Mass enhancements and band shifts in strongly hole overdoped Fe-based pnictide superconductors: KFe$_2$As$_2$ and CsFe$_2$As$_2$

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Abstract  The interplay of high and low-energy mass renormalizations with band-shifts reflected by the positions of van Hove singularities (VHS) in the normal state spectra of the highest hole-overdoped and strongly correlated AF$_2$As$_2$ (A122) with A=K, Cs is discussed phenomenologically based on ARPES data and GGA band-structure calculations with full spin-orbit coupling. The big increase of the Sommerfeld coefficient $\gamma$ from K122 to Cs122 is ascribed to an enhanced coupling to low-energy bosons in the vicinity of a quantum critical point to an unknown, yet incommensurate phase different from the commensurate Mott one. We find no sizeable increase in correlations for Cs122 in contrast to F. Eilers et al., PRL 116, 237003 (2016) [3]. The empirical (ARPES) VHS positions as compared with GGA-predictions point even to slightly weaker correlations in Cs122 in accord with low-$T$ magnetic susceptibility $\chi(T)$ data and a decreasing Wilson ratio $\propto \chi(0)/\gamma$.

Keywords Pnictides · ARPES · van Hove singularity

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Fig. 1 (Color) Schematic general doping phase diagram of Fe pnictides ignoring nematicity. Blue (red) magnetic (superconducting) regions, respectively. Phase I - a combined charge, orbital, and spin ordered phase responsible for the vicinity of the critical point as discussed in the text. The yellow line at isovalent or no doping stands for such systems as Li(Na)FeAs and P-doped Ba(Sr)-122 where the competing magnetic SDW magnetic stripe-phase is absent or strongly suppressed. Phase II has been observed but not been yet characterized experimentally. The outermost hypothetical SDW or ferromagnetic (FM) phase around Fe$^+$ is our suggestion. The bright (dark) red regions stand for 122 and H doped La-1111 (under pressure) FeSC compounds, respectively.
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Detailed maps 80eV

![Detailed maps 80eV](image)

**Fig. 2** (Color) ARPES data for K$_{0.96}$Cs$_{0.04}$Fe$_2$As$_2$. Upper panel: general map with visible ε-FSS, Lower panel: Cuts (white arrows) for the linearly polarized spectra (left and middle); 3$d_{xz}$/3$d_{yz}$ derived saddle-point VHS (right).
1 Introduction

To achieve a better qualitative and quantitative understanding of the rich doping phase diagram and the strength of correlation effects in the electronic and magnetic properties of Fe-based superconductors and related compounds is one of the most challenging and central issues (see e.g. Fig. 1 and 1). The two isomorphic compounds AFe$_2$As$_2$ with $A=K$, Cs with the same strongly hole-overdoped state but with surprisingly different thermodynamic properties in the vicinity of a recently proposed quantum critical point (QCP) 3 provide a good opportunity to get deeper insight into the interplay of high- and low-energy physics by a comparative analysis of the underlying electronic structure. In Sects. 3-5 we present densities of states (DOS) around the Fermi level and discuss band shifts as marked by the positions of van Hove singularities (VHS). The very presence of VHS for one of them was first qualitatively detected in STM 1 on K122 surfaces 1 (its shape is similar to that shown Figs. 2-4). The same group did, however, not succeed in observing an expected analogous feature in Cs122 5. From the theoretical DFT side a clear identification of the VHS was previously lost due to a too scarce $k$-mesh 1. In Sect. 5 we report the observation of VHS for both compounds by means of ARPES. Controversial aspects of the magnetic susceptibilities, $\chi(T)$, and the Wilson ratios of the title compounds are discussed in Sect. 4. The present paper builds on the recent multiband Eliashberg theory based analysis of Fe-based superconductors of Refs. 16 supplemented, here, with new ARPES and thermodynamic experimental findings for A122 ($A=K$, Cs) including also the less strongly K-overdoped Ba$_{1-x}$K$_x$Fe$_2$As$_2$ system with $0.7 \leq x < 1$.

2 Sample preparation and characterization

For the ARPES (angular resolved photoemission spectroscopy) measurements reported in Sect. 5 (see Fig. 2 ) K$_{0.96}$Cs$_{0.04}$ and Cs$_{0.94}$K$_{0.06}$Fe$_2$As$_2$ single crystals have been grown from corresponding AAs ($A=K$, Cs) mixed fluxes 78910. The electronic structure and the normal state properties of both samples, we focus here, are considered to be very close to those of the corresponding stoichiometric cases. Both as grown crystals exhibit a plate-like morphology, these crystals were characterized by SEM (scanning electron microscopy) and EDX (energy-dispersive X-ray analysis) diffraction measurements. The weak disorder produced by the slight deviations from stoichiometry causes however an expected and observed reduction of $T_c$ generic for unconventional nodal superconductivity, similarly as in the case of Na-doped K122 6 generic for an $d$-wave superconducting order parameter. Also in the cases of less strongly hole-overdoped samples Ba$_{1-x}$K$_x$Fe$_2$As$_2$ shown in Figs. 6 and 7 the self-flux method for the crystal growth 10 have been used resulting in high-quality single crystals with low values for the residual resistivity $\rho_0$. The doping level was determined by x-ray diffraction using the known dependence of the $c$-axis lattice constant versus K doping (see Fig. 3 in Ref. 9 and Fig. S1 in the Suppl. of Ref. 8). The specific heat and electric transport measurements of single crystals were done in a Quantum Design physical property measurement system (PPMS) and the magnetization measurements in a commercial superconducting quantum interference device magnetometer (SQUID) from Quantum Design. Part of the magnetization, transport and specific heat data shown here have been presented already in Ref. 22.

3 Mass enhancement from the density of states

Here we will consider the electronic DOS, $N(0)$, at the Fermi energy $\varepsilon_F = 0$ and several related thermodynamic properties such as the Sommerfeld coefficient $\gamma$ of the linear in temperature $T$ electronic specific heat at low $T$ (see Fig. 4), the magnetic susceptibilities $\chi(T)$ (see Figs. 5 and 6), as well as the positions of saddle-point VHS generic for quasi-2D electronic systems. In the present case, these derive from Fe-3$d_{xz}/d_{yz}$ electronic states and, owing to the strong hole-doping level occurs only slightly below $\varepsilon_F$ (see Figs. 2, 3, and 4), as compared to the parent compounds AFe$_2$As$_2$ with...
$A = \text{Ba, Sr, Ca or isovalent P-doped Ba122 or Sr122}$ (see Fig. 1) with Fe$^{2+}$ ($d^{6}$). However, all these quantities are strongly affected by the presence of non-negligible many-body effects which become evident when compared with traditional density functional theory (DFT) based results, within the framework of the local density approximation (LDA) and the general gradient approximation (GGA) (for details see Ref. [1]) employed here as an effective "bare" description of the electronic structure, when ignoring the weak exchange and correlation effects implemented in present day DFT functionals.

There are two observations providing direct evidence for significant many-body effects in the strongly hole-doped end members of the so-called 122 compounds $A$Fe$_2$As$_2$ with $A = K, Rb, Cs$: (i) the mass enhancement of various bands crossing the Fermi energy and (ii) a shifting of these bands resulting in different filling factors. The latter effect is sensitive to approaching a filling ratio closer to half-filling for the most strongly correlated Fe-3$d_{xy}$ states which form the outermost Fermi surface sheet (FSS) centered around the $\Gamma$-point of the Brillouin zone (BZ). The el-el interaction affects also the position of various orbital-dependent VHS: In the present case they stay closer to the Fermi energy by a factor of 3 as compared to the best DFT predictions, (see Fig. 3). Here we will focus briefly on the closest to $\varepsilon_F$ Fe 3$d_{xz}/d_{yz}$ VHS which occurs in the middle of the $\Gamma$-X line in the BZ. The latter is the center of the blade/propeller-like $\varepsilon_F$-FSS [1,11,12,13] clearly visible in Fig. 2. The corresponding band has been suggested to dominantly bear superconductivity, although, both, nodeless [12,13] and $d_{x^2-y^2}$-nodal type [1,5,7,9] characters have been proposed.

$^2$ In our calculations of the DOS, see Fig. 3, we have used that of Perdew et al. [15,16].

4 Thermodynamic puzzles

We start with an analysis of the available specific heat data shown in Fig. 5. Using our bare DOS $N(0)$ GGA-derived values shown in Fig. 3, one arrives at a total mass enhancement of about 8.9 for K122, rather similar to about 9 for Rb122, whereas in Cs122 an enhanced value $\approx 12$ is realized [1]. With the low-energy bosonic weak coupling constant $\lambda \approx 0.7$ taken into account, one is left with a dominant high-energy renormalization exceeding five. With the same or slightly reduced high-energy renormalization, but enlarged low-energy coupling, the Cs122 data can be understood in qualitative accord with the somewhat reduced shift of the VHS considered in Sect. 5 dominated by the high-energy interactions $U$ and $J$ (see below). The magnetic susceptibilities $\chi(T)$ of K122 and Cs122 show a broad maximum at low $T_{\text{max}}$. This has been considered as the hallmark for strong correlations ascribing it to the freezing temperature $T_f$ generic for bad metals with well-defined quasi-particles and Fermi liquid-like behavior below $T_f$, only. Then the observed systematic downshift of $T_{\text{max}}$ on going from K122 via Rb122 to Cs122 could be a signature of increased correlation strength [13,20]. However, our experimental data for
the less strongly hole-overdoped samples, exhibit only a very moderate downshift and an anomalous behavior of the Wilson ratios $R_W$ (see Figs. 6 and 7). This points to a more complex scenario, probably related to the multiband nature of these compounds with rather different correlation regimes in the various subsystems. Indeed, our low-energy bosonic scenario [1] mentioned above could also be helpful in resolving these puzzles related to the smaller $\chi(0)$ of Cs122 in comparison to Rb122 and K122, as well as to their Wilson ratios $R_W$. Noteworthy, a large and even an increased $R_W \approx 4$ was recently observed in Cs122 [24]. This is the first counter-intuitive observation. Since this values is in obvious conflict with the notion that stronger correlations are present in Cs122 and Rb-122 when compared to K122.

5 Van Hove singularities as seen by ARPES

To determine the position and the correct orbital nature of the VHS of both single crystals mentioned in Sect. 2, angle-resolved photoemission spectroscopy (ARPES) data have been collected at the I05 beamline of Diamond Light Source. Single-crystal samples were cleaved in situ in a vacuum better than $2 \times 10^{-10}$ mbar and measured from 5.7 to 270 K. These measurements were performed using linearly polarized synchrotron light, utilizing a Scienta R4000 hemispherical electron energy analyzer with an angular resolution of 0.2 to 0.5° and an averaged energy resolution of about 3 meV. (see Fig. 2 for the case of K122). The position of the Fe 3d$\sz$/3d$\gy$ VHS as derived from our ARPES measurements of about -15 ± 1 meV and -11±1 meV for K-122 and Cs-122, respectively, significantly differs as expected from the DFT values by a factor of four which clearly points to strong many-body effects. Also the GW-approximation in the present form does not yield a good description, caused probably by overscreened Coulomb interactions. Its future combination with a DMFT-like approach might resolve this problem. We admit that a fully relativistic GGA-based code might reduce the deviations from the ARPES data. The order of magnitude of the VHS-shifts can be approximately reproduced by the slave spin and/or the DMFT theory using appropriate phenomenological parameters for the Hubbard $U = 2.7$ to 4 eV and the Hund’s exchange $J = U/4$. Both are responsible also for the high-energy renormalizations for the DOS and the Sommerfeld coefficient $\gamma$. In

3 We mention that among a large number of known (until 2000) heavy-fermion superconductors, only three of them (CeCu$_2$Si$_2$, UPt$_3$, and UBe$_{13}$) exhibiting surprisingly formally “free electron” Wilson ratios $R_W \approx 1$.

4 Note that our results differ quantitatively by a systematic shift of nearly 10 meV for the entire spectrum as compared to Ref. [4], and even qualitatively in that previous Cs122-STM [5] showed no VHS at all. We speculatively ascribe this to surface reconstructions and charging in those samples most detrimental for STM. The position in STM of the VHS was given as -5 to -6 meV for K122.

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Fig. 6 Low-$T$ maximum of the magnetic susceptibility in hole-overdoped K-doped Ba-122 single crystals vs. doping ratio, from our data and from those of Liu et al. [21].

Fig. 7 Wilson ratio in h-overdoped K-doped Ba-122 vs. doping from our data and that of Refs. [21][13]. Notice the moderate but non-monotonous dependence with a minimum near the the Lishitz point where the two electron pockets near the corner of the BZ disappear, and the seemingly weakly correlated values well below 2.
general, one may expect the following decomposition of the VHS-shift relative to standard non-relativistic DFT
\[ \delta \mu_{\text{VHS}} = \delta \mu_{\text{so}} + \delta \mu_{\text{high}}(U, J) + \delta \mu_{\text{lowb}}. \] (2)
where the three terms stand for the SO coupling, the high- and low-energy bosonic contributions, respectively. According to Fig. 2, and Ref. [1] the 1st terms amount to \( \approx 18.3 \) (12.2, 8.75) meV for K(Cs,Rb)122, respectively. Then one is left with empirical shifts of many-body origin of \( \approx 45 \) meV for K122 and 37 meV for Cs122, yet to be understood theoretically. The 2nd term in Eq. (2) is the high-energy contribution. It should scale with the matrix element of the high-energy self-energy \( \Sigma_{\text{el-el}} \propto (U + \alpha J)^2 \) where \( \alpha \) is a value in between -1 for Fe\(^{3+}\)(d\(^5\)) and \( \alpha = +4 \) for full 3d Mott systems at half filling (i.e. at Fe\(^{3+}\)(3d\(^5\))) realized in some Mn or Cr systems. For simplicity we adopt \( \alpha = 1.5 \) and an often used \( J = 0.25U \) ratio. Anyhow, it should be nearly the same for K122 and Cs122 and will therefore not affect our main conclusion. This contribution reads
\[ \rho_{\text{high}}(U, J) \propto (U + \alpha J)^2 \approx 1.89U^2, \] (3)
and provides a convenient measure of the effective Hubbard interaction \( U_{\text{eff}} = U + \alpha J \) or of its relative change from K122 to Cs122 at the same doping but at fixed ratio \( J/U = 0.25 \). It is expected to be dominant since the low-energy bosonic contribution should be much weaker, although not necessarily the same for a coupling to soft critical modes and this way different for the three compounds (see below). Ignoring it to first approximation and using the empirical absolute shifts, one would arrive at a ratio of about 1.216 or at \( U_{\text{K122}} \approx 1.103U_{\text{Cs122}}, \) i.e. at weaker correlations for Cs122 in accord with the reduced \( \chi \) and the Wilson ratio, but in sharp contrast to opposite claim of Ref. [3] where an increase of \( U \) of \( \approx 20\% \) has been suggested for Cs122. A reduced \( U \)-value for Cs122 might be due to the larger polarizabilities of the larger Cs\(^{1+} \) cations (by \( \approx \) a factor of 3) as compared to K\(^{1+} \), leading to more screened \( U \)-values. Note that a significantly higher energy of the VHS by \( \approx 8 \) meV i.e. at \(-3 \) meV[ for Cs122 would be required to arrive at the same effective \( U \) in the present estimate. In the scenario of Ref. 3 the VHS would even occur above or at \( E_F \).

Indeed, adopting an effective two-band model by dividing the total system into one subsystem containing the Fe-3d\(_{xz}/3d_{yz} \) electrons (which produce the VHS considered here) and a second for the remaining part of electrons, one might estimate the bosonic shift for the chemical potential following Ref. [27] as
\[ \delta \mu_{\text{lowb}} \propto \lambda_b \omega_b. \] (4)

Using \( \lambda_b \text{K122} = 0.7 \) [1] and \( \hbar \omega_b = 7 \) meV from inelastic neutron scattering (INS) data [28]. The order of the experimental difference of \( \approx 4 \) meV can be readily understood, if a stronger coupling to low-energy bosons for Cs122 due to the closer vicinity to a QCP [3] (see Fig. 1) is taken into account. The incommensurate spin fluctuations seen in the INS [28] and NMR data for Cs122 [29] point to a phase different from the AFM commensurate Mott one. Measurements of the VHS for Rb122 and other Fe-pnictides are highly desirable.

6 Summary and outlook

Shifts of van Hove singularities relative to DFT-predictions provide a direct measure of the high-energy el-el interaction. There is no obvious increase of the Hubbard \( U \) and the Hunds’s exchange \( J \) ongoing from K122 to Cs122 by analyzing phenomenologically the 3d\(_{xz} - 3d_{yz} \) VHS (closest to \( E_F \)). Its shift is affected by the spin-orbit coupling which cannot be ignored (as done previously in the literature) for a reliable estimate of many-body effects. For a full description, also the VHS at larger binding energies related to the Fe-3d\(_{xy} \) and the 3d\(_{z^2} \) orbitals should be studied experimentally. More results will be given elsewhere. In general, a combined theoretical and ARPES study of VHS shifts provides a valuable general tool to study many-body effects in quasi-2D systems in addition to those reflected in the mass enhancements.

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Note added for the readers of arXiv

Within a very recent preprint: arXiv:1807.00193v1 (submitted 30 June 2018) devoted to a chemical pressure tuning of the van Hove singularities in KFe\(_2\)As\(_2\) and CsFe\(_2\)As\(_2\) revealed by an ARPES study by P. Richard, A. van Roekeghem, X. Shi, P. Seth, T.K. Kim, X.-H. Chen, S. Biermann, and H. Ding, very similar positions of the saddle-point van Hove singularities have been found: -15 meV to -12 meV as well as -10 meV as compared to -15 \( \pm \) 1 meV and -11 \( \pm \) 1 meV, respectively, reported above.

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