Nesting between hole and electron pockets in Ba(Fe_{1−x}Co_{x})_{2}As_{2} (x=0−0.3) observed with angle-resolved photoemission

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We present a comprehensive angle-resolved photoemission study of the three-dimensional electronic structure of Ba(Fe_{1−x}Co_{x})_{2}As_{2}. The wide range of dopings covered by this study, x=0 to x=0.3, allows to extract systematic features of the electronic structure. We show that there are three different hole pockets around the Γ point: the two inner ones being nearly degenerate and rather two-dimensional, the outer one presenting a strong three-dimensional character. The structure of the electron pockets is clarified by studying high doping contents, where they are enlarged. They are found to be essentially circular and two-dimensional. From the size of the pockets, we deduce the number of holes and electrons present at the various dopings. We find that the net number of carriers is in good agreement with the bulk stoichiometry but that the number of each species (holes and electrons) is smaller than predicted by theory. Finally, we discuss the quality of nesting in the different regions of the phase diagram. The presence of the third hole pocket significantly weakens the nesting at x=0, so that it may not be a crucial ingredient in the formation of the spin-density wave. On the other hand, superconductivity seems to be favored by the coexistence of two-dimensional hole and electron pockets of similar sizes.

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I. INTRODUCTION

The newly discovered iron pnictides superconductors, 1, 2 are characterized by small hole and electron pockets, containing few carriers. 3, 4 This semimetallic band structure is rather unusual and contrasts with that of many correlated systems, where exotic properties are mostly found near half-filling of the bands. Many of the different properties observed in the iron pnictides family are thought to depend crucially on the interactions between these pockets. 3–5 For the magnetic phases (x<0.07 and low dopings, see phase diagram on Fig. 7), the good nesting between hole and electron pockets should stabilize the spin-density-wave ground state. For the superconducting phases, a nonconventional mechanism based on the exchange of spin fluctuations, with an order parameter changing sign between the hole and electron pockets has been put forward. 4 Angle-resolved photoemission spectroscopy is the best suited tool to observe the shape and size of the different pockets and how they evolve with doping, thanks to its unique ability to map the electronic structure in the reciprocal space. This is an exciting challenge that has triggered a tremendous activity in the past year. 6–22

It was soon confirmed that the electronic structure is made out of hole pockets at the Γ point and electron pockets at the Brillouin-zone (BZ) corners, as predicted from band-structure calculations. This was shown for the so-called 1111 family, in LaFeOP (Ref. 9) and NdFeAsO_{1−x}F_{x} 11 and, much more extensively due to the higher sample quality, for the 122 family, AFe_{2}As_{2} (A=Ba, Sr, Ca). In this family, the size of these pockets was found to change with hole 12 or electron 19 doping, confirming one can transfer rather simply electron and holes to the Fe bands. For the hole-doped family Ba_{1−x}K_{x}Fe_{2}As_{2}, two different hole pockets were clearly resolved. They exhibit different superconducting gaps, evidencing that these bands may have different roles in the electronic properties. 7 However, there are still missing pieces of the puzzle to establish a global view of the electronic structure of these systems. In particular, the number of hole pockets, their degeneracy, the shape of the electron pockets, the two-dimensional (2D) or three-dimensional (3D) character of the different bands are not totally clarified. This task is actually not trivial, as the bands often overlap and may be difficult to resolve. In this paper, we establish these facts as clearly as possible for the electron-doped family Ba(Fe_{1−x}Co_{x})_{2}As_{2}. Our aim is to discuss the quality of nesting between the different pockets as a function of x and compare this to the evolution of electronic properties in the phase diagram.

Ba(Fe_{1−x}Co_{x})_{2}As_{2} has not yet been as extensively studied as Ba_{1−x}K_{x}Fe_{2}As_{2}. Sekiba et al. 19 reported Fermi surface (FS) for x=0.15 and Terashima et al. 20 reported the opening of a superconducting gap for x=0.075. Vilmercati et al. showed that the hole pocket at x=0.1 exhibits strong photon energy dependence. 21 Such a photon energy dependence is suggestive of 3D effects, as an angle-resolved photoemission spectroscopy (ARPES) experiment at a fixed photon energy maps the electronic structure at one particular k_{F} value. 22 If there is significant dispersion as a function of k_{F} (i.e., perpendicular to the FeAs slab), measurements at different photon energies map inequivalent sections of the electronic structure and it will be necessary to study this dependence to get a correct three-dimensional map of the pockets. We find that it is indeed the case here and report detailed measurements for a wide range of photon energies (20–100 eV) and dopings: x=0 (T_{SDW}=139 K), x=0.045 (T_{SDW}=63 K), T_{c}
When the five bands are included, there is significant rehybridization between all of them. The electron pockets, for example, acquire significant $d_{xz}$ character and a slightly more oval shape. More strikingly, bands of mainly $d_{xy}$ or $d_{yz}$ symmetry are found very near the Fermi level and may even form an additional hole pocket (sketched in blue on Fig. 1). This disrupts the symmetry between the hole and electron pockets and therefore destroys the perfect nesting for the undoped system. Moreover, this pocket appears extremely sensitive to the structure of the FeAs slab, particularly the As height, and can be more 2D or 3D depending on its character. It also seems to be different in the 1111 or 122 families. Nekrasov et al. predicted it to be smaller than the other 2D hole pockets in LaFeAsO and larger in BaFe$_2$As$_2$. Other studies predict it to be already filled in BaFe$_2$As$_2$. It is then an important parameter of the electronic structure that is difficult to predict theoretically and should be determined experimentally.

Two different BZ can be considered, the “unfolded BZ” based on the Fe square (1 Fe/BZ) or the “folded BZ” based on the true structural unit cell (2Fe/BZ). The structural unit cell is twice as large as the Fe square to account for the inequivalent positions of the As above or below the Fe plane (see Fig. 1). In this paper, we quote all results in the folded BZ. The electronic structure in the folded BZ can essentially be obtained by folding all bands with respect to the new BZ boundaries [Fig. 1(b)]. One ends up with three hole pockets at the $\Gamma$ point and two electron pockets at the BZ corners. One can expect the two bands arising from the folding to be nearly degenerate and mostly 2D, while the third hole pocket may be more 3D.

Single crystals were grown using a FeAs and CoAs self-flux method. Chemical analyses were performed with an electron probe (Cameca SX50) on several crystals for each Co doping (yielding the Co content within 0.5% absolute accuracy). All experiments were carried out at the CASSIOPEE beamline from the SOLEIL synchrotron, with a Scienta-R4000 analyser, an angular resolution of 0.2°, and an energy resolution better than 15 meV. Samples were cleaved in ultra-high vacuum (better than $4.1 \times 10^{-10}$ mbar), which exposes flat and shiny surfaces.

II. 3D STRUCTURE OF THE HOLE POCKETS

Figure 2 presents the hole band structure for different $x$ values at 35 eV (left) and 45 eV (right). The data were taken at 30 K, hence, in the SDW state for $x=0$ and $x=0.045$. However, we do not consider here the changes associated to the SDW, which will be briefly discussed in Sec. V. Surprisingly, the band structure appears extremely different at the two photon energies, which is very unusual, and this has to be understood before anything can be said on the band structure. One would, for example, conclude that the hole pocket is already almost filled at $x=0$ looking at the 45 eV data, and that it is not yet filled at $x=0.15$, looking at the 35 eV data.

At 35 eV, two bands are clearly distinguished, forming two hole pockets with distinct Fermi velocities and Fermi crossings. Their dispersion is sketched by red and blue lines, for bands called hereafter A and B, respectively. These two
NESTING BETWEEN HOLE AND ELECTRON POCKETS IN…

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**FIG. 2.** (Color online) Near $E_F$ electronic structure around the $\Gamma$ point for the indicated dopings, measured at 35 eV (left) or 45 eV (right) photon energy and a temperature of 30 K. On the left part, lines sketch the dispersion of inner band A (red) and outer band B (blue). On the right part, black line is a sketch for a cosine dispersion for the two merged bands A+B (see text).

In sharp contrast, only one band is apparently observed at 45 eV, with a more rounded shape. At $x=0$, it barely touches the Fermi level and sinks below it for higher $x$. Here again, the shape is roughly similar for all $x$. We describe it by a cosine function $E = 0.18 \cos(k^*a)$, and shift it by 0.1 eV between $x=0$ and $x=0.3$.

There are a priori two possible ways to explain the difference between 35 and 45 eV. The first one is that the intensity of band B is strongly suppressed at 45 eV by matrix-element effects, so that it becomes undetectable and that band A dominates the spectrum. Note, however, that the dispersion at 45 eV is already quite different from that of band A at 35 eV (especially, the region at $k=0$ appears filled). The second one is to assume that the two bands have shifted with photon energy and have merged together at 45 eV. This is possible if there is significant dispersion of the electronic structure perpendicularly to the surface, as different photon energies correspond to cuts of the electronic structure at different $k_z$ values. These two possibilities would have very different implications for the understanding of the electronic structure. For example, the number of holes contained in these pockets would be quite different. They can be distinguished by observing these dispersions over a large photon energy window. If this behavior is related to perpendicular dispersion, it should display oscillations with a well-defined periodicity related to $k_z$, whereas no such periodicity is automatically expected for matrix-element effects. In Fig. 3, the $k_F$ positions as a function of photon energy are shown for $x=0.08$ and $x=0.15$. They were extracted by linear fits, similar to those of Fig. 2. They indeed display well-defined oscillations as a function of the photon energy. This periodicity matches very well that expected for $k_z$. This was recognized before, but the inner structure of A and B bands was not resolved. In BaFe$_2$As$_2$, there are two FeAs slabs per unit cell, so that the distance between two slabs is $c^*/c=2=6.5$ Å and the periodicity expected for the perpendicular dispersion is $2\pi/c^*$. At the $\Gamma$ point, the value of $k_z$ can be estimated by

$$k_z = 0.512 \frac{h\nu - W + V_0}{c^*},$$

where $h\nu$ is the photon energy, $W$ is the work function of the material ($W \sim 4.4$ eV), and $V_0$ is an inner potential. It is usually on the order of 10 eV but is in practice adjusted to get a reasonable agreement with the data. Using $V_0=14$ eV, we obtain $k_z=1$ for the maxima of $k_F$ at 34 eV (7$/pi/c^*$), 62 eV (9$/pi/c^*$), and 98 eV (11$/pi/c^*$) and $k_z=0$ for the minima at 22 eV (8$/pi/c^*$), 48 eV (8$/pi/c^*$), and 79 eV (10$/pi/c^*$). This describes very well the experimental minima and maxima, which supports this interpretation.

The 3D behavior is the same in all the samples we have investigated. Recently, Liu et al. claimed that the 3D structure was characteristic of the orthorhombic (magnetic) phase of BaFe$_2$As$_2$ and disappeared at high temperature in the tetragonal phase. At the various dopings studied here, the structure changes from orthorhombic to tetragonal, and the properties from magnetic to superconducting to simply metallic, so that if there is a change in dimensionality as a function of temperature, it is not likely associated to structural or magnetic transitions.

A more detailed variation of $k_F$ with $k_z$ is shown in Fig. 4 for $x=0.045$. Panel (a) shows the positions of the two bands extracted by linear fits as a function of $k_z$, while panel (b) directly images the shrinking of the cylinders as a function of

![Image](https://example.com/figure3.png)

**FIG. 3.** (Color online) (a) Fermi surface measured at 35 eV and 30 K, for $x=0.08$. Red points and blue diamonds indicate Fermi-level crossings for A and B bands, respectively, and the circles, the corresponding FS. (b) Fermi wave vector for the two bands as a function of photon energy for $x=0.08$ and $x=0.15$. Vertical dotted line shows positions corresponding to $k_z=1$. Solid lines are guides for the eyes.
We find that this evolution can be best described by a shift of B toward A from \( k_z = 1 \) to \( k_z = 0 \), although the overlap between bands A and B does not allow to definitely rule out that B could mainly lose weight toward \( k_z = 0 \). Assuming the shift of B, we obtain a moderate increase of \( k_F \) from \( k_z = 0 \) to \( k_z = 0.6 \), followed by a steep increase for band B toward \( k_z = 1 \) [see Fig. 4]. This shows that the band B has a more pronounced 3D character than A. At low \( k_z \), it is difficult to determine whether both bands move to lower \( k_F \) or only one. From the qualitative arguments presented in the introduction, it is tempting to associate this more 3D band with the third hole pocket and, consequently, the band A with the two folded 2D pockets.

Band-structure calculations for BaFe\(_2\)As\(_2\) further support this assignment.\(^{4,30}\) In Ref. 30, two nearly circular hole pockets are indeed found nearly degenerate around the \( \Gamma \) point, with modest \( k_z \) dispersion, while a third hole pocket, also circular, is much more 3D. It is nearly degenerate with the first two pockets at \( k_z = 0 \), but increases abruptly near \( k_z = 1 \).

This behavior corresponds qualitatively very well to that of \( k_z \) toward A from \( k_z = 1 \) to \( k_z = 0 \), although the overlap between bands A and B does not allow to definitely rule out that B could mainly lose weight toward \( k_z = 0 \). Assuming the shift of B, we obtain a moderate increase of \( k_F \) from \( k_z = 0 \) to \( k_z = 0.6 \), followed by a steep increase for band B toward \( k_z = 1 \) [see Fig. 4]. This shows that the band B has a more pronounced 3D character than A. At low \( k_z \), it is difficult to determine whether both bands move to lower \( k_F \) or only one. From the qualitative arguments presented in the introduction, it is tempting to associate this more 3D band with the third hole pocket and, consequently, the band A with the two folded 2D pockets.

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III. SHAPE OF THE ELECTRON POCKETS

The case of electron pockets is more simple because, as we will show, the effect of \( k_z \) dispersion is nearly negligible. On the other hand, their shape is more complicated and has been the subject of some debate. At low dopings, Zabolotnyy et al. measured a “propellerlike structure” for these pockets, with sharp “blades” oriented along the BZ diagonals.\(^{15}\) They argued that this was due to a large reconstruction of these pockets due to a \( \alpha(\pi/2, \pi/2) \) interaction with the hole pockets. On the contrary, Yi et al. argued that the complicated structure can be understood from the interactions between four bands present in the LDA near the Fermi level.\(^{10}\) Figure 5 shows that the shape simplifies when the band fills up and the Fermi level moves away from the bottom of the band. At \( x=0.08 \), the electron parabola is still very shallow and emerges from a high intensity background only in a 40 meV window below \( E_F \), while at \( x=0.3 \), it becomes very clear over 150 meV. Note that this doping is much higher than the highest doping previously studied \([x=0.15 \ (Ref. \ 19)] \), which is very helpful to determine the trend in \( k_F \) variations (Fig. 7). The Fermi velocity changes from \( V_F = 0.38 \) eV Å at \( x=0.08 \) to \( V_F = 0.76 \) eV Å at \( x=0.3 \). This can be simply understood by a shift of \( E_F \) near the bottom of the band. Both values correspond to about the same effective mass \( m^* = 3.5 m_e \) (\( m_e \) is the mass of the electron). We have quoted similar values of \( V_F \) and \( k_F \) for the hole pockets in Sec. II, so that \( m^* \) is comprised between \( 2 m_e \) and \( 4 m_e \), depending on the doping, the band A or B, and \( k_z \).

The FSS shown in Figs. 5 are clearly defined, with simple shapes, quite similar at the two dopings (this is identical at \( x=0.15 \), not shown). They can be reasonably well described by circles, although some segments appear more straight, especially at \( x=0.08 \). We always observe a higher intensity on the sides of the circle away from the diagonal direction. This is probably due to the fact that these sides have, respec-
tively, $d_{xz}$ or $d_{yz}$ symmetry and, consequently, obey different matrix-element effects. The strong dependence of these pockets on the polarization was already noted before and is an additional complication to determine the true shape of the electronic pockets.

Figure 6 shows that we do not observe strong changes of $k_F$ as a function of photon energy. This confirms the 2D character of these bands, similar to that of the hole A bands. We do observe variation in intensity and peak width as a function of photon energy, which may be due to an internal structure of the pockets, with two bands that are not exactly degenerate at all $k_F$. As an example, Fig. 6 shows spectra near the Fermi level at two different photon energies. At 92 eV, the peaks are very sharp, with $0.08 \pi/a$ half width at half maximum (HWHM), and centered at $0.43 \pi/a$. They broaden at 55 eV but can be well fitted by two peaks of $0.08 \pi/a$ HWHM, positioned at $x=0.35 \pi/a$ and $0.5 \pi/a$. In band calculations, the two electron pockets are degenerate and nearly circular for $k_F=0.5$ but become more oval and less degenerate toward $k_F=0$ and 1. This would explain these variations quite well. Previous studies at $x=0.15$ (Ref. 19) and $x=0.06$ (Ref. 10) attempted fits with two different oval shapes. This would also be possible with these data but seems to us beyond experimental accuracy. Even though such variations of $k_F$ are not negligible, they do not affect much the average area of the pockets, which is the main quantity we want to determine, so that we neglect them in the following.

IV. EVOLUTION WITH DOPING OF $k_F$ AND OF THE NUMBER OF HOLES AND ELECTRONS

Finally, Fig. 7 summarizes the evolution of $k_F$ as a function of doping. For the hole pockets, maximum values of $k_F$ are reported (i.e., those for $k_F=1$). We add results for magnetic phases ($x=0$ and 0.045), although we do not address the details of the reconstruction of the electronic structure in the magnetic phase in this paper. For the hole pockets, we use low-temperature data (20 K) to be able to resolve the two different bands but fit the dispersions to linear models, ignoring possible gaps (see Fig. 2). For the electron pockets, we use data taken at temperatures above the magnetic transition to avoid this problem. For low dopings, $k_F$ for the electron pockets is just indicative, as their shape may differ significantly from a circle.

We first note that $k_F$ varies almost linearly with doping. The slopes are quite similar for the hole and electron bands, reflecting that the properties of the two types of carriers are not very different. We are not in a situation of heavy holes and light electrons (or the inverse), except, possibly, at some singular points of $k_z$ and dopings. We add in Fig. 7 two points measured by Ref. 6, corresponding to hole-doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$, with $x=0.2$ (0.1 holes/Fe) and $x=0.4$ (0.2 holes/Fe). They extrapolate quite well with $k_F$ determined for the electron-doped side, which strongly suggests to identify the so-called $\alpha$ and $\beta$ hole pockets with our A and B pockets. In Sec. II, we argued that the A sheet is probably doubly degenerate and the B sheet singly degenerate because of its more 3D character. Xu et al. also concluded that the inner $\alpha$ sheet must be doubly degenerate and the outer $\beta$ sheet singly degenerate to satisfy the Luttinger theorem. This correspondence further supports these assignments. No $k_F$ dependence was ever reported for the $\beta$ band, in contrast with the B band, but it may indeed be more 2D in the K case.

To be more quantitative, it is instructive to estimate the number of carriers in the different pockets, as we propose in Fig. 8. In a 2D system, the Luttinger theorem states that the number of carriers contained in one pocket is proportional to its area compared to that of the BZ, even in the presence of strong correlations. The BZ is here approximately a square of side $2\pi/a$ with $a=3.96$ Å in the tetragonal phase of BaFe$_2$As$_2$. This does not change much with Co doping. It contains two holes (or two electrons) and two Fe, hence, 1 carrier per Fe. A pocket of area $S$ then contains $S/S_{BZ}$ carriers per Fe in this 2D analysis. In a 3D system, the number of carriers should be integrated over the entire volume, which is possible knowing the evolution of $k_F$ with $k_z$, as determined in Fig. 4 for the hole pockets.

For the electron pockets, we compute the number of electrons $n_{el}$ by assuming two nearly degenerate 2D and circular
pockets, yielding $n_{\text{el}} = \pi k_F^2 / 2$. We caution that at low dopings, deviation from a circular shape may be important. The simplest case is that of high Co doping, when the hole pocket is completely filled. In this case, the electron pocket should contain all electrons brought by Co. This is in good agreement with the value $n_{\text{el}} = 0.29$ that we measure at $x = 0.3$. This number decreases with decreasing percentage of Co. However, it seems to converge to a lower value than the 0.15 electrons/Fe predicted by Ref. 25 at $x = 0$ and also shown in Fig. 8. Interestingly, a very similar evolution of the number of electrons with Co doping was deduced from Hall measurements (Ref. 24). Hatched areas indicate likely values for the number of holes and electrons, including possible experimental errors. Thick solid lines are prediction for the evolution of number of holes and electrons reproduced from Ref. 25.

For the hole pockets, the general trend of Fig. 7 extrapolates to $k_F^A = 0.14 \pi / a$ and $k_F^B = 0.28 \pi / a$ at $x = 0$ and $k_F = 1$. This is significantly smaller than in the calculation of Ref. 30, where $k_F^A = 0.2 \pi / a$ and $k_F^B = 0.5 \pi / a$ at $k_F = 1$. Consequently, our measurement also correspond to a smaller number of holes at $x = 0$ than predicted theoretically. This confirms the tendency obtained for electrons, which is self-consistent, as charge neutrality requires $n_{\text{el}}(0) = n_{\text{el}}(0)$. The $k_F$ values at $k_F = 1$ correspond to $\sim 0.015$ holes/Fe in one band A and $\sim 0.06$ holes/Fe in band B, adding to a total of 0.09 holes/Fe, assuming double degeneracy of A. This should be taken as a maximum estimate for the number of holes since the holes cylinders in fact shrink at lower $k_x$ values, especially for B. Integrating these numbers over $k_x$ with the dependence determined on Fig. 4, reduces these numbers to 65% for band A ($\sim 0.01$ holes/Fe) and 25% for band B ($\sim 0.015$ holes/Fe). Note that almost half of the holes are contained in band B, meaning both bands are equally important to consider. The total number of holes is very small $[n_{\text{el}}(0) = 0.035$ with this estimation] and this might mean that the integration on $k_x$ underestimate this number (with these small $k_F$ values, small changes will affect significantly the results). In Fig. 8, we report both the maximum and integrated values, for the different dopings. Comparison with the electron case indicates $n = 0.06 \pm 0.02$ as a likely value for the number of carriers at $x = 0$. A similar shrinking of hole and electron pockets compared with band theory was also observed by de Haas–van Alphen experiments in the non-magnetic LaFeAsO (Ref. 33) and appears therefore as a common feature of pnictide that we will discuss in conclusion.

V. DISCUSSION OF THE NESTING

One major interest of such a study is to estimate the degree of nesting between the different pockets. As the pockets are roughly circular, they will exhibit good nesting at the wave vector $(\pi / a, \pi / a)$, if they have similar $k_F$. It is immediately clear from Fig. 7 that a good nesting on the electron-doped side will only be found between electron pockets and the B hole pocket in the region $x < 0.07$. As this is indeed the region where the SDW is observed, one could conclude that this supports the role of nesting in driving this instability. However, it seems quite counterintuitive that the 3D pocket alone contributes to the nesting. Also, the good nesting would exist only in a limited $k_x$ range, due to the strong dispersion of this band. The nesting appears therefore much worse than in the initial naive two-band model, in the absence of the 3D pocket. It is also interesting to keep in mind that this third hole pocket seems quite different in other iron pnictides, although the SDW transition temperature is quite similar. $k_F$ can be as large as 0.8 $\pi / a$ for LaFeAsO (Ref. 9) or 0.5 $\pi / a$ for NdFeAsO$_2$ (Ref. 11), so that it is unlikely that the SDW critically depends on how it is nested with the electron pocket. Note that this very large pocket has sometimes been assigned to surface effects (Ref. 33) but that the 3D effects we probe are incompatible with surface effects.

Such a simple view of FS nesting is however probably not very relevant to describe such phases. Johannes and Mazin showed that the reconstruction of the electronic structure in the magnetic phase extends over almost the entire bandwidth and not just in a small energy window below $E_F$. Such changes cannot be captured by simple nesting arguments. Indeed, there is no obvious gap opening detected by ARPES at the magnetic transition, as would be expected for a simple SDW, at least not for the A bands (see Fig. 2). One rather observes a splitting of the electrons and holes bands and new bands folded with $(\pi / a, \pi / a)$ periodicity, testifying for the new antiferromagnetic (AF) BZ boundaries (see Fig. 1). This behavior can also be observed at $x = 0$ in Fig. 2, where a weak electronlike band, shown as a white dotted line, becomes visible at the $\Gamma$ point. It is much larger than in the nonmagnetic phase ($k_F = 0.4 \pi / a$) due to the splitting, and interacts with both hole bands when they cross.
Although this does not result in a straightforward gap at the Fermi level. As a result, the magnetic phase is characterized by a complicated pattern of residual metallic pockets. The origin of the splitting has been discussed in terms of exchange splitting\textsuperscript{17} or anisotropic gaps in different domains\textsuperscript{18} and is not yet fully clarified, in our opinion. A better observation of the location and sizes of the magnetic gaps would be needed to fully understand the reconstruction of the electronic structure in the magnetic phase.

It is also interesting to compare the relative sizes of the pockets in the superconducting phase, as interband transitions are supposed to play an active role in superconductivity.\textsuperscript{3} Figure 8 immediately suggests that the disappearance of superconductivity on the electron-doped side coincides with the filling of the hole bands. This was indeed suggested in Ref. 20. More precisely, we have shown in Fig. 3 that the pocket is not yet totally filled but exists only at particular \( k_z \) values. As it seems very convincing, it is interesting to note that the symmetric behavior on the hole-doped size is not as obvious. There is a very clear asymmetry of \( T_c \) on the hole and electron sides. \( T_c \) is higher with K doping \( (T_{c,\text{max}}=38 \, \text{K}) \) than Co doping \( (T_{c,\text{max}}=24 \, \text{K}) \) and also extends on a much wider doping range (up to 0.5 holes/Fe with K doping). If superconductivity also disappears when the two carriers cease to coexist, this means that the electron pocket survives up to \( x=0.5 \), a much higher doping than on the electron-doped side. This may be possible, if they survive as "blades\textsuperscript{19,20}" containing very few electrons, but still supporting superconductivity. A detailed investigation is likely to reveal interesting aspects on essential ingredients for superconductivity in these systems.

A big difference between the hole and electron sides is that the electron pocket is of the same size as the inner pocket for hole doping and as the outer pocket for electron doping. As the degeneracy and dimensionality of the inner and outer pockets are not the same, this is quite a different situation. On the hole-doped side, the superconducting gap was found similar on the two pockets of similar size (electron and hole A pockets) but smaller on the B pocket.\textsuperscript{7} This agrees very well with the idea that superconductivity is stabilized by interband transitions. Following these ideas, one would expect it to be destabilized on the electron-doped case, when the pocket sizes are more different, which might indeed be the reason for the lower \( T_c \). At \( x=0.075 \), Terashima et al.\textsuperscript{20} reported a superconducting gap stronger on the hole B pocket than on the electron pocket. They assumed that the hole A band was already filled. We show here that it is not the case and a complete investigation of the different gaps as a function of \( k_z \) could reveal interesting aspects of the role of 3D effects and FS nesting in the superconducting properties.

VI. CONCLUSION

Our investigation clarifies the internal structure of the hole and electron pockets in Ba\textsubscript{1−}\( x \)Co\textsubscript{1−}\( x \)Fe\textsubscript{2}As\textsubscript{2}. This study is complicated by the overlap between the different bands and strong polarization and photon energy dependence. Disentangling these different effects is however a prerequisite for an insightful study of the evolution of the electronic structure in the magnetic and superconducting states. The way each band participates in these transitions is indeed a key to understand the nature of the ground states. Our study identifies three different hole pockets, the outer one exhibiting strong photon energy dependence. We attribute this to a stronger 3D character of this band, in good agreement with band calculations. We caution that a further study of matrix-element effects is required to definitely establish this fact. At large electron doping, we observe 2D electron pockets, with rather circular shapes. The continuity of these structures with the hole-doped side (in Ba\textsubscript{1−}\( x \)K\textsubscript{1−}\( x \)Fe\textsubscript{2}As\textsubscript{2}) suggests a unified structure, where the third hole pocket always play an important role and the electron pocket survives deep in the hole-doped side because of an increasingly anisotropic shape.

Figures 7 and 8 summarize the results of this study. The nesting between hole and electron pockets is not as strong as usually expected, even at \( x=0 \), and especially when 3D effects are taken into account. On the other hand, the presence of hole and electron pockets seems crucial to stabilize superconductivity. It disappears when the hole pockets are nearly filled and the different \( T_c \) on the hole-doped and electron-doped sides may be related to the quite different relative sizes of the pockets. Our study suggests directions to investigate in order to better understand the role of the coupling between hole and electron pockets in superconductivity. It would, for example, be interesting to compare the size of the third hole pocket, which effectively controls the mismatch between the 2D hole and electron pockets, with the maximum \( T_c \) value in the 1111 family, which strongly varies from \( T_c=26 \, \text{K} \) with La to \( T_c=52 \, \text{K} \) with Sm.

The total number of carriers is found in good agreement with the overall bulk stoichiometry. This gives confidence that the measured electronic structure is that of the bulk. On the other hand, we find a number of carriers of each species at \( x=0 \) that is smaller by about a factor of 2 than predicted theoretically.\textsuperscript{25} This tendency was already suggested to interpret transport data in Ba\textsubscript{1−}\( x \)Co\textsubscript{1−}\( x \)Fe\textsubscript{2}As\textsubscript{2} (Ref. 24) or de Haas–van Alphen oscillations in the nonmagnetic LaFeOP,\textsuperscript{33} so that it is probably an intrinsic feature of these systems. It implies shifts of the electronic bands compared to the LDA, not a simple renormalization. The presence of a third hole pocket in most of the phase diagram promoted by our analysis also implies similar shifts to be consistent with some of these calculations. This is a consequence of the multiorbital character of these compounds, which is one of their originality. It may play an important role in the electronic properties but is often neglected in minimal modeling of these compounds. The origin of these shifts involves fine tuning of structural parameters and interorbital correlations. Ortenzi et al.\textsuperscript{35} suggested that the shrinking of the pockets could be attributed to strong interband scattering\textsuperscript{35} and therefore reveals important feature of the physics of these materials.

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