Electronic dispersion anomalies in the iron pnictide superconductor \(\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2\)

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The pairing mechanism in the iron-pnictide superconductors is still unknown. However, similarities to the cuprate high-temperature superconductors suggest that a similar mechanism may be at work. Recently, careful experimental studies of the spin excitation spectrum revealed, like in the cuprates, a strong temperature dependence in the normal state and a resonance feature in the superconducting state. Motivated by these findings, we develop a model of electrons interacting with a temperature dependent magnetic excitation spectrum based on these experimental observations. We apply it to analyse angle resolved photoemission and tunnelling spectra in \(\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2\). We reproduce in quantitative agreement with experiment a renormalisation of the quasiparticle dispersion both in the normal and the superconducting state, and the dependence of the quasiparticle linewidth on binding energy. We estimate the strength of the coupling between electronic and spin excitations. Our findings support the possibility of a pairing mechanism based dominantly on such a coupling.

Shortly after the discovery of high-temperature superconductivity in Fe-based pnictide compounds,\(^1\) a magnetic Cooper-pairing mechanism was proposed\(^2\), while electron-phonon interaction as primary pairing mechanism was found to be unlikely\(^3\). This conjecture is supported by the proximity of antiferromagnetism and superconductivity in the phase diagram\(^4\)\(^5\). The spin excitation spectrum in pnictides shows pronounced similarities with other superconductors where a magnetic pairing mechanism is under debate. In particular, the strong temperature dependence of the normal state spin excitations studied recently by Inosov et al.\(^9\), as well as the presence of a spin resonance feature in the superconducting state\(^10\) are prominent features also present in cuprates, as well as in some heavy fermion superconductors.

Furthermore, angle resolved photoemission (ARPES) measurements reveal a sharp Fermi surface consisting of electron-like and hole-like pockets that exhibit comparable superconducting order parameter amplitudes and are nearly nested by the antiferromagnetic wave vector \(Q\)\(^11\)\(^12\), a reason to believe that magnetic and electronic order are closely connected\(^13\). This raises the question how strongly electrons couple to spin fluctuations, as those lead to an effective electron-electron attraction, if the order parameter changes the sign on the different pockets\(^14\)\(^16\). Investigating the low energy dispersion anomalies, whose position and shape can be traced back to a coupling of bosonic modes, has proven to be a powerful method for obtaining this information\(^17\)\(^19\). Recent experimental studies on the superconducting state spectral function of \(\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2\) measured by ARPES find such an anomaly, which appears as a kink in the dispersion relation at about 25 meV\(^19\). On the other hand, inelastic neutron scattering (INS) studies of this compound reveal the development of a resonant spin excitation in the superconducting state\(^10\). The temperature dependence of both neutron intensity and the self-energies extracted from ARPES follow an order parameter like evolution. This strongly indicates that the spin resonance indeed accounts for the observed anomaly.

Below, we present a theoretical model that explains the anomalous features in the dispersion relation by a coupling of electrons to a spin fluctuation spectrum that (a) reproduces the experimentally observed temperature dependent spectrum in the normal state and (b) features a low energy resonance in the superconducting state. We show that coupling to such a spin-fluctuation spectrum leads to a renormalisation of the quasiparticle dispersion even in the normal state and can account for the renormalisation factor necessary to match density functional theory (DFT) calculations to experiment. Furthermore, taking into account the resonance in the superconducting state, we are able to quantitatively reproduce experimental ARPES results, including low-energy and high-energy renormalisation of the dispersion and the energy dependence of the quasiparticle linewidth. Our theoretical SIN tunnelling spectra obtained for the same parameter set are consistent with recent experimental observations that show an asymmetric lineshape of the tunnelling conductance\(^20\).

**Spin fluctuation spectrum and resonance mode**

The appearance of a resonance in the dynamic magnetic susceptibility upon entering the superconducting state is well known from cuprate superconductivity. It is situated at an energy below the particle-hole continuum and is peaked around the antiferromagnetic wavevector.
Although there are various theoretical models for the spin-spin response function, here we prefer to not rely on a specific theoretical model, but rather use a semi-phenomenological approach where the spin susceptibility near the antiferromagnetic wavevectors \( q \in \{ Q_{1}, Q_{2} \} \) can be described by the Ornstein-Zernicke form

\[
\chi(q) = \frac{\chi_0(T + \theta)}{1 + \xi_q^2 |q - Q_\alpha|^2},
\]

where \( \chi_0 = \chi_0(T + \theta) \) controls the strength of magnetic correlations, \( \Omega_{max} \) sets the typical spin-fluctuation energy scale, \( \xi_q = \xi_0 \sqrt{T + \theta} \) is the magnetic correlation length and \( \theta \) is the Curie-Weiss temperature.

With decreasing temperature, spectral weight is shifted towards lower energies. Below \( T_c \) the spectrum becomes gapped and a resonance appears at an energy that follows approximately an order parameter like evolution, i.e. \( \Omega_{res}^T = \Omega_T \sqrt{1 - T/T_c} \). In order to model the quasiparticle continuum below the quasiparticle continuum we assume a (sharply peaked) Lorentzian in energy and a separable form for the momentum dependence,

\[
\chi_{r,n}(\omega,q) = \frac{w_{n}(q)}{\pi} \frac{2\Omega_{res}^T}{(\Omega_{res}^T)^2 - (\omega + \Gamma_{res}^T)^2},
\]

with the weight functions

\[
w_{n}(q) = \sum_{\alpha=1,2} b_{n,\alpha} \frac{w_T(q)}{1 + \xi_q^2 |q - Q_\alpha|^2}.
\]

In order to take care of the periodicity in reciprocal space we replace the factors \(|q - Q_\alpha|^2\) in Eqs. (1) and (3) by \(4|\sin^2(\frac{q_x}{2} - \frac{Q_{1,x}}{2}) + \sin^2(\frac{q_y}{2} - \frac{Q_{1,y}}{2})|\), and we neglect the dependence on \( q_z \) for our purpose as it varies weakly [21, 22]. The resulting momentum dependence at the resonance energy is shown in Fig. 1(b), with the two antiferromagnetic wavevectors \( Q_1 = (\pi, 0) \) and \( Q_2 = (0, \pi) \). These wavevectors connect Fermi surface sheets with same orbital character (\( n = 1,2 \cdots 5 \) corresponding to...
the five Fe orbitals \(d_{xz}, d_{yz}, d_{xy}, d_{x^2-y^2}, d_{3z^2-r^2}\), as illustrated in Fig. 1(a). In our model we consider only the main orbital contributions to quasiparticle scattering resulting from the \(n = 1, 2, 3\) orbitals and describe the different momentum variations with the help of the parameter \(b_{n,α}(= 1/2 \text{ for } nα = 11, 22, 31, 32 \text{ and } = 0 \text{ else})\).

For the gapped continuum (in the absence of detailed experimental data) we make the approximation that for \(ω\) above a temperature dependent continuum threshold, \(ω > 2\Delta(T)\), it is identical to its normal state value, Eq. 1, at the respective temperature. We note that this approximation is excellent except possibly close to the continuum threshold. Here, \(Δ\) is the mean superconducting gap at the nested Fermi surfaces. Thus, denoting the imaginary part \(\text{Im}\chi\) of the retarded dynamical susceptibility with \(\chi''\), we approximate the superconducting state spectrum of the susceptibility by

\[
\chi''_{sc,n}(ω, q) = \begin{cases} 
\chi''_{n}(ω, q) \quad |ω| < 2\Delta \\
\chi''_{c,n}(ω, q) \quad |ω| ≥ 2\Delta 
\end{cases}
\]

and calculate the real part by exploiting Kramers-Kronig relations. In order to reduce the number of parameters we employ a local sum rule to determine the ratio between resistance and continuum part, \(w_T/\chi_T\). It is chosen so that the energy and momentum integrated spin structure factor, \(\int_{-∞}^{∞} dω \int d\mathbf{q} S(\mathbf{q}, ω)\), with \(S(\mathbf{q}, ω) = 2\hbar \chi''(q, ω)/(1 – e^{-\hbar ω/κ_BT})\) remains temperature independent in the normal as well as the superconducting phase (for technical details see the Methods section). The overall weight \(\chi_0\) will be combined with the coupling constant \(g\) below, and it is only the combined quantity \(g^2\chi_0\) that is of relevance for our results. However, as discussed below, from experimental values of \(\chi_0\) and from a determination of the fit parameter \(g^2\chi_0\) an estimate of the coupling constant can be obtained.

We apply this model to hole-doped \(\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2\), where data are available both for spin excitations as well as for electronic excitations, and where also the most detailed experimental angle resolved photoemission data exist. In FIG. 1(a) the momentum and energy dependence for the parameter set in TABLE 1 is presented. The resonance in the spin excitation appears at an energy \(\Omega^*_c ≈ 14 \text{ meV}\) below the quasiparticle continuum \(ω < 2\Delta(15K) ≈ 24 \text{ meV}\) [11]. In momentum space the mode is peaked around the wave vectors \(\mathbf{Q}_1 = (π, 0, q_z)\) and \(\mathbf{Q}_2 = (0, π, q_z)\) with correlation length \(ξ_r\) of nearly twice the lattice constant [FIG. 1(b)]. The momentum dependence in \(z\)-direction is assumed to vary weakly as motivated by [21][22].

### TABLE I: Parameter Set used for \(\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2\)

| Parameter | Value |
|-----------|-------|
| \(w_T/\chi_T\) | 15.6 meV |
| \(Ω_c\) | 0.375 meV |
| \(T^*\) | 2 K |
| \(Δ\) | 15.5 meV |
| \(Γ\) | 3 meV |

Comparing the energy-momentum distribution in the normal and the superconducting state [FIG. 1(c)], we see that low-energy spectral weight is shifted into the resonance when the continuum gap opens below \(2\Delta\). In addition, the sharpened momentum distribution leads to an enhancement of the resonance spectral weight. In FIG. 1(e) we show the numerically calculated ratio \(w_T/\chi_T\), which features this evolution and is in excellent agreement with the functional form \(w_T/\chi_T = w_T/\chi_T\) [\(1 = T^2/T^2\)]. As we will see later on, such a modelling will lead to an effect on the electronic dispersion that fits well with experimental observations.

### Coupling to spin fluctuations

We are interested in the renormalisation of the fermionic dispersion as a result of the coupling of electrons to the spin fluctuation mode. The idea is to extract the influence of the resonance by comparing the superconducting and normal state dispersion from which self-energy effects are directly inferred. This allows for an immediate comparison with experiment. Following the approach for the cuprates [17], one could assume that the momentum dependence in Eq. 1 and Eq. 2 exclusively chooses the Fermi surface sheets that are coupled by the mode. However, fluctuation exchange (FLEX) approaches have shown that the magnetic mode predominantly scatters between states with the same orbital character [27][28].

To take this into account, we employ a tight-binding fit in orbital basis which was obtained from the DFT band structure of \(\text{BaFe}_2\text{As}_2\) by Graser et al. [26]. Details are discussed in the Methods section.

In FIG. 1(a) we show the bare Fermi surface for \(k_z = -π, -π/2\) and 0, corresponding to a bc tetragonal unit cell and the I4/mmm symmetry of the crystal. The hole pockets at \((0, 0, k_z)\) and \((π, π, k_z)\) are nearly nested to each other. The electron pockets at \((0, π, k_z)\) and \((π, 0, k_z)\) by the wave vectors \(\mathbf{Q}_1\) and \(\mathbf{Q}_2\), even when taking into account the orbital characters [23][28]. We couple electrons to the spin fluctuation spectrum with a coupling constant \(g\), which is assumed to be independent of energy, momentum and orbital number.

In ARPES experiments the intensity of photo electrons is proportional to \(f(ε)A(ε, k)\), where \(f\) is the Fermi distribution function. Dispersions obtained from those usually differ from DFT calculations by an renormalisation factor of 2 [22][31]. In the upper panel of FIG. 2 we present the influence of a coupling to spin fluctuations in the normal state. It shows an intensity plot of the spectral function \(A(ε, k)\) along a cut in the 1st Brillouin zone, obtained numerically as explained in the Methods section. The band maxima and minima as well as the Fermi velocity very well align with experimentally observed values [29]. By choosing the coupling constant \(g\) to be the same for all orbitals the band curvature becomes strongly enhanced leading to the observed...
FIG. 2: **Electronic spectral intensity.** On top: spectral function in the normal state for $T = 50\, K$ along a cut in the 1st Brillouin zone for $k_z = 0$. At bottom: the same for the superconducting state at $T = 15\, K$ for the square regions indicated (a) and (b) in the top panel. The black lines show MDC-derived dispersions for the (a) $\alpha_1$ and $\alpha_2$ band and the (b) $\beta_1$ band. At the lower right the renormalised Fermi surfaces including the group notations are shown.

shallow electron pocket at the $X$-point. One clearly sees that the bands are bent by a factor $1.5 - 2$ and that the quasiparticle width increases with energy. Thus coupling to spin fluctuations gives an essential contribution to the above mentioned renormalisation factor. However the Fermi surface remains nearly unaffected as can be seen by comparing the Fermi surface at 50K on the right bottom of FIG. 2 with the bare one in FIG. 1(a).

**Superconducting order**

The origin of the pairing instability may well be related to the spin fluctuation continuum, as demonstrated by a recent FLEX calculation [23]. Our model is restricted to the low energy region in the spin excitation spectrum, and does not precisely treat the incoherent high-energy part. However, this part considerably contributes to pairing, whereas the energy range of interest here ($|\omega| < \omega_c = 200\, \text{meV}$) gives only a partial contribution (about 40-50%) to the value of the superconducting order parameter. Thus, we add in our theory a contribution $\Delta_k$ to the order parameter that results from the incoherent high-energy part of the spin-fluctuation spectrum beyond 200 meV.

The order parameter is chosen to have an $s^\pm$-symmetry (here and in the following the unit of length is the in-plane lattice constant $a$)

$$\Delta_k(T) = \Delta_0(T) \cos(k_x) \cos(k_y). \quad (5)$$

This pairing state is supported by experiment as well as numerical calculations [11, 12, 24–26]. The magnitude of the superconducting gap was observed to be $\Delta(15K) \approx 12\, \text{meV}$ at the inner hole-like pocket as well as the corresponding nested pockets [11, 12]. We choose $\Delta_0$ in Eq. (5) so that the renormalised gap reaches the experimentally observed value at these particular points in the Brillouin zone, which gives $\Delta_0(0) = 18.1\, \text{meV}$. The renormalised gap is obtained by taking into account a renormalisation factor as discussed in the Methods. For the temperature dependence (in the absence of detailed data) we assume the form $\Delta_0(T) = \Delta_0(0) \sqrt{1 - T/T_c}$.

**Dispersion and linewidth: self-energy effects**

In the superconducting state the dispersion features in FIG. 2(a) are modified due to (a) the appearance of the superconducting gap, and (b) the modifications in the spin excitation spectrum that is coupled to the conduction electrons. In the lower panel of FIG. 2 extracts from the hole-like and electron-like pockets at the $\Gamma$- and $X$-point are presented for 15 K, well in the superconducting state. At first glance the intensity plots show no clear hint of the bosonic resonance, in contrast to the eye-catching break features in the cuprates [32]. In order
to extract a quantitative effect we need to analyse differences between the dispersions and linewidths in the normal and superconducting state in detail.

Because in the case of pnictides multiple orbitals are involved in the electronic spectra, the linewidth function and the renormalisation of the dispersion cannot be related in an easy way to theoretically obtained self energies as it has been possible in the case of the cuprates. For this reason we follow here a different path and extract quantities from theoretically obtained spectral functions exactly as they are extracted in the ARPES experiments [18, 19] from measured spectra. For fixed energy the momentum dependence of the spectral function (a so-called momentum distribution curve, or MDC, see inset to FIG. 3) is peaked, with the peak often well approximated by a Lorentzian. If the self energy does not vary much as a function of momentum over the width of such an MDC peak, the MDC spectral function is of the form

$$A_r(k) = \frac{1}{\pi} \frac{\Sigma''(\epsilon)}{(\epsilon - \epsilon_r(k))^2 + (\Sigma''(\epsilon))^2},$$  \hspace{1cm} (6)$$

where $k_r$ determines the maximum point of the MDC, and $v_r = (\partial \epsilon_r / \partial \epsilon)^{-1}$ [33]. In the bottom panel of FIG. 2 we show dispersions obtained from MDC maxima of the $\alpha_{1,2}$ and the $\beta_1$ band as black curves. Furthermore, we obtain the linewidth in analogy to experiment by fitting a Lorentzian to the theoretically obtained ARPES spectra.

We now discuss the thus obtained quantity $\Sigma''(\epsilon) \equiv \Sigma''(\epsilon, k_r)$ that determines the linewidth of the MDC. Assuming that it weakly depends on momentum in a small region around $k_r$ it is given by $\Sigma''(\epsilon, k_r) \approx v_r \delta k_r$, and $\delta k_r$ is the full width at half maximum (FWHM) of the Lorentzian in reciprocal space in direction of $v_r$. We underline that it is impossible to distinguish between the calculated self-energy $\Sigma''(\epsilon)$ for the $n^{th}$ orbital, as discussed in the Methods, and the experimentally motivated quantity $\Sigma''(\epsilon)$ extracted by fitting a Lorentzian to the theoretically obtained ARPES spectra. Since the Green’s function matrix in orbital space cannot be inverted analytically there is no simple correspondence between the two quantities above. We will call the experimentally motivated quantity $\Sigma(\epsilon)$ imaginary part of the effective self energy below.

As can be seen in FIG. 3 the imaginary part of the effective self-energy exhibits a linear dependence for higher energies, i.e. $\Sigma''(\epsilon) \propto \epsilon$, consistent with marginal Fermi liquid theory [34]. This results from the coupling to the continuum, in particular from the slow decay of the spin fluctuation spectrum towards high energies. We note that the correct magnitude of the linear in $\epsilon$ high-energy part of $\Sigma''(\epsilon)$ restricts the coupling strength $g^2 \chi_0$. We are able to reproduce the experimental observations [19] with a coupling strength $g^2 \chi_0 = 1.17 \times 10^3 \mu_B^2 \text{eV K}$. With this, all parameters of the theory are fixed by the high-energy behaviour of the electronic spectra, and consequently the magnitude of all low-energy features are true predictions of the theory.

The spin resonance leads to a hump feature in $\Sigma''(\epsilon)$ for excitation energies between 20 – 30 meV at the $\alpha_2$-band, which is apparently observed in experiment [19]. This feature is washed out in the $\alpha_2$-band. However the actual position of the resonance can not be obtained from such a vague energy range. In order to give a convincing quantitative statement, one has to consider the modification of the dispersion upon entering the superconducting state, which we do now.

The values $k_r$ determine an MDC-derived dispersion $\epsilon = \epsilon_{k_r}$, as can be seen as black curves in FIG. 2(a) and (b). The modification of the bare dispersion $\xi_k$ to $\epsilon_k$ can be expressed in terms of the real part of the effective self-energy, $\Sigma'$, that is defined by $\epsilon_k = \xi_k + \Sigma'(\epsilon_k, k)$. The bare dispersion is not a measurable quantity. However, as the bare dispersion is temperature independent, any changes of $\Sigma'(\epsilon_k, k) \equiv \Sigma_k'$ with temperature can be extracted experimentally by taking the difference between two MDC-derived dispersions at fixed $k$, provided again the momentum dependence of the self energy is weak. Comparing the normal and superconducting state dispersion, the influence of the resonance can then be quantified using e.g. the relation

$$\Sigma_k'^{15K} - \Sigma_k'^{50K} = \epsilon_k^{15K} - \epsilon_k^{50K}. \hspace{1cm} (7)$$
the β respectively inset feature a broad maximum at shown. The real part of the effective self energies in the as well as a peak at lower energies. This peak appears due to coupling to the resonance at energy ∆

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FIG. 4: MDC-derived dispersions, obtained from the cen-
tres of the Lorentzian fits as shown in the inset of Fig. 3 of the α₁ (red) and α₂ (green) band as well as the β₁ band (magenta) in the superconducting state at T = 15 K. The blue curves are the dispersions in the normal state at T = 50 K respectively. The insets show the real part of the effective self energy Σ′(ε) = Σ′(ε, k). For temperature dependent results see Fig. 9.

It is common to plot Σ′(ε) = Σ′(ε, k) − Σ′(ε, k) for a given reference temperature Tref well inside the normal phase.

In FIG. 4 the MDC-derived dispersions of the α₁,₂ and the β₁ band in the normal and superconducting state are shown. The real part of the effective self energies in the respective inset feature a broad maximum at ≈ 50 meV as well as a peak at lower energies. This peak appears due to coupling to the resonance at energy ΔQ + Ω, where ΔQ is the gap at the corresponding Fermi surfaces that are nested by an antiferromagnetic wavevector. The shape as well as the absolute value of the real part of the effective self energy agree with experimental data [18, 19].

Tunnelling spectra
Another useful tool to obtain information on the density of states (DOS) is the scanning tunnelling spectroscopy (STS). Apart from the magnitude of the superconducting gap, also features due to the interaction with spin excitations can be expected [17]. Since we calculate the spectral function in the en-
tire Brillouin zone, the evaluation of tunnelling spec-
tra of superconductor-insulator-normal metal (SIN) and superconductor-insulator-superconductor (SIS) tun-
nelling junctions is straightforward. The SIN tunnelling current I(V) is given by

\[ I(V) = \sum_{k} |M_k|^2 \int_{-\infty}^{\infty} \frac{dc}{2\pi} A(\epsilon, k)[f(\epsilon + eV) - f(\epsilon)]. \] (8)

For incoherent (momentum non-conserving) tunnelling we assume a constant |M_k|^2 = |M_0|^2. The results for the differential SIN tunnelling conductance \( \rho_{SIN} = dI/dV \) is shown in the top panel of FIG. 6 for varying coupling strength. With increasing coupling constant a dip-hump structure develops and weight is shifted into the peak at the occupied side. Furthermore, the hump position moves towards the chemical potential. Analogously to the cuprates, coupling predominantly influences the occupied side [17, 31].

For a SIS junction and the case of incoherent single particle tunnelling we have with \( A(\epsilon) = \sum_{k} A(\epsilon, k) \)

\[ I(V) = |T_0|^2 \int_{-\infty}^{\infty} \frac{dc}{2\pi} A(\epsilon, k) A(\epsilon + eV)[f(\epsilon) - f(\epsilon + eV)]. \] (9)

and again calculate the differential tunnelling conduc-
tance dI/dV, which is shown in the bottom panel of FIG. 6. Due to the symmetry of Eq. 9, the dip-hump feature is now strong on both sides.

However, in both junctions we see no well pronounced dip for the coupling strength \( g^2 \chi_0 = 1.17 \times 10^3 \mu_B^2 \) eV K which is the value we obtain from our comparison with ARPES experiments.

Discussion
From the knowledge of the experimental value of \( \chi_0 \) it is possible to extract the coupling constant g. This value is not known for Ba₁₋ₓKₓFe₂As₂, however it has been determined for optimally doped BaFe₁₅Co₀₁₅As₂ [31]. In order to obtain a rough estimate of the coupling constant g, we insert this experimentally determined value \( \chi_0 = (3.8 \pm 1.0) \times 10^4 \mu_B^2 \text{eV}^{-1} \) and obtain \( g \approx 0.15 - 0.2 \) eV. We also have performed extended calculations of the temperature dependence of the self energy effects discussed above, which are presented in the appendix. From our results we conclude that the experimentally observed modifications of the electronic dispersion when entering the superconducting state can be explained within a model where a continuum of strongly incoherent high-energy spin fluctuations provide the pairing interaction, whereas the low-energy spin-fluctuation modes lead to the observed electronic dispersion features. The coupling strength that is required to explain the experimental data is large enough to allow for a magnetic pairing scenario in iron-pnictide superconductors.
The largest contribution to the density of states comes from the DFT band structure of BaFe$_2$As$_2$. Here we assume that the set of five eigenvectors for each $k$ is orthonormal,

$$\sum_{\mu,n} a_{\mu n}^m(k) a_{\mu n}^m(k') = \delta_{mn},$$

and completeness,

$$\sum_{\mu,n} a_{\mu n}^m(k) a_{\mu n}^m(k') = \delta_{mn}.$$  

In order to simulate hole doping we apply a rigid shift of the chemical potential by an amount of $\delta \mu_c = -50 \text{meV}$. This leads to the appearance of additional hole pockets around $(\pi, \pi, k_z)$ that favour an $s^\pm$-state.

The unperturbed Green’s function is diagonal in band index, with normal (diagonal) and anomalous (off-diagonal) components $G^{(0)}_{\mu\nu}(\epsilon, k)$ and $F^{(0)}_{\mu\nu}(\epsilon, k)$. The renormalised Green’s functions, $G_{\mu\nu}$ and $F_{\mu\nu}$, are not diagonal in band index due to interband interactions introduced by spin fluctuations. The Green’s functions in an orbital basis, $G_{mn}$ and $F_{mn}$, are related to those in a band representation, $G_{\mu\nu}$ and $F_{\mu\nu}$, by

$$G_{mn}(\epsilon, k) = \sum_{\mu,\nu} a_{\mu n}^m(k) a_{\mu n}^m(k') G_{\mu\nu}(\epsilon, k),$$

$$F_{mn}(\epsilon, k) = \sum_{\mu,\nu} a_{\mu n}^m(k) a_{\mu n}^m(-k) F_{\mu\nu}(\epsilon, k).$$

Note that due to $\xi_{mn}(-k) = \xi_{mn}(k)^*$ the eigenvectors can be chosen such that $a_{\mu n}^m(-k) = a_{\mu n}^m(k)^*$ holds.

Magnetic excitations can be described in terms of the dynamic spin susceptibility $\chi_{\mu\nu}^{mn}$, where the measured susceptibility $\chi$ is the sum over all orbital contributions $\chi = \sum_{mn} \chi_{\mu\nu}^{mn}$ [25]. Since the magnetic susceptibility is in particular enhanced for intra-orbital coupling [25], we assume that the elements $\chi_{\mu\nu}^{mn}$ of the susceptibility dominate, neglect in our model all inter-orbital contributions, i.e. $\chi \approx \sum_{mn} \chi_{\mu\nu}^{mn}$, and take only those orbitals into account where the coupling is most pronounced ($n = xy, yz, xy$). The neglected contributions have a small spectral weight in the considered energy range $\omega < 100 \text{meV}$, and are thus nearly unaffected by superconductivity. Taking them into account leads to a simple energy and momentum independent renormalisation of the low-energy electronic spectra (see below). In order to determine the relative weight between $w_{xz} = w_{yz}$ and $w_{xy}$ we studied the behaviour of the electronic dispersion near the X point of the Brillouin zone. We find that experiments are best reproduced when the weight is roughly equal. We thus performed our calculations for $w_{xz} = w_{yz} = w_{xy} = \omega_T$ and $\chi_T^x = \chi_T^y = \chi_T^y = \chi_T^y$. In order to determine the ratio between $\chi_T$ and $\omega_T$ we employ the total moment sum rule for the dynamical structure factor, as the temperature variation of the total moment is negligible. With the above assumptions, we can separate the sum-rule into its orbital parts. Employing the fluctuation dissipation theorem that connects the dynamical spin structure factor with the susceptibility, $S(q, \omega) = 2\pi \sum_{\nu} \chi_{\nu\nu}^{mn}(q, \omega)/(1 - e^{-\hbar \omega/k_BT})$, the ratio $\omega_T/\chi_T$ is determined by the equality

$$\int_{-\Delta}^{\Delta} d\omega \int d^3 q S_{\nu\nu}(q, \omega) = \int_{-\Delta}^{\Delta} d\omega \int d^3 q S_{\nu\nu}(q, \omega),$$

with $S_{\nu\nu}(q, \omega) = 2\pi \hbar \chi_{\nu\nu}^{mn}(q, \omega)/(1 - e^{-\hbar \omega/k_BT})$ and a temperature dependent order parameter $\Delta \propto \sqrt{1 - T/T_c}$. 

Methods

We employ a tight-binding fit in orbital basis that was obtained from the DFT band structure of BaFe$_2$As$_2$ by Ref. 27. The largest contribution to the density of states comes from the five Fe-d-orbitals in the energy region we consider, which allows to reduce the Hamiltonian

$$H_0 = \sum_{k\sigma, m} d_{m}(k) \left[ \xi_{mn}(k) + \delta_{mn} \epsilon_n \right] d_{m}(k\sigma),$$

to this basis. Here $d_{m}(k)$ creates an electron with momentum $k$ and spin $\sigma$ [we denote $k = (k, \sigma)$] in the orbital $m$, where $m = 1 \ldots 5$ corresponds to the five orbitals $d_{xx}, d_{y^2}, d_{xy}, d_{x^2-\Delta^2}, d_{z^2}$. The parameters $\xi_{mn}$ and $\epsilon_n$ are listed in Ref. 27. The chemical potential at zero temperature in the undoped state is at $\mu_c = 0$. The canonical transformation $d_{m}^\dagger(k\sigma) = \sum_{m} a_{m}^\dagger(k) d_{m}^{\dagger}(k\sigma)$, where $a_{m}^\dagger(k) = \langle m|k\mu(k)\rangle$, diagonalises the Hamiltonian, leading to eigenvalues $\xi_{m}(k)$ and eigenvectors $a_{m}^\dagger(k)$, where $\mu$ represents the band index.
We couple electrons to the spin fluctuation spectrum with an energy and momentum independent coupling constant $g$ (instantaneous and local coupling). The retarded diagonal and off-diagonal self-energies are then given by

\[ \Sigma_{mn}^R = \delta_{mn} \Sigma_{nn}^R, \quad \Phi_{mn}^R = \delta_{mn} \Phi_{nn}^R, \]

written in terms of retarded ($R$) and Keldysh ($K$) Green's functions,

\[ \Sigma_n^R = -\frac{i}{2} g^2 \left( G_{nn}^K \chi^R_n + G_{nn}^R \chi^K_n \right), \]
\[ \Phi_n^R = -\frac{i}{2} g^2 \left( F_{nn}^K \chi^R_n + F_{nn}^R \chi^K_n \right), \]

with $(A + B)(\epsilon, k) = \sum_{\omega, q} A(\epsilon - \omega, k - q) B(\omega, q)$ as explained in Ref. [17], and with the diagonal susceptibility, $\chi_n \equiv \chi_{nn}^R$. In the normal and superconducting state the susceptibility is given by $\chi_n = \chi_c$ and $\chi_n = \chi_{sc}$ respectively, where $n = 1, 2, 3$. We calculate the convolutions numerically by fast Fourier transform, using bare Green's functions (a procedure supported by the numerical studies in Ref. [25]) with a broadening parameter $\delta = 4$ meV.

Using the completeness relation $\sum_{\mu} a_{\mu}^m a_{\mu}^m = \delta_{mn}$, we can write the Dyson equation for the renormalised retarded Green's function in Nambu-Gor'kov space,

\[ G_{mn}^{R^{-1}}(\epsilon, k) = G_{mn}^{(0)R^{-1}} - \Sigma_{mn}^R = \sum_{\mu} a_{\mu}^m a_{\mu}^m(k) \left( G_{\mu \mu}^{(0)R^{-1}} - \tilde{\Sigma}_n \right) \]

in the following way

\[ G_{mn}^{R^{-1}}(\epsilon, k) = \sum_{\mu} a_{\mu}^m(k) a_{\mu}^m(k)^* \]
\[ \times \left[ \left( Z^n(\epsilon, k) \right)(\epsilon + i\delta) \hat{1} - \xi_{\mu}(\epsilon, k) \hat{\sigma}_z - \Delta^n(\epsilon, k) \hat{\sigma}_x \right]. \]

where $\hat{1}$ and $\hat{\sigma}_z$ are the 2×2 unit matrix and the Pauli matrices in Nambu space, respectively. The renormalised dispersion and order parameter as well as the renormalisation function are given in terms of the retarded diagonal and off-diagonal self energies,

\[ \xi_{\mu}(\epsilon, k) = \xi_{\mu}(k) + \frac{\Sigma_{\mu}^R(\epsilon, k) + \Sigma_{\mu}^R(-\epsilon, -k)^*}{2}, \]
\[ \Delta^n(\epsilon, k) = \Delta_k + \Phi_{n}^R(\epsilon, k), \]
\[ Z^n(\epsilon, k) = 1 - \frac{\Sigma_{\mu}^R(\epsilon, k) - \Sigma_{\mu}^R(-\epsilon, -k)^*}{2(\epsilon + i\delta)}, \]

using the fact that $\Phi_{n}^R(\epsilon, k) = \Phi_{n}^R(-\epsilon, -k)^*$.

The equation for $G_{mn}^{R^{-1}}(\epsilon, k)$ is inverted numerically to obtain $G_{mn}^{R}(\epsilon, k)$. The spectral function is then obtained from the retarded Green's function via

\[ A(\epsilon, k) = -\frac{1}{\pi} \text{Im} \left( \sum_m \left[ G_{mn}^{R}(\epsilon, k) \right]_{11} \right). \]

For the numerical calculations we use a $2^3 \times 2^3 \times 2^3$ k-mesh and 200 points in energy space.

A high-energy cutoff of $\omega_c = 200$ meV was introduced in the spectrum of spin excitations. The exact value of this cutoff, as well as spectral weight beyond this cutoff and the precise variation of the spin susceptibility in the vicinity of the cutoff energy are however not of importance, as any change in the high-energy contributions only leads to an additional renormalisation factor $Z^{HE}$ for the low-energy electronic excitations. Thus as the high-energy part of the susceptibility varies with temperature, so does $Z^{HE}$. Taking the dispersion relation $\epsilon_k$ and the imaginary part of the effective self energy $\Sigma_{n}^R(k)$ as obtained from Eq. (6) in the main text, the spectral function in the superconducting state can be well approximated by

\[ A_s(k) = -\frac{1}{\pi} \text{Im} \left( \frac{1}{Z_s(k)(\epsilon + i\delta) - \epsilon_k + \Delta_s(k)/2} \right); \]

where $\Delta_s(k)$ is the renormalised order parameter. The renormalised value of the gap is obtained by considering the quantity $\Delta_s(k)/Z_s(k)$. The total renormalisation factor $Z_s(k)$ can be expressed as a product of high- and low-energy renormalisations, $Z_s(k) = Z^{HE}(k)Z^{LE}(k)$, with an energy-independent (on the low energy scale) $Z^{HE}(k)$, and with $Z^{LE}(k) = 1 - \Sigma_{n}^R(k)/(\epsilon + i\delta)$. In order to compare the results for different temperatures we have to include the high energy contributions to the renormalisation of the electronic dispersions, i.e. $\epsilon_k^{new} = \epsilon_k/Z^{HE}(k)$. The high-energy renormalisation factor is only weakly momentum dependent due to the weak momentum dependence of the susceptibility at high energies, and consequently we neglect this momentum dependence in our calculation. We are able to reproduce the experimentally observed high-energy part of the dispersions with $Z^{HE}(T = 50K) = 1$, and determine $Z^{HE}$ for the other temperatures so that the dispersions merge the normal state dispersion at $T = 50K$ for high energies. For the temperatures $T = 15 - 35K$ $Z^{HE}$ varies slowly between 0.9 - 1 as is shown in Fig. 6. Its value is < 1 to account for the overestimate of $\chi'_{\omega_c}$ near $\omega_c$ at lower temperatures.

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TEMPERATURE DEPENDENCE OF THE SPIN FLUCTUATION SPECTRUM AND THE RESONANCE MODE

We model the spin fluctuation spectrum by the procedure explained in the main article. The functional form of \( \chi''(\omega, q) \) is given by Eqs. (1) and (2) in the paper. In FIG. 7 the temperature dependence of the bosonic mode is shown. We present the energy dependence of the dynamic spin susceptibility at fixed momentum \( q = Q \), where \( Q \) is the antiferromagnetic wave vector, as well as the energy-momentum dependence of the spectrum. With decreasing temperature, spectral weight of the two-particle excitation spectrum is shifted into the energy region \( |\epsilon| < 2\Delta(T) \), leading to a well pronounced resonance feature that is sharp both in momentum and energy. Near \( T_c \) the resonance disappears and the energy dependence obeys the same shape as the normal state dispersion at \( T = 50K \).

FIG. 7: Dependence of the spin fluctuation spectrum on temperature. On the left of each panel the shape of the dynamic spin susceptibility at the antiferromagnetic wave vector, \( \chi''(\omega, Q) \), is shown (red line). The blue curve corresponds to the normal state spectral function at \( T = 50K \). On the right hand side the energy and momentum dependence around the wave vector \( Q \) is presented.
INFLUENCE OF THE BOSONIC SPECTRAL SHAPE ON THE ELECTRONIC SPECTRA

In addition to the results in the paper, which are given for the temperatures $T = 15K$ and $T = 50K$, we performed the same calculations for various temperatures ($T = 6.8 - 36.6K$). The appearance of the bosonic resonance leads to an effect on the electronic dispersion which is characterised by the development of a peak in the real part of the effective self energy as well as a hump feature in the imaginary part of the effective self energy. Both effects clearly show the same temperature dependence as the resonance in the bosonic spectrum as presented in FIG 8 and FIG 9.

FIG. 8: Temperature dependence of the real part of the effective self energy at the $\beta_1$-band. With increasing temperature, the self energy shows the development of a broad hump and a peak appearing at low energies.
FIG. 9: Temperature dependence of the imaginary part of the effective self energy at the $\alpha_1$-band. We present the results for each temperature (red line) compared to the normal state imaginary part of the effective self energy at $T = 50K$ (blue line). The black curve presents the difference of both, scaled by a factor of 3.