optimally doped systems ($x = 0.4$), where the sizes of the electron and hole FSs are roughly equal, $\text{KFe}_2\text{As}_2$ has only the hole pockets centered at $\Gamma$ point [$k = (0, 0)$] but no electron pockets according to the angle-resolved photoemission spectroscopy (ARPES) measurements [11–13]. The absence of the electron pockets makes the $s_\pm$ superconducting mechanism, which is mediated by the interband spin fluctuations between the hole and electron pockets, questionable in these heavily overdoped systems. A functional renormalization group study [27] suggests a $d$-wave superconducting state, while a random-phase-approximation (RPA) analysis [28] shows that the $s_\pm$-wave pairing is dominant but the $d$-wave is very close in energy. Based on the leading angular harmonic approximation of the effective pairing interaction from RPA calculation, Maiti et al also find that the $s$-wave and $d$-wave solutions are comparable [29]. Experimentally, the
thermal conductivity [14–16] and magnetic penetration-depth [17] measurements support the $d$-wave symmetry. However, the recent laser ARPES experiment observes a nodal $s$-wave state with an exotic FS-dependent multi-gap structure [11]: a nodeless gap with the largest magnitude on the inner FS, an unconventional gap with °octet-line nodes on the middle FS, and an almost-zero gap on the outer FS. These ARPES results are supported by thermodynamic experiments [18, 19], though certain inconsistencies of the exact position of gap nodes are shown in some experiments [30, 31]. Moreover, the more recent ARPES experiment [20] finds that the gap anisotropy on these FSs drastically changes with a small amount of electron doping. In particular, the gap on the middle FS becomes nodeless when the electron concentration is slightly increased, while the gap structure on the outer FS remains unchanged [20]. By assuming the dominant interaction at small momentum transfers, a particular kind of $s$-wave state was proposed [32], but it is hard to explain the evolution of gap structure with doping. Besides the multi-gap structures, the spin fluctuation also exhibits differences from that in optimally doped systems, where spin fluctuations are observed at the same $q$ position $(\pi, 0)$ as the collinear SDW order wavevector at low energies [33]. By contrast, the spin fluctuation in overdoped BaK122 is incommensurate with the wavevector $(\pi \pm 0.32, 0)$ as found by the recent inelastic neutron scattering (INS) experiments [21, 22].

These anomalous phenomena in heavily overdoped BaK122 raise the following issues: (i) How can we understand the complicated octet-node structures of the SC gap and its evolution with doping? (ii) What is the possible origin of the incommensurate spin fluctuations? (iii) Whether is the spin fluctuation mechanism applicable to these systems in which the electron pockets are absent. In this paper, we provide a unified picture for the incommensurate spin fluctuations and the resulting unusual octet-node structures of the SC gap and its evolution with doping based on a weak-coupling calculation of the five-orbital Hubbard model. We propose a Fermi-patch mechanism different from the conventional Fermi-surface-nesting picture. We find that the incommensurate spin fluctuation originates from the intra-orbital particle-hole excitations. Though the inter-orbital spin fluctuation does not show up in the physical spin susceptibility, it plays a role in the determination of the FS-dependent exotic SC gap structure. Besides the FS nesting, we find that the scatterings of electrons related to the Fermi patches play an essential role both in the incommensurate spin fluctuation

Figure 1. (a) FS in the unfolded BZ for KFe$_2$As$_2$ with $n = 5.5$ at $k_z = 0$. The dominant orbital weights along the FS are highlighted by colors (red: $d_{xz}$, green: $d_{yz}$, blue: $d_{xy}$). The grayscale image in the background shows the intensity of the spectral function $A(k)$. The lines with an arrow indicate the transferred wave vectors for the dominant particle-hole scatterings. The four sets of FSs are labeled by $\alpha$, $\beta$, $\gamma$ and $\delta$. Here, the $\gamma$ FS corresponds to the outer FS in the folded BZ observed by ARPES experiment according to its orbital characteristic. (b) FS in the folded BZ for KFe$_2$As$_2$. The red FS is the $\gamma$ FS which is folded from that around $M$ point as shown in (a). (c) Energy band structure. The dashed line indicates the Fermi level for KFe$_2$As$_2$. (d) Density of state along the FS for KFe$_2$As$_2$. 
and SC gap structures, since the Fermi level is close to the flat band. In addition, although the $s$-wave pairing is the dominant pairing symmetry in a large doping range, a $d$-wave pairing state will be more favored around the Lifshitz transition point. Therefore, the long sought $s + id$ state is probably realized around this transition point.

II. Model and method

The model Hamiltonian consists of two parts:

$$H = H_0 + H_{\text{int}}.$$  \hspace{1cm} (1)

$H_0$ is the effective five-orbital tight-binding model in the unfolded Brillouin zone (BZ) developed by Graser et al [34] to describe the energy band structure of the BaK122. It reads

$$H_0 = \sum_{k,\sigma, \mu, \nu} c_{\mu\sigma}^\dagger(k)c_{\nu\sigma}(k)c_{\mu\sigma},$$  \hspace{1cm} (2)

where $c_{\mu\sigma}^\dagger$ ($c_{\mu\sigma}$) creates (annihilates) an electron with spin $\sigma$ and momentum $k$ in the orbital $\mu$. The details of $H_{\text{int}}(k)$ can be found in [34]. The FS for the chemical potential $\mu = -0.26$ eV at $k_z = 0$ is shown in figure 1(a), which corresponds to the FS observed in ARPES experiments for KFe$_2$As$_2$ [11–13]. The relation between $x$ and the electron concentration $n$ is $n = 6 - 0.5x$, so KFe$_2$As$_2$ corresponds to $n = 5.5$. Also shown in figure 1(a) is the intensity map of the bare single-particle spectral function $A(k) = -\text{Im}[\text{Tr}\hat{G}(k, \omega = 0)]/\pi$ with $\hat{G}(k, \omega)$ the Green’s function. We find that the orbital characters of the FS are consistent with the experimental results [11] and only a point-like FS appears around the X point. Here, the $\gamma$ FS corresponds to the outer FS observed by the ARPES experiment [11] according to its orbital characteristic, though it is not exactly the outer FS according to its size as shown in figure 1(b). A characteristic of the electronic structure is that there is a flat band (saddle point) close to the Fermi level around $X$ (figure 1(c)), which results in four Fermi patches (a region in the $k$ space with a spectral intensity comparable to that on the FS) at $(\pi, 0, 0)$ and $(0, \pm \pi, 0)$ as shown in figure 1(a) and a large density of state (DOS) on the $\delta$ FS as shown in figure 1(d). We note that recent ARPES experiment on heavily over-hole-doped BK122 do observe similar large spectral intensity around $X$ [30]. The interactions between electrons in $H_{\text{int}}$ are the standard multi-orbital on-site interactions, i.e.

$$H_{\text{int}} = U \sum_{i\mu} n_{i\mu}n_{i\mu} + U' \sum_{i,\mu < \nu} n_{i\mu}n_{i\nu}$$

$$+ J_1 \sum_{i,\mu < \nu, \sigma \sigma'} c_{i\mu \sigma}^\dagger c_{i\nu \sigma} c_{i\nu \sigma'} c_{i\mu \sigma'},$$

$$+ J' \sum_{i,\mu < \nu} c_{i\mu \sigma}^\dagger c_{i\nu \sigma} c_{i\nu \sigma'} c_{i\mu \sigma'},$$  \hspace{1cm} (3)

where $n_{i\mu\sigma} = c_{i\mu\sigma}^\dagger c_{i\mu\sigma}$ is the density operator at site $i$ of spin $\sigma$ in orbital $\mu$, $U$ ($U'$) is the intra-orbital (inter-orbital)
Coulomb interaction, $J$ and $J'$ are the Hund’s coupling and the pairing hopping respectively. In this paper, we choose $U = 0.6 \text{ eV}$, $U' = 0.3 \text{ eV}$ [34], and use the relations $J = J'$ and $U = U' + 2J$. We have checked the results for $U = 0.2 \sim 0.7 \text{ eV}$ and found no qualitative difference.

Based on the scenario that the pairing interaction in the FeSCs arises from the exchange of spin and charge fluctuations, we can calculate the effective electron-electron interaction using the RPA. The singlet pairing interaction is given by

$$
\hat{V}(q) = \frac{3}{2} \hat{U}^\dagger \hat{\chi}^s(q) \hat{U} \frac{1}{2} \hat{U}^\dagger \hat{\chi}^c(q) \hat{U} + \frac{1}{2} \left( \hat{U} \hat{U}^\dagger - \hat{U}^\dagger \hat{U} \right),
$$

(4)

where $\hat{\chi}^s$ ($\hat{\chi}^c$) is the spin (charge) susceptibility and $\hat{U}$ ($\hat{U}^\dagger$) is the interaction matrix for the spin (charge) fluctuation. $\hat{\chi}^s$ and $\hat{\chi}^c$ are expressed as $\hat{\chi}^s(q) = [1 - \hat{\chi}^o(q) \hat{U}^\dagger]^{-1} \hat{\chi}^o(q)$ and $\hat{\chi}^c(q) = [1 + \hat{\chi}^o(q) \hat{U}^\dagger]^{-1} \hat{\chi}^o(q)$ respectively. The non-interacting susceptibility is given by $\chi^0_{\nu \sigma}(q) = -\frac{1}{2} \sum_{\omega} G_{\nu \sigma}(k + q) G_{\nu \sigma}(k)$ with the number of lattice sites $N$ and temperature $T$. The Green’s function is given by $G(k) = \left[i\omega_n - H_0(k) + \mu\right]^{-1}$. In the

Figure 3. Dominant gap functions $g(k)$ and their sign structures along the FSs for different electron concentrations: (a) and (b) $n = 5.5$, (c) and (d) $n = 5.55$, (e) and (f) $n = 5.63$. In (a), (c) and (e), the signs of $g(k)$ are shown by the following colors: red (positive) and blue (negative). The arrows in (a) and (c) indicate the typical vectors related to the peaks of the spin fluctuations. (b), (d) and (f) show $g(k)$ as a function of the angular $\theta$ indicated in (c). The fittings of $g(k)$ are shown as the solid lines (see text).
above, \( k \equiv (\mathbf{k}, i\omega_n) \) with \( \omega_n = \pi T (2n + 1) \). In the following calculations, we use the retarded Green’s function and susceptibility by performing a Wick rotation \( i\omega_n \to \omega + i\eta \). \( U^i(\Omega') \) is given by: for \( \mu = \nu = \eta = \varphi, U^\mu_{\nu\varphi\eta} = U(U^\mu_{\nu\varphi\eta} = U) \); for \( \mu = \nu = \eta = \varphi, U^\mu_{\nu\varphi\eta} = J(U^\mu_{\nu\varphi\eta} = 2U^i - J) \); for \( \mu = \eta, \nu = \varphi \) and \( \nu \neq \nu, U^\mu_{\nu\varphi\eta} = U(U^\mu_{\nu\varphi\eta} = -U^i + 2J) \); for \( \mu = \varphi, \nu = \eta \) and \( \mu = \nu, U^\mu_{\nu\varphi\eta} = J(U^\mu_{\nu\varphi\eta} = J) \); for other cases, \( U^\mu_{\nu\varphi\eta} = 0 \) (\( U^6_{\nu\varphi\eta} = 0 \)).

In the orbital representation, the linear superconducting gap equation (the ‘Eliashberg’ equation) is given by

\[
\lambda \Delta_{\mu \nu}(k) = -\frac{T}{N} \sum_{\eta \not= \mu \not= \eta} \sum_{\mu \not= \nu} \sum_{\mu \not= \mu} V^{\mu \nu}_{\eta \mu \nu}(q) G_{\mu \nu}(k - q) \times G_{\nu \mu}(q - k) \Delta_{\mu \nu}(k - q).
\]

We confine our considerations to the dominant scattering occurring in the vicinity of the FS. Thus, we can reduce the effective interaction (4) and the ‘Eliashberg’ equation (5) to the FS. The scattering amplitude of a Cooper pair from the state \((\mathbf{k}, -\mathbf{k})\) on the FS \(i\) to the state \((\mathbf{k}', -\mathbf{k}'')\) on the FS \( j \) is calculated from the projected interaction [7, 35]

\[
\Gamma_{ij}(\mathbf{k}, \mathbf{k}') = \sum_{\mu \not= \nu} b^\mu_j(\mathbf{k}) b^\nu_j(\mathbf{k}') \text{Re}[V_{\mu \nu}(\mathbf{k} - \mathbf{k}', \omega = 0)] \times b^\nu_j(\mathbf{k}') b^\mu_j(-\mathbf{k}'),
\]

where \( b^\mu_j(k) = (\mu, |j|, k) \) projects the band basis \(|j|, k\) to the orbital basis \(|\mu, k\). Here, \( i \) and \( j \) are the band and orbital index respectively. We then solve the following eigenvalue problem:

\[
-\sum_{ji} \frac{dE_i}{4\pi^2 N E_i(\mathbf{k})} \Gamma_{ij}(\mathbf{k}, \mathbf{k}') g_{ij}(\mathbf{k}') = \lambda g_{ij}(\mathbf{k}),
\]

where \( E_i(\mathbf{k}) \) is the energy of the tight-binding Hamiltonian (2) for the band \( j \) at the momentum \( \mathbf{k} \) and \( g_{ij}(\mathbf{k}) \) is the normalized gap function along the FS \( i \). The integral in equation (7) is evaluated along the FSs. The most favorable SC pairing symmetry corresponds to the gap function with the largest eigenvalue \( \lambda \). One merit of this method is that it can adequately include the effect of DOS on the FS, which is very important in overdoped BaK122.

To resolve the eigenvalue equation (7), we use 256 points along every hole-like FS around \( \Gamma \) (and \( M \)) point and 16 to 128 points along every FS around \( X \) point depending on the size of this FS. The temperature is set at \( T = 0.005 \text{eV} \), and the calculation of the susceptibility is done with uniform 128 \times 128 meshes.

### III. Results

We will only discuss the spin fluctuations in the following because of the negligible role of charge fluctuation. In figure 2, we present the spin susceptibility for \( n = 5.5 \). Figure 2(a) is the static physical spin susceptibility \( \chi^s(q) = \sum_{\alpha} \chi_{\alpha \alpha}(q, \omega = 0) \), for which the structure of peaks can be reflected by the result of the neutron scattering experiments. It shows eight peaks located at the incommensurate wave vectors \((\pi \pm 0.34\pi, 0)\) and their symmetric points, which is consistent with the INS experiments on KFe2As2 [21, 22] and the previous theoretical result [28]. We find that \( \chi^s \) is governed primarily by the intra-orbital spin fluctuations, and those within the \( d_{xy} \), \( d_{zx} \) and \( d_{yz} \) orbitals contribute mainly to it, since the electronic states near the FS basically come from these three orbitals (figure 1(a)). In figures 2(b) and (c), the intra-orbital spin fluctuations in the \( d_{xy} \) (that in the \( d_{yz} \) orbital is rotated by 90 degrees) and \( d_{zx} \) orbitals are presented. Usually, the spin fluctuations in the weak-coupling scheme is resulted from the particle-hole scatterings of electrons between the nesting FS. From the FS shown in figure 1(a), one can find that there is no nesting condition for the intra-\( d_{zx} \)-orbital spin fluctuation with the wavevector \( \mathbf{q}_c \) (figure 2(b)). Instead, we find that it is the scatterings of electrons between the \( \beta \) FS and the Fermi patches at \((0, \pm \pi)\) (figure 1(a)) contribute essentially to \( \chi_{d_{zx}d_{zx}} \). Whereas, the intra-\( d_{xy} \)-orbital spin fluctuation with \( \mathbf{q}_2 \) (figure 2(c)) is resulted from the nesting of the \( \gamma \) FS as shown in figure 1(a). The consequence of the Fermi-patch mechanism is that the peaks of \( \chi \) in the \( d_{xy} \) orbital is much broader than those in the \( d_{yz} \) orbital. Another character is that in this doping level \( \mathbf{q}_2 \approx 2\pi - \mathbf{q}_p \), so the peaks of the intra-orbital spin fluctuations in the \( d_{xy} \) and \( d_{yx} \) orbitals appear basically at the same wave vectors. Besides, we find that the inter-orbital spin fluctuation \( \chi_{d_{zx}d_{yz}} \) where \( \mu = d_{zx} \) (or \( d_{yx} \)) and \( \nu = d_{yz} \) with the wavevector \( \mathbf{q}_3 \) also has a comparable magnitude with the intra-orbital spin fluctuations as shown in figure 2(d). It mainly comes from the scatterings of electrons between the \( \gamma \) FS and the Fermi patches near \((0, \pm \pi)\) as indicated by \( \mathbf{q}_3 \) in figure 1(a). Though not showing up in the physical spin susceptibility, this inter-orbital spin fluctuation is an important ingredient in determining the pairing symmetry.

The dominant pairing functions \( g(\mathbf{k}) \) and their sign structures obtained from equation (7) for three different electron concentrations are shown in figure 3. Figures 3(a) and (b) show the results at \( n = 5.5 \) corresponding to the case of KFe2As2. An obvious feature is that the gap function exhibits an unusual FS-dependent multi-gap structure. The gaps on the \( \beta \) and \( \gamma \) FSs reveal an eightfold sign reversal (figure 3(a)), whereas that on the \( \alpha \) FS (the inner pocket) is nodeless. In addition, the magnitude of the gap on the \( \gamma \) FS is much smaller than those on the \( \alpha \) and \( \beta \) FSs (figure 3(b)), and the magnitude on the \( \alpha \) FS is the largest. We note that a similar octet-node structure of the gap on the \( \beta \) FS has also been proposed in [32], but the largest

| \( n \) | FS | \( a_0 \) | \( a_1 \) | \( a_2 \) |
|---|---|---|---|---|
| 5.5 | \( \alpha \) | 0.61 | 0.23 | 0 |
| 5.5 | \( \beta \) | 0.34 | -0.15 | 0.07 |
| 5.5 | \( \gamma \) | 0.005 | 0.25 | 0 |
| 5.63 | \( \beta \) | 0.64 | 0.32 | 0 |
| 5.63 | \( \gamma \) | 0.022 | 0.057 | -0.005 |

Note: The fitting function is \( g(k) = \Delta_{\alpha}(a_0 + a_1 \cos 4\theta + a_2 \cos 8\theta) \) with \( i \left(= \alpha, \beta, \gamma \right) \) representing one of the hole Fermi surfaces (FSs).
magnitude of gap is on the $\beta$ FS, which is not consistent with the ARPES experiment [11]. With a slight increase of the electron concentration, we find that the gap anisotropy on these FS drastically changes, as shown in figures 3(c)–(f) for $n = 5.55$ ($x = 0.9$) and $n = 5.63$ ($x = 0.74$). The octet node structure on the $\beta$ FS disappears completely, and the gaps on both the $\beta$ and $\alpha$ FSs are nodeless. While the gap on the $\gamma$ FS still has the octet nodal structure. The obtained gap structure for KFe$_2$As$_2$ and its doping dependence are consistent with the recent laser ARPES results [11, 20]. Furthermore, the pairing functions on all three FSs can be well fitted in an unified manner with the function $\theta(k) = \Delta + g_0 \cos^4 \theta_i$, where $i$ ($= \alpha$, $\beta$ or $\gamma$) represents one of the hole FSs, as shown by the solid lines in figures 3(b), (d) and (f) with the fitting parameters given in table 1.

Within the spin-fluctuation mechanism, the pairing interaction in the spin-singlet channel is positive (repulsive) (see equation (4)). Thus, the most favorable SC gap should satisfy the condition $g(k)\theta(k + Q) < 0$, where $Q$ is the typical wavevector at which the spin fluctuation has a peak. As the $\delta$ FS is very tiny for $n = 5.5$, it doesn’t play a role in determining the gap signs. According to the general gap equation shown in equation (5), the scattering of a Cooper pair mediated by the intra-orbital spin fluctuation will happen between the FSs with the same orbital character. Due to the orbital weights of the $\alpha$ and $\beta$ FSs shown in figure 1(a), three typical wavevectors $q_1^\alpha$, $q_1^\beta$ and $q_1^\gamma$, which correspond to the broad peak of the intra-$d_{xz}$-orbital spin fluctuation resulting from the scatterings of electrons in the Fermi patches, connect the FS pieces with the $d_{xz}$ orbital character. Due to the symmetry constraint for the spin singlet pairing, the gap on the FS pieces connected by $q_1^\alpha$ should change sign. While, those on the FS pieces connected by $q_1^\beta$ and $q_1^\gamma$ should not change sign. Thus, it leads to the anomalous gap structures on the $\alpha$ and $\beta$ FSs. This analysis is also applied to the sign change of $\theta(k)$ within the $\beta$ FS connected by $q_2^\alpha$ which is the characteristic wavevector of the intra-$d_{yz}$-orbital spin fluctuation. While, the sign change between the $\beta$ and $\gamma$ FSs connected by $q_3^\alpha$ is required by the inter-orbital spin fluctuation as shown in figure 2(d).

With the increase of electron density, such as for $n = 5.55$ and $n = 5.63$, the Fermi level will be pushed towards the flat band. Consequently, the $\delta$ FS as well as the DOS on it will be enlarged. Though we do not find noticeable change in spin fluctuations correspondingly, the essential change is that now the $\delta$ FS plays an important role in determining the sign structure of $g(k)$. In figure 3(c), we plot the typical vectors by which the gaps on the connected FS change signs for $n = 5.55$. The same situation happens for $n = 5.63$. In these cases, the gap function on the $\beta$ FS is nodeless, while the sign structure of $g(k)$ on the $\gamma$ FS remains the same as that for $n = 5.5$.

![Figure 4.](image-url)
In fact, between \( n = 5.55 \) and \( n = 5.63 \), there is a Lifshitz transition from the small off-X-centered hole FS pocket lobes to that centered around the \( X(0, \pi) \) point, as can been seen from a comparison between figures 3(c) and (e). This Lifshitz transition has also been confirmed by the ARPES experiment [30]. Interestingly, we find that a \( d \)-wave pairing state will prevail over the \( s \)-wave state around the transition point, as seen from figure 4(a) where the most favorable gap structure for \( n = 5.6 \) is shown. The reason is that the DOS on the \( \delta \) FS near \( X \) point is divergent at the transition point, which makes the gap function of the \( \delta \) FS changes its signs between \( (\pi, 0) \) and \( (\pi, \pi) \) points according to equation (7). Besides this requirement, in fact, the typical vectors by which the gaps on the connected FS change signs are the same as those at \( n = 5.5 \) shown in figure 3(c). The only difference is that the sign structure is antisymmetric along the \( k_x \) and \( k_y \) directions in this case, while it is symmetric at \( n = 5.5 \) and \( n = 5.63 \). Without the addition requirement, in the latter case the nodeless gap on both the \( \alpha \) and \( \beta \) FSs is favored energetically.

A detailed evolution of the gap symmetry with doping is presented in figure 4(c), where the two leading eigenvalues of the gap function equation (7) is shown (the optimal doping is \( n = 5.8 \)). We can identify five regions according to the symmetry and sign structure of the gap. In region (I), the gap is \( s \)-wave with octet nodes on both \( \beta \) and \( \gamma \) FSs (figure 3(a)). In regions (II) and (IV), the gap is \( s \)-wave with octet nodes only on the \( \gamma \) FS (figure 3(c) and (e)). In region (III), the gap is \( d \)-wave (figure 4(a)); In region (V), the gap is nodeless \( s_\pm \)-wave as shown in figure 4(b) and the peaks of spin fluctuations are at \( (0, \pm \pi) \) and \( (\pm \pi, 0) \) [34]. Considering the near degeneracy of the \( s \) and \( d \) wave, we propose that the long sought \( s + id \) pairing state in FeSC [36–42] would be probably realized in the heavily overdoped BaK122 around the Lifshitz transition point.

Finally, we note that the above investigations are based on the tight-binding energy band fitted from the first-principle calculations [34]. In this case, the Fermi level is determined by the nominal density of the electrons. Consequently, the theoretical energy band gives a tiny electron-like \( \delta \) FS for KFe2As2 \( (x = 1.0) \) as shown in figure 1(a). However, the \( \delta \) FS observed by the experiments is hole-like for KFe2As2 \( (x = 1.0) \) [13, 24]. To check the effect of this difference, we shift down the Fermi level by 0.03 eV compared to that in figure 1(c), to produce this kind of hole-like FS as shown in figure 5(a). The physical spin susceptibility calculated in this case is presented in figure 5(b). It shows similar eight peaks located at the incommensurate wave vectors \( (\pi, \pm 0.34\pi, 0) \) as that in figure 2(a). The sign structure of the dominant pairing functions \( g(k) \) and the variation of its value along the FS are presented in figure 5(c) and figure 5(d) respectively. One can find that the results are similar as those in figures 3(a) and (b), and also consistent with the ARPES experiments [11, 20]. The physical origin of this gap structure is the same as that used to explain the results presented in figures 3(a) and (b). Another
important point is that, to produce the octet-nodal gap along the $\beta$ and $\gamma$ FSs, the size of the $\delta$ FS in this case can be much larger than that in the case where the $\delta$ FS is electron-like, because the Fermi level is farther away from the saddle point at $X$ in this case and the DOS on the $\delta$ FSs is correspondingly much smaller.

IV. Conclusion

In summary, the pairing symmetry in the heavily overdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ is studied based on the spin-fluctuation mechanism. The exotic octet nodes of the superconducting gap and the unusual evolution of the gap with doping observed by the recent experiments are explained in the Fermi-patch mechanism, which is different from the conventional Fermi-surface-nesting picture. The scattering of electrons related to the Fermi patches is demonstrated to be mainly responsible for the incommensurate spin fluctuations and consequently the gap structure. This Fermi-patch scenario provides a new viewpoint based on the large density of states resulting from the flat band, instead of the usual Fermi-surface-nesting picture where the Fermi surface topology is essential.

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