A shadow gap in the over-doped (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ compound

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Abstract
The electron band around the $M$ point in the (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ compound, which is completely lifted up above the Fermi level for $x > 0.7$ and hence its Fermi surface (FS) disappears, can still play the role of the main pairing resource by exchanging inter-band repulsive interaction with the main hole band ($h_1$) around the $\Gamma$ point. This hidden electron band, which develops the superconducting order parameter (OP) $\Delta_e$ but has no FS, displays a shadow gap feature which is easily detected by various experimental probes such as angle-resolved photo-emission spectroscopy (ARPES) and tunneling measurements. We also show that the formation of the nodal gap $\Delta_{nodal}$ with $A_{1g}$ symmetry on another hole pocket ($h2$) around the $\Gamma$ point with a larger FS is stabilized due to the balance of the inter-band repulsive interactions from the main hole band ($h1$) with the OP $\Delta_{b1} = \Delta_e$, and the hidden electron band with the OP $\Delta_e = \Delta_\pi$.

Keywords: Fermi surface instability, iron-based superconductor, pairing symmetry, Fe$_2$As$_2$, nodal gap

1. Introduction

The superconducting (SC) transition is the most well known example of Fermi surface (FS) instability along with other density wave instabilities such as spin density wave (SDW), charge...
density wave (CDW), etc. Mathematically, it is summarized by a pairing susceptibility
\( \chi (T) = \lambda \ln \left[ \frac{\Lambda_{hi}}{T} \right] \) of a conduction band of the Bloch states [1], where \( \lambda \) is a dimensionless coupling constant and \( \Lambda_{hi} \) is the high energy cut-off of the pairing interaction (for example, \( \Lambda_{hi} = \alpha_{D} n \), Debye frequency, for phonon interaction). For the conduction band with a FS, the low energy cut-off is zero because the presence of FS allows zero energy excitations, which is replaced by \( T \) at finite temperature in the above formula. This susceptibility displays a logarithmic divergence with lowering temperature, hence no matter how weak the pairing interaction \( \lambda \) is, the instability condition, \( \chi (T) \to 1 \), is achieved by decreasing the temperature \( T \to T_c = \Lambda_{hi} \exp \left[ -1/\lambda \right] \). This is called FS instability. However, if there exists a finite low energy cut-off \( \Lambda_{low} \), for example, because there is no FS, then the pair susceptibility becomes \( \chi \sim \lambda \ln \left[ \frac{\Lambda_{hi}}{\Lambda_{low}} \right] \) and the instability condition \( \chi (T) \to 1 \) can only be satisfied when the coupling strength \( \lambda \) becomes sufficiently strong, i.e. \( \lambda > \lambda_{crit} = \frac{1}{\ln \left[ \frac{\Lambda_{hi}}{\Lambda_{low}} \right]} \). This hypothetical exercise shows that the instability can still occur with Bloch states without the FS if the coupling is strong enough. However, notice that the susceptibility \( \chi \) becomes temperature independent in this case, hence this mechanism cannot derive a phase transition in a real system by decreasing temperature. Therefore, we reconfirm the common knowledge: no FS, no phase transition with Bloch states.

In this paper, however, we demonstrate that the presence of the low energy cut-off in the pairing susceptibility does not prohibit the SC phase transition in the multi-band SC pairing model mediated by an interband pairing interaction, as most probably realized in the Fe-based superconductor [2–4]. In particular, in the case of the hole over-doped \((\text{Ba}_{1-x}\text{K})_x\text{Fe}_2\text{As}_2\) compound, it is known that the electron band is completely lifted up above the Fermi level, hence the FS of the electron pocket disappears, for \( x > 0.7 \) [5]. Even in this case, we show that the SC order parameter (OP) should still be formed both in the electron band, which has no FS, and in the hole band, maintaining the general structure of the sign-changing s-wave pairing state mediated by antiferromagnetic (AFM) spin fluctuations.

The formation of a SC OP in the band without FS is an unprecedented SC state and its identification will be ‘smoking-gun’ evidence, proving the pairing mechanism of the iron-based superconductors mediated by interband repulsive interaction [4, 6–9]. This SC gap state without FS will display a shadow gap feature in various physical properties and this shadow gap feature can be easily detected by experiments such as angle-resolved photoemission spectroscopy (ARPES), tunneling, etc. Finally, the formation of the SC pairing condensate in the electron band, although it is not visible at the Fermi level, is the main driving force in determining the SC transition temperature \( T_c \) and also plays an important role in stabilizing a nodal SC gap on the second and/or third hole pocket with a larger FS area. Our scenario can provide a natural explanation of the \( T_c \) variation and evolution of a nodal gap of \((\text{Ba}_{1-x}\text{K})_x\text{Fe}_2\text{As}_2\) with K doping [10–12, 14].

2. \( T_c \) with the electron band lifted above Fermi level

For the purpose of demonstration, we start with a minimal two band model [8]: one hole band around the \( \Gamma \) point and one electron band around the \( M \) point in the folded Brillouin zone (BZ). The pairing interaction is assumed to be a simple phenomenological form induced by the AFM spin fluctuations defined as
\[ V_{\text{AFM}}(k, k') = V_0 \frac{\kappa^2}{|\vec{k} - \vec{k}'| - \vec{Q} + \kappa^2} \]  \hfill (1)

where the AFM correlation wave vector \( \vec{Q} \) is assumed to be \( \vec{Q} = (\pi \pm \delta, \pi \pm \delta) \) to incorporate an incommensurability [15]. The coupled gap equations are written as

\[
\Delta_h(k) = -\sum_{k'} \left[ V_{hh}(k, k') \chi_h(k') \Delta_h(k') + V_{hh}(k, k') \chi_e(k') \Delta_e(k') \right],
\]

\[
\Delta_e(k) = -\sum_{k'} \left[ V_{ee}(k, k') \chi_h(k') \Delta_h(k') + V_{ee}(k, k') \chi_e(k') \Delta_e(k') \right],
\]

where \( V_{hh}(k, k') = V(k_h, k_h'), V_{he}(k, k') = V(k_h, k_e') \), etc are the interactions defined in equation (1). For the convenience of the analysis of \( T_c \), we introduced the FS averaged pairing potential \( \langle V_{he}(k_h, k_e) \rangle_{\text{FS}} = \bar{V}_{he} = \bar{V}_{eh} \), etc and the coupled \( T_c \)-equations are written as

\[
\Delta_h = -\left[ \bar{V}_{hh} N_h \chi_h \right] \Delta_h - \left[ \bar{V}_{he} N_e \chi_e \right] \Delta_e,
\]

\[
\Delta_e = -\left[ \bar{V}_{ee} N_e \chi_e \right] \Delta_e - \left[ \bar{V}_{eh} N_h \chi_h \right] \Delta_h
\]

where the pair susceptibility is defined as

\[
\chi_{h,e}(T) = \int_0^{\Lambda_{hi}} \frac{d\xi}{\xi} \tanh \left( \frac{\xi}{2T} \right) \approx \ln \left[ \frac{1.14 \Lambda_{hi}}{T} \right].
\]

and \( N_{h,e} \) are the density of states (DOS) of the hole band and electron band, respectively. For simplicity of demonstrating the mechanism, we temporarily drop the intra-band interactions \( \bar{V}_{hh} \) and \( \bar{V}_{ee} \), which are always much weaker than \( \bar{V}_{he} = \bar{V}_{eh} \). Then the \( T_c \)-equations can easily be combined to be

\[
\Delta_h = \left[ \bar{V}_{hh} N_e \chi_e \right] \Delta_h - \left[ \bar{V}_{he} N_h \chi_h \right] \Delta_e.
\]

\[
\approx \left[ \bar{V}_{he} N_e \chi_h \right] \left[ \ln \left( \frac{1.14 \Lambda_{hi}}{T} \right) \right] \Delta_h,
\]

hence we can read off the critical temperature as

\[
T_{c0} \approx 1.14 \Lambda_{hi} \exp \left[ -1/\lambda_{\text{eff}} \right]
\]

with \( \lambda_{\text{eff}} = \sqrt{\bar{V}_{he} N_e \bar{V}_{eh} N_h} \). Now if the electron band does not cross the Fermi level and the bottom of the band is lifted above the Fermi level by \( \epsilon_b \), the only modification of the above analysis is to replace the susceptibility of the electron band as follows

\[
\chi_e = \int_{\epsilon_b}^{\Lambda_{hi}} \frac{d\xi}{\xi} \tanh \left( \frac{\xi}{2T} \right) \approx \ln \left[ \frac{1.14 \Lambda_{hi}}{\epsilon_b} \right],
\]
and the coupled $T_c$-equation, equation (7), changes as follows

$$
\Delta_h \approx \left[ \bar{V}_{he} N_e \bar{V}_{eh} N_h \right] \left[ \ln \left( \frac{1.14 \Lambda_{hi}}{\epsilon_b} \right) \right] \left[ \ln \left( \frac{1.14 \Lambda_{hi}}{\epsilon_b} \right) \right] \Delta_h. \tag{10}
$$

The critical temperature is then reduced as

$$
T_c(\epsilon_b) \approx 1.14 \Lambda_{hi} \exp \left[ -1/\tilde{\Lambda}_{eff}(\epsilon_b) \right]
$$

with $\tilde{\Lambda}_{eff} = \left[ \bar{V}_{he} N_e \bar{V}_{eh} N_h \right] \cdot \ln \left[ \frac{1.14 \Lambda_{hi}}{\epsilon_b} \right].$ Notice that this analysis is accurate only when $\epsilon_b > T_{c0}$, and in the other limit the susceptibility $\chi$ of equation (9) should be numerically calculated. Nevertheless, this simplified analysis clearly demonstrates the fact that in the multiband pairing model, where the main pairing interaction is the inter-band scattering, the FS instability still operates even if the FS of the electron band disappears and the $T_c(\epsilon_b)$ will continuously decrease as the bottom of the electron band $\epsilon_b$ is lifted up above the Fermi level.

In Figure 1, we show the numerical results of $T_c$ calculated with equation (4) and the pair susceptibilities equations (5) and (9) numerically calculated. We also include both interband ($\bar{V}_{eh}$ and $\bar{V}_{he}$) and intraband ($\bar{V}_{ee}$ and $\bar{V}_{hh}$) interactions. The FS averaged interaction can still be defined when the FS of the electron band disappears, for example, as follows

$$
\bar{V}_{he} = < V_{he}(k_h, k_e) >_{FS} = \frac{\int_{-\Lambda_{hi}}^{\Lambda_{hi}} d\epsilon_h(k_h) \int_{\epsilon_b}^{\Lambda_{hi}} d\epsilon_e(k_e) V_{AFM}(k_h, k_e)}{\int_{-\Lambda_{hi}}^{\Lambda_{hi}} d\epsilon_h(k_h) \int_{\epsilon_b}^{\Lambda_{hi}} d\epsilon_e(k_e)}, \tag{12}
$$

where the high energy cut-off $\Lambda_{hi}$ can be understood to be the high energy cut-off of the AFM spin fluctuations mediated pairing interaction $\omega_{AFM}$. The above formula explicitly shows that the pairing interaction exists as far as $\epsilon_b < \Lambda_{hi}$ and its strength only depends on the average distance.
of the momenta $k_h$ and $k_e$. The effective pairing interaction, of course, is proportional to the volume of the phase space connected by the interaction as

$$\frac{1}{N_{tot}} \sum_{k_{e\text{pairing}}} = N_e \int_{\epsilon_e}^{\Lambda_{hi}} d\epsilon_e(k_e)$$

and this information is absorbed in the definition of the pair susceptibility (equation (9)) and $N_e$, the average DOS of the electron band in the region of $\epsilon_h < \epsilon_e(k_e) < \Lambda_{hi}$, is a constant to a good approximation because the band dispersion $\epsilon_e(k_e)$ is a quasi-2-dimensional parabolic band near the bottom of the band.

The above defined repulsive inter-band interaction $V_{inter} = \tilde{V}_{eh} = \tilde{V}_{he} > 0$ will induce the $\Delta_\pm$ gap solution [8] and its precise value need not be specified because the final results are normalized as $T_c/T_{c0}$ vs. $\epsilon_b/\Lambda_{hi}$ in figure 1. Also, instead of using the actual values of the intra-band interactions $\tilde{V}_{hh}, \tilde{V}_{ee}$, we treat them as free parameters for the purpose of demonstration. With this freedom and for generality, we considered both repulsive and attractive intra-band interaction in figure 1; the attractive intra-band interaction can possibly be caused by phonons [16]. When the intra-band interaction $V_{intr}$ is sufficiently attractive (the case $V_{intr} = -0.4V_{inter}$ in figure 1, for example), the $T_c$ finally converges to the limit where only the hole band develops a SC transition with the attractive interaction. The gap symmetry does not change in this evolution because it evolves as $\Delta_\pm \rightarrow 0$.

In figure 1, we show the calculations starting from the negative value of $\epsilon_b < 0$, which means that the electron band sinks slightly below the Fermi level and hence has a small FS. The positive $\epsilon_b > 0$ value means that the bottom of electron band is lifted above the Fermi level by $\epsilon_b$. The overall behavior of $T_c(\epsilon_b)$ in figure 1 is similar for all cases; a linear decrease for small $\epsilon_b$ value and then exponential decrease for large $\epsilon_b$ value in accord with equation (11). This behavior is in qualitative agreement with the experimental observation of $T_c$ variation of $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ compound with K doping [10–12, 14]. It should be desirable to have a good estimate of the model parameter $\epsilon_b(x)$ vs. the K-doping $x$. Sato et al [5] found that the band structures of $(\text{Ba}_{0.6}\text{K}_{0.4})\text{Fe}_2\text{As}_2$ and $\text{KFe}_2\text{As}_2$ are pretty well matched by a rigid band model and the chemical-potential shift of 20–25 meV. They also estimated $\epsilon_b(x = 0.4) \approx -18$ meV, hence we estimate $\epsilon_b(x = 1) \sim 2-7$ meV. However, in the real system, the K-doping will not only lift the electron band but also cause many other changes such as the hole FS sizes, the spin fluctuations strength, etc. Nevertheless, our calculations of figure 1 strongly suggest that the continuous lifting of the bottom of the electron band with K-doping ($x$) and its distance $\epsilon_b(x)$ from $E_F$ can be the leading factor for controlling $T_c$ in the $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ compound. This pairing state in the lifted or sunken band close to the Fermi level was also considered in previous works [9, 13], but there the systematic investigations for understanding the phase diagram and other physical signatures were not carried out. Finally, during the calculations of figure 1, we assumed that the pairing symmetry maintains the same pairing state $\Delta_\pm$. In section 4, we will show that this is the most natural, and also consistent, assumption.
3. The shadow gap in the electron band

Here we solve the coupled gap equations, equations (2) and (3), for $T \ll T_c$ with the realistic tight binding bands [8] and the fully momentum dependent phenomenological pairing interaction of equation (1). We used two model bands:

$$
\epsilon_+ = t^h_{22} \cos k_x \cos k_y + \epsilon_h \quad \text{and} \quad \epsilon_- = t^e_{12} \cos k_x + \epsilon_e \quad \text{with the band parameters as (0.30, 0.24, -0.6) for the hole band and (1.14, 0.74, \epsilon_e) for the electron band with the notation (t^i, t^j, \epsilon).}$$

The electron band located in the $M$ points $(\pi, \pi)$ in the folded BZ is artificially lifted by shifting the parameter $\epsilon_e$. The overall pairing strength $V_0$ (equation (1)) need not be physically accurate since all results are normalized by the gap values.

In figure 2, we show the calculated DOSs, $N_h(\omega)$, $N_e(\omega)$, and the total $N_{\text{total}}(\omega)$. Figure 2(A) is the case when $\epsilon_e = 0.0$. In the normal state, the electron band and its DOS $N^\text{normal}_e(\omega)$ exists only above the Fermi level. Nevertheless, in the SC state, the Bogoliubov quasiparticles are formed above and below the Fermi level, hence the DOS $N^\gamma_e(\omega)$ is created both for $\omega > 0$ and for $\omega < 0$. However, the shape of $N^\gamma_e(\omega)$ is very asymmetric for above and below $\omega = 0$ as seen in the right inset of figure 2(A). It should be contrasted with $N^\gamma_h(\omega)$ in the left inset which is symmetrical, as a typical SC DOS. The total DOS, $N_{\text{total}}(\omega)$, displays this clear signature of the asymmetric DOS due to the electron band above the Fermi level.

Figure 2(B) is the case $\epsilon_e = |\Delta_e|$. In this case the gap size in $N^\gamma_e(\omega)$ becomes $\sqrt{\epsilon_h^2 + \Delta_e^2}$ and the shapes of $N^\gamma_e(\omega)$ and $N^\gamma_h(\omega)$ become even more asymmetric than the $\epsilon_e = 0$ case. This predicted asymmetric DOS could be detected by STM or tunneling measurements although the multiple peaks due to the multiband nature of the Fe-based superconducting compounds might obscure a clear separation of the predicted asymmetric DOS due to the shadow gap from other features. However, next we predict that a more direct and unambiguous signature of the shadow gap can be measured in the ARPES experiment.
In figure 3, we showed the quasiparticle spectral density of the electron band $\epsilon_{\mathbf{k}}(k)$ near the $M$ point. This is calculated by $\omega = \pi I m G(\omega, k) = \frac{1}{2} I m \frac{\omega + \epsilon_{\mathbf{k}}(k)}{\omega^2 - [\epsilon_{\mathbf{k}}(k) + \Delta]}$. These results are another manifestation of the shadow gap feature of the electron band which does not have FS. Figures 3(A) and (B) are the normal state and the SC state of the case $\epsilon_b = 0.0$, respectively, and figures 3(C) and (D) are the corresponding results of the case $\epsilon_b = |\Delta|$. In the normal state, the quasiparticles do not appear below the Fermi level both in figures 3(A) and (C) simply because the band does not exist there. However, when temperature decreases below $T_c$, the quasiparticle spectral density appears below the Fermi level both in figures 3(B) and (D). This shadow band behavior should appear only when the lifted electron band—hence having no FS pocket—participates in pairing of the $\Delta$ gap state, otherwise it would not. This dramatic effect should be easy to detect by the ARPES measurement and in fact it seems to have already been detected in the $\text{FeTe}_{0.6}\text{Se}_{0.4}$ compound by Shin and coworkers [17] although there the lifted electron band (about $\sim 7$ meV above $E_F$) occurs at the $\Gamma$ point and these authors’ interpretation is different from ours.

4. Evolution of a nodal gap in $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$

$\text{KFe}_2\text{As}_2$, the end member of $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ with $x = 1$, has been considered the strongest candidate for a nodal gap superconductor among the iron-based superconductors [18–21]. However, the optimal doped $(\text{Ba}_{0.6}\text{K}_{0.4})\text{Fe}_2\text{As}_2$ compound is confirmed to have isotropic full s-wave gaps [3]. Therefore, the evolution from a full gap to a nodal gap in the $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$ compound has been of great interest over the years [10–12, 14, 22].
In this section, in order to study the gap evolution in \((\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2\), we introduce the minimal three band model. We added one more hole band \((h2)\) around the \(\Gamma\) point, 
\[
e_{h2}(k) = t^{h2}_1 \cos k_x + \cos k_y) + t^{h2}_2 \cos k_x \cos k_y + t^{h3}_3 \cos 2k_x + \cos 2k_y) + \epsilon_{h2},
\]
to the two band model introduced in the previous section, so that we have two hole bands \(h1\) and \(h2\) and one electron band \(e\). The second hole band \(h2\) is tuned to have a larger FS than the \(h1\) hole band; we used parameters \((0.7, -0.1, 0.3, \epsilon_{h2})\) and varied \(\epsilon_{h2}\). With K doping, the FS sizes of both \(h1\)- and \(h2\)-bands will increase but the FS of the \(e\)-band will decrease and then disappear for \(x > 0.6\)–0.7. The spin fluctuations will also change with K doping; the neutron scattering study of [14] showed that the strong and well defined spin fluctuations continue to exist up to KFe\(_2\)As\(_2\) but develops the incommensurability of \((\pi \pm \delta, \pi \pm \delta)\) with \(\delta \approx 0.32\) while the optimal doped \((\text{Ba}_{0.6}\text{K}_{0.4})\text{Fe}_2\text{As}_2\) has \(\delta \approx 0\). Its overall strength will also change.

However, our intention in this section is to focus on and investigate the correlation between the FS size and the anisotropic or nodal gap evolution in the most clear manner and therefore we ignore the above mentioned changes of the real system except the FS size variation. Further, because we have already shown in the previous section that the main hole band \((h1)\) and the electron band \((e)\)—whether it has a FS or not—maintain the \(\Delta\)-pairing state via the inter-band repulsive interaction, we also fix the FSs of the \(h1\) and \(e\) bands and only vary the FS size of the \(h2\) band. The spin fluctuation interaction \(V_{AFM}(\mathbf{q})\) given by equation (1) is also fixed with \(\kappa = 0.2\pi\) and \(\delta = 0.32\pi\) [15] for all calculations. Therefore, our model calculations in this section should be considered a theoretical experiment designed for revealing the possible role of the FS size of a hole band for developing a nodal gap when all other conditions are fixed.

We have solved the coupled gap equations with three bands, generalizing equations (2) and (3) by adding one more band to them, with the interaction potential \(V_{AFM}(\mathbf{q})\) of equation (1) as inter-band and intra-band interactions among all three bands. We didn’t impose any constraint on the shapes and signs of the gap functions \(\Delta_{h1,h2,e}(k)\) except \(C_{\pi}\) symmetry. In figure 4, we showed the gap solutions for the several different sizes of the \(h2\)-hole pocket. In the left panel, the FSs of three bands are drawn for different values of \(\epsilon_{h2}\) in the folded BZ. In the case of \(e\)-band, a tiny \(e\)-band pocket is drawn only for indication but in real calculations its size was chosen to be zero with \(\epsilon_{e} = 0\). As expected, when the \(h2\)-hole pocket and the \(h1\)-hole pocket have similar sizes as in figure 4(A), the corresponding gap solution shown in the right panel is basically a \(\pm s\)-wave state with some anisotropy. The reason why the \(\Delta_{e2}\) gap has the same sign as the \(\Delta_{e1}\) gap is simply because the average distance between the \(h2\)-FS and the \(e\)-FS is closer to the AFM peak momentum \((\pi \pm \delta, \pi \pm \delta)\) than the distance between the \(h2\)-FS and the \(h1\)-FS to \((\pi \pm \delta, \pi \pm \delta)\). Increasing the \(h2\)-FS size in figure 4(B), these distances become comparable (including the weighting factors of the DOSs, \(N_{h1}, N_{h2}\) and \(N_{e}\)) so that the inter-band interaction from the \(h1\)-band (which tends to develop a \(-\Delta\) gap on the \(h2\)-band) and the inter-band interaction from the \(e\)-band (which tends to develop a \(+\Delta\) gap on the \(h2\)-band) almost cancel each other out on the \(h2\)-FS. As a result, the gap size of \(\Delta_{h2}\) becomes vanishingly small as seen in figure 4(B). Although this happens with a fine tuning of the FS size of the \(h2\)-band in our model calculation, this vanishingly small gap should naturally occur as a horizontally vanishing gap—like a horizontal line node—when the FS size continuously increases along the \(k_{c}\)-direction, as observed in the \(\alpha\)-band of BaFe\(_2\)(As\(_{0.7}\)P\(_{0.3}\))\(_2\) by ARPES measurement [23].

Further increasing the \(h2\)-FS in figure 4(C), both the \(h1\)-band \((+\Delta\) gap) and the \(e\)-band \((\pm\Delta\) gap) exert similar strength but opposite pairing interactions on the \(h2\)-band which do not exactly
Figure 4. (left panel) The FS evolution of the three band model ((A)–(D)); only the \( h_2\)-FS (green line) size varies in the whole calculation. Also the \( e\)-FS (blue line) is shown only for indication and in real calculations it has zero size by choosing \( \epsilon_0 = 0 \). The pink line is the magnetic BZ as a guide for the eyes. (right panel) The corresponding gap solutions \( \Delta_{h1} \) (red line), \( \Delta_{h2} \) (green line), and \( \Delta_e \) (blue line), respectively. The Fermi surface angle is measured from the \( x \)-axis.
cancel out at each point of the $h2$-FS. Therefore the $h2$-band maximizes the condensation energy gain by mixing $-\Delta$ gap and $+\Delta$ gap on the different sections of the $h2$-FS, hence developing accidental nodes but keeping $A_{1g}$ symmetry because of the $C_4$ crystal symmetry. Increasing the $h2$-FS size even further in figure 4(D), the average distance between the $h2$-pocket and the $h1$-pocket increases and therefore the repulsive interaction from the $h1$-pocket also increases, hence $\Delta_{h2}$ develops more negative lobes.

Figure 5 shows the same calculations as in figure 4 but choosing a finite value $\epsilon_b = 0.2 \omega_{AFM}$, hence the electron pockets are completely lifted above the Fermi level. A choice of this value $\epsilon_b = 0.2 \omega_{AFM}$ is to simulate the fully doped KFe$_2$As$_2$. According to Sato et al [5], $\epsilon_b$ of KFe$_2$As$_2$ was roughly estimated to be 2–7 meV, so we assumed it to be $\sim 5$ meV and the spin fluctuation energy scale $\omega_{AFM} \sim 25$ meV. We emphasize that these values are not intended to be precise but only to give some ball-park guideline.

As explained in section 2, the main cause changed by increasing the $\epsilon_b$ value is the reduction of the pair susceptibility of the electron band $\chi_\epsilon (\epsilon_b) \approx \ln \left[ \frac{1.14 \Lambda}{\epsilon_b} \right]$. As a consequence, the effective repulsive interactions exerted from the $e$-band onto the $h1$- and $h2$-pockets become weakened, and the other conditions are almost the same as in figure 4. Therefore, the evolution of the gap solutions from (A) to (D) is qualitatively similar to the case of figure 4 but we notice two quantitative changes: (1) the overall gap sizes ($\Delta_{h1}, \Delta_{h2}$, and $\Delta_e$) are reduced because of the weakened pair susceptibility $\chi_\epsilon (\epsilon_b)$; (2) the negative portion of the $\Delta_{h2}$ gap function relatively increases again because the effective repulsion from the electron band—which itself forms a negative sign gap ($\Delta_e < 0$)—becomes weakened. For example, comparing figure 4(B) and figure 5(B), a tiny positive $\Delta_{h2}$ in figure 4(B) becomes a nodal gap $\Delta_{h2}$ with a mixture of tiny positive and negative portions in figure 5(B). Similarly, the magnitudes—relative magnitudes to the average gap size of each case—of the negative lobes of $\Delta_{h2}$ in figures 5(C) and (D) become bigger than the ones in figures 4(C) and (D), respectively.

In our simple model, the pairing interaction equation (1) is oversimplified and even orbital degrees of freedom is completely ignored, therefore our gap solution results cannot be quantitatively compared to the real compounds. However, this dramatic gap evolution with only a small variation of the FS size demonstrates that the subtle balance of the inter-band repulsive interactions between bands can be the crucial mechanism for developing and stabilizing the nodal gap solution. In this regard, the most important role is still played by the hidden electron band. Although its FS disappears, the $e$-band develops the largest gap $\Delta_e$ (see the right panel in figure 4)—which is the inevitable consequence of the interband paring mechanism ($\Delta_e N_e \approx \Delta N_e$) [8]—and therefore this hidden $e$-band, although lifted above the Fermi level, continues to play the important role of balancing the overall $\Delta_e$ gap state and inducing a nodal gap on the $h2$-band with a larger FS. Finally, if we consider that the $h2$-pocket in our model corresponds to the outer or middle hole pocket of (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$, the overall gap anisotropy of $\Delta_{h2}$ and its systematic development of the nodal gap structure is surprisingly similar to the recent ARPES measurements on (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ with K doping.

The intra-band repulsive interaction $V_{i2,i2}(q)$ also contributes but it mainly shifts the balance in the parameter space. When the $h2$-FS size becomes very large, the intra-band interaction $V_{i2,i2}(q)$ itself tends to drive a $d$-wave nodal gap rather than the $A_{1g}$-nodal gap as found here.
Figure 5. The same calculations as in figure 4, except choosing $\epsilon_0 = 0.2\omega_{AFM}$. Hence the electron band is lifted above the Fermi level by $0.2\omega_{AFM}$ and the electron pockets have completely vanished in the left panel. Notice, however, that the electron band still forms a gap solution $\Delta_e$ as shown in the left panel.
by Shin and coworkers [14, 24]. As has been repeatedly stated, quantitative comparisons such as the magnitude of the gap sizes with doping etc should not be done using our model calculations.

5. Conclusion

We showed that the absence of a FS does not prohibit FS instability of the SC transition in the multi-band model mediated by inter-band pairing interaction. Although we used a simplified model calculation ignoring realistic details, it is a proof of principle. Applying this pairing mechanism with a missing FS to the two band model where the electron band is lifted up by $e_b$ above the Fermi level, we also showed that the $T_c$ evolution vs. $e_b$ qualitatively captures the experimental $T_c$ evolution of (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ with K doping. As proof that our scenario forms the SC gap in the hidden electron band, we predicted the shadow gap features using both ARPES and tunneling measurements, which can be easily tested experimentally. Finally, we demonstrated that the presence of the hidden electron band plays a crucial role in developing a nodal gap on the larger hole pocket ($h2$) in the three band pairing model. This result might contribute to the understanding of nodal gap development in (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ [14, 24] as well as BaFe$_2$(As$_{0.7}$P$_{0.3}$)$_2$ [23] compounds.

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