Consequences of Orbital Selectivity for Magnetism and Superconductivity in Fe-based Superconductors

Andreas Kreisel
Institut für Theoretische Physik, Universität Leipzig

Brian Andersen
Niels Bohr Institute, University of Copenhagen, 2100 København, Denmark
Peter Hirschfeld
Department of Physics, University of Florida, Gainesville, FL 32611, USA

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A. Kreisel, et al.
Phys. Rev. B **95**, 174504 (2017)

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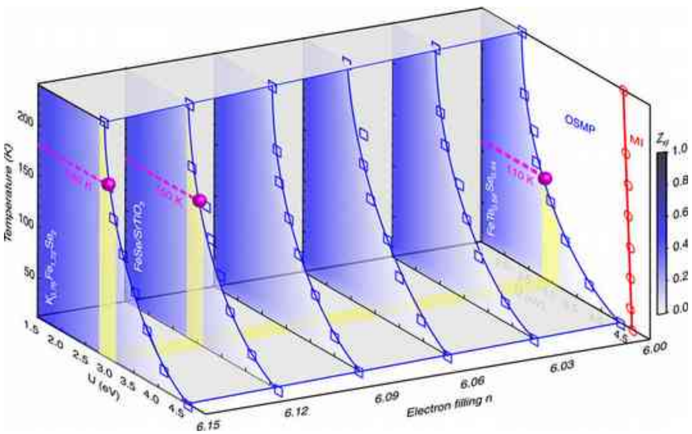
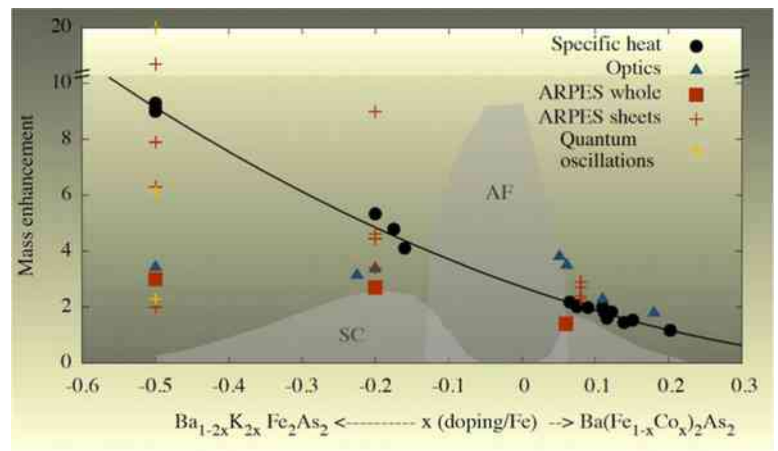
Orbital selectivity

- Fe based materials: multiband systems
  electrons in some orbitals less coherent





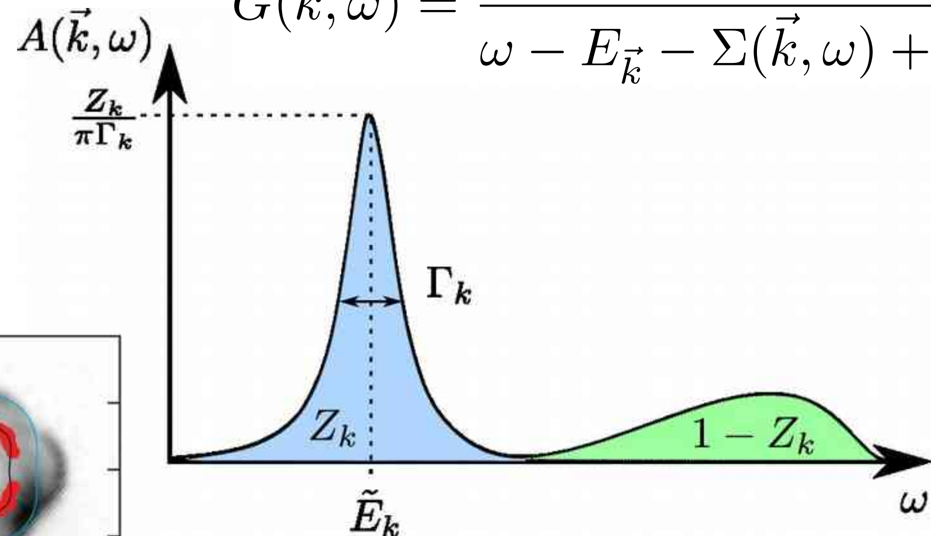
Relevant for Fe based SC:
Yin, Haule, Kotliar, Nat. Mat. **10**, 932 (2011)
de' Medici, Giovannetti, Capone. Phys. Rev. Lett. **112**, 177001 (2014)
M. Aichhorn, et al., Phys. Rev. B **82**, 064504 (2010)
Liu et al., Phys. Rev. B **92**, 235138 (2015)
Yi et al., Nat. Comm. **6**, 7777 (2015)
...

- FeSe: nematic order, no magnetism
  opportunity to study unequal states in d_{xz}/d_{yz}

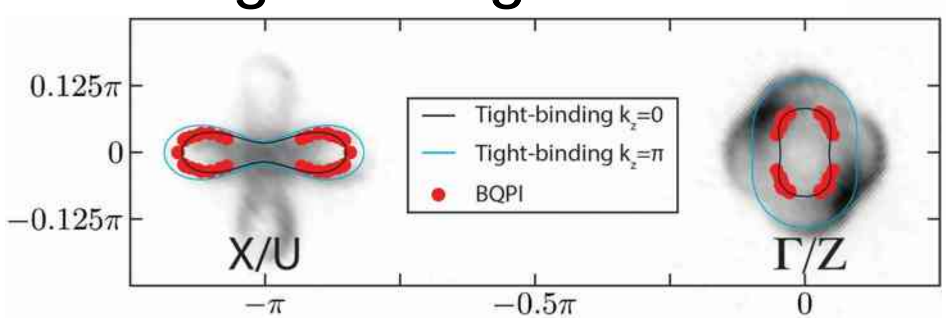
Theoretical approach

- Dressed Green's function

$$G(\vec{k},\omega) = \frac{1}{\omega - E_{\vec{k}} - \Sigma(\vec{k},\omega) + i0^+}$$



- Parametrization
  - true eigenenergies



  - quasiparticle weights

Watson, et al., PRB **94**, 201107(R) (2016)
Watson, et al., PRB **90**, 121111(R) (2014)
Suzuki, et al., PRB **92**, 205117 (2015)
Maletz, et al., PRB **89**, 220506(R) (2014)
Fedorov, et al., Sci. Rep. **6**, 36834 (2016)
Watson, et al., New J. Phys. **19**, 103021 (2017)
Peter O. Sprau, et al., Science, **357**, 75 (2017)
Liu, et al., arXiv:1802.02940

geometric mean of quasiparticle weights
(phenomenological/measured/calculated)

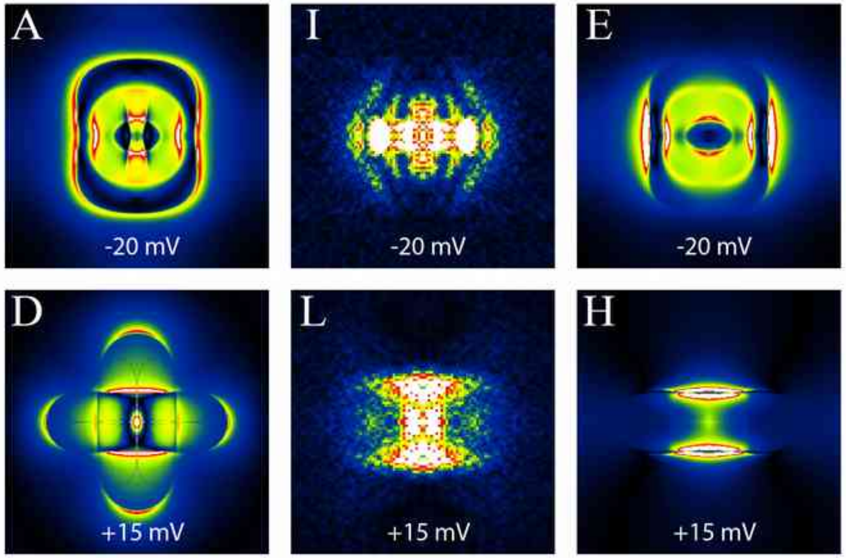
$$\tilde{G}_{\ell\ell'}(\mathbf{k},\omega_n) = \sqrt{Z_\ell Z_{\ell'}} \sum_\mu \frac{a^\ell_\mu(\mathbf{k}) a^{\ell'*}_\mu(\mathbf{k})}{i\omega_n - \tilde{E}_\mu(\mathbf{k})}$$

measured true
eigenenergies

Normal state properties: Spectroscopy

- Normal state QPI

A. Kostin et al., arXiv:1802.02266

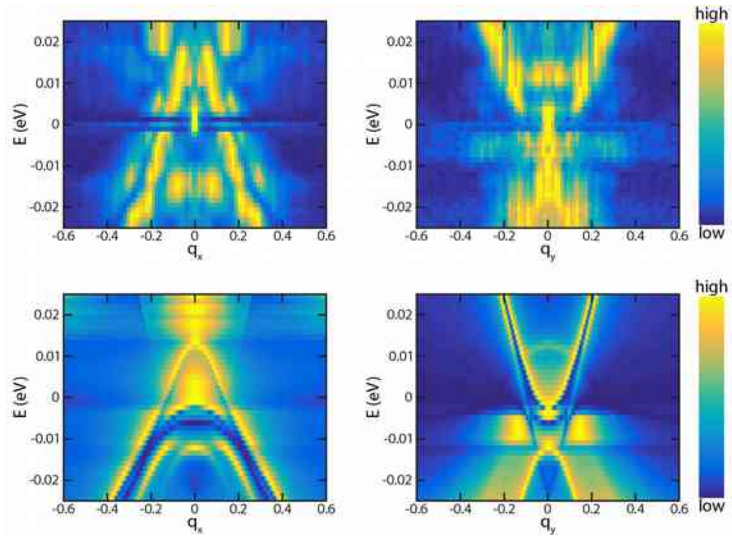


T-matrix: no orbital selectivity Z=1

experiment

T-matrix: orbital selectivity (Z as for superconductivity)

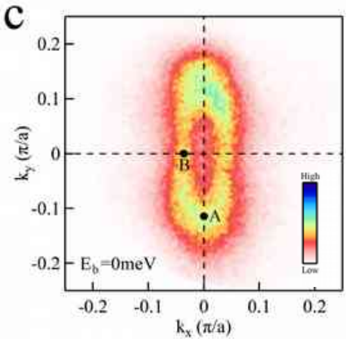
Cuts along axis: experiment

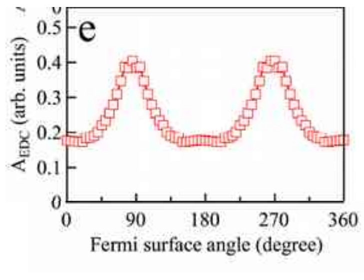


T-matrix with orbital selectivity

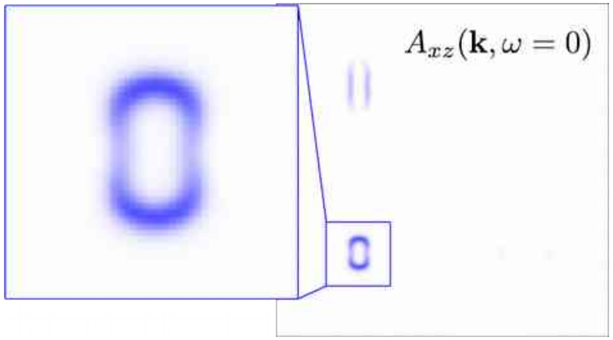
- ARPES

Liu, et al., arXiv:1802.02940





Orbitally resolved spectral function



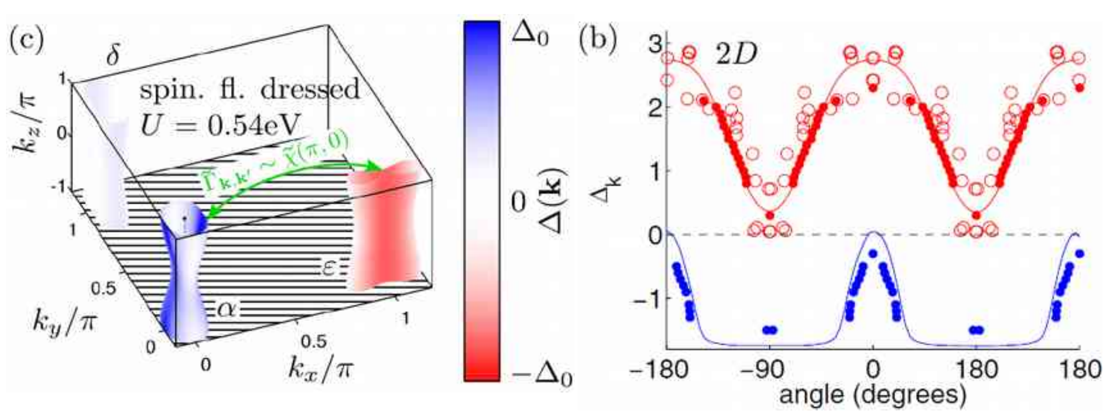
Superconducting state: gap function

- Modified spin-fluctuation theory

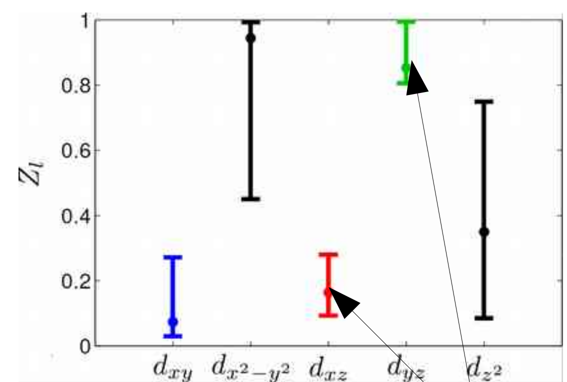
$$\tilde{\Gamma}_{\nu\mu}(\mathbf{k},\mathbf{k}') = \mathrm{Re} \sum_{\ell_1\ell_2\ell_3\ell_4} \sqrt{Z_{\ell_1}}\sqrt{Z_{\ell_4}}\, a_{\nu}^{\ell_1,*}(\mathbf{k}) a_{\nu}^{\ell_4,*}(-\mathbf{k}) \tilde{\Gamma}_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}')\ \sqrt{Z_{\ell_2}}\sqrt{Z_{\ell_3}}\, a_{\mu}^{\ell_2}(\mathbf{k}') a_{\mu}^{\ell_3}(-\mathbf{k}'$$

- Solve linearized gap equation $-\sum_{\mu}\int_{\mathrm{FS}_\mu} dS' \frac{\tilde{\Gamma}_{\nu\mu}(\mathbf{k},\mathbf{k}') g_i(\mathbf{k}')}{V_G |v_{\mathrm{F}\mu}(\mathbf{k}')|} = \lambda_i g_i(\mathbf{k})$

Quasiparticle weights (same trends found in microscopic calculations)

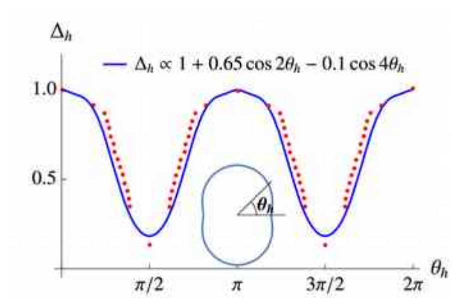


$$\{\sqrt{Z_l}\} = [0.2715, 0.9717, 0.4048, 0.9236, 0.5916]$$

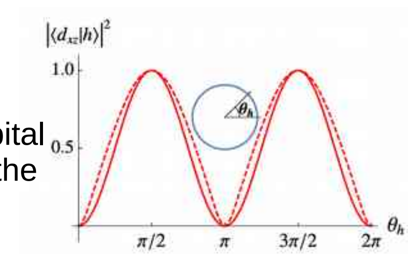


Strong splitting required!

Picture challenged: Kang, Fernandes, Chubukov arXiv:1802.01048
Talk: B14.00007



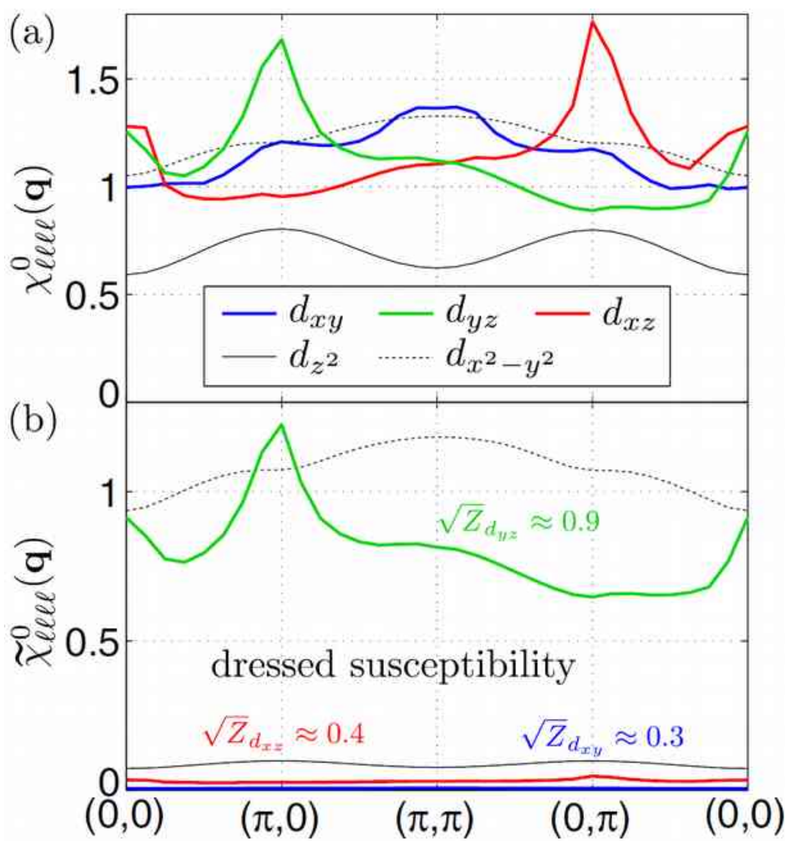
But:
different orbital content on the hole-pocket

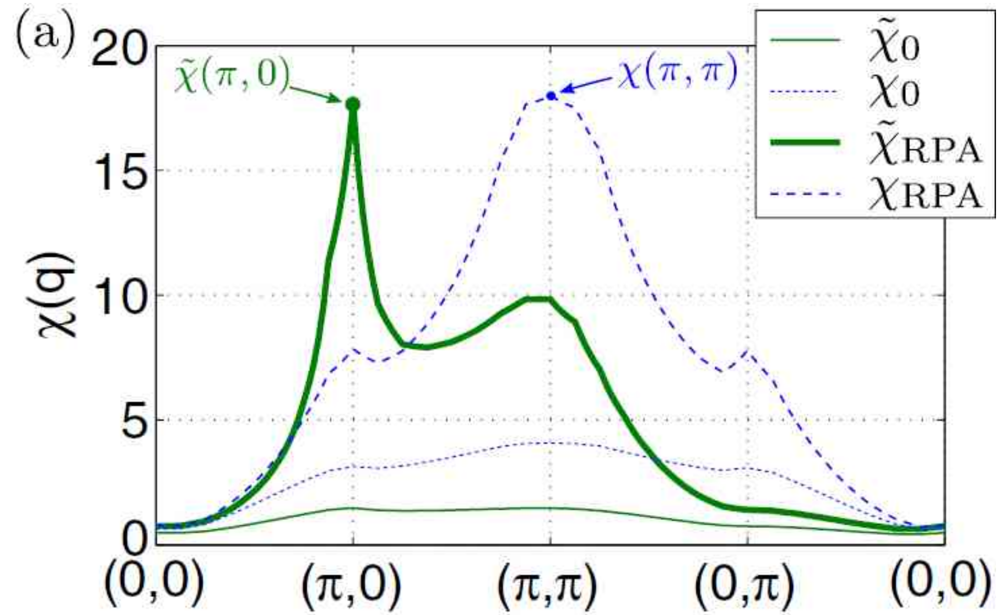


Static spin fluctuations

- Use parametrization of Green's function

$$\tilde{\chi}^0_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{q}) = \sqrt{Z_{\ell_1} Z_{\ell_2} Z_{\ell_3} Z_{\ell_4}}\, \chi^0_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{q}),$$

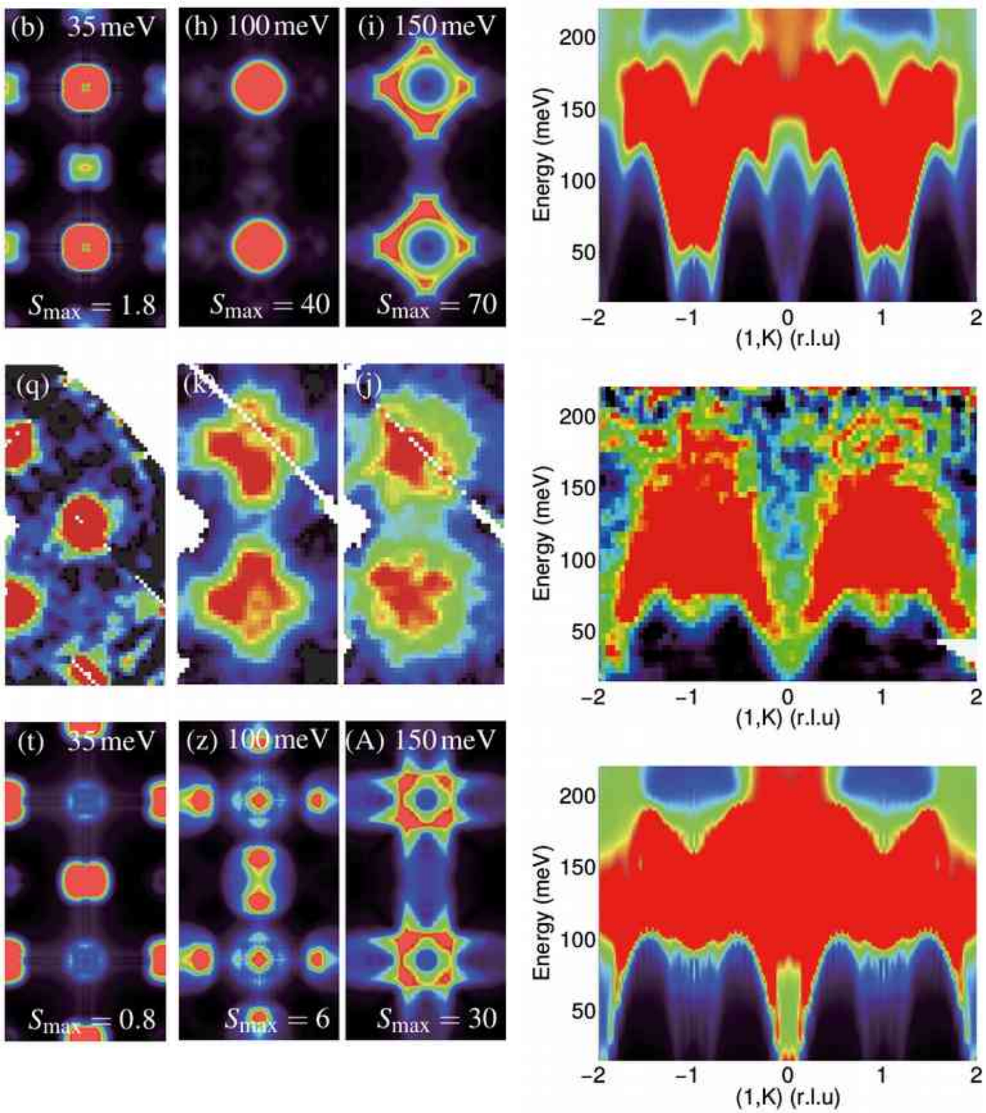




Strong renormalization of d_{xy}:
suppression of (π,π) weight

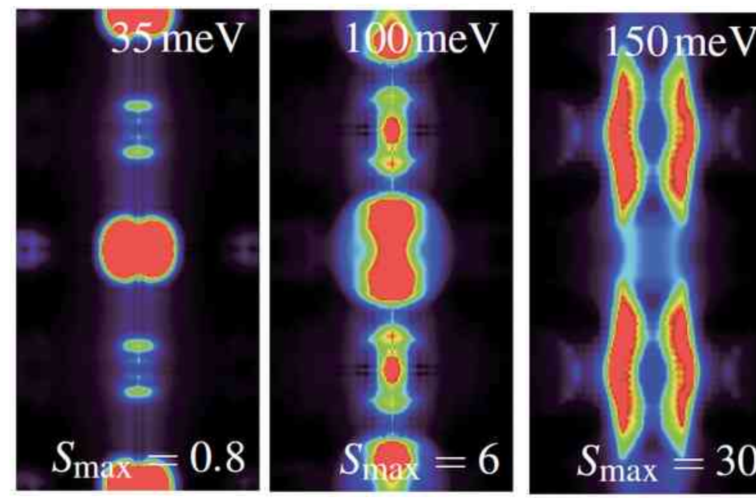
Spin fluctuations: Inelastic neutron scattering

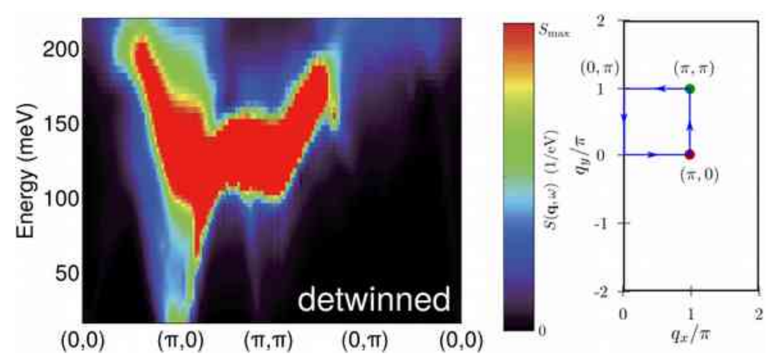
twinned



Wang, et al., Nat. Commun. **7**, 12182 (2016)

detwinned





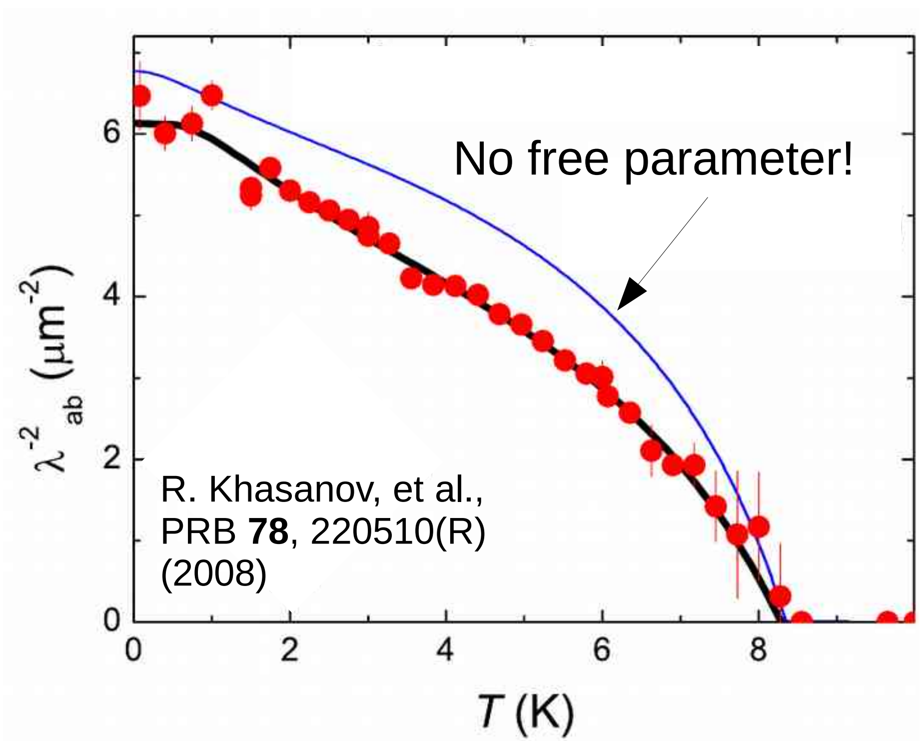
Band structure with reduced coherence

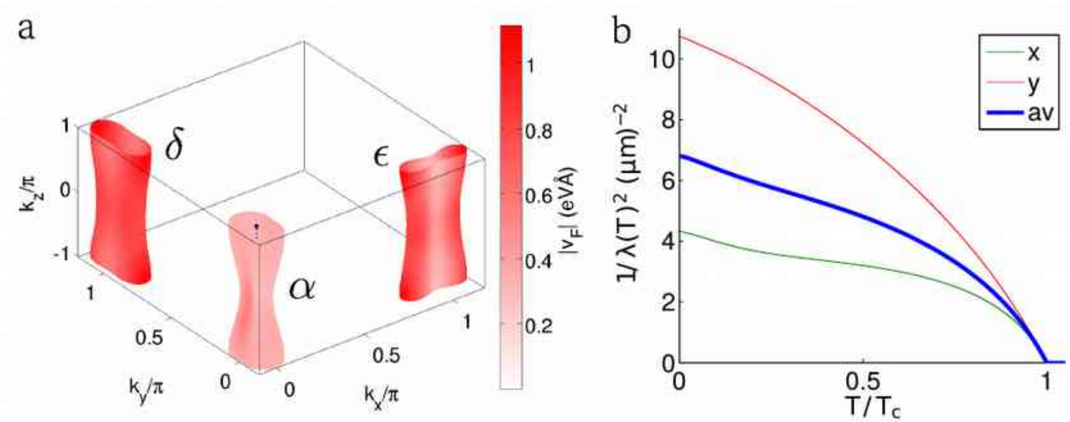
Magnetic penetration depth

- Penetration depth from tight binding model

$$\frac{1}{\lambda_i^2} = \frac{4\pi e^2}{c^2\hbar^2}\sum_{\mathbf{k},\nu}\frac{d\tilde{E}_\nu(\mathbf{k})}{dk_i}\left(\frac{d\tilde{E}_\nu(\mathbf{k})}{dk_i}|\Delta_\mathbf{k}|^2 - \frac{d|\Delta_\mathbf{k}|}{dk_i}|\Delta_\mathbf{k}|\tilde{E}_\nu(\mathbf{k})\right)$$
$$\times \frac{\tilde{Z}_\nu(\mathbf{k})}{E_{\nu,\mathbf{k}}^2}\left(\frac{1}{E_{\nu,\mathbf{k}}}\tanh\left(\frac{E_{\nu,\mathbf{k}}}{2k_BT}\right) - \frac{1}{2k_BT}\operatorname{sech}\left(\frac{E_{\nu,\mathbf{k}}}{2k_BT}\right)^2\right)$$

M. V. Eremin, et al., J. Phys.: Condens. Matter **22**, 185704 (2010).





P. Biswas, et al. (in preparation)

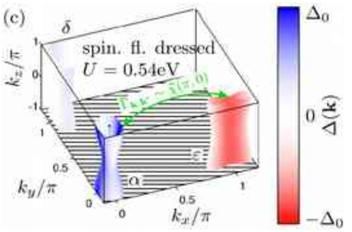
A. Kreisel, et al.
Phys. Rev. B **95**, 174504 (2017)
A. Kostin et al., arXiv:1802.02266

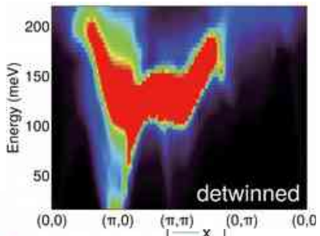
Summary

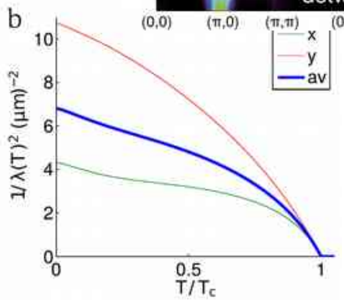
- Phenomenological, but microscopic approach: including low-energy renormalizations

$$\tilde{G}_{\ell\ell'}(\mathbf{k},\omega_n) = \sqrt{Z_\ell Z_{\ell'}} \sum_\mu \frac{a_\mu^\ell(\mathbf{k}) a_\mu^{\ell' *}(\mathbf{k})}{i\omega_n - \tilde{E}_\mu(\mathbf{k})}$$

- Consequences
  - Anisotropic quasiparticle scattering in FeSe
  - Pairing: modified spin-fluctuation theory (stabilization of s-wave pairing, anisotropic order parameter for FeSe)
  - Magnetism, spin-fluctuation spectrum: suppression of (π,π) spectral weight, prediction for INS on detwinned FeSe
  - Penetration depth: anisotropies (elongated vortices), magnitude fixed by parameters







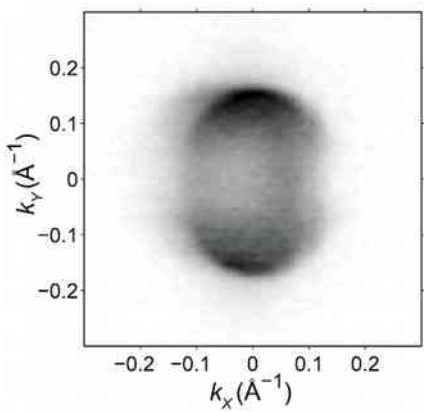
- Microscopic calculation of $\sqrt{Z_\ell}$

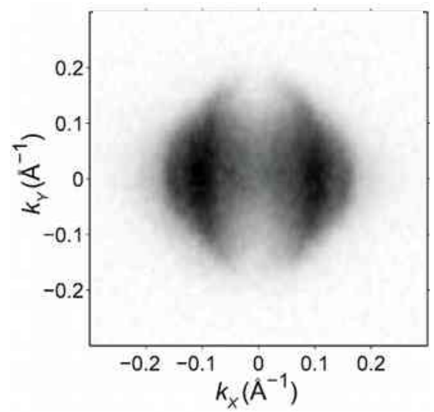
  E14.00006 : Orbitally Resolved Quasiparticle Weight Renormalization Factors in Fe-based Superconductors
  Tue 9:24, 304B

ARPES on FeSe

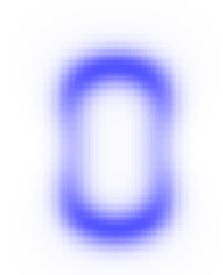
d_xz

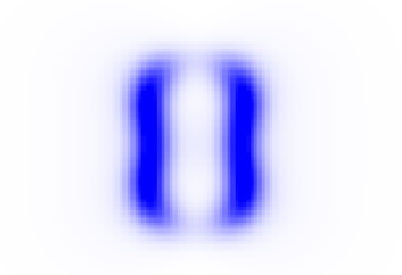
d_yz





Watson, et al., New J. Phys. **19**, 103021 (2017)





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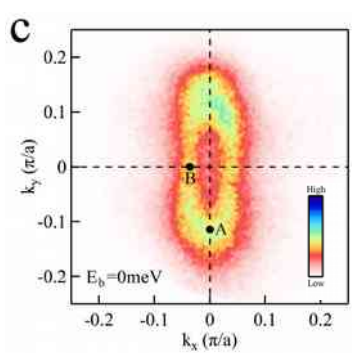

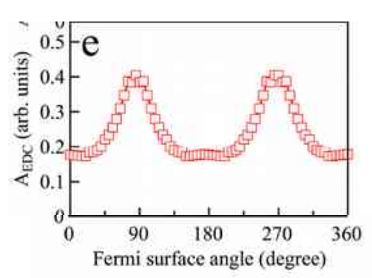

Liu, et al., arXiv:1802.02940