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Supplementary Materials for

Tuning across the BCS-BEC crossover in the multiband superconductor $Fe_{1+y}Se_xTe_{1-x}$: An angle-resolved photoemission study

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Supplementary Materials

Comparison between superconducting and normal state ARPES data

In fig. S1 we compare data for the $\varepsilon_F = 10\,\text{meV}$ sample with $T_c = 14\,\text{K}$ in the normal and superconducting states. In panels (A) and (B) we show raw data at 1K and at 22K. The data is normalized by the intensity above the Fermi-level produced by the second order light. The asymmetric intensity of the bands on positive and negative momenta at 22K is due to the circular polarization used at high temperatures. The dispersion of α_2 was extracted from both data sets. We find the maxima in the MDC peaks using a gaussian model. The band dispersion and ε_F were found to be identical in the normal and SC states within the experimental error bars. The dashed line in panels a and b represents the dispersion.

In panels c and d we show three EDC taken at the Γ point and at $k = 0.1\text{Å}^{-1}$ and $k = 0.15\text{Å}^{-1}$, at the same two temperatures.

At low temperatures the coherence peaks can be seen in all three EDC while above T_c there are no coherence peaks. The α_1 band, although not crossing the Fermi-level, contributes to the spectral weight up to the Fermi-level. The EDC in Fig. 4 of the main text show clearly that the top of the α_1 band is about 25meV below the Fermi-level. But due to the finite life-time of the quasiparticles associated with α_1 this band does contribute some spectral weight at the Γ point up to the Fermi-level, as can be seen in panel d. Below T_c a sharp coherence peak emerges on top of the normal state EDC.

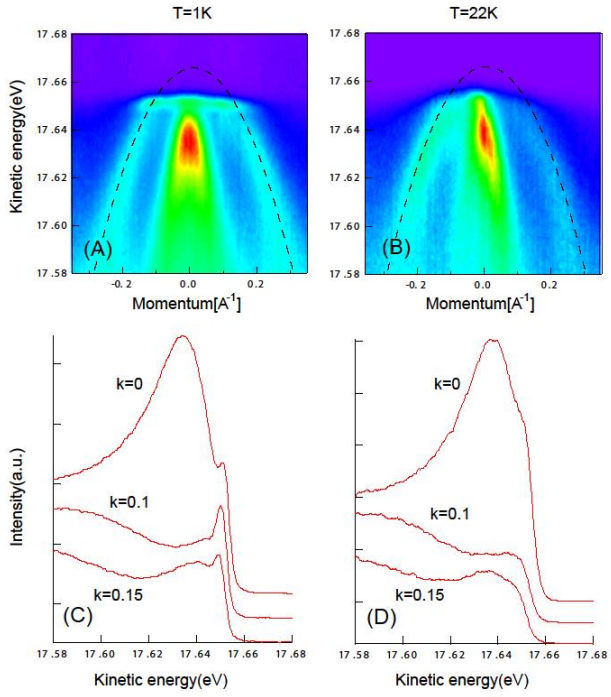

fig. S1. ARPES spectra above and below T_c. (**A** and **B**) ARPES spectra of a $\varepsilon_F = 10\,\text{meV}$ sample at T=1K and T=22K. The dashed line is the same parabolic dispersion from Fig. 4e in the main text. (**C** and **D**) Three EDCs at $k = 0$, $k = 0.1\text{Å}^{-1}$ and $k = 0.15\,\text{Å}^{-1}$ at the same temperatures.

Modeling the spectral function

In Fig. 1 (D-F) in the main text we plotted the spectral function $A(k,\omega)$ based on a simple model of the BCS-BEC crossover and it captures the qualitative features -- both dispersion and spectral weight -- of our ARPES data. ARPES probes only the occupied part of this spectral function, since it measures **k** -dependent matrix elements multiplying $f(\omega)A(k,\omega)$ convolved with resolution functions, where $f(\omega)$ is the Fermi function.

Here we carefully explain our modeling procedure focusing on the following points that we did not discuss in the main text.

(1) Line width broadening, (2) the renormalization of the chemical potential across the BCS-BEC crossover, and (3) the crucial negative signs that are important in modeling a hole band. We pay careful attention to the last point since most theory papers on the BCS-BEC crossover deal with "electron bands" with positive curvature.

We use a BCS-inspired form for the Green's function $G(k,\omega)$ and include a phenomenological line width broadening Γ in the self energy (*38*) with

$$G^{-1}(k,\omega) = \omega - \xi_k + i\Gamma - \frac{\Delta^2}{\omega + \xi_k + i\Gamma} \qquad (S1)$$

Here $\xi_k = \varepsilon_k - \mu$ is the dispersion ε_k measured with respect to μ, the chemical potential, ω is the energy, Δ the pairing gap and Γ the broadening (taken to be independent of ω for simplicity).

The spectral function $A(k,\omega) = -\operatorname{Im} G(k,\omega)/\pi$ is given by

$$A(k,\omega) = \frac{v_k^2}{\pi}\frac{\Gamma}{(\omega - E_k)^2 + \Gamma^2} + \frac{v_k^2}{\pi}\frac{\Gamma}{(\omega + E_k)^2 + \Gamma^2} \qquad (S2)$$

Where $1 - u_k^2 = v_k^2 = \frac{1}{2}(1 - \xi_k / E_k)$ and $E_k = \sqrt{\xi_k^2 + \Delta^2}$. ARPES measurements will be dominated by the second term which is centered at $\omega = -E_k$ on the occupied side.

To model the α_2 hole band in our ARPES data, we use

$$\varepsilon k = -\frac{k^2}{2m^*} \text{ with } m^* = 3.2 m_e \qquad (S3)$$

We also use a phenomenological $\Gamma = 3\,\text{meV}$.

It is crucial to take into account the renormalization of the chemical potential μ as one goes through the BCS-BEC crossover. Note that in our simple model we do not make a distinction between μ and $\tilde{\mu}$, where $\tilde{\mu}$ takes into account *additional* renormalization, beyond that which enters the thermodynamic μ specific to the excitation spectrum (*6*,*34*,*39*).

We next use the results of the mean field theory of the BCS-BEC crossover in 2D which yield analytical results (*3*) $\Delta = \sqrt{2\varepsilon_F E_A}$ and $\mu = \varepsilon_F - E_A/2$ that are valid across the entire crossover at $T = 0$. (The μ result quoted here is for an electron-like band; see below).

Here E_A is the binding energy of the two-body bound state in vacuum with $E_A/\varepsilon_F \ll 1$ corresponding to the weak-coupling BCS limit and $E_A/\varepsilon_F \gg 1$ to the extreme BEC limit.

Next we see, via a particle-hole transformation, that for a hole-band, with a negative curvature as in eq. S3, we must set μ to $-\mu$ in the equation above. We then eliminate (the experimentally unknown quantity) E_A between the two equations to obtain

$$\mu = -\varepsilon_F + \Delta^2/4\varepsilon_F \qquad (S4)$$

It is easy to see that this is the correct sign convention, since in the noninteracting limit ($\Delta = 0$), the dispersion goes to the correct limit $\xi_k = (\varepsilon_k - \mu) \to -k^2/2m^* + \varepsilon_F$.

Finally, let us comment on the minimum gap locus and the spectral weights of the two Bogolyubov quasiparticle peaks as one goes through the BCS to BEC crossover. In the BCS regime, which for the hole band corresponds to $\mu < 0$ (note sign!), the minimum of the spectral gap $E_k = \Delta$ occurs at $\xi_k = 0$ corresponding to $k^* = \sqrt{2m^*|\mu|}$.

In this case the spectral weights $v_{k^*}^2 = u_{k^*}^2 = 1/2$. This is, of course, very well known in the extreme BCS limit with $\Delta \ll \varepsilon_F$, where $k^* \simeq k_F$.

In the BEC regime when $\mu > 0$ for a hole band, the minimum spectral gap $E_k = \sqrt{\mu^2 + \Delta^2}$ occurs at $\mathbf{k} = 0$. This is the collapse of the minimum gap locus discussed in the main text. The spectral weights at the gap edge $\mathbf{k} = 0$ are given by $v_{k=0}^2 = \frac{1}{2}\left(1 + \mu/\sqrt{\mu^2 + \Delta^2}\right)$ which is (much) greater than $u_{k=0}^2 = \frac{1}{2}\left(1 - \mu/\sqrt{\mu^2 + \Delta^2}\right)$. It is instructive to look at the extreme BEC limit $\mu \gg \Delta \gg \varepsilon_F$, where $v_{k=0}^2 \simeq 1$ while $u_{k=0}^2 \simeq \mu^2/4\Delta^2 \ll 1$.

Thus there is a large spectral weight v_k^2 on the occupied side that can be measured by ARPES for a hole-band in the BEC regime. In contrast, the roles of u_k^2 and v_k^2 are interchanged for an electron band, and one would have a tiny occupied spectral weight in the BEC regime. In this sense, the BCS-BEC crossover in the hole band investigated in this paper is ideally suited for being probed by ARPES.

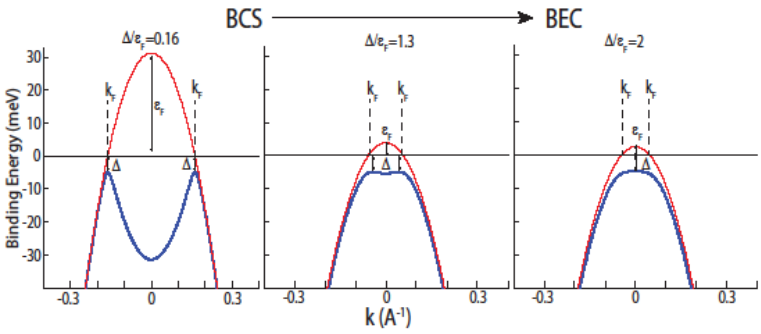

fig. S2. Bogoliubov dispersion from BCS to BEC. Evolution of the Bogoliubov dispersion from BCS state, where the bending-back at kF can be seen to the BEC state where the minimum of the gap is found at k=0.