Mobility spectrum analytical approach for intrinsic band picture of Ba(FeAs)$_2$

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Abstract

Unconventional high temperature superconductivity as well as three-dimensional bulk Dirac cone quantum states arising from the unique d-orbital topology have comprised an intriguing research area in physics. Here we apply a special analytical approach using a mobility spectrum, in which the carrier number is conveniently described as a function of mobility without any hypothesis, both on the types and the numbers of carriers, for the interpretations of longitudinal and transverse electric transport of high quality single crystal Ba(FeAs)$_2$ in a wide range of magnetic fields. We show that the majority carriers are accommodated in large parabolic hole and electron pockets with very different topology as well as remarkably different mobility spectra, whereas the minority carriers reside in Dirac quantum states with the largest mobility as high as 70,000 cm$^2$(Vs)$^{-1}$. The deduced mobility spectra are discussed and compared to the reported sophisticated first principle band calculations.

Keywords: iron pnictide superconductors, Fermi surface, magnetotransport
1. Introduction

Rich physics in the transport properties of iron pnictide (FePn) materials is the consequence of the complex d-orbital energy bands with unique topology \[1, 2\], and the unconventional high temperature superconductivity \[3\] and the intriguing quantum transport phenomena resulting from Dirac cones forming via spin density wave (SDW) band folding \[4–9\] have been reported so far. Despite various experimental observations as well as theoretical calculations, debate continues in understanding the real band picture of FePns. There are many experimental challenges in differentiating various bands in this complex multiple band system of the materials, in which both electrons and holes with a wide range of relaxation times are present at various points of the Fermi surface in momentum space. In addition, the existence of Dirac-like quantum states that have an extremely small number of carriers with short-circuit cyclotron motions but markedly high mobilities makes the story more complex.

The first experimental observations of the Dirac-cone states were successfully made by angle-resolved photoemission spectroscopy measurements (ARPES) \[10\] just after the theoretical implications \[1\]. However, the complete picture on this complex multiple band energetics has yet been fully elucidated, because the energy scale of the Dirac-cone is not sufficiently large and the information of the different $k_z$ dependencies is not feasible to access in high enough accuracy for ARPES observations. Generally quantum oscillations have become very useful in examining the electronic states at the Fermi level. Unfortunately, however, they are not sufficiently sensitive to detect tiny pockets of holes and electrons of the Dirac cone quantum states. Electrical transport of both longitudinal and transverse directions in a wide-range of temperature and magnetic fields ($B$) in principle contains rich information and provides versatile experimental information for understanding the real multiple band nature as a sum of various electron and hole pockets. In order to deduce the important band picture from experimental electric-transport observations, however, one generally needs to hypothesize a large number of parameters, such as the number of carrier types, in order to analyze the experimental data in question. This becomes the essential problem when the electric transport parameters are determined from the limited experimental information available in a multi-carrier system.

In this paper, we apply the technique of mobility ($\mu$) spectrum analysis to the longitudinal and transverse transport of Ba(FeAs)$_2$ (structure shown in the inset of figure 1), an important parent compound in an FePn system, under a wide range of $B$ up to 50 $T$ in a facility of high magnetic fields. This \textit{ab initio} analysis, originally developed for semiconductor physics, is applicable to transport data of a high quality Ba(FeAs)$_2$ (ratio-of-residual-resistance $RRR = R(300 K)/R(2 K) \approx 25$) and gives a physically reasonable and intrinsic interpretation on the electronic states of the low temperature phase without any assumptions on the number of carrier types. We describe how effectively this special approach can clarify the intrinsic multiple band nature, including Dirac cones and other parabolic pockets, without making any special assumptions. There is a sharp contrast between the electron and the hole regions. The conclusion is discussed by referring to theoretical calculations; the importance of the anisotropic band picture in Ba(FeAs)$_2$ which shows a projected unique negative curvature existing in the Fermi surface, is exaggerated.
2. Experiments and results

High quality single crystals of Ba(FeAs)\textsubscript{2} were synthesized using a modified self-flux method described in detail in a recent literature \cite{11}. In this synthesis technique, a temperature gradient is employed to separate the grown crystals from the employed FeAs flux in place of the usual decanting process in order to avoid possible thermal shocks. As-grown crystals were annealed for 3.5 days in BaAs atmosphere to annihilate the effects of vacancies and the microscopic strain on the electric transport properties \cite{12}. After annealing, the quality of the crystal was greatly improved. As shown in figure 1, RRR = \( R(300\, \text{K})/R(2\, \text{K}) \), increased from 3.5 in the as-grown samples to nearly 25 in the annealed samples. The high value of RRR guarantees the quality of the annealed crystals used in the subsequent magnetotransport measurements. The magnetoresistance (MR) and Hall resistance were measured using a Quantum Design Physical Properties Measurement System (PPMS) up to magnetic field \( B < 9\, \text{T} \). More importantly, in order to clearly observe the transport properties of the entire Fermi pocket, the measurements were carried out under \( B \) up to 50\,T with the help of the pulsed magnet at the Center for Advanced High Magnetic Field Science, Osaka University.

Figure 2 shows the \( B \)-dependences of electric transport of an annealed sample up to \( B \leq 50\, \text{T} \), including the longitudinal resistivity \( \rho_{xx} \) and Hall resistivity \( \rho_{yx} \). Under high \( B \), the MR showed a \( B^2 \)-dependence, being in contrast to the \( B \)-linear dependence found in the as-grown samples, because the influence of the Dirac quantum states was comparatively hidden by the improved parabolic bands occupied by a major number of carriers. However, as shown in figure 2(b), the MR revealed a more complex behavior under lower \( B \). In fact, using the 1st \( B \)-derivative of \( \rho_{xx} \) \( (d\rho_{xx}/dB) \) in the low-\( B \) region, a saturation in its evolution as a function of \( B \) was clearly indicated in a very small \( B \)-window (figure 2(c)). The saturation behavior exactly mimics the linear magnetoresistance previously found as evidence of Dirac cones in as-grown Ba(FeAs)\textsubscript{2} \cite{5} and therefore can be interpreted as the transport phenomenon strongly indicative of the quantum regime of the Dirac cone \cite{5, 13}.

In general, important information on the Fermi surface can be deduced from these accurate experimental transport data by means of a multi-carrier analysis in a semiclassical description.
However, for the analysis one has to postulate the number of carrier types, and therefore the resulting conclusion frequently becomes ambiguous. In order to interpret the accurate transport data without any prejudiced or biased conclusions, we have performed the special \textit{ab initio} analyses by employing a mobility spectrum method on the $B$-dependent conductivity tensor.

\textbf{Figure 2.} Experimental magnetotransport data of the annealed Ba(FeAs)$_2$ single crystal. (a) Magnetic field ($B$) dependence of $\rho_{xx}$ at 4.2 K. The inset shows the measurement setting. (b) $B$-dependence of $\rho_{xx}$ under low $B \leq 9$ T. (c) The 1st order derivative $d\rho_{xx}/dB$ in the low $B$ region, highlighting the saturated-like behavior. (d) $B$-dependence of $\rho_{yx}$ at 4.2 K. The inset shows a complex sign change in the slope of $\rho_{yx}$ at low-$B$. Figures (a) and (d) show the experimental data whereas the lines exhibit the analytic models representing the data obtained from the fitting of the $B$-dependent conductivity tensor (see figure 3 and section 3.2). It is clear that the experimental data can be well described by the analytical model.
3. Analyses of magnetotransport properties

3.1. The mobility spectrum description of the transport properties

In this paper, the analysis on the magnetotransport properties will be mainly carried out in terms of the reduced conductivity tensor, in which the longitudinal \((X(B))\) and the transverse \((Y(B))\) components are normalized to the conductivity at \(B = 0\):

\[
X(B) = \frac{\sigma_{xx}(B)}{\sigma_{xx}(0)} = \frac{1}{\sigma_0} \cdot \frac{\rho_{xx}(B)}{\rho_{xx}^2(B) + \rho_{yx}^2(B)}; \\
Y(B) = \frac{\sigma_{xy}(B)}{\sigma_{xx}(0)} = \frac{1}{\sigma_0} \cdot \frac{\rho_{yx}(B)}{\rho_{xx}^2(B) + \rho_{yx}^2(B)}.
\]

Here \(\sigma_0\) is the conductivity at \(B = 0\); \(\sigma_{xx}(B)\) and \(\sigma_{xy}(B)\) are the longitudinal and transverse conductivities, respectively.

Instead of assuming the number of electron and hole pockets \([14]\), one can define the two continuous distributions of normalized conductivity versus mobility \(s^{(n)}(\mu)\) and \(s^{(p)}(\mu)\) in relation to the total number of electron-like \((n)\) and hole-like \((p)\) carriers:

\[
K = \sigma_0 \int_0^\infty \frac{s^{(k)}(\mu)}{e\mu} d\mu,
\]

where \(e\) is the elementary charge, \(k = n, p\) and \(K = N, P\), the total number of the \(k\)-like carriers. Using the notations of \(s^{(n)}\) and \(s^{(p)}\), \(X(B)\) and \(Y(B)\) can be reformulated as follow \([15–17]\):

\[
X(B) = \int_0^\infty \frac{s^{(n)}(\mu)}{1 + \mu^2 B^2} d\mu + \int_0^\infty \frac{s^{(p)}(\mu)}{1 + \mu^2 B^2} d\mu \\
\equiv X^{(n)}(B) + X^{(p)}(B) \\
Y(B) = -\int_0^\infty \frac{s^{(n)}(\mu)\mu B}{1 + \mu^2 B^2} d\mu + \int_0^\infty \frac{s^{(p)}(\mu)\mu B}{1 + \mu^2 B^2} d\mu; \\
\equiv Y^{(n)}(B) + Y^{(p)}(B).
\]

In equations (3a)–(3d), each pair of \([X^{(k)}(B), Y^{(k)}(B)]\) separately describes the partial longitudinal and transverse conductivities of only electron-like \((k = n)\) or hole-like \((k = p)\) carriers. These equations connect the experimental data \(X(B)\) and \(Y(B)\) to the responses against a specific \(B\) from all possible electron-like and hole-like carriers.

3.2. Kramer–Kronig transformation of the semiclassical magnetoconductivity

Importantly, by employing the reformulations described in the earlier section, \(X(B)\) and \(Y(B)\) can be proven to be connected to each other via the famous Kramer–Kronig (KK) causality principle \([15]\). More practically, the application of the KK-transformation allows one to obtain individual contributions of hole-like and electron-like carriers from the experimental data as follows:
\[
\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dB'}{B-B'} X(B) = Y^{(p)}(B) - Y^{(n)}(B), \quad (4a)
\]
\[
\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dB'}{B-B'} Y(B) = -X^{(p)}(B) + X^{(n)}(B). \quad (4b)
\]

Here \( P \) denotes the principal part of the integral, and \( X^{(k)} \) and \( Y^{(k)} \) are the individual longitudinal and transverse reduced conductivities of the \( k \)-like carriers, respectively. By using equations (4a–4b), \([X^{(n)}(B), Y^{(n)}(B)]\) and \([X^{(p)}(B), Y^{(p)}(B)]\) can be distinctly deduced from the \([X(B), Y(B)]\) datasets. This separation between holes and electrons effectively allows one to extract the \( \mu \)-spectrum \( \mu_X^{(k)}(\mu) \) of the \( k \)-like carrier category solely from its own conductivities \( X^{(k)}(B) \) and/or \( Y^{(k)}(B) \) without worrying about the mixing of other complementary components.

In equations (4a) and (4b), the \( K \& K \) transformation needs an impractical \( B \)-range from 0 to \( \infty \). In order to bypass this difficulty, we have tried to find a representation of the data, on which the \( K \& K \) transformation can be analytically carried out. This can be done by fitting the real data of \( X(B) \) and \( Y(B) \) to the linear combinations of Lorentzian components [16]:

\[
X'(B) = \sum_{i} \frac{\alpha_i}{1 + \mu_{\alpha,i}^2 B^2}, \quad (5a)
\]
\[
Y'(B) = \sum_{i} \frac{\beta_i B}{1 + \mu_{\beta,i}^2 B^2}. \quad (5b)
\]

It is noted here that the parameters \( \mu_{\alpha,i} \) and \( \mu_{\beta,i} \) in (5a) and (5b) have no physical meaning other than as a set of analytic representations for the experimental data [16]. In the case of the experimental data shown here, a linear combination composed of six Lorentzian components has been used as the representation of \( X(B) \), whereas up to nine components were necessary to reproduce \( Y(B) \). The models of \( X'(B) \) or \( Y'(B) \) with minimal number of Lorentzian components that can give a good representation of the data were selected. We note that models of \( X'(B) \) or \( Y'(B) \) containing larger numbers of terms do not affect the quality of the representations; the additional Lorentzian terms generally have very small amplitudes. This is due to the fact that the experimental \( X(B) \) and \( Y(B) \) data approached almost zero values at the highest \( B \), leaving no degree of freedom for the fitting parameters.

The parameters of the Lorentzian terms are listed in table 1. In figure 3, we compare the experimental data with their analytic representations. It is clear in the figure that the two kinds of datasets are almost identical to each other. In order to make sure that the analytic conductivities \( X'(B) \) and \( Y'(B) \) are actually capable of representing the experimental data, we have employed them to simulate \( \rho_{xx}(B) \) and \( \rho_{xy}(B) \) in a reversed process. A comparison between the simulated and the experimental resistivity tensors is shown in figures 2(a) and (d). The \( K \& K \) transformations were performed on the analytic representations with the help of the computer software Maxima [18]. The partial conductivities for electron-like and hole-like carriers, \([X^{(n)}(B), Y^{(n)}(B)]\) and \([X^{(p)}(B), Y^{(p)}(B)]\), obtained from the calculations are shown in figure 3 as the blue and the orange curves, respectively.

### 3.3. Calculations of mobility spectrum

Employing the partial conductivities separated via the \( K \& K \) transformation at hand, we can now extract the \( \mu \)-spectra of electron-like and hole-like carriers in Ba(FeAs)\(_2\).
Figure 3. $B$-dependencies of longitudinal ($a$) and transverse ($b$) reduced conductivities of \( \text{Ba(FeAs)}_2 \). The black points and the red curves denote the experimental data and their analytic representing curves, respectively. The blue and the orange solid curves denote the partial normalized conductivities of electron-like (superscripted ($n$)) and hole-like (superscripted ($p$)) carrier types obtained from the KK transformation, respectively. Whereas both $X^{(n)}(B)$ and $X^{(p)}(B)$ positively contribute to $X(B)$, $Y(B)$ result from the competition between $Y^{(n)}(B)$ and $Y^{(p)}(B)$. The contrast between the $B$-dependence of electron-like conductivities and that of hole-like conductivities can also be clearly seen.

Table 1. Lorentzian components.

| No.($i$) | $\mu_{\alpha,i}^a$ | $\alpha_i$ | No.($i$) | $\mu_{\beta,i}^a$ | $\beta_i$ |
|---------|-----------------|--------|---------|-----------------|--------|
| 1       | 0.0279          | 0.0051 | 1       | 1.0287          | −0.1151|
| 2       | 0.0547          | 0.1747 | 2       | 1.9207          | −0.0936|
| 3       | 0.0955          | 0.1988 | 3       | 2.9050          | −0.0048|
| 4       | 0.1835          | 0.5146 | 4       | 0.1965          | −0.0004|
| 5       | 1.0519          | 0.0835 | 5       | 0.6265          | −0.0702|
| 6       | 4.7153          | 0.0220 | 6       | 0.4913          | 0.0102 |
| −       | −               | −      | 7       | 0.8181          | 0.0207 |
| −       | −               | −      | 8       | 0.3837          | 0.0136 |
| −       | −               | −      | 9       | 2.9047          | −0.0185|

\(^a\) In \( \text{m}^2/(\text{V} \cdot \text{s})^{-1} \).
In a logarithmic equally-spaced grid of the $\mu$-space, the normalized conductivities $X^{(k)}(B)$ and $Y^{(k)}(B)$ in (3a) and (3b) can be approximated as follow:

$$X^{(k)}(B) = \sum_{i=0}^{N} \frac{1}{1 + \exp\left(2(m_i + b)\right)} \times e^{m_i S^{(k)}(m_i)} \Delta m$$

$$Y^{(k)}(B) \left| = \sum_{i=0}^{N} \frac{1}{2 \cosh (m_i + b)} \times e^{m_i S^{(k)}(m_i)} \Delta m \right.$$  

$$= \sum_{i=0}^{N} \frac{1}{2 \cosh (m_i + b)} \times h_i,$$  

$$= \sum_{i=0}^{N} \frac{1}{2 \cosh (m_i + b)} \times h_i,$$  

where $\mu = e^m$, $B = e^b$, and $h_i = e^{m_i S^{(k)}(m_i)} \Delta m$. Here $N$ is the total number of points used in the approximation and $\Delta m$ is the distance between two $m_i$ points. In the calculation of the $\mu$-spectrum, a set of $h_i$ values at each $m_i$ point is the quantity that one needs to estimate.

In terms of analysis, (6a) and (6b) are much more convenient than equations (3a–3b). Thanks to the KK separations, these equations contain the separated contributions only from the single type of electron-like ($k = n$) or hole-like ($k = p$) quasi particles, and therefore the complex mixing of the contribution between electrons and holes can be avoided. This transformation greatly simplifies the process of extracting the $\mu$-spectra $S^{(n)}(\mu)$ and $S^{(p)}(\mu)$ from the experimental data. Moreover, (6a) and (6b) provide two alternate models for deriving $h_i$ and thus can be used to test the validity of the result spectra. For instance, one can try to extract $S^{(k)}(\mu)$ from $X^{(k)}(B)$ (or $Y^{(k)}(B)$). These spectra in turn can be employed to simulate a transverse (longitudinal) conductivity $Y^{(k)}(B)$ ($X^{(k)}(B)$) using (6a) and (6b). If the obtained $\mu$-spectrum is correct, then $Y^{(k)}(B)$ and $X^{(k)}(B)$ ($X^{(k)}(B)$ and $X^{(k)}(B)$) should be consistent with each other. One can also try to estimate two $\mu$-spectra from both $X^{(k)}$ and $Y^{(k)}$ and compare them.

In order to estimate the $\mu$-spectra, some initial flat $h_i$ spectra including up to 1000 points of $m_i$ were generated by (6a) and (6b). The initial $\mu$-spectra were then independently fitted to the $X^{(k)}(B)$ or $Y^{(k)}(B)$ datasets using the program fikyk [19]. For either $k = n$ or $k = p$, the $S^{(k)}(\mu)$ extracted from $X^{(k)}(B)$ is identical with that obtained from $Y^{(k)}(B)$, confirming the validity of our analyses. The continuous $\mu$-spectrum obtained from these calculations is shown in figure 4. The structure of the $\mu$-spectrum is discussed in relation to the FS of Ba(FeAs)$_2$ in the next section.

4. Discussion

Taking the advantages of the KK hole–electron separation, a contrast between the two complementary categories of carriers can unambiguously be visualized when plotting the conductivities in the logarithmic scale. In figure 3(a), the value of $X^{(n)}(B = 0)$ is about 0.6, which is considerably larger than about 0.4 of $X^{(p)}(0)$, suggesting that electrons are larger either in number or in mobility than holes [2]. As $B$ increases, however, $X^{(n)}(B)$ starts to fall down at a certain $B$ as small as 0.1 T, and furthermore arrives at the drop-down step at a smaller $B$ than
Importantly, as seen in figure 3(b), \( Y^{(n)}(B) \) displays an asymmetrically broadened peak located at \( B \approx 3 \) T with a large shoulder in the low-B side, which eventually develops into a long tail extending very far to the \( B = 0 \) T limit. In comparison, \( Y^{(p)}(B) \) displays a simple, almost symmetrical peak centered at \( B \approx 5 \) T, although a very small asymmetry can be recognized at the low-B side. In the framework of a semiclassical transport description, the longitudinal or the transverse conductivity of one type of carriers is correspondingly stepped or peaked at a value of \( B \), which is inversely proportional to the mobility \( \mu \) of that carrier type [21]. Due to this \( \mu = 1/B \) relationship, the carriers that have a long relaxation time \( \tau \) and a small effective mass \( m^* \) make their contributions at low \( B \)'s, whereas the ones with a short \( \tau \) and a large \( m^* \) respond at relatively larger \( B \)'s. The small but sharp decrease in \( X^{(n)}(B) \) and the long tail of \( Y^{(n)}(B) \) at very low \( B \)'s thus are the evidences for the existence of a small number of electron-like carriers with very high mobility, i.e. the Dirac cones. On the other hand, the major weights of both \([X^{(n)}(B), Y^{(n)}(B)]\) and \([X^{(p)}(B), Y^{(p)}(B)]\) come from other electron-like and hole-like carriers with much larger numbers and much lower mobilities, which can be more plausibly assigned to the large parabolic hole-like and electron-like pockets.

**Figure 4.** The \( \mu \)-spectrum \( s^{(k)}(\mu) \) estimated from the magnetotransport properties of Ba(FeAs)\(_2\) in comparison with a schematic picture of its electronic band structure. (a) \( \mu \)-spectra of electron-like (negative \( \mu \)) hole-like (positive \( \mu \)) carriers in Ba(FeAs)\(_2\) displayed in semi-logarithmic scale. The vertical axis shows the carrier density per unit of \( \mu \) \( (\sigma_{0} s^{(k)}/e\mu) \). The mobility spectrum of electron-like carriers is in striking contrast to that of hole carriers. Note the large differences in the carrier numbers. (b) A schematic \( (k_x, k_y) \) projection of the low temperatures 1st BZ in adapted from the DFT + DMFT calculations found in [2]. The orange circle depicts the large hole pocket at the \( \Gamma \) point, whereas the blue bean-like shapes represent the non-trivial morphology of the large electron pockets. The Dirac cones are plotted in green and red colors. (c) The larger Dirac cone (green) is connected to the smaller one (red) through the interlayer hopping along \( k_z \); therefore these two DC's locate at almost the same \( (k_x, k_y) \) position. (d) Effects of FSs shape on the transport properties. Under \( B \), a segment of an electron-like FS can behave as if it were a hole-like Fermi pocket when its curvature is negative; hence it gives a positive contribution to \( \rho_{xy}(B) \) and \( \sigma_{xy}(B) \) [20]. The other segment with positive curvature makes a conventionally negative contribution to the transverse measurements.
From the partial conductivities \([X^{(n)}(B), Y^{(n)}(B)]\) and \([X^{(p)}(B), Y^{(p)}(B)]\), we have successfully evaluated the \(\mu\)-spectra \(s^{(k)}\) for both electron-like and hole-like carriers in Ba(FeAs)\(_2\) as shown in figure 4(a). Here we have conventionally represented electrons as the carriers with negative and holes as those with positive \(\mu\)’s, respectively. Surprisingly, the electron-like and the hole-like sides of the figure show a striking contrast to each other. Although the two highest peaks in \(s^{(n)}(\mu)\) and \(s^{(p)}(\mu)\) are both located in the low |\(\mu|\) region, the two spectra evolve very differently as |\(\mu|\) increases. In the hole side, \(s^{(p)}(\mu)\) is characterized by the three isolated delta-like peaks at 0.13, 0.82, and 2.85 m\(^2\)(Vs\(^{-1}\)). On the other hand, \(s^{(e)}(\mu)\) is composed of a very sharp peak at \(\mu = -0.11\) m\(^2\)(Vs\(^{-1}\)) (marked as A in the figure), which is continuously connected with a very broad tail ending up with the |\(\mu|\) as high as 8 m\(^2\)(Vs\(^{-1}\)). The latter can be divided into a shoulder centered at \(\mu = -2\) m\(^2\)(Vs\(^{-1}\)) (marked as B) and a wide hump ranging from around −4 to −8 m\(^2\)(Vs\(^{-1}\)) (marked as C). While both spectra of B and C appear in the high \(\mu\) spectrum region, their magnitudes of around 10\(^{-2}\) m\(^{-5}\)Vs and 10\(^{2}\) m\(^{-5}\)Vs are very small in comparison with the value of 10\(^{2}\) m\(^{-5}\)Vs of the peak A. Whereas the sharp peaks in \(s^{(p)}(\mu)\) are interpreted in terms of isotropic FSs, being similar to the \(\mu\)-spectra reported for conventional semiconductors [22], the features in \(s^{(p)}(\mu)\) are very unconventional and have not been reported so far. Since a \(\mu\)-spectrum originates from the response of FSs under external \(B\), the features are actually the representations of the intriguing Fermiology of Ba(FeAs)\(_2\), as discussed in the next paragraph.

Ba(FeAs)\(_2\) is a nearly compensated semi-metal, in which the total volumes of electron-like and hole-like pockets are almost equivalent in size to each other at the Fermi level \((E_F)\) [2]. At low temperatures, antiferromagnetic spin density wave (AF-SDW) band nesting generates a complex structure with many pockets of different sizes via the band reconstruction at low temperatures. Linear band crossing particularly occurs near \(E_F\) due to the restriction of the odd and even parity of orbital symmetry, and thus Dirac pockets form at certain \(k\)-points that accommodate a small number of carriers [1, 10, 23]. Although these crossings do not reside at any symmetric positions in the Brillouin zone, they are topologically protected with well-defined vorticity quantum numbers [4]. On the other hand, a majority of carriers still remain as the trivial large hole- or electron-like pockets, which are located at the center or at the corners of the first Brillouin zone (BZ), respectively. The emergence of the Dirac pockets promises distinct carriers with an extremely long relaxation time (\(\tau\)) [4, 9], originating from the great suppression of backward scatterings [7] as well as other intriguing transport phenomena [5, 6]. In contrast, the relaxation of the majority carriers in the large parabolic FSs is determined by the inter-pocket AF scatterings, which may directly connect the emergence of superconductivity to the magnetic origin in a multiple-band system of FePns. It is also notable that despite the existence of the non-trivial colinear AF-SDW state at low temperatures, the reported dc transport properties of high quality annealed samples are almost isotropic [12, 24]. This is distinguished from the extrinsic anisotropy observed in as-grown Ba(FeAs)\(_2\) crystals [25], which can be virtually removed by the annealing process [24]. The annealing thus helps to eliminate extrinsic effects that may hinder the observation of the band structure by transport properties. Experimental measurements of the electronic structures in both kinds of samples are generally in good agreement with each other [26–28], yet it is still unclear whether fine details of the energy band are affected by the annealing process.

In figure 4(b) we show a schematic FS structure in agreement with the DFT+DMFT band calculations by Yin et al [2]. This unusual band picture consists of a hole-like FS located at the center of the BZ and three electron-like pockets residing along the FM and the AFM directions.

New J. Phys. 16 (2014) 093062

K K Huynh et al

10
in accordance with the $C_2$ symmetry. Whereas the simple ellipsoidal shape of the hole pocket $\eta$ is well-agreed in both theoretical calculations and experimental measurements, the electron FSs are much more complex and remain in question [2, 23, 26, 27, 29]. In the current band picture for instance, two small FSs $\delta$ and $\epsilon$ form via the SDW band folding with different parities [1], and therefore are characterized by a linear dispersion $E = \hbar v_F k$, i.e. Dirac cone (pockets). These two Dirac pockets, being very different in size, are connected to each other via the interlayer hoping along $k_z$, as shown in figure 4(c), and hence appear at almost the same $(k_x, k_y)$ positions [2, 27]. On the other hand, the large parabolic $\alpha$ pocket along the FM direction shows a curious cashew-like shape featured by both convex and concave segments of the surface. Intriguingly, the distinct contrast described here between the hole-like and electron-like FSs is similar to what was described earlier between $s^{(p)}(\mu)$ and $s^{(n)}(\mu)$. We will show that our $\mu$-spectra are actually in very good agreement with this band picture and therefore are the first observations of the intrinsic transport properties.

Let us focus first on the sharp peak $H$ in $s^{(p)}(\mu)$. In the context of the $\mu$-spectrum, such a sharp peak can be interpreted by an isotropic band with parabolic dispersion. Considering its large peak height, which is in principle proportional to the pocket size, the $H$ peak in $s^{(p)}(\mu)$ can reasonably be assigned to the large hole pocket $\eta$ of the calculated band. Similarly, the $A$ peak in $s^{(n)}(\mu)$ can also be assigned to the large $\alpha$ pocket. However, the curious shape of $\alpha$ gives a clue for understanding the additional unexpected transport phenomenon. Ong [20] proposed that during a cyclotron motion on a FS under $B$, an electron can interestingly behave not only like a hole but also like an electron, depending on whether the local curvature of the FS is negative or positive (see figure 4(d)). It is natural to consider that the cashew-like $\alpha$ pocket can be responsible both for the $A$ peak in $s^{(n)}(\mu)$ of the electron side and for the $A$ peak in $s^{(p)}(\mu)$ of the hole-side. Consequently, the $A$ peak in $s^{(n)}(\mu)$ can be attributed to the cyclotron motions of electrons on the convex part and the $A$ to those on the concave part of the $\alpha$ cashew band. From the band curvature, the concave part has higher mobility than that of the convex part.

Next, we consider the features of the high mobility $B$ and $C$ in $s^{(n)}(\mu)$. Keeping in mind that the high mobility is reasonably considered to be one of the intriguing quantum properties of Dirac fermions, one could naively ascribe these features to the two Dirac pockets $\delta$ and $\epsilon$. However, taking into account the experimental fact that $B$ and $C$, continuously extending to a very wide range of mobilities, have not been observed in any $\mu$-spectrum analyses so far, a more careful discussion is necessary. As we mentioned above, the $\mu$-spectrum analysis technique aimed at understanding the conduction under $B$ of conventional metals and semiconductors where the scattering time $\tau$ and the effective mass $m^*$ do not change with respect to $B$. In the case of a Dirac cone, however, this simple picture may not be valid. As has been shown in [13], the transport of a Dirac cone obeys the Abrikosov model of linear MR (LMR), in which the longitudinal conductivity of a single Dirac cone is inversely proportional to $B$, i.e. $\sigma_{xx}^{(D)}(B) \propto 1/B$. This interesting quantum transport phenomenon has been clearly observed in the Ba(FeAs)$_2$ as-grown samples [5] as well as other Dirac cone systems [30, 31].

In the case of the optimally annealed samples studied in this paper, as shown in figure 2(b), $d\text{MR}/dB$ exhibited a clear saturation in a small window of $B$. This is clearly indicative to the LMR contribution of the Dirac cones to the electric transport. The $\mu$-spectrum of the Dirac cone can be deduced by combining the $1/B$ dependence of $\sigma_{xx}^{(D)}$ and the semiclassical definition 3a of a $\mu$-spectrum:
From (7), one can judge that the $\mu$-spectrum $s^{(D)}(\mu)$ of the Dirac cone is constant against $\mu$. Figure 5 shows such a schematic plot of $s^{(D)}(\mu)$ and $s^{(D)}(\mu)/\mu$, the latter of which is directly proportional to the carrier density of the Dirac cone. Interestingly, this constant spectrum produces a long tail up to the high $\mu$ region in $s^{(D)}(\mu)/\mu$, being well consistent with C and B in the experimentally extracted $s^{(n)}(\mu)$ shown in figure 4(a). The long tails C and B therefore can be qualitatively interpreted as the effects of quantum transport of the Dirac cones being observed from the semiclassical description point of view. The intrinsic $\mu$ of the smaller Dirac cone can be estimated to be around 70,000 cm$^2$(Vs)$^{-1}$ at the peak of C.

5. Conclusions

The $\mu$-spectra described in the present paper provided a remarkable overview of the unusual band picture of Ba(FeAs)$_2$ from the viewpoint of electric transport phenomena. The topology of the FSs played an important role in understanding the electric transport of Ba(FeAs)$_2$. The broad features in the mobility spectrum of the Dirac cones qualitatively indicated that the relaxation time of the Dirac carriers is greatly $B$-dependent. We also noted that the Dirac pockets in Ba(FeAs)$_2$ have finite tight binding-like dispersions along $k_z$, and hence may be very different from the 2D ones found in graphene as well as in the surface-state Dirac cones of topological insulators. It will be very interesting to see in the future whether the $\mu$-spectra of Ba (FeAs)$_2$ deduced in the present study can be rationalized by other experiments, as well as further sophisticated and deeper theoretical band calculations.

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