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

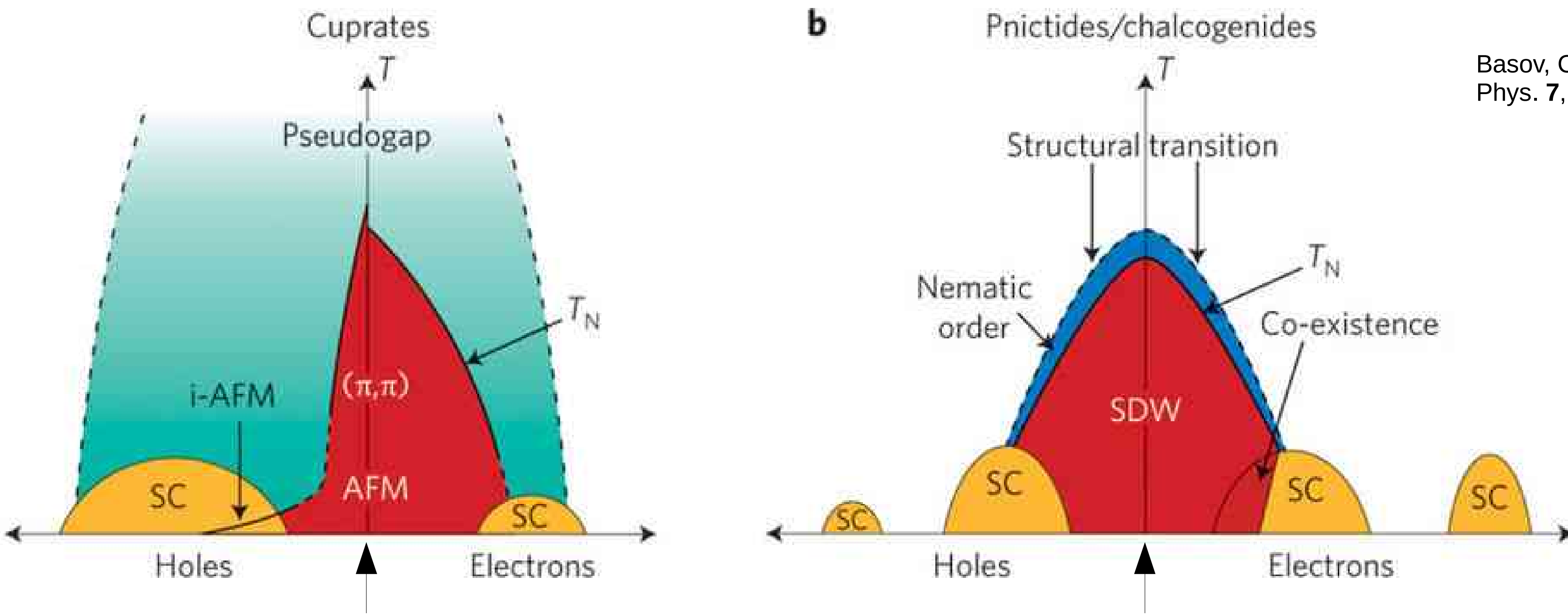
UF UNIVERSITY of FLORIDA
The Foundation for The Gator Nation

UNIVERSITÄT LEIPZIG

A. Kreisel, et al.
Phys. Rev. B **95**, 174504 (2017)
Peter O. Sprau, et al.,
Science, **357**, 75 (2017)
A. Kostin, et al., arXiv:1802.02266

KØBENHAVNS UNIVERSITET

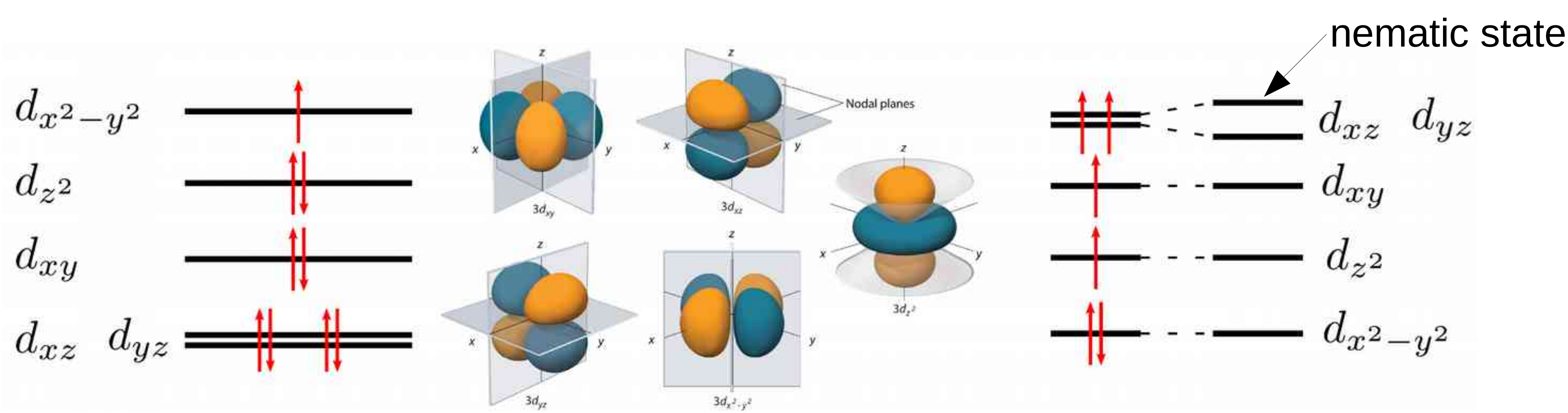
Correlated superconductivity



Basov, Chubukov, Nat. Phys. **7**, 272 (2011)

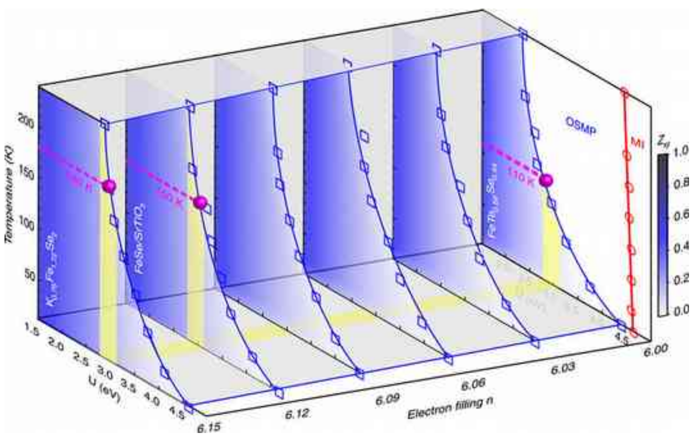
Single band: Mott insulator

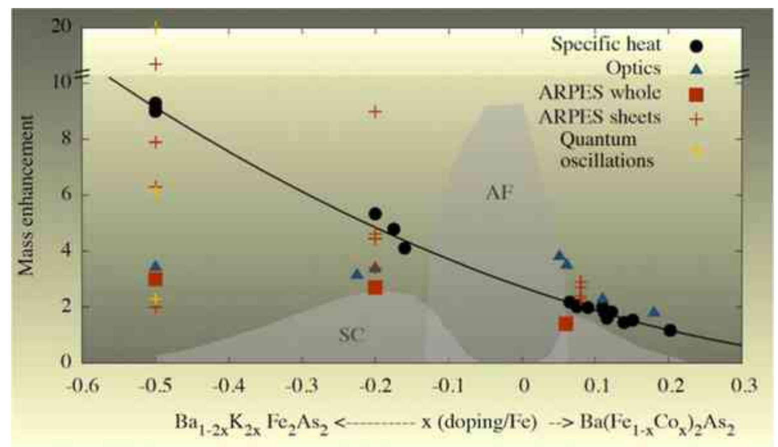
Multiband system: Bad metal



Orbital selectivity

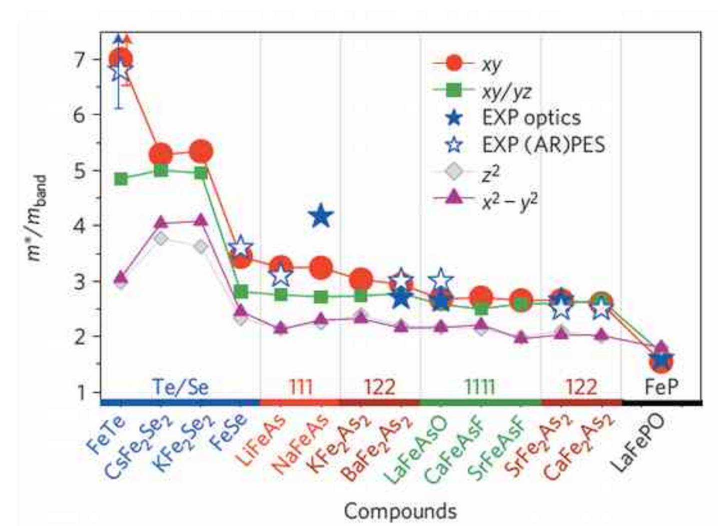
- Fe based materials: multiband systems
  electrons in some orbitals less coherent





Relevant for Fe based SC:
Yin, Haule, Kotliar, Nat. Mat. **10**, 932 (2011)
Greger, Kollar, Vollhardt, Phys. Rev. Lett ***110***, 046403 (2013)
Yu, Si, Phys. Rev. Lett ***110***,146402 (2013)
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}

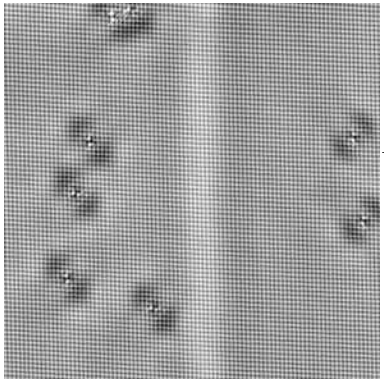


Orbital selectivity
Normal state properties

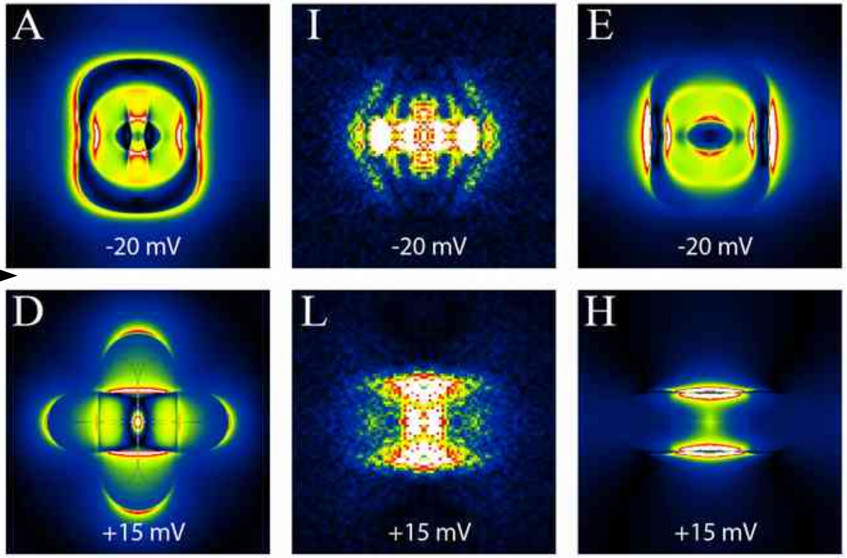
- Normal state QPI

A. Kostin et al., arXiv:1802.02266

STM: conductance map



FT

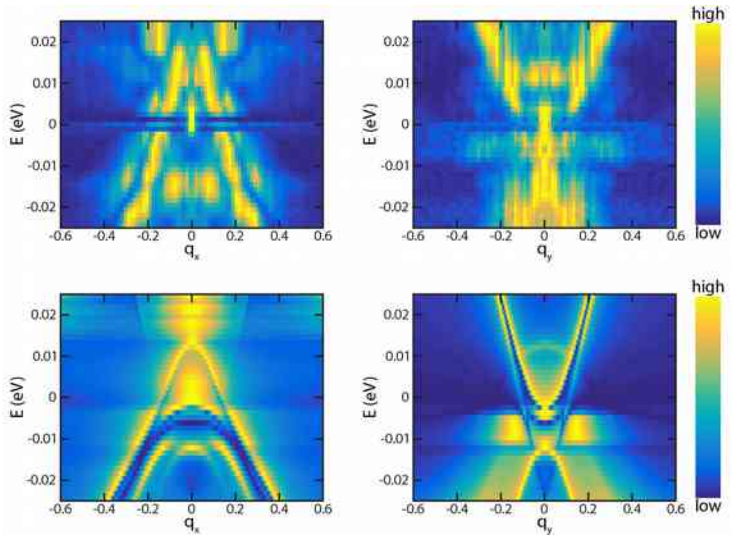


T-matrix: no orbital selectivity Z=1

experiment

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

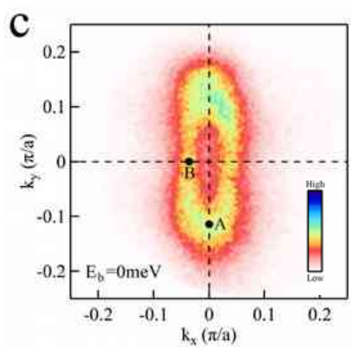
Cuts along axis: experiment

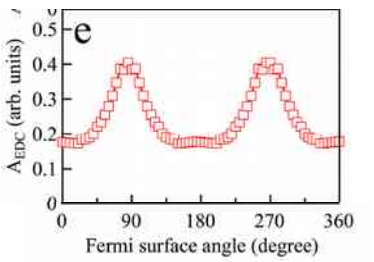


T-matrix with orbital selectivity

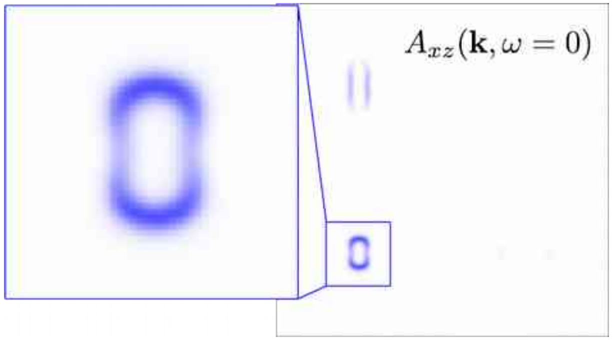
- ARPES

Liu, et al., arXiv:1802.02940





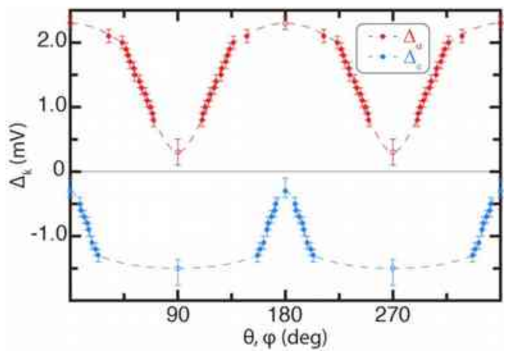
Orbitally resolved spectral function

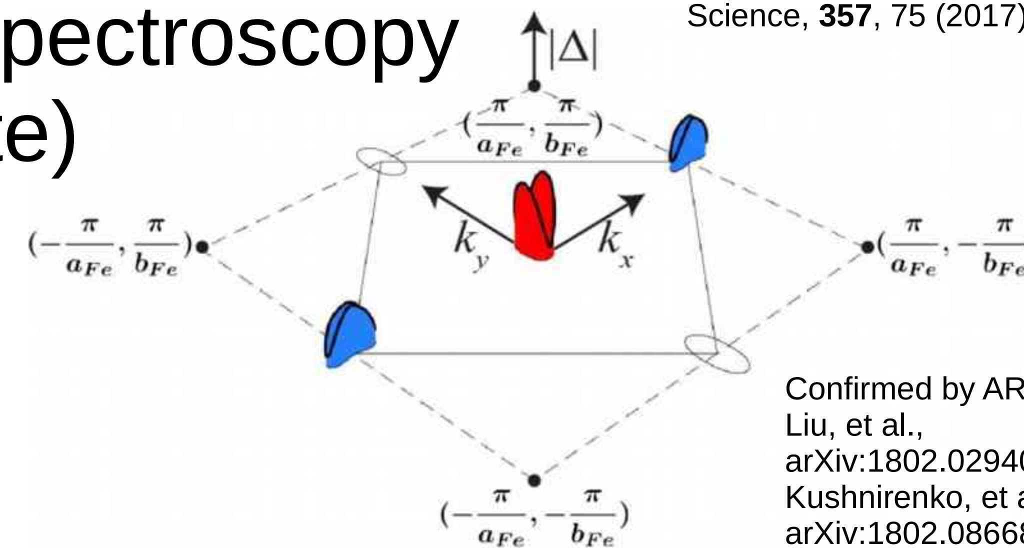


Orbitally selective superconductivity

Sprau, Kostin, Kreisel, et al., Science, **357**, 75 (2017)

- Scanning tunnelling spectroscopy (superconducting state)



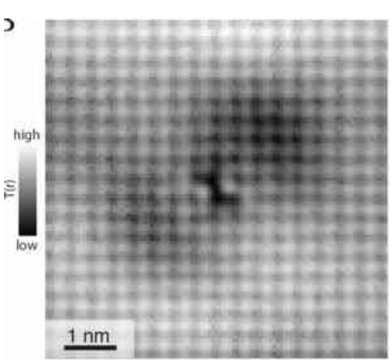


Confirmed by ARPES:
Liu, et al., arXiv:1802.02940
Kushnirenko, et al., arXiv:1802.08668

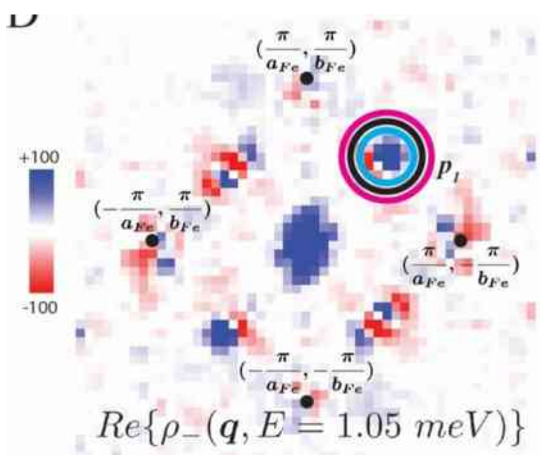
- Sign change

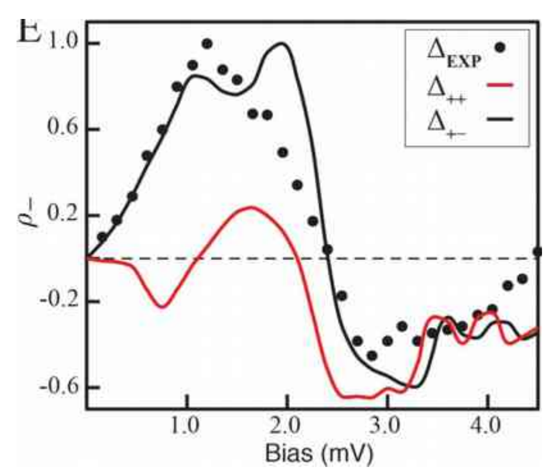
$$\rho_-(\vec{q},\omega) = Re\{g(\vec{q},+\omega)\} - Re\{g(\vec{q},-\omega)\}$$

Hirschfeld et al., PRB **92**, 184513 (2015)
J. Martiny, A. Kreisel, et al.
Phys. Rev. B **95**, 184507 (2017)



FT

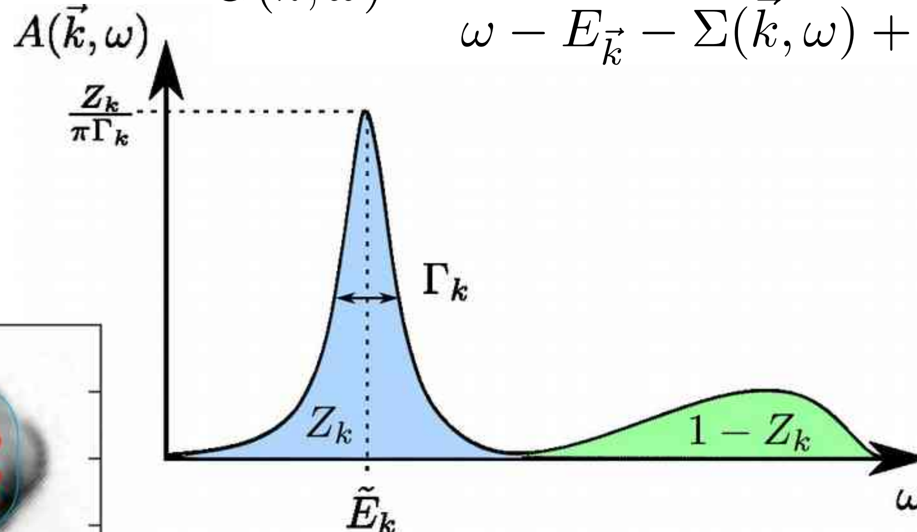




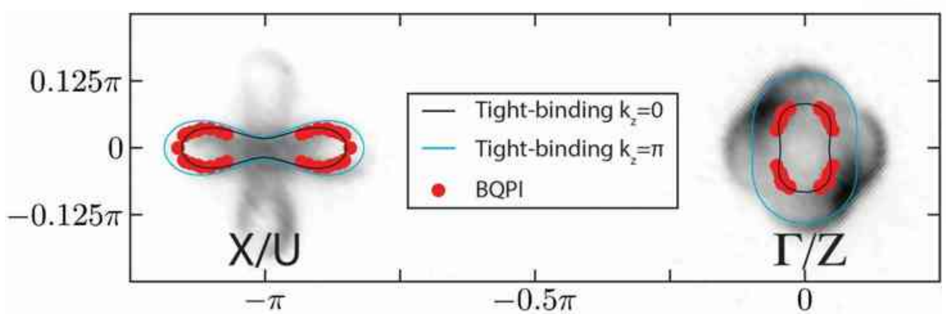
Theoretical approach

- 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

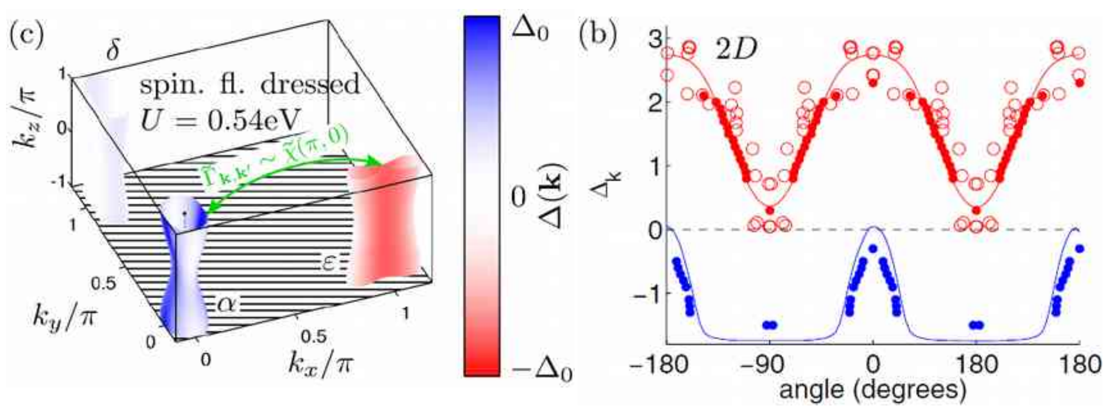
Superconducting state: gap function

- Modified spin-fluctuation theory

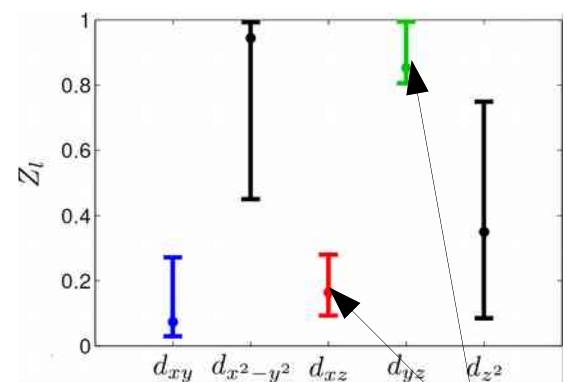
$$\tilde{\Gamma}_{\nu\mu}(\mathbf{k},\mathbf{k}') = \mathrm{Re} \sum_{\ell_1\ell_2\ell_3\ell_4} \sqrt{Z_{\ell_1}}\sqrt{Z_{\ell_4}} a_\nu^{\ell_1,*}(\mathbf{k}) a_\nu^{\ell_4,*}(-\mathbf{k}) \tilde{\Gamma}_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}') \sqrt{Z_{\ell_2}}\sqrt{Z_{\ell_3}} a_\mu^{\ell_2}(\mathbf{k}')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

- 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)



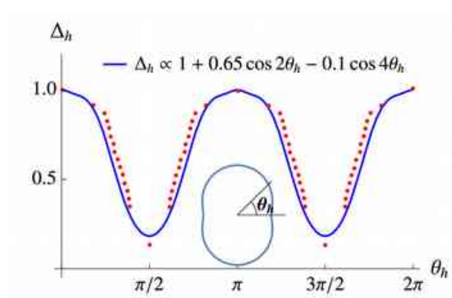
$$\{\sqrt{Z_l}\} = [0.2715, 0.9717, 0.4048, 0.9236, 0.5916]$$



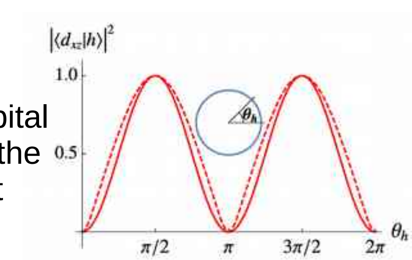
Strong splitting required!

Picture questioned:
Kang, Fernandes, Chubukov
arXiv:1802.01048

but: orbital selectivity in d_{xy}



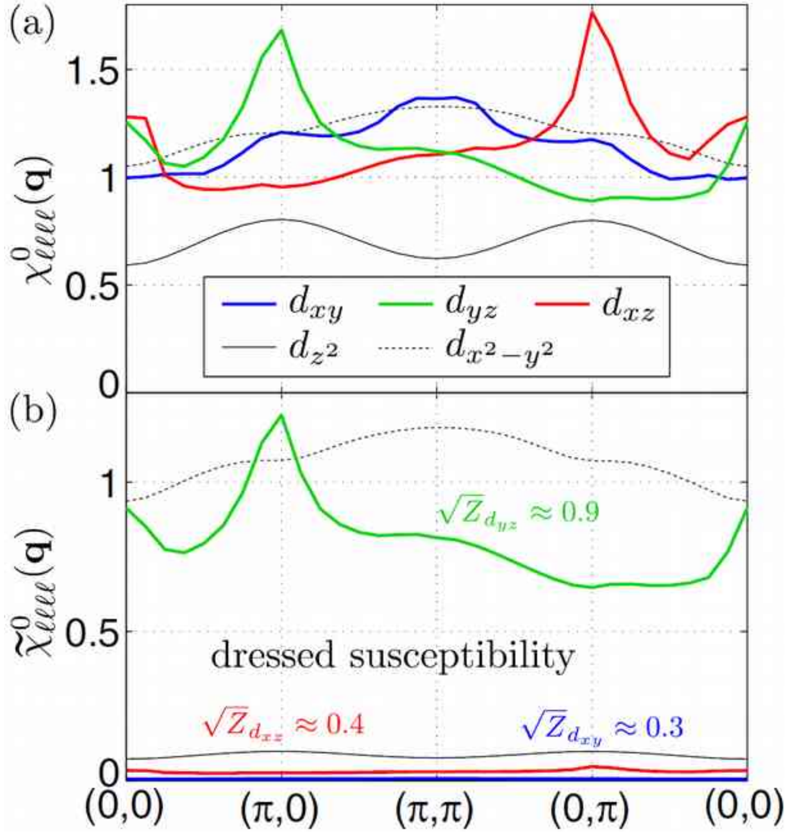
But:
different orbital content on the hole-pocket

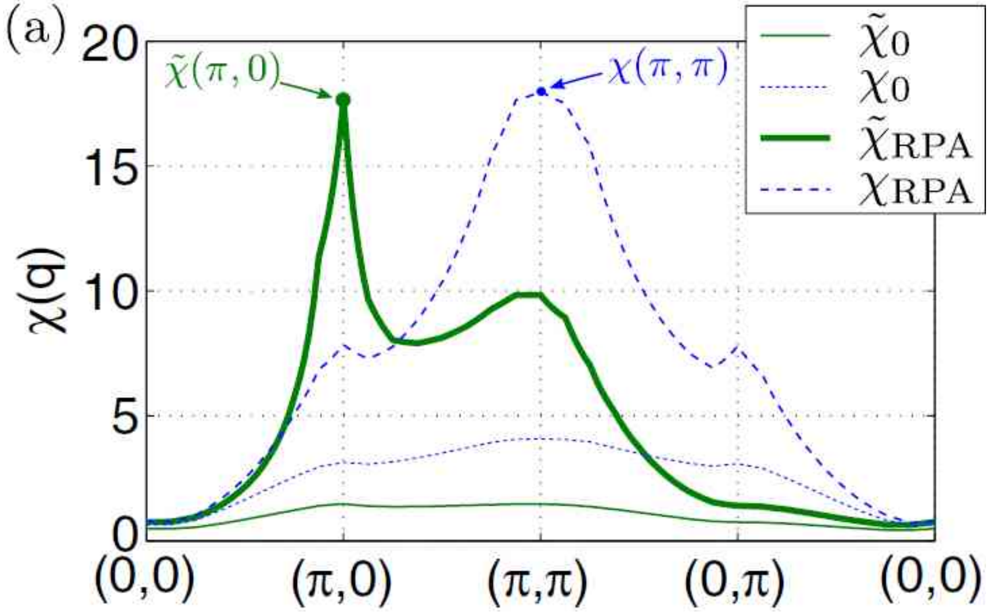


Static spin fluctuations

- Use parametrization of Green's function

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

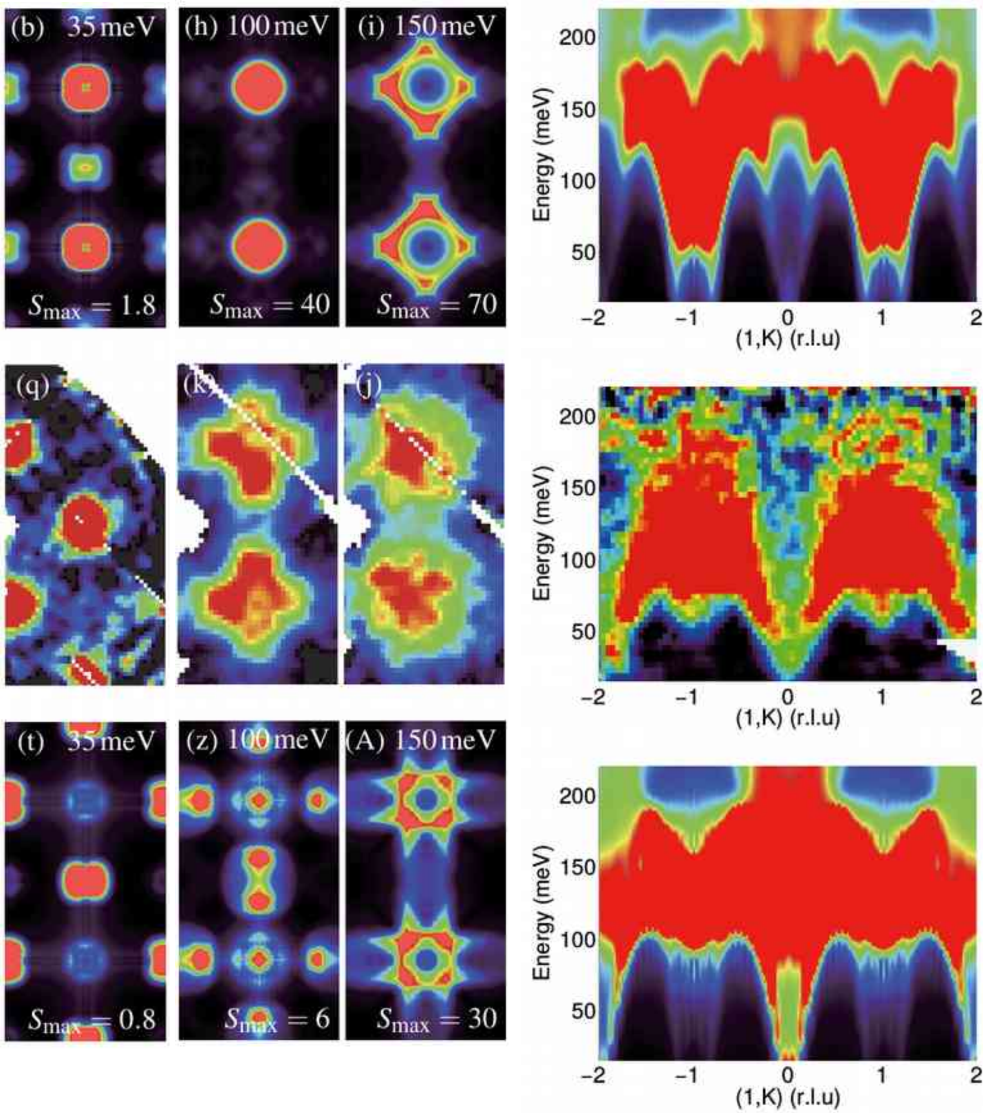




Strong renormalization of d_{xy}: suppression of (π,π) weight

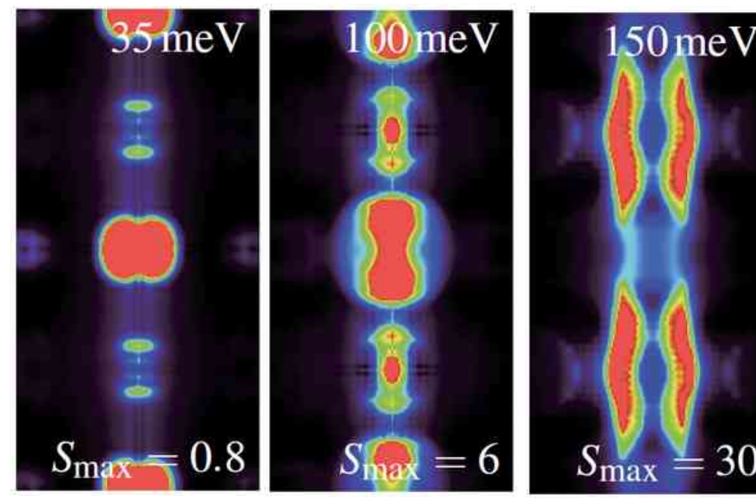
Spin fluctuations: Inelastic neutron scattering

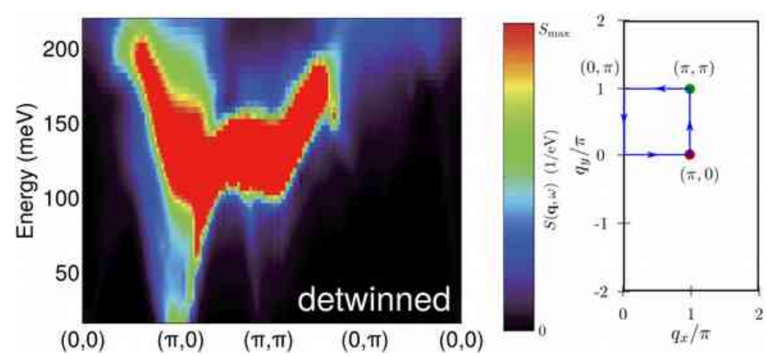
twinned



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

detwinned





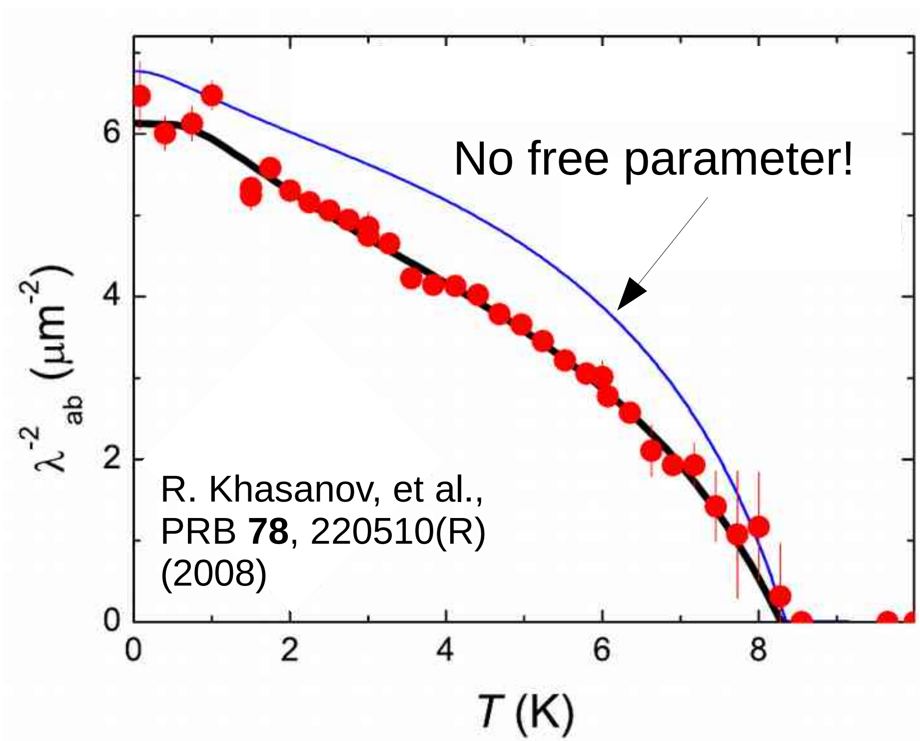
Band structure with reduced coherence

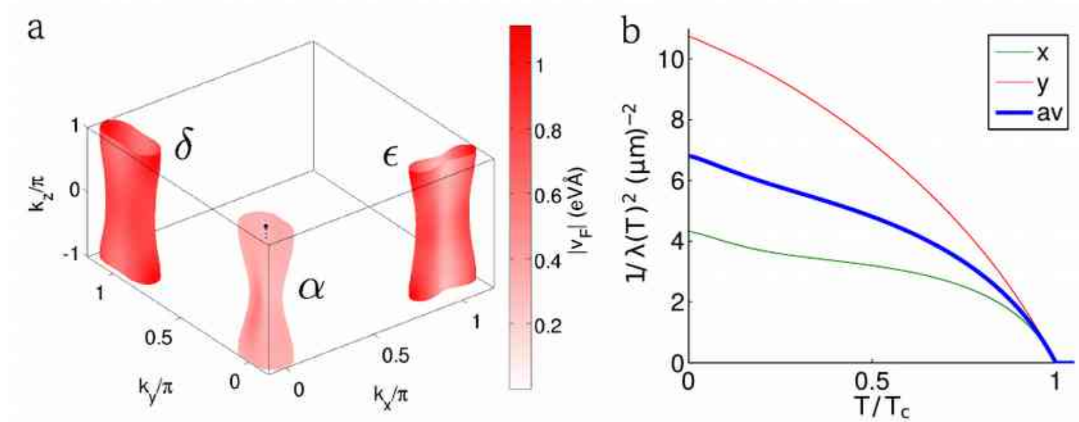
Magnetic penetration depth

- Penetration depth from tight binding model

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

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





P. Biswas, et al. (in preparation)

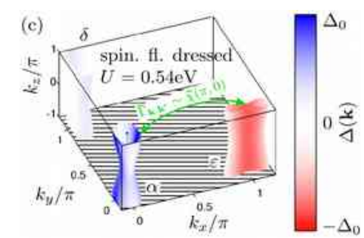
A. Kreisel, et al.
Phys. Rev. B **95**, 174504 (2017)
Sprau, Kostin, Kreisel, et al.,
Science, **357**, 75 (2017)
Kostin, Sprau, Kreisel, et al.,
arXiv:1802.02266

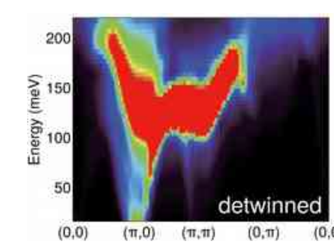
Summary

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

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

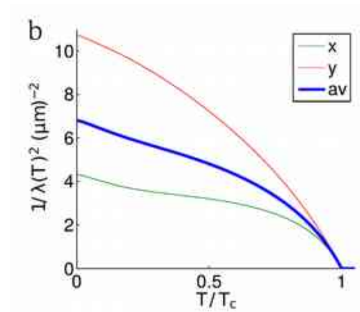
- Consequences
  - Anisotropic quasiparticle scattering in FeSe
  - Pairing: modified spin-fluctuation theory (stabilization of s-wave pairing, anisotropic order parameter for FeSe)
  - Magnetism, spin-fluctuation spectrum: suppression of (π,π) spectral weight, prediction for INS on detwinned FeSe
 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





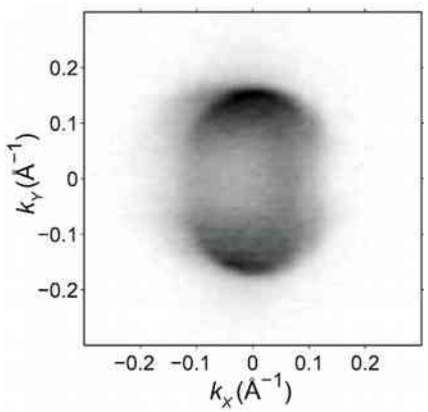
- Microscopic calculation of $\sqrt{Z_\ell}$

  RPA approach → Bhattacharyya et al. (in preparation)
  slave boson approach → Chatzieleftheriou (unpublished);
  Yu, Zhu, Si, arXiv:1803.01733

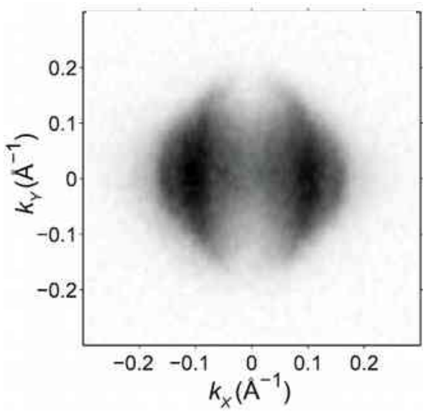


ARPES on FeSe

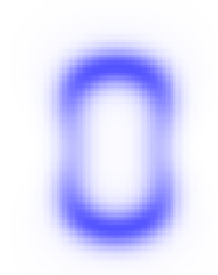
d_xz

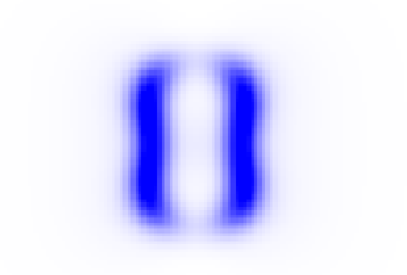


d_yz

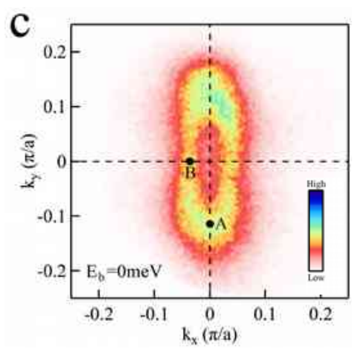


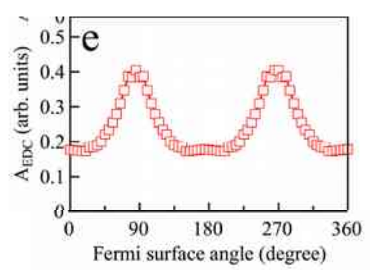
Watson, et al., New J. Phys. **19**, 103021 (2017)





Orbitally resolved spectral function
A. Kreisel, et al.
Phys. Rev. B **95**, 174504 (2017)





Liu, et al., arXiv:1802.02940