

Dispersion kinks from electronic correlations in an unconventional iron-based superconductor

Corresponding Author: Professor Heike Pfau

This file contains all reviewer reports in order by version, followed by all author rebuttals in order by version.

Version 0:

Reviewer comments:

Reviewer #1

(Remarks to the Author)

The manuscript by M.-H. Chang et. al. reports two distinct kink structures in RbFe_2As_2 by ARPES and DMFT which is purely originated from electronic correlations. The kink structure in ARPES spectrum often holds very important information in understanding the interactions in correlated materials, especially that in unconventional superconductors, the observation of the kink structure might indicate the electron coupling to certain boson modes which is crucial to the electron pairing.

In the manuscript, the two kink energies are located at 23 meV and 330 meV, respectively. The high energy kink at 330 meV is beyond the phonon energy range and is thought to be a correlation induced effect which connects coherent quasiparticle component with the incoherent Hubbard band. And the low energy kink at 23 meV is thought to be primarily from electronic origin by checking the temperature dependent behavior of this kink. And the authors discussed about the possible origin of the spin fluctuation since the low energy link has the same energy scale which has a strong impact on understanding the superconducting pairing symmetry.

The correlation induced kink in the dispersion has already been discussed widely theoretically and visualized experimentally in a lot of materials such as cuprates, ruthenates, transition metal oxides etc, and iron-based superconductors is well known electronic system with moderate electronic correlations. Though the main conclusion of the manuscript is solid, I don't the originality and importance of the observation can fit the high standard of Nature Communications. the authors should present the data more clearly for better understanding, for example:

1. In Fig.1 a, the author should mark the high symmetry points in the schematic of the BZ to show which direction the cut is.
2. In Fig.1b, the authors mention "It shows a 3-peak structure that is...". It is not clear to me how the spectrum fits the 3-peak structure. It will be better to mark the 3 peaks.
3. What is the difference between Fig.2a and Fig.1a, is it the same energy cut but with different energy range? Similar case for Fig.3a when the authors show the temperature dependent behavior of the kink, they use a "different momentum cut than those in Fig. 2a." Then what cut direction it is? Why use a different cut? The author should specify all these details clearly.
4. Also, when discuss about Fig.1d, the authors mention "The EDC in Fig. 1d shows the same three-peak structure of the incoherent spectral weight... However, the peak around -1 eV is absent in DFT calculations". This is also confusing. From Fig.1d, one can see the 3-peak structure with 3 peaks at (-0.5,-1), (-2,-2.5) and (-3.5,-4). If the peak at "-1 eV is missing, I don't understand how the spectrum fits the 3-peak structure.
5. "The FWHM in Fig. 2g shows a step at each kink energy indicating a substantial increase in lifetime." I cannot see where the step is and how it matches the kink energy.

Reviewer #2

(Remarks to the Author)

Authors have investigated the electronic structure of iron-based superconductor RbFe_2As_2 using ARPES and DFT+DMFT and argued that the 'two kinks' – kinks of electronic dispersion at relatively low- and high-energy, respectively – can be primarily electronic-correlation-induced and possible importance of the coincidence of the kink and spin fluctuation energy scales. While the kink structure of electron dispersion at a few tens of meV low-energy range (as well as high-energy kink) is ubiquitously observed in strongly correlated normal metallic states of unconventional superconductors such as cuprates, ruthenates, and iron-based superconductors, the origin of kink structure and its possible role in the superconducting pairing

mechanism is still on debate.

In this context, the authors investigated the low-energy electronic structure of RbFe_2As_2 using ARPES and DFT+DMFT complementarily and found out that the DFT+DMFT calculation could precisely reproduce the observed two kink structures and their energy scales by implementing only the electronic origins, which could sufficiently rule out the other bosonic contribution and emphasize the electronic origin as well as the possible role of spin fluctuation (as concluded in the manuscript) in 122 compound family.

We support the significance of this work, but it would be beneficial to provide additional clarification on the analysis in the manuscript and supplemental materials to ensure that readers can fully understand the authors' study. We recommend the publication of this manuscript, upon appropriate responses to the following questions and comments.

1. Adding some content would help to ensure a comprehensive understanding of the DFT+DMFT calculation results.

A. What is the distribution of Fe d orbitals in DFT and DFT+DMFT fat bands? Could the authors also show the total band structure? Do other orbitals exhibit similar phenomena as the xz band?

B. It seems that the xz bands are almost fully filled. How is the condition of the Hund correlation effect satisfied?

C. In Fig. 1e, the authors presented atomic model results to designate the characteristics of Hubbard multiplet bands, which seems opposite to our usual expectation that the ground state should have the largest weight. How are the spectral weights obtained? Since the authors performed calculations using CTQMC, the atomic state probability would be more straightforward to compare with DMFT EDC in Fig. 1d.

2. Regarding the comparison of three-peak structure between ARPES and DFT+DMFT, in Fig. 1b and 1d, unlike the EDC curve from the ARPES spectrum, which shows dominant QP weight near zero frequency and relatively small Hubbard bands (HB) weight at around -2.5 eV, DFT+DMFT shows strong suppression of the overall QP weight, so it could be quite far from the Hund regime.

A. Similarly, how can we understand the strong suppression of DMFT EDS at zero frequency in Fig. 1d?

Reviewer #3

(Remarks to the Author)

The present work reports ARPES and DMFT study of the hole-doped iron-based superconductor RbFe_2As_2 . They mainly focus on the two kink features observed on the ARPES band dispersions near EF. By a systematic comparison with the DMFT calculations, these kinks are suggested to originate from the strong electron correlations. The manuscript is clearly written, the good agreement between ARPES and DMFT well supports the authors' arguments and conclusions. I believe the presented results provide important information for the understanding of unconventional superconductivity and other emergent phenomena in the strongly-correlated iron-based superconductors. Before I can recommend the publication in Nature Communications, I would like the authors to address the following comments and questions:

1. In Fig. 2, instead of the FWHM of MDCs, I suggest to present the imaginary part of the self-energy; accordingly, a comparison with the real part of the self-energy would increase the readability of the manuscript.
2. To demonstrate the orbital characters of the concerned bands, the geometry of the experiment is suggested to be further clarified, and the ARPES matrix element analysis should be included.
3. What is the momentum dependence of these two kinks? Also, the momentum direction of the cut in Fig. 2a needs to be clarified.
4. Are the similar two kink features observable on the band dispersions around the zone corner?
5. In page 4, to estimate the electron-phonon coupling strength, instead of using the change of band velocities, more comprehensive Eliashberg function analysis with calculating both the real part and imaginary part of the self-energy should be performed.

Reviewer #4

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I co-reviewed this manuscript with one of the reviewers who provided the listed reports. This is part of the Nature Communications initiative to facilitate training in peer review and to provide appropriate recognition for Early Career Researchers who co-review manuscripts.

Version 1:

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Reviewer #1

(Remarks to the Author)

I appreciated the authors' changes in the manuscript according to my suggestions. I agree with the authors that the observation of such a dispersion kink gives information in understanding the unconventional superconductivity and other emergent phenomena in the strong correlated iron-based superconductors, especially that the low energy kink indicates that the spin fluctuations might be the pairing glue. However, as I mentioned before, the correlation induced kink in the dispersion has already been discussed widely theoretically and visualized experimentally in a lot of materials. And in iron-based superconductors, spin resonance mode observed by neutron scattering experiment do support the spin fluctuation scenario. In this sense, I don't think the authors convinced me about the uniqueness and importance of this observation in RbFe₂As₂ and I feel it cannot match the high standard of Nature Communications.

Reviewer #2

(Remarks to the Author)

All questions have been thoroughly addressed, and this paper is ready for publication as it stands.

Reviewer #3

(Remarks to the Author)

My concerns have been well addressed, and I recommend the publication in Nature Communications.

Minor points:

1. For the self-energy derived from the ARPES data (Fig. S3d,e), I suggest to use the real part and imaginary part of the self-energy for the labels, as in Fig. S3a,b.
2. In the section DMFT SPECTRAL FUNCTION FOR ALL 3d ORBITALS: "(a) to (e)" --> "(b) to (f)"; "(f)" --> "(a1) and (a2)".

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Response to the Referees

We thank all referees for their time to review our manuscript and for their valuable comments. We reply to them in detail below and marked changes in the manuscript in red text.

Reviewer #1

The manuscript by M.-H. Chang et. al. reports two distinct kink structures in RbFe₂As₂ by ARPES and DMFT which is purely originated from electronic correlations. The kink structure in ARPES spectrum often holds very important information in understanding the interactions in correlated materials, especially that in unconventional superconductors, the observation of the kink structure might indicate the electron coupling to certain boson modes which is crucial to the electron pairing.

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The correlation induced kink in the dispersion has already been discussed widely theoretically and visualized experimentally in a lot of materials such as cuprates, ruthenates, transition metal oxides etc, and iron-based superconductors is well known electronic system with moderate electronic correlations. Though the main conclusion of the manuscript is solid, I don't the originality and importance of the observation can fit the high standard of Nature Communications.

The strong coupling to electrons found in our study indicates that spin excitations may serve as the superconducting pairing glue. The majority of unconventional superconductors are strongly correlated electron systems, such as cuprates, nickelates, iron-based materials and heavy fermions. Our study identifies RbFe₂As₂ as a model system that points to a deep relationship between unconventional superconductivity and electronic correlations. We believe that our results provide a clear advance in our scientific understanding of unconventional superconductivity and will likely stimulate the interest of a broad physics community. As Referee #3 pointed out: "The presented results provide important information for the understanding of unconventional superconductivity and other emergent phenomena in the strongly-correlated iron-based superconductors."

The authors should present the data more clearly for better understanding, for example:

We thank the referee for guidance on how to improve our data presentation. We implemented the suggested changes in our manuscript.

1. In Fig.1 a, the author should mark the high symmetry points in the schematic of the BZ to show which direction the cut is.

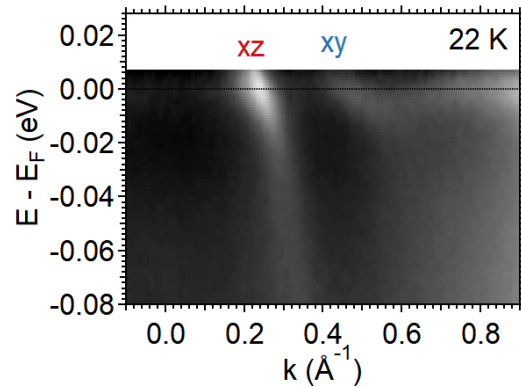
We updated Figure 1a and included the assignment of high-symmetry points.

2. In Fig.1b, the authors mention “It shows a 3-peak structure that is...”. It is not clear to me how the spectrum fits the 3-peak structure. It will be better to mark the 3 peaks.

We updated Figure 1b and 1d and included markers to point out the three peaks described in the main text.

3. What is the difference between Fig.2a and Fig.1a, is it the same energy cut but with different energy range? Similar case for Fig.3a when the authors show the temperature dependent behavior of the kink, they use a “different momentum cut than those in Fig. 2a.” Then what cut direction it is? Why use a different cut? The author should specify all these details clearly.

We updated Fig 2a and Fig 3b to include a sketch of the momentum cut and labels for high symmetry points. Indeed, the spectrum in Figure 2a is taken along the same momentum direction as Fig. 1a, but in a smaller energy window and slightly different momentum range to highlight the kinks in the dispersion. The momentum direction for Fig 3 is equivalent to Fig. 2. But it is in the second Brillouin zone in order to monitor both the xz and xy band dispersion (see spectrum below). The latter has favorable matrix elements in the second Brillouin zone. Detailed analysis of the data revealed that the intensity of the xy band is insufficient for an in-depth MDC analysis and we therefore excluded it from our discussion in the manuscript.



4. Also, when discuss about Fig.1d, the authors mention “The EDC in Fig. 1d shows the same three-peak structure of the incoherent spectral weight... However, the peak around -1 eV is absent in DFT calculations”. This is also confusing. From Fig.1d, one can see the 3-peak structure with 3 peaks at (-0.5,-1), (-2,-2.5) and (-3.5,-4). If the peak at “-1 eV is missing, I don’t understand how the spectrum fits the 3-peak structure.

The referee pointed out the three peaks in Fig. 1d correctly. These are the same three peaks as seen in ARPES in Fig. 1b. However, DFT calculations (Supplementary Material Fig. 1) do not predict a state at the energy of the first peak around 1eV. Therefore, we conclude that it appears due to electronic correlations that are explicitly included in DMFT but not in DFT.

5. “The FWHM in Fig. 2g shows a step at each kink energy indicating a substantial increase in lifetime.” I cannot see where the step is and how it matches the kink energy.

The step in the FWHM occurs at the same energy as the kink in the dispersion. To highlight the steps in the FWHM, we marked the kink energy with arrows in Fig. 2g and h as well.

Reviewer #2

Authors have investigated the electronic structure of iron-based superconductor RbFe₂As₂ using ARPES and DFT+DMFT and argued that the ‘two kinks’ – kinks of electronic dispersion at relatively low- and high-energy, respectively – can be primarily electronic-correlation-induced and possible importance of the coincidence of the kink and spin fluctuation energy scales. While the kink structure of electron dispersion at a few tens of meV low-energy range (as well as high-energy kink) is ubiquitously observed in strongly correlated normal metallic states of unconventional superconductors such as cuprates, ruthenates, and iron-based superconductors, the origin of kink structure and its possible role in the superconducting pairing mechanism is still on debate.

In this context, the authors investigated the low-energy electronic structure of RbFe₂As₂ using ARPES and DFT+DMFT complementarily and found out that the DFT+DMFT calculation could precisely reproduce the observed two kink structures and their energy scales by implementing only the electronic origins, which possible role of spin fluctuation (as concluded in the manuscript) in 122 compound family.

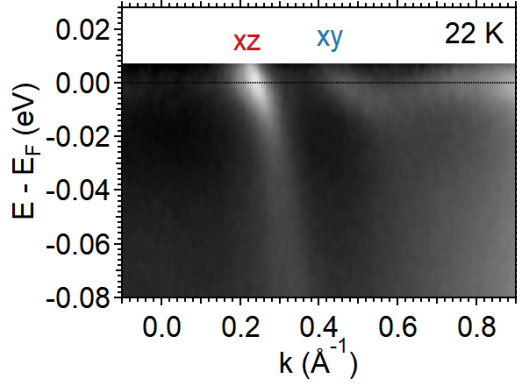
We support the significance of this work, but it would be beneficial to provide additional clarification on the analysis in the manuscript and supplemental materials to ensure that readers can fully understand the authors’ study. We recommend the publication of this manuscript, upon appropriate responses to the following questions and comments.

We appreciate the suggestions by the Referees to provide a comprehensive picture of our study to readers. Accordingly, we implemented the suggested changes and provide further details below.

1. Adding some content would help to ensure a comprehensive understanding of the DFT+DMFT calculation results.

A. What is the distribution of Fe d orbitals in DFT and DFT+DMFT fat bands? Could the authors also show the total band structure? Do other orbitals exhibit similar phenomena as the xz band?

We added a complete set of DFT and DMFT calculations into the Supplementary information (Figure S1, S2). Indeed, the kinks observed in the xz orbital appear in other orbitals as well within our DMFT calculations. The xz orbital provides us with the best case to study the kinks. In particular, the experimental geometry at the ARPES end station at SSRL can be chosen such that we predominantly and strongly photoemit from xz without substantial interference from other orbital contributions around Gamma. In addition, the xz hole band provides an advantageous band dispersion with a large band width to clearly see both kinks in ARPES and in DMFT. Below is an ARPES spectrum that contains both the xz and xy hole band. One can see a similar kink-like feature in the xy band, however the overall intensity of the band is very weak. Therefore, we cannot perform such an in-depth analysis of the ARPES data for the xy orbital as we carried out for the xz orbital in the manuscript.



B. It seems that the xz bands are almost fully filled. How is the condition of the Hund correlation effect satisfied?

From the shown spectra it indeed might appear that the xz band is almost filled, but this is misleading because it only shows a small part of the Brillouin zone. In fact, integrating the electronic charge over the full Brillouin zone results in a filling close to half-filling (0.59) for the xz orbital, and similar values for the other Fe 3d orbitals. When comparing to the filling from the DFT calculation, we indeed find that the filling is pushed closer to half filling by the electronic correlations, indicative of Hund's correlation physics trying to maximize the spin.

We have added a table comparing the fillings from DFT and DMFT with a discussion in the supplementary material.

C. In Fig. 1e, the authors presented atomic model results to designate the characteristics of Hubbard multiplet bands, which seems opposite to our usual expectation that the ground state should have the largest weight. How are the spectral weights obtained? Since the authors performed calculations using CTQMC, the atomic state probability would be more straightforward to compare with DMFT EDC in Fig. 1d.

The atomic model is a basic description of electron removal states of an atomic configuration, i.e. it serves as an approximation of the real system in the limit of strong interactions, where the hybridization with the atomic environment is negligible. As such, it does not include metallic quasiparticle-like excitations around the Fermi level. We calculate the spectral weights by diagonalizing the atomic Hamiltonian and calculating the spectral function from the Green's function in Lehmann representation

$$G_{ab}(\omega) = \frac{1}{Z} \sum_{n,m} (e^{-\beta E_n} + e^{-\beta E_m}) \frac{\langle n | c_a | m \rangle \langle m | c_b^\dagger | n \rangle}{w + i\delta + E_n - E_m}$$

where Z is the partition function, a, b labels the orbital index, and the sum is performed over the n, m Eigenstates of the atomic Hamiltonian. As the system does not hybridize with an environment, it does not show a metallic ground state. But it includes the full set of atomic multiplets, i.e. the spectral satellite features that correspond to the Hubbard bands in the DFT+DMFT calculation. Therefore, we use it only to identify possible Hubbard peaks in the spectral function.

2. Regarding the comparison of three-peak structure between ARPES and DFT+DMFT, in Fig. 1b and 1d, unlike the EDC curve from the ARPES spectrum, which shows dominant QP weight near zero frequency

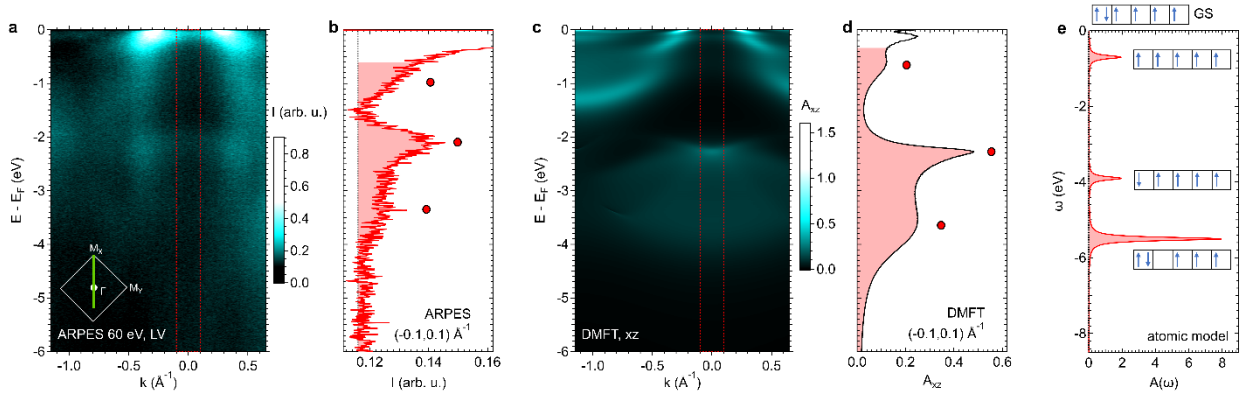
and relatively small Hubbard bands (HB) weight at around -2.5 eV, DFT+DMFT shows strong suppression of the overall QP weight, so it could be quite far from the Hund regime.

A. Similarly, how can we understand the strong suppression of DMFT EDS at zero frequency in Fig. 1d?

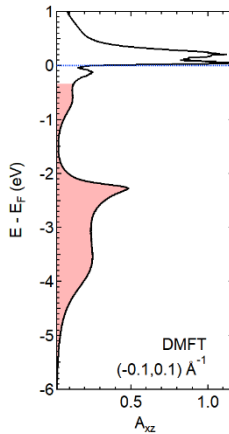
Indeed, the EDC in Fig. 1d, which is derived from the DMFT spectral function, does not contain a large quasiparticle peak below the Fermi level. The reason is the momentum integration window $(-0.1, +0.1)\text{\AA}^{-1}$ chosen for this EDC. Here, the quasiparticle peak is centered at an energy above E_F . We show below a plot of the EDC from Fig. 1d but extended to a larger energy range to illustrate this point. The momentum integration window is the same for ARPES (Fig. 1b) and DMFT (Fig. 1d). The quasiparticle peak is broader in ARPES than in DMFT and therefore appears in the EDC in Fig. 1b. In the revised version of the manuscript, we added boxes to Fig. 1a and Fig. 1c to highlight the integration window.

In general, a suppression of spectral weight in a small part of momentum range does not imply that the system is far away from the Hund's regime, as the correlations induced via Hund's physics is a local correlation effect. The data shown comprises only a small momentum window around Gamma, so it is not indicative for the strength of Hund's correlations.

Figure 1 from the manuscript:



Extended energy range for Fig. 1d:



Reviewer #3

The present work reports ARPES and DMFT study of the hole-doped iron-based superconductor RbFe₂As₂. They mainly focus on the two kink features observed on the ARPES band dispersions near EF. By a systematic comparison with the DMFT calculations, these kinks are suggested to originate from the strong electron correlations. The manuscript is clearly written, the good agreement between ARPES and DMFT well supports the authors' arguments and conclusions. I believe the presented results provide important information for the understanding of unconventional superconductivity and other emergent phenomena in the strongly-correlated iron-based superconductors. Before I can recommend the publication in Nature Communications, I would like the authors to address the following comments and questions:

1. In Fig. 2, instead of the FWHM of MDCs, I suggest to present the imaginary part of the self-energy; accordingly, a comparison with the real part of the self-energy would increase the readability of the manuscript.

The real and imaginary part of the self-energy are a product of our DMFT calculations and we present them in the Supplementary Figure S3. To extract the self-energy from ARPES involves the assumption of a bare band dispersion. This is a non-trivial task and is approached in various ways in literature. Two common strategies are approximating the bare band by the high-temperature data or by a linear or parabolic band. The combination of ARPES and DMFT in our work offers us a unique way of directly comparing experiment and theory: Since DMFT provides the spectral function, we can use the same MDC fitting routines as we do for ARPES and avoid the extra assumption of a bare band. Instead of comparing the real and imaginary part of the self-energy, we therefore chose to compare the dispersion and FWHM in the main text of the manuscript. We believe that this type of direct comparison adds to the strength of the presented work.

We described the reason for our approach in the main text as follows: “Typically, a self-energy is extracted from such an MDC analysis to compare with theoretical predictions. It requires the assumption of a bare-band dispersion, which would need to extend over more than 0.5eV in our analysis and certainly involves a-priori unknown non-linear contributions. To circumvent this ambiguity, we instead perform the same MDC analysis on the spectral function obtained from our DFT+DMFT calculations as we did for the ARPES data.”

In the revised version, we extended Figure S3 in the Supplementary information, which now also shows the self-energy derived from our ARPES data using a linear approximation of the bare band dispersion. This approach allows us to identify kink signatures, but absolute values as well as values of the slope will be affected by the precise choice of the bare band. We added the sentence “A complementary self-energy analysis of the ARPES data can be found in the Supplementary Material [54].” into the main text that guides readers to the self-energy analysis in the supplement.

2. To demonstrate the orbital characters of the concerned bands, the geometry of the experiment is suggested to be further clarified, and the ARPES matrix element analysis should be included.

We added a graph of the ARPES photoemission matrix elements for the present geometries in Supplementary Figure S5. We added the sentence “A sketch of the geometry and calculations of the photoemission matrix elements [81–83] can be found in the Supplementary Material [54]” into the Methods

section of main text to guide the reader to this additional material. The matrix element calculations were performed in the length gauge using the approximation of a free electron removal state and Fe3d hydrogen-like wave functions as initial states. A sketch of the photoemission geometry was included in the same Figure.

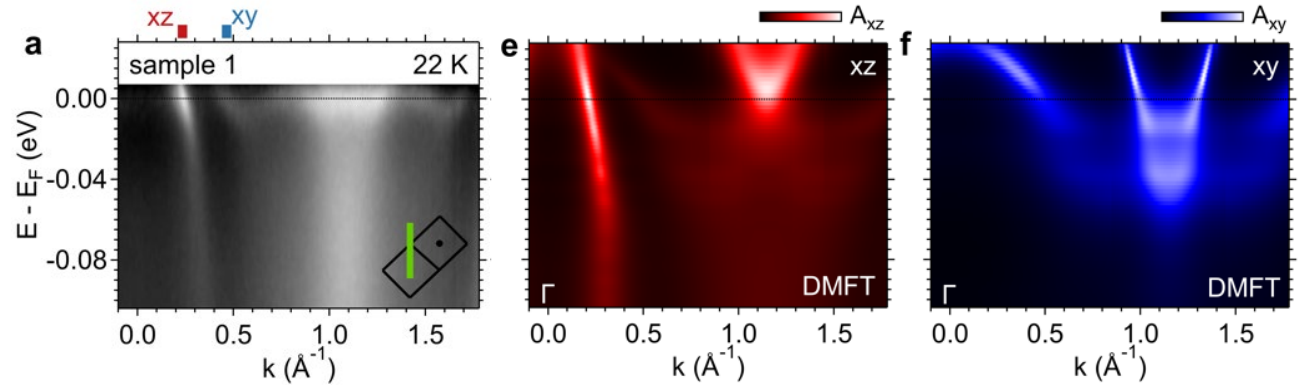
3. What is the momentum dependence of these two kinks? Also, the momentum direction of the cut in Fig. 2a needs to be clarified.

While the momentum dependence of the kink is certainly extremely interesting, such a study goes beyond the present work. The main focus here is identifying the existence of the kinks and their origin.

We included sketches of the Brillouin zone and added labels for high symmetry points into Fig. 1a, 2a, 3b.

4. Are the similar two kink features observable on the band dispersions around the zone corner?

This would indeed be very interesting. However, the electron bands at the zone corner are very shallow in RbFe2As2. Below are the ARPES (a) and the DMFT (e,f) spectral functions around the Brillouin zone corner. A dip in the intensity of the spectral function is visible for the xy electron band in DMFT and in ARPES. However it is not feasible to perform an MDC analysis in the same detail as in the main manuscript.



5. In page 4, to estimate the electron-phonon coupling strength, instead of using the change of band velocities, more comprehensive Eliashberg function analysis with calculating both the real part and imaginary part of the self-energy should be performed.

From the ARPES point of view, the most common analysis in literature to obtain an estimate for the strength of electron-boson coupling is a comparison of the velocities above and below the kink. We therefore chose this metric to compare to literature data. In general, an analysis within an Eliashberg function formalism is certainly desirable, but it requires a derivation of the self-energy with the same caveats as described above.

From the theoretical perspective, solving the Eliashberg equation is computationally already quite demanding for a one orbital system, especially when a lot of Matsubara frequency points are needed. Solving the Eliashberg equations for a realistic 5 orbital system like the one we investigated here, would be an extremely challenging task, requiring significant further numerical developments and improvements, and would be out of the scope of the current manuscript.

We believe that our analysis from the band velocities suffices to provide a qualitative estimate. We leave a more elaborate analysis via the Eliashberg formalism for a future work.

Reviewer #4

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Response to the Referees

We thank all referees for their time to review our manuscript and for their valuable comments. We reply to them below and changed the manuscript accordingly.

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Minor points:

1. For the self-energy derived from the ARPES data (Fig. S3d,e), I suggest to use the real part and imaginary part of the self-energy for the labels, as in Fig. S3a,b.

We added the connection between the self-energy and the plotted experimental quantities explicitly into the caption of the figure.

2. In the section DMFT SPECTRAL FUNCTION FOR ALL 3d ORBITALS: "(a) to (e)" --> "(b) to (f)"; "(f)" --> "(a1) and (a2)".

We corrected the Figure labels in the supplementary text.

Reviewer #4

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