Orbital-Selective Pairing and Gap Structures of Iron-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

Peter O. Sprau, Andrey Kostin, J.C. Séamus Davis

LASSP, Department of Physics, Cornell University, Ithaca, NY 14853, USA

Peter O. Sprau, …, A. Kreisel, et al.
arXiv:1611.02134
A. Kreisel, et al.
arXiv:1611.02643

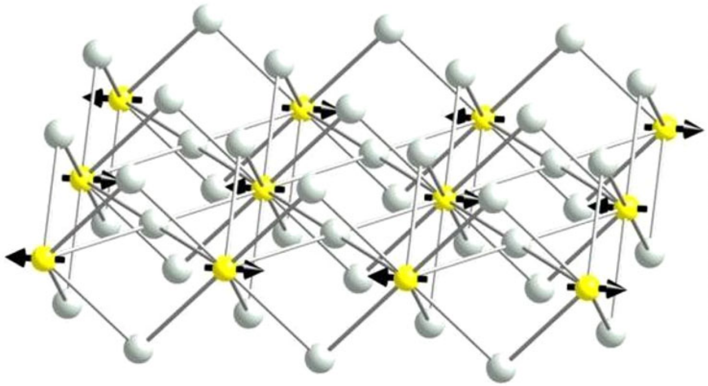
Outline

- Unconventional superconductivity
  - some “big questions”
- Example of Fe-based SC: FeSe (bulk)
  - Why interesting?
  - Nematic order
  - Superconducting gap structure
  - Orbital selectivity
- Other materials: FeSe (monolayer), LiFeAs

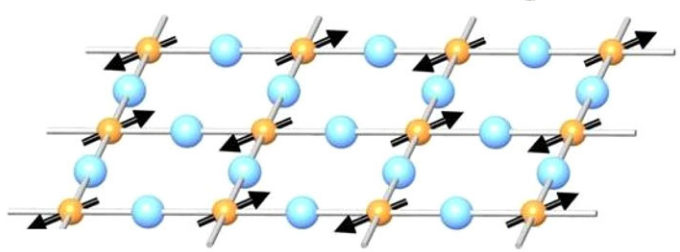
Unconventional superconductivity

2d active layers, antiferromagnetic spin orders (undoped compounds)

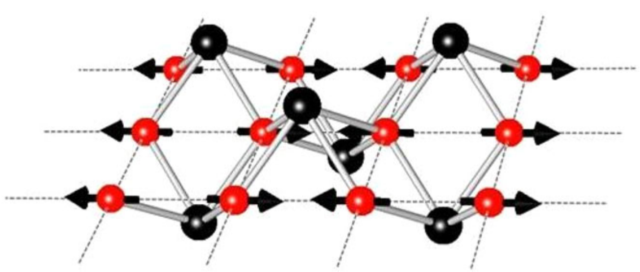
$CeIn_3$



CuO_2

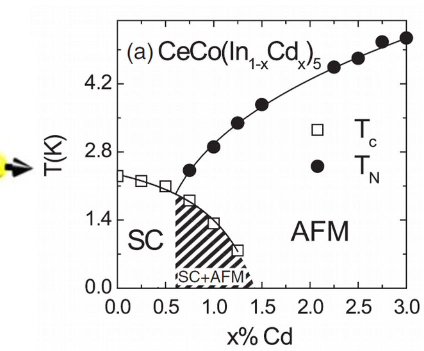


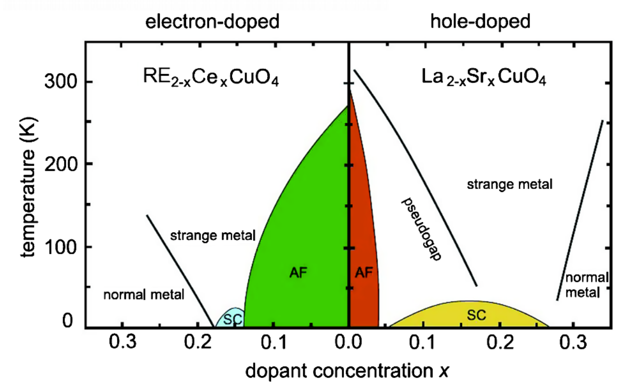
FeAs



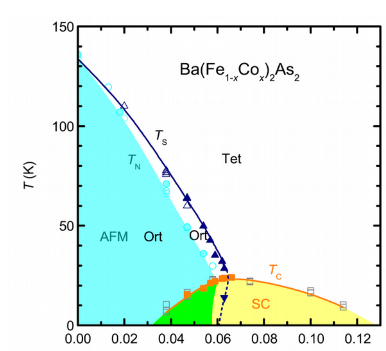
D. J. Scalapino
Rev. Mod. Phys. **84**, 1383 (2012)

Phase diagram: close proximity of antiferromagnetism and superconductivity





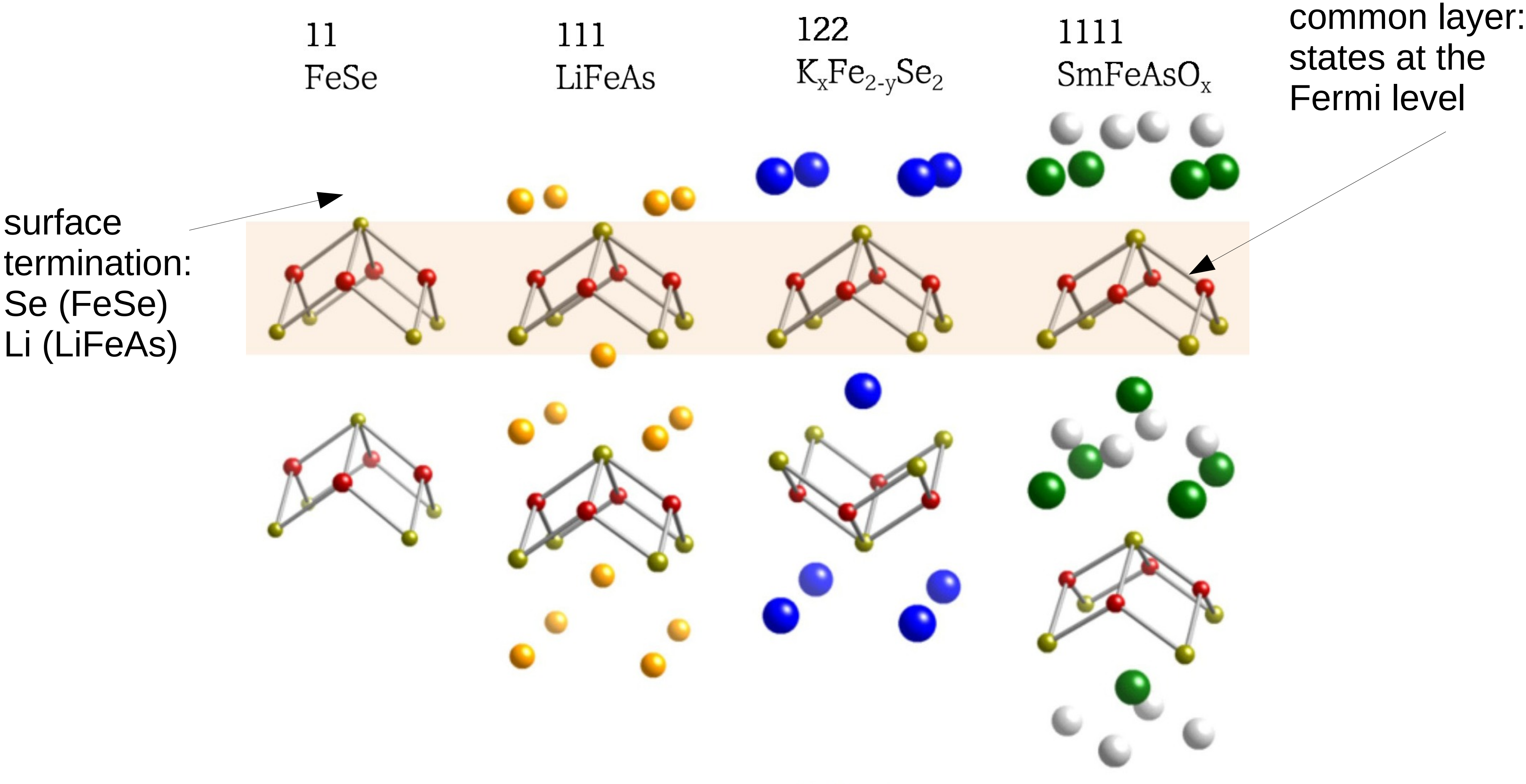
other interesting phases:
·charge density wave
·C_4 symmetric magnetic phases
·Nematic phase



Similarities in physical mechanisms?

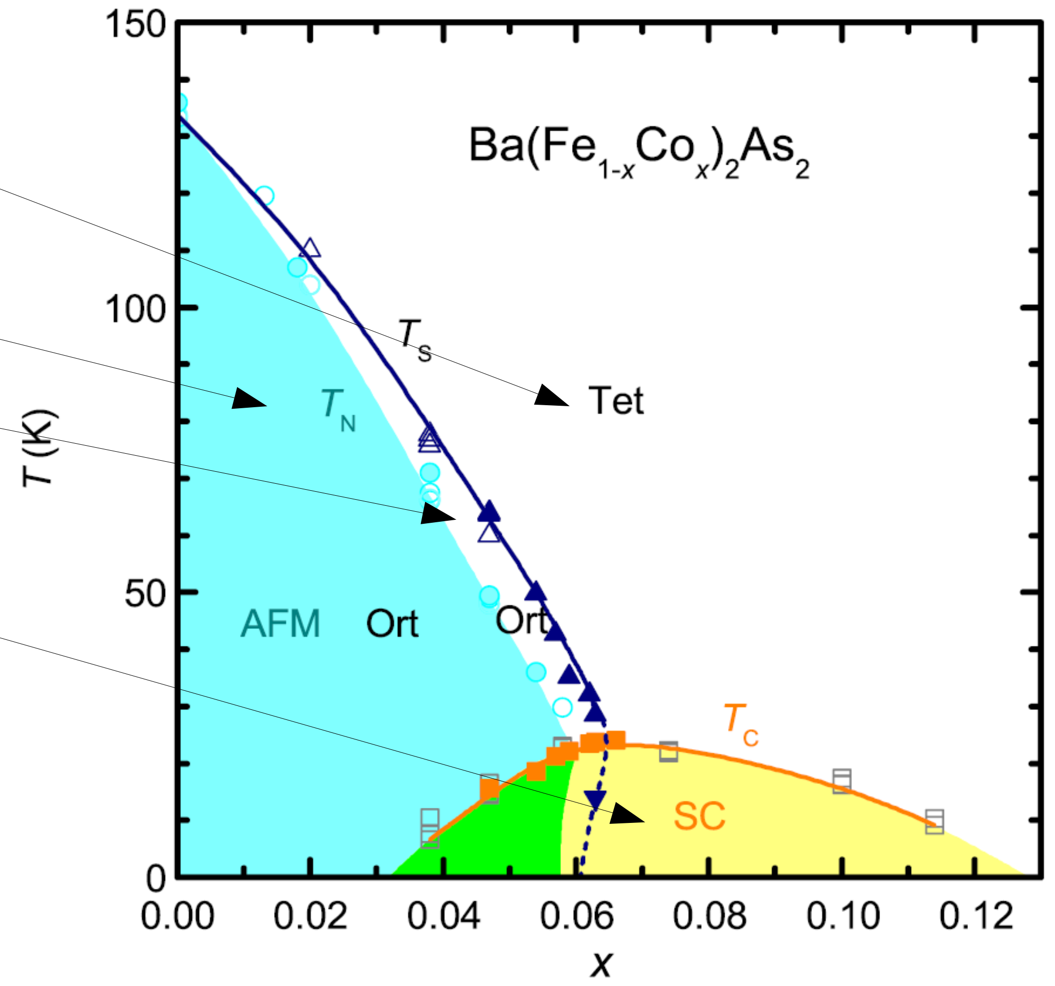
Fe based superconductors

- 2d layered materials: active states Fe(d)



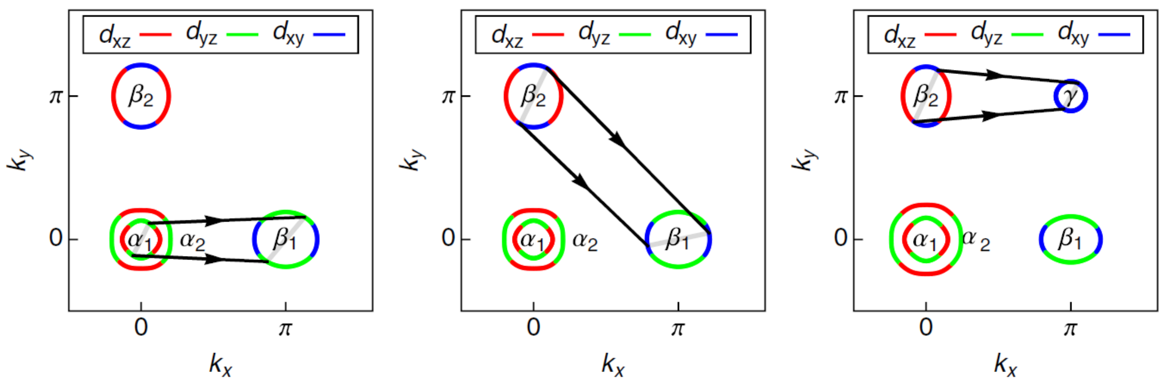
Fe based superconductors

- Band structure
- Magnetism
- Nematicity
- Superconductivity (gap structure)

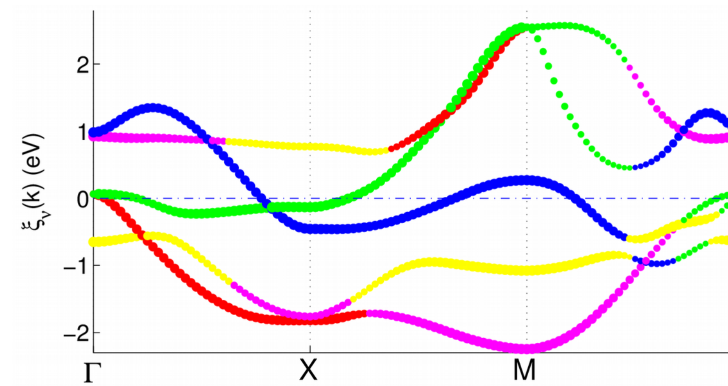


Band structure / Magnetism

- Fe(d) orbitals: quasi 2D electronic structure: 5 orbital model

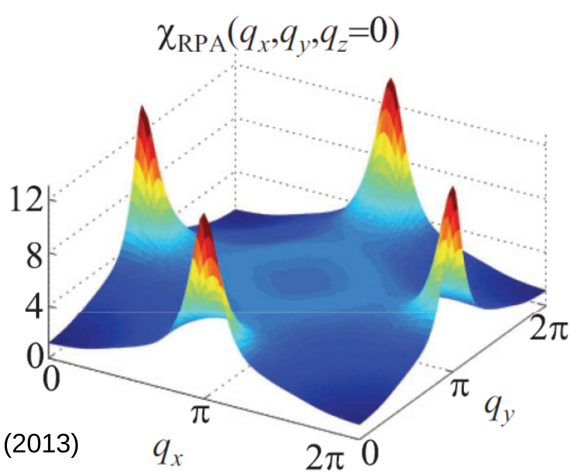


D. J. Scalapino Rev. Mod. Phys. **84**, 1383 (2012)

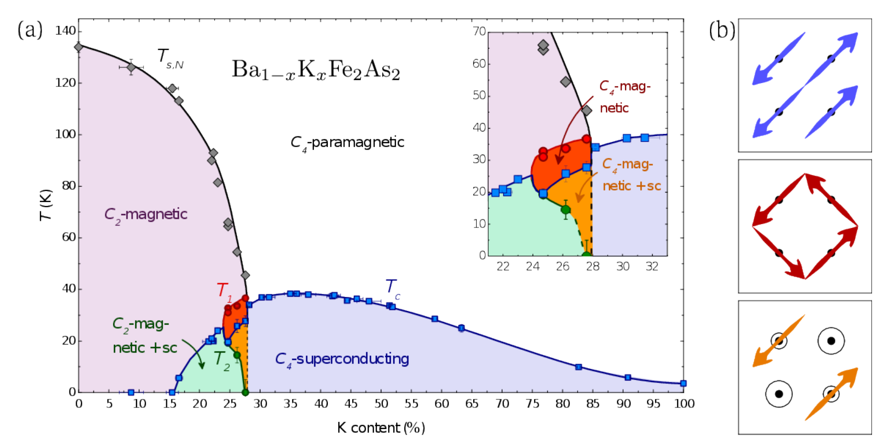


Chi et al., PRB **94**, 134515 (2016) [LiFeAs]

- Tendency towards (pi,0), (0,pi) magnetism



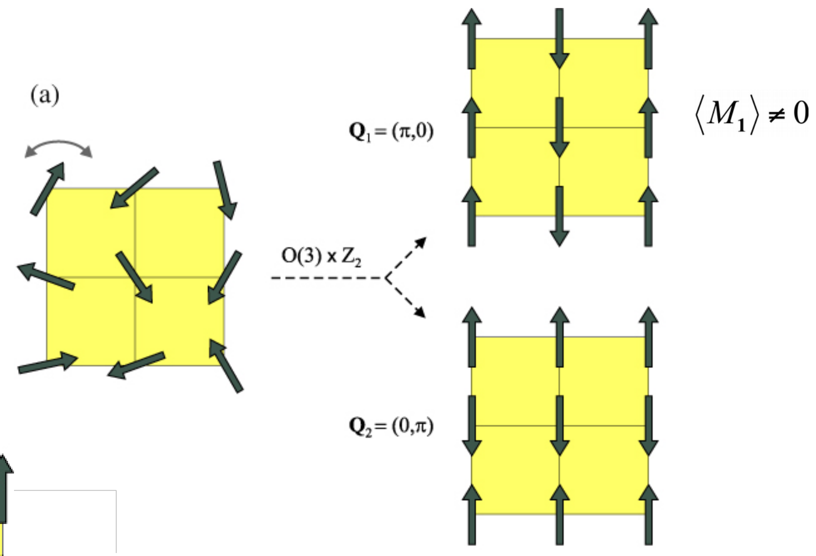
Wang, et al., PRB **88**, 174516 (2013)



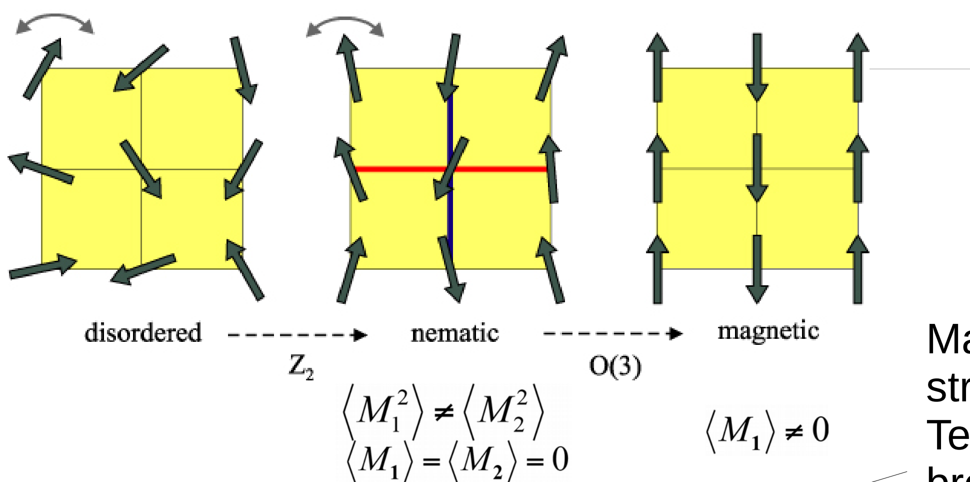
Böhmer, et al., Nat. Commun. **6**, 7911 (2015)
Gastiasoro, Andersen, PRB **92**, 140506 (2015)

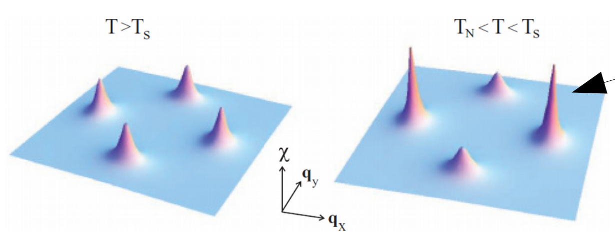
Nematicity

- Magnetic ordering

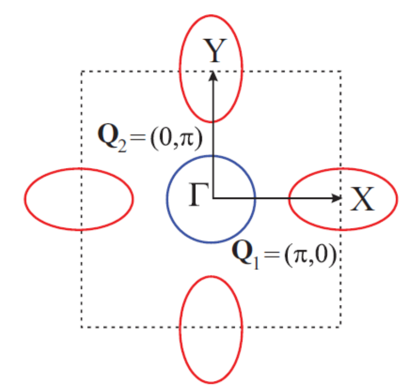


- Nematic state





Magnetic fluctuations stronger in x-direction
Tetragonal symmetry breaking



Itinerant approach to nematic state

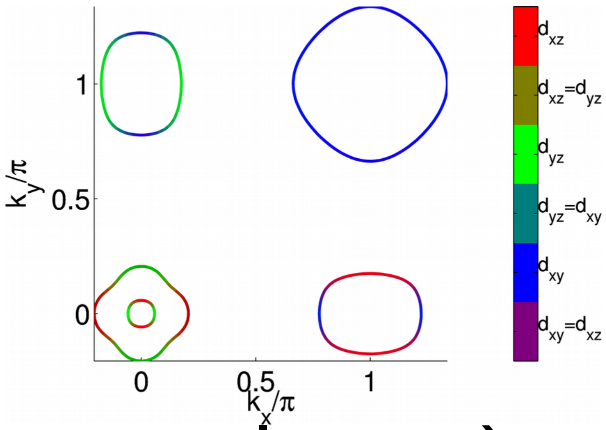
$$\chi_{\mathrm{nem}} \sim \chi_{\mathrm{mag}}^2$$

Fernandes, Schmalian, Supercond. Sci. Technol. **25** 084005 (2012)

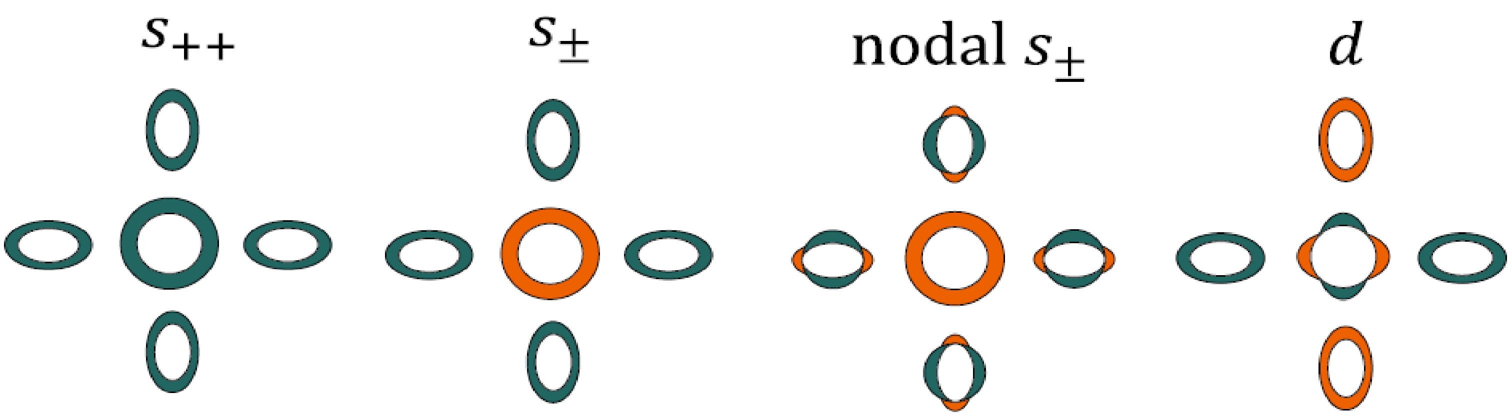
Fernandes, et al., PRB **85**, 024534 (2012)

Superconductivity: gap structure

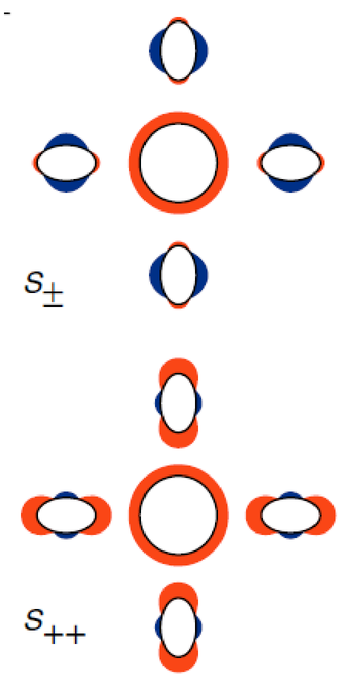
- Fermi surface



- Possible order parameters (tetragonal state)



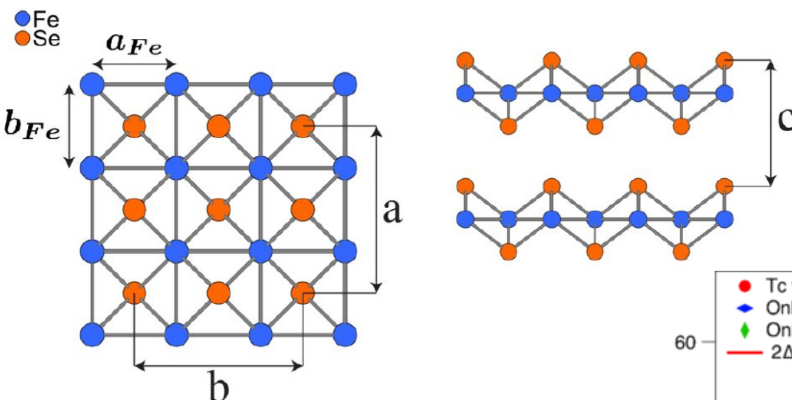
Hirschfeld, Korshunov, Mazin
Rep. Prog. Phys. **74** 124508 (2011)



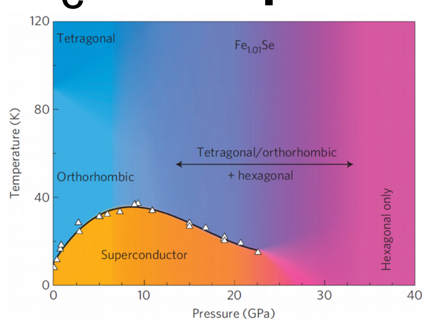
Mizukami, et al.
Nat. Commun. **5**, 5657 (2014)

FeSe: Why interesting?

- 11 compound

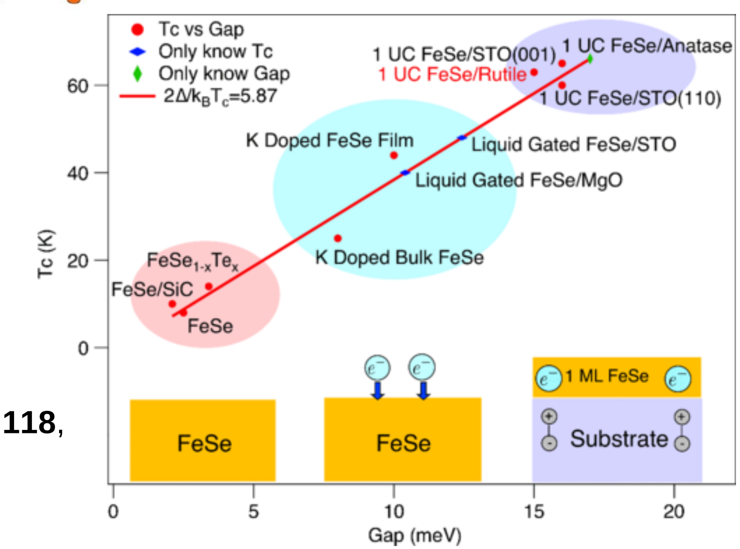


- T_c 8K, pressure,doping ~40K

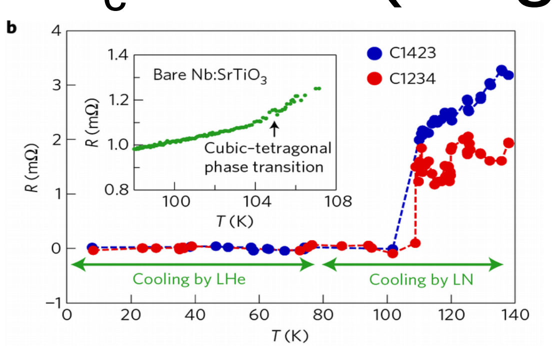


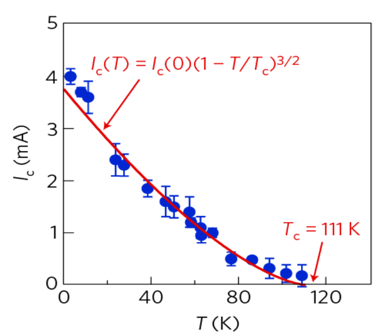
Medvedev, et al. Nat. Mater. **8**, 630 (2009)

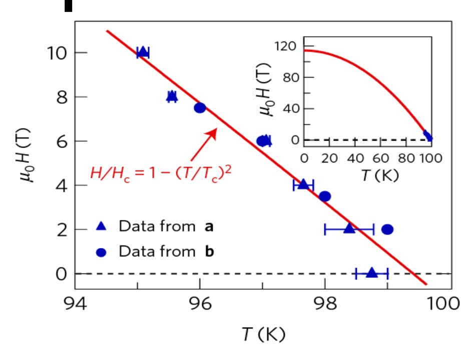
Rebec, et al., PRL **118**, 067002 (2017)



- T_c 100K (single layer) transport measurement





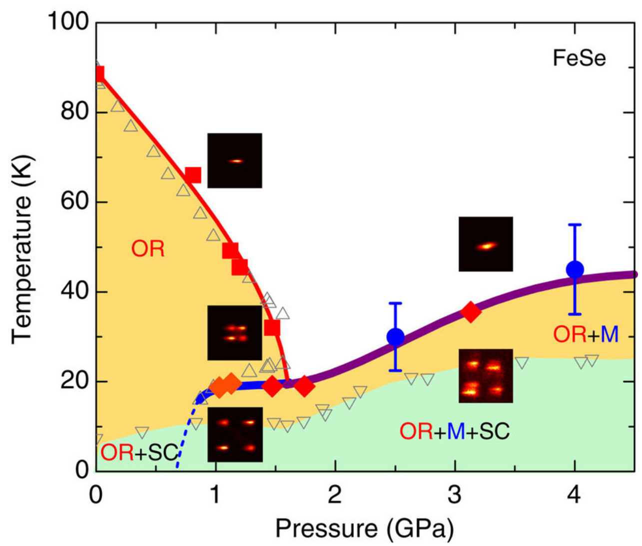


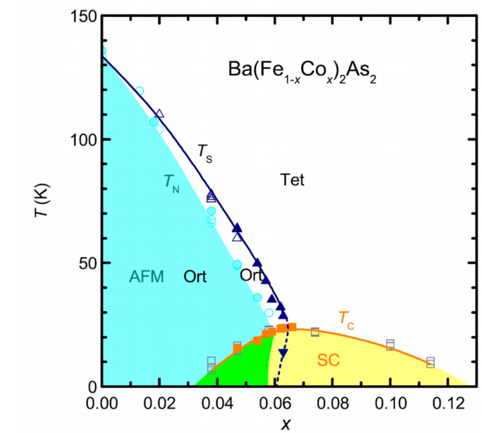
Ge et al. Nat. Mater. **14**, 285 (2015)

FeSe: Why interesting?

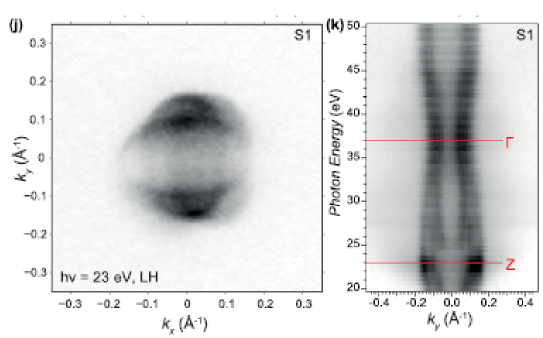
- nematic phase
  no magnetism
  (p=0)

K. Kothapalli, et al.,
Nat. Commun. **7**, 12728 (2016)

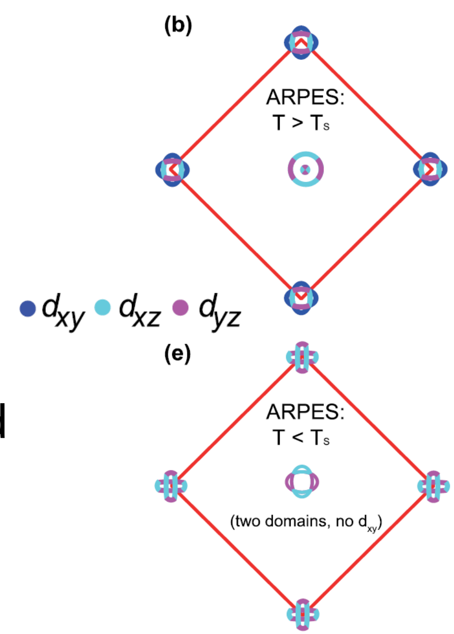




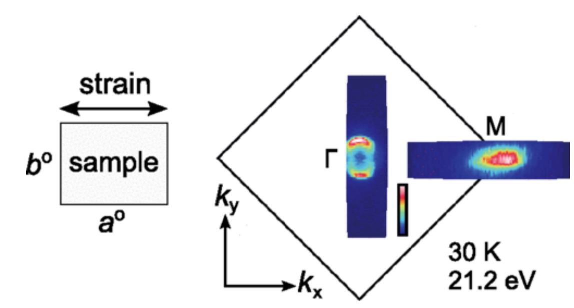
- ARPES
  measured band structure
  tiny Fermi surface
  (far from ab initio results)



Measured
orbital
splitting



detwinned ARPES



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)

FeSe

- Origin of nematic order
  - Orbital order
    Baek et al., Nat. Mat. **14**, 210 (2015)
    Yamakawa, Onari, Kontani, Phys. Rev. X **6**, 021032 (2016)
  - Quantum paramagnet
    Wang, Kivelson, Lee, Nat. Phys. **11**, 959 (2015)
  - Spin ferroquadrupolar / antiferroquadrupolar order
    Wang, Hu, Nevidomskyy PRL **116**, 247203 (2016)
    Lai, et al., arXiv:1603.03027
  - Longer-range Coulomb interactions
    Jiang, et al., PRB **93**, 115138 (2016) Scherer, et al., Phys. Rev. B **95**, 094504 (2017)
  - Competition between magnetism and charge current order
    Chubukov, Fernandes, Schmalian, PRB **91**, 201105(R) (2015)

FeSe

- Origin of nematic order
  - Orbital order
    Baek et al., Nat. Mat. **14**, 210 (2015)
    Yamakawa, Onari, Kontani, Phys. Rev. X **6**, 021032 (2016)
  - Quantum paramagnet
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    Lai, et al., arXiv:1603.03027
  - Longer-range Coulomb interactions
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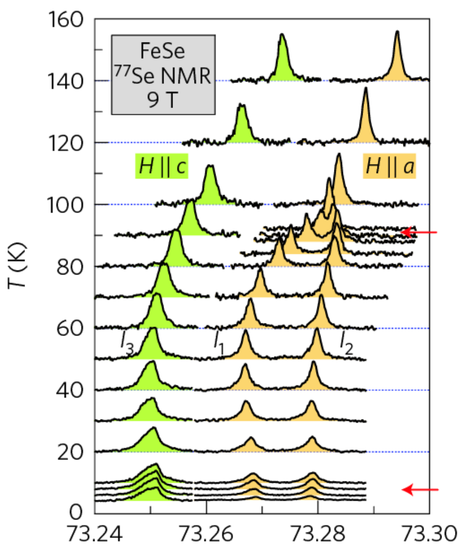
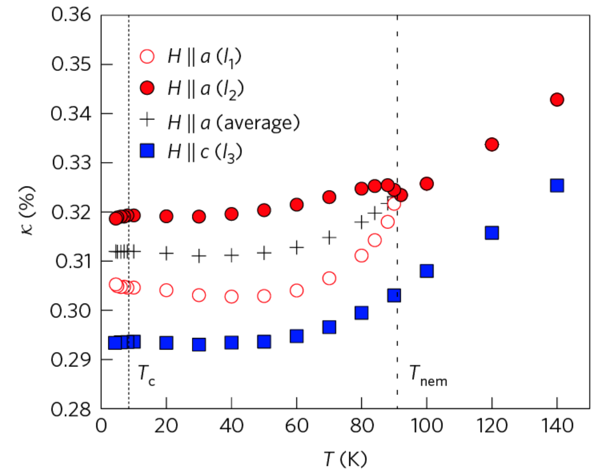
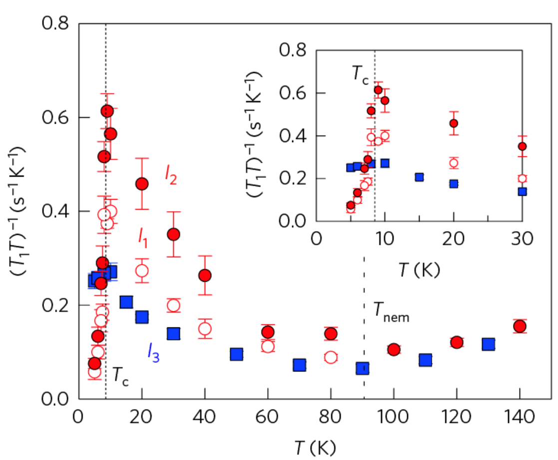
  - Competition between magnetism and charge current order
    Chubukov, Fernandes, Schmalian, PRB **91**, 201105(R) (2015)

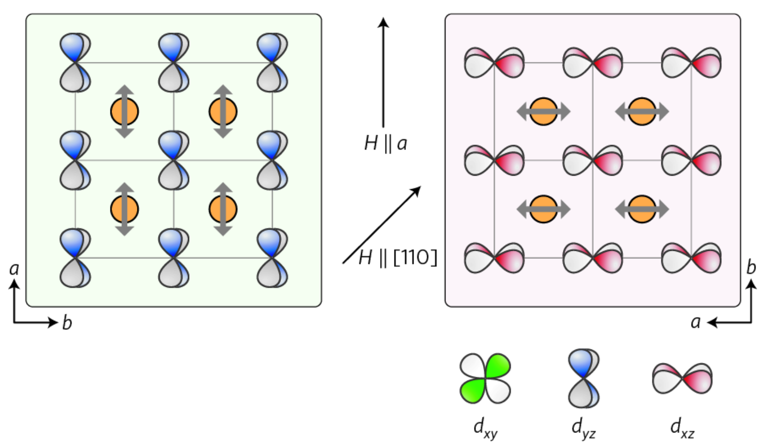
Nematic order

- NMR on FeSe splitting of the Se line
- No enhanced spin fluctuations below T_s







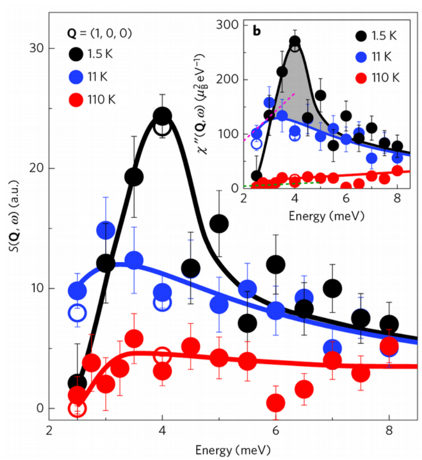


→ not caused by lattice distortion
→ evidence for orbital order (ferro)

Baek et al., Nat. Mat. **14**, 210 (2015)

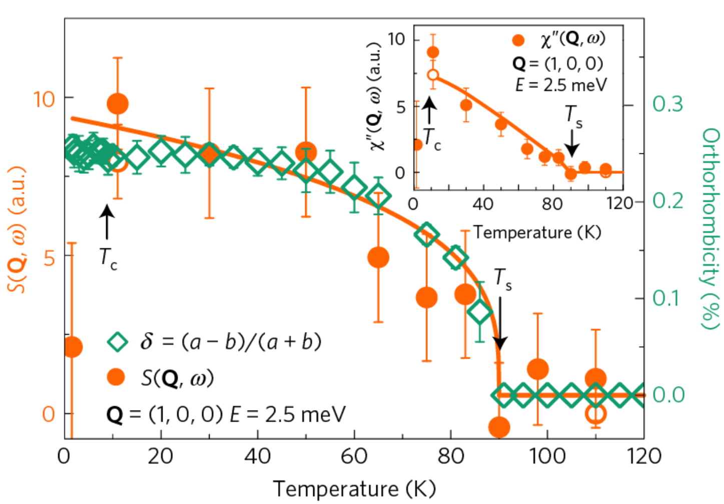
Spin excitations and magnetism

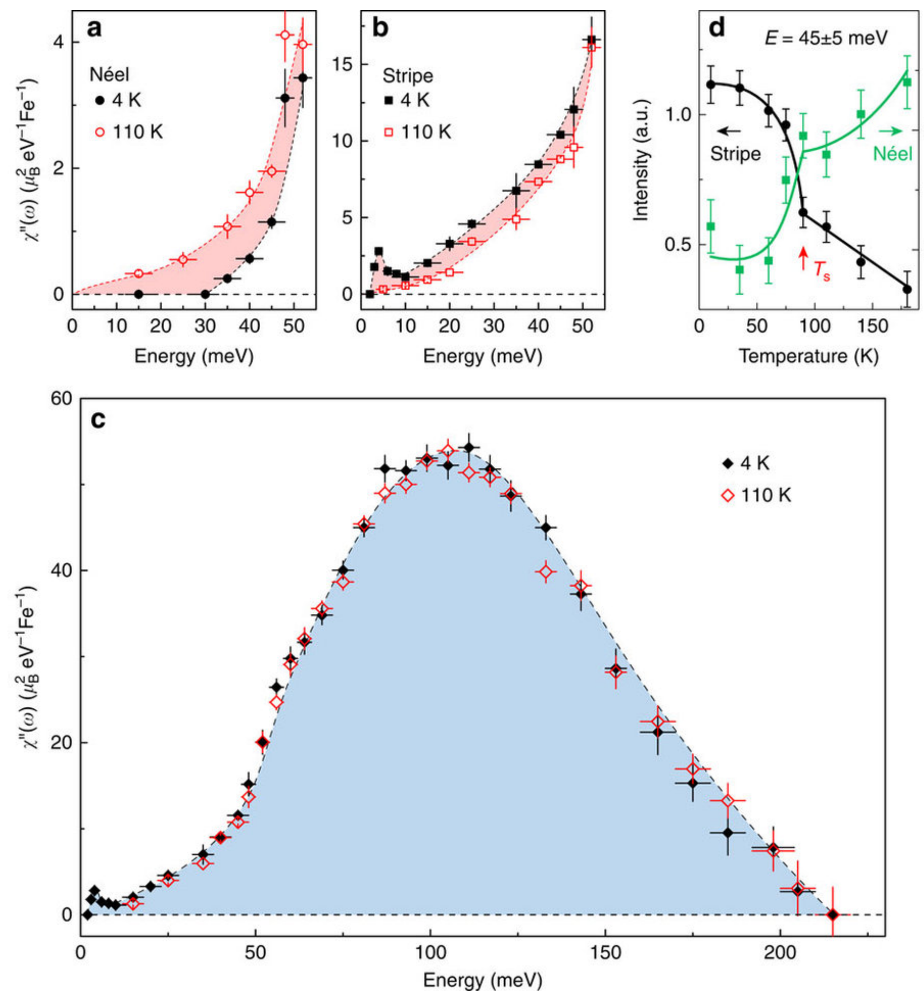
- Competition between stripe and Néel fluctuations



"spin resonance" at (pi,0)

Wang et al., Nat. Mat., **15**, 159 (2016)

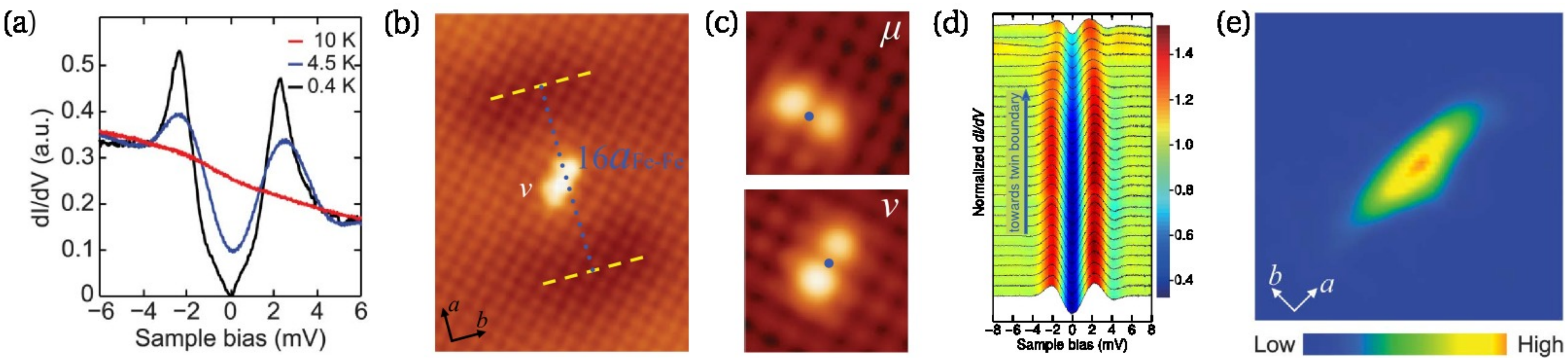




Wang et al., Nat. Commun. **7**, 12182 (2016)

Superconducting gap structure

- consequences: nodal gapstructure, anisotropy



Song et al., PRL **109**, 137004 (2012)

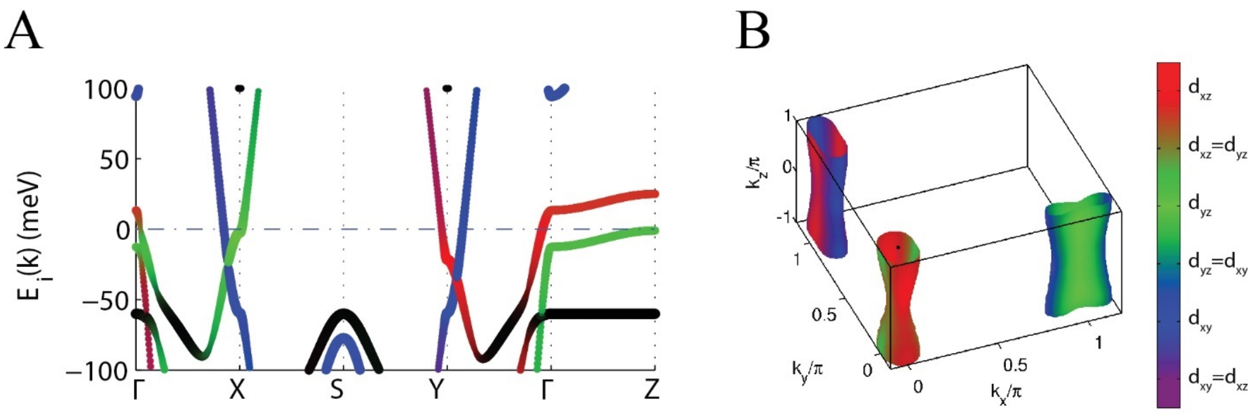
Song et al., Science **332**, 1410 (2011)

Modelling

- Band structure:
  measured spectral function

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

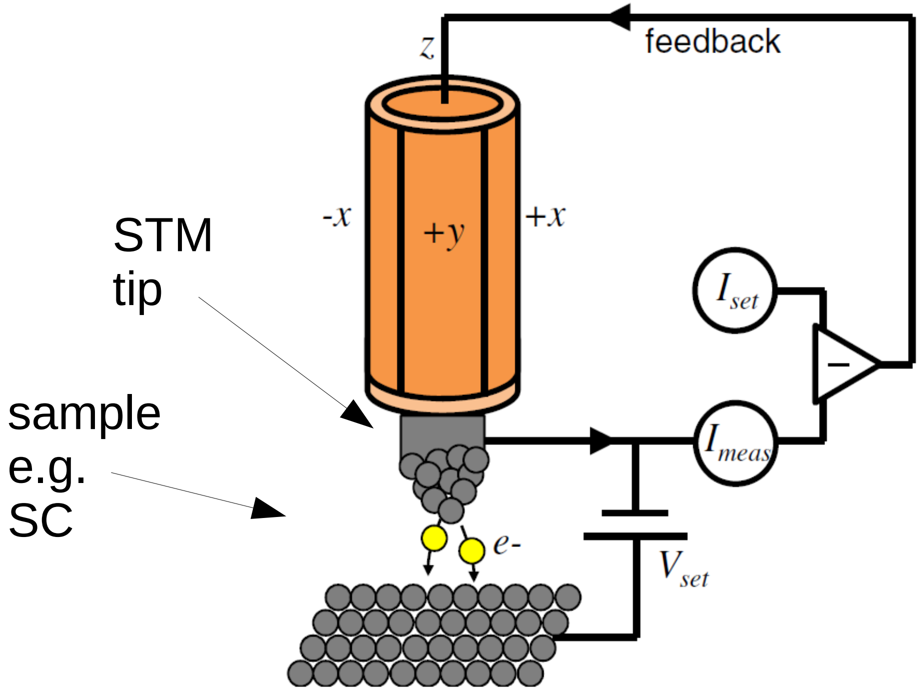
$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G(\vec{k},\omega)$$



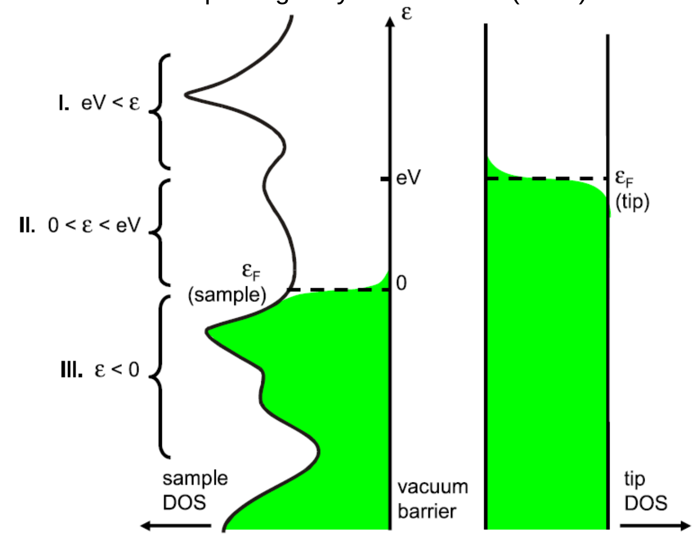
- ARPES
- Quantum oscillations
- Scanning tunnelling microscopy

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)

Scanning tunnelling microscopy



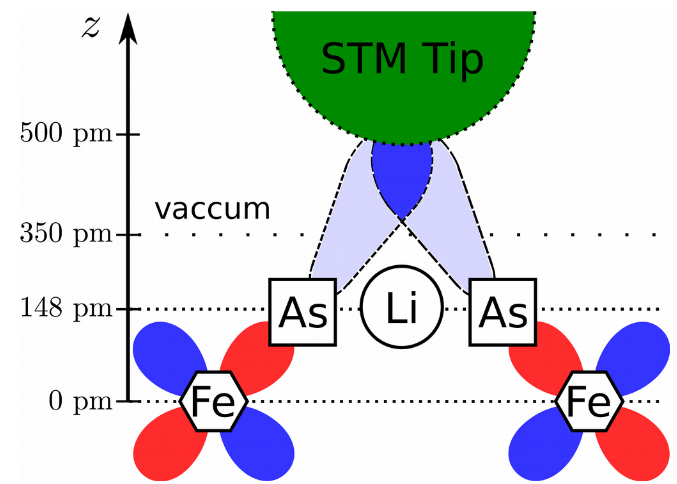
J. Hoffman Rep. Prog. Phys. **74** 124513 (2011)



Tunnelling current:

$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2\int_0^{eV}\rho(x,y,z,\epsilon)d\epsilon$$

Local Density Of States (LDOS)
of sample at given energy at the tip position

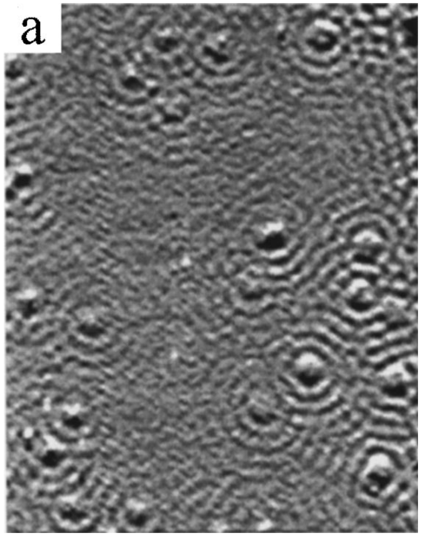


A. Kreisel, et al., Phys. Rev. B **94**, 224518 (2016)

J. Tersoff and D. R. Hamann, PRB **31**, 805 (1985)

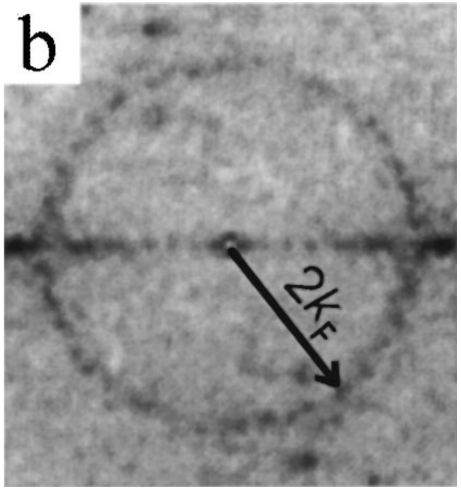
Quasiparticle Interference (QPI)

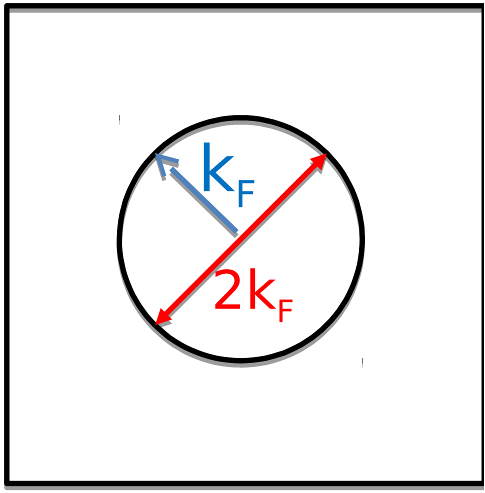
- STM on normal metal (Cu)
  - impurities
  - Friedel oscillations



L. Petersen, et al.
PRB **57**, R6858(R)
(1998)

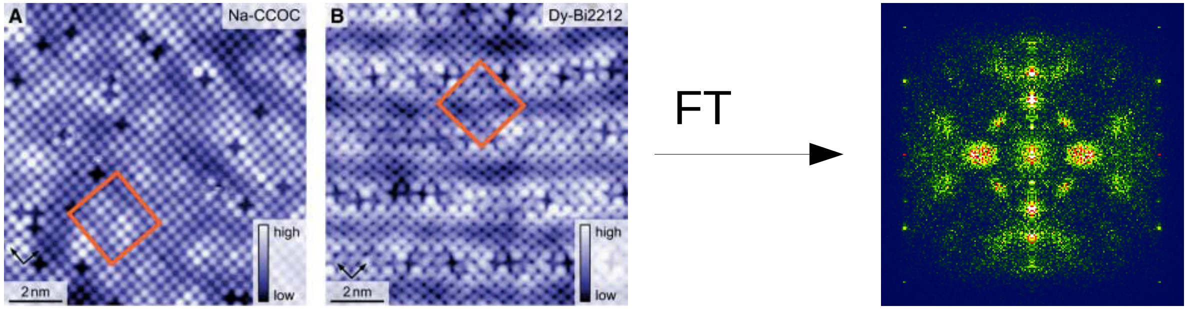
- Fourier transform of conductance map
  - mapping of constant energy contour

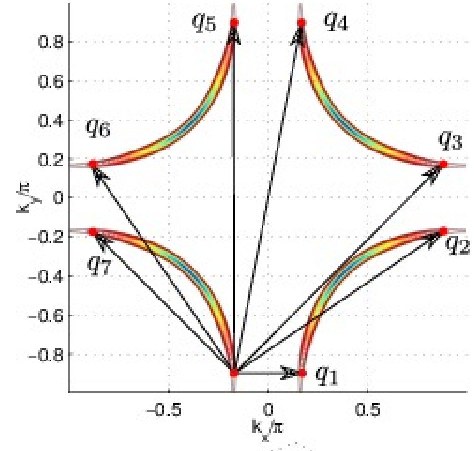




QPI in superconductors

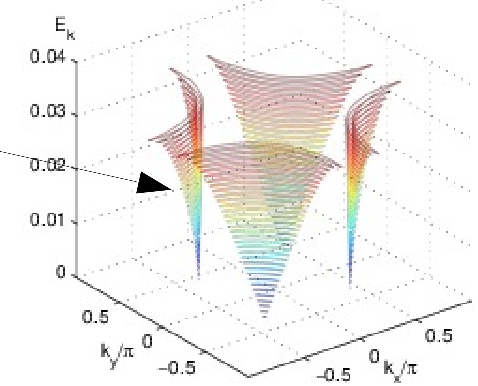
- Fourier transform of differential conductance maps

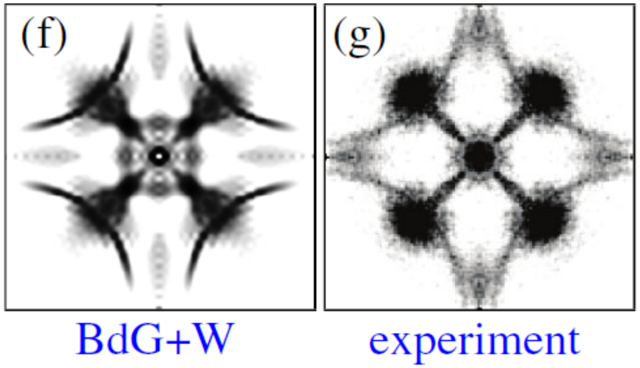




K Fujita et al. Science **344**, 612 (2014)

$$E_{\mathrm{k}} = \pm\sqrt{\epsilon_{\mathrm{k}}^2 + \Delta_{\mathrm{k}}^2}$$





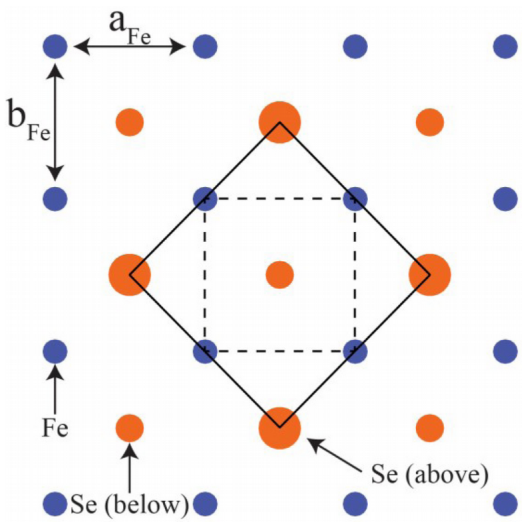
A. Kreisel, et al., PRL **114**, 217002 (2015)

Trace back Fermi surface+measure superconducting gap function

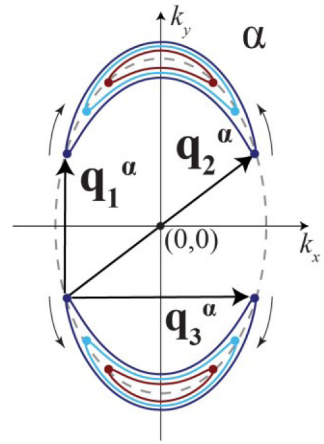
octet model: 7 scattering vectors between regions of high DOS

Peter O. Sprau, …, A. Kreisel, et al.
arXiv:1611.02134

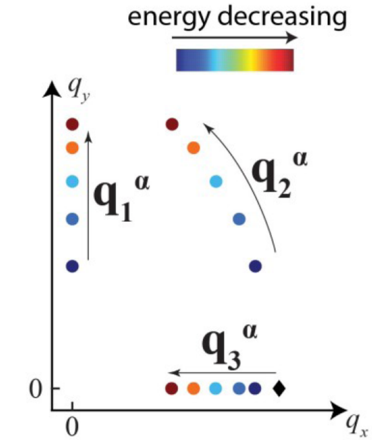
FeSe BQPI



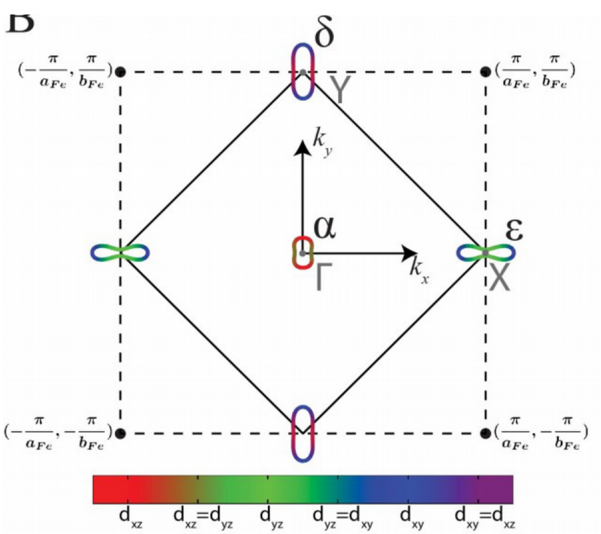
Coordinate system,
expected Fermi surface



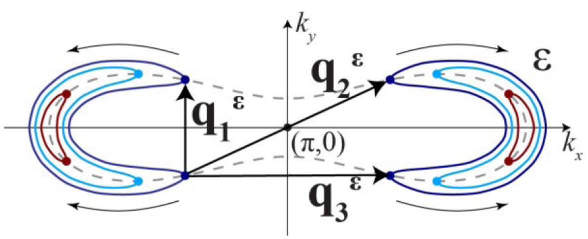
CEC: constant energy contour
Expected scattering vectors

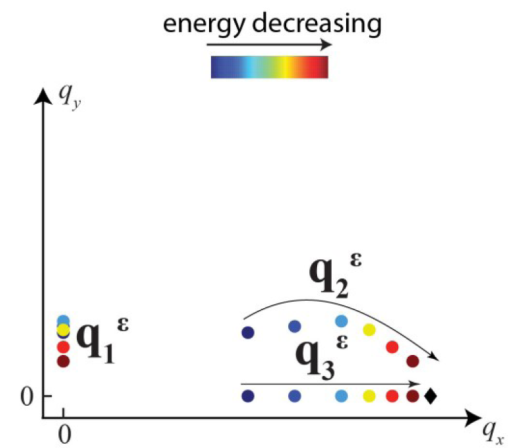


Dispersion of QPI peaks
q(E) → k(E) → E(k)

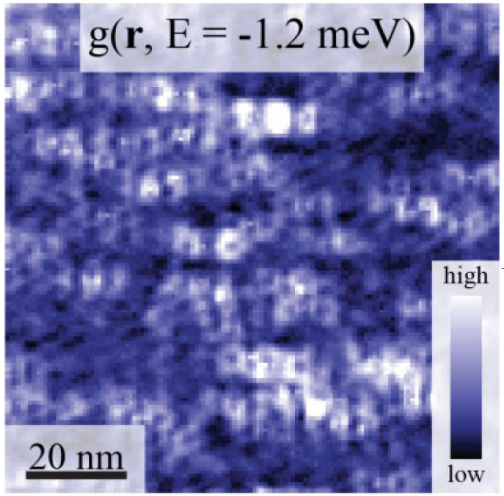


$$E_k = \pm\sqrt{\epsilon_k^2 + \Delta_k^2}$$

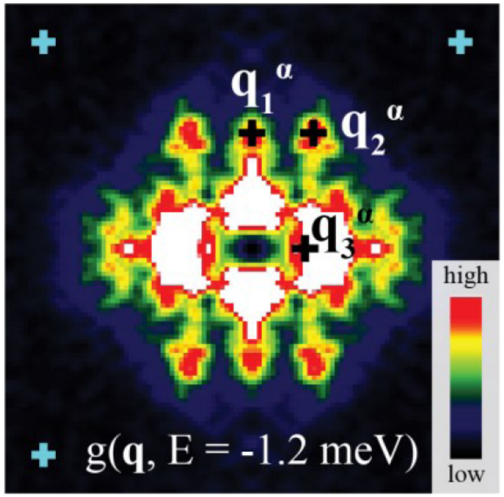




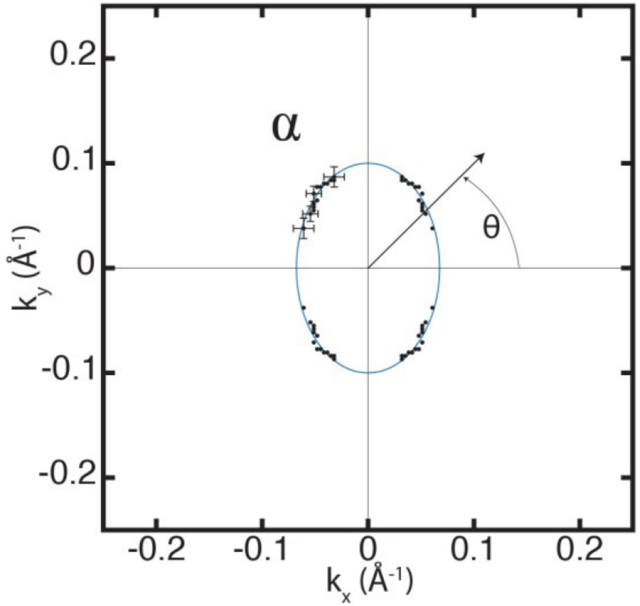
FeSe measurement



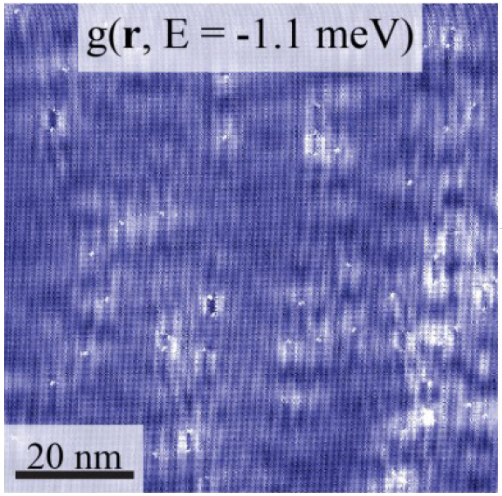
FT



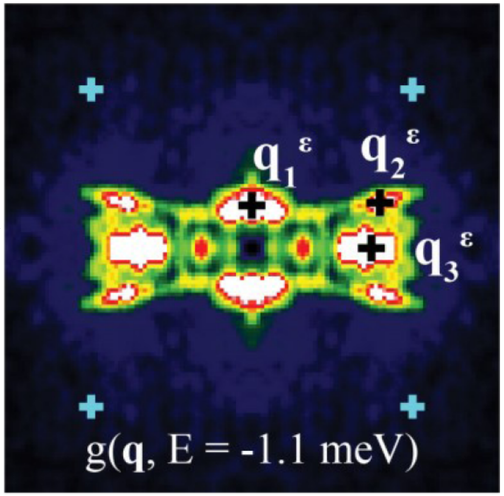
Conductance maps

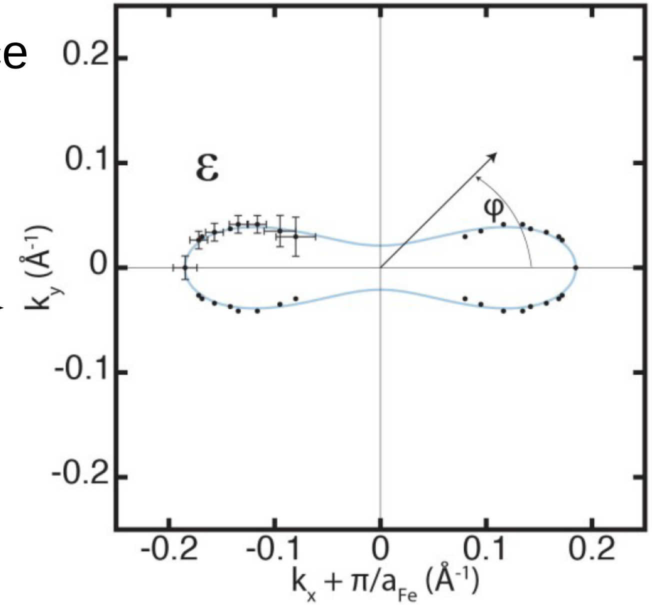


Trace back Fermi surface



FT





Band structure modelling

- Tight binding model

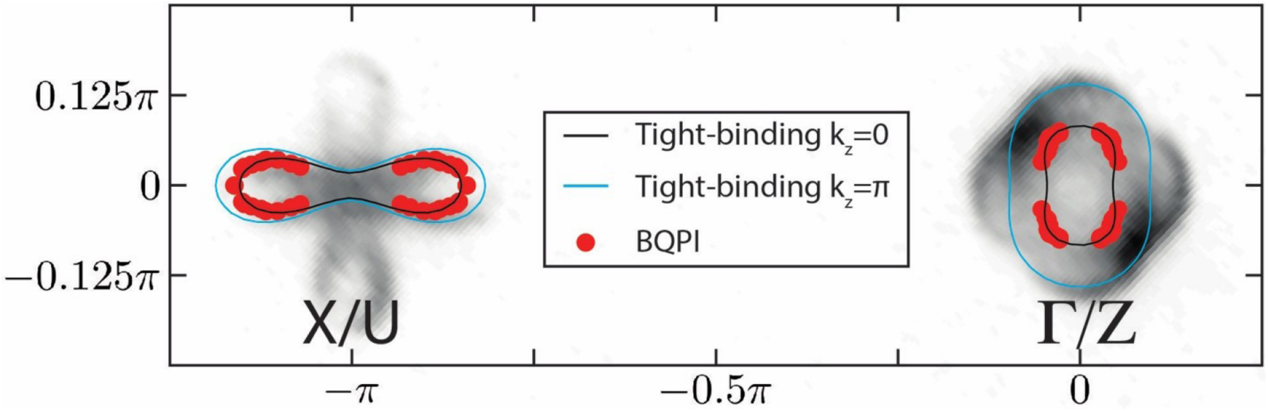
$$H_N = H_0 + H_{OO} + H_{SOC}$$

$$H_0 = \sum_{\boldsymbol{r},\boldsymbol{r}',a,b} t^{ab}_{\boldsymbol{r}-\boldsymbol{r}'} c^\dagger_{a,\boldsymbol{r}} c_{b,\boldsymbol{r}'}$$

site+bond centered orbital order

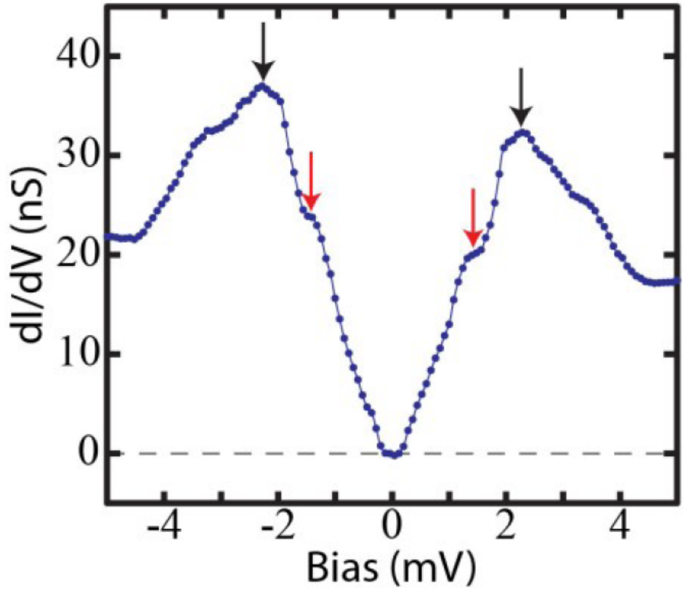
$$H_{SOC} = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

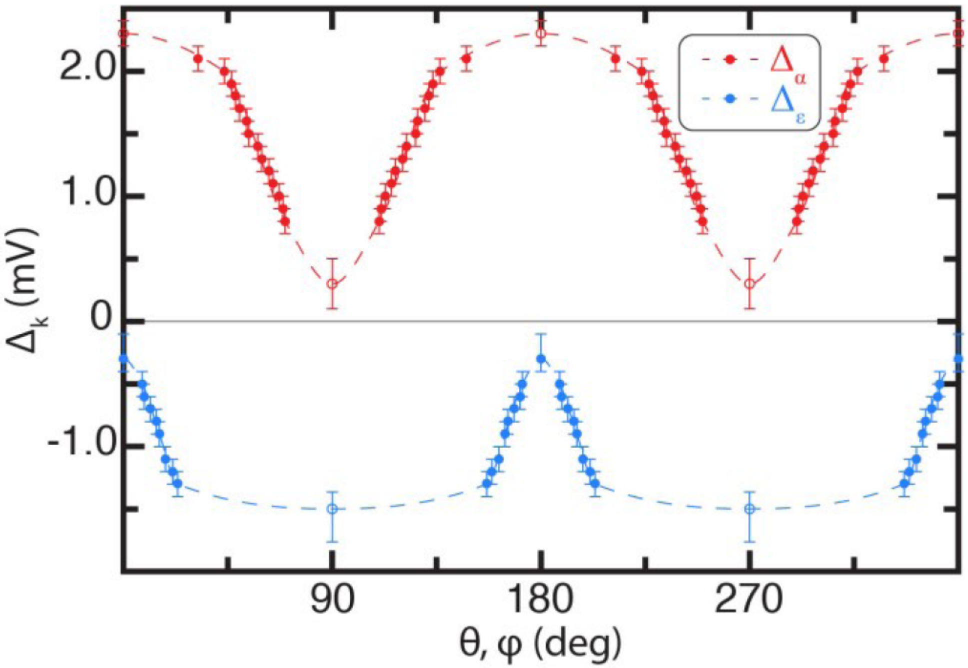
needed for consistent splitting at Gamma

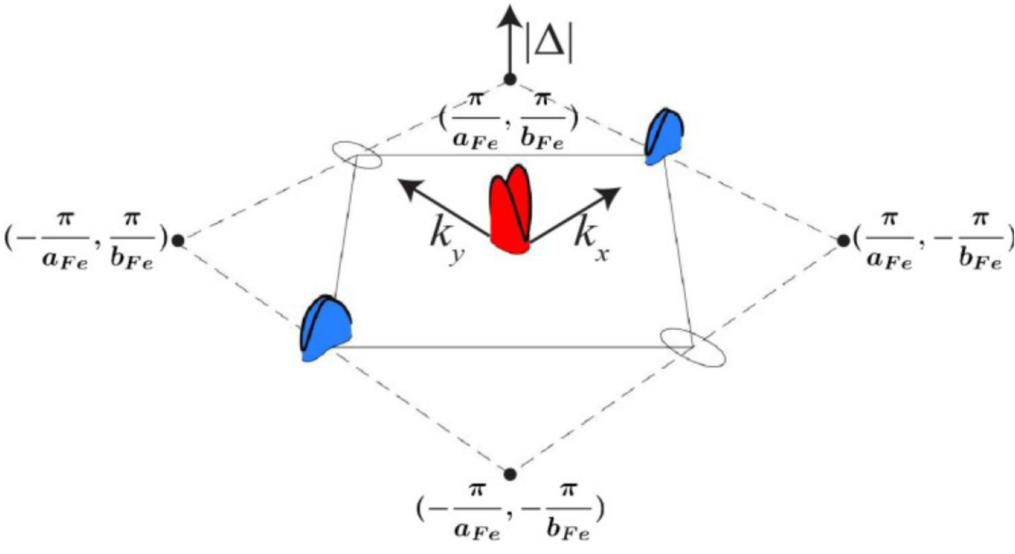


Superconducting gap

- highly anisotropic order parameter, 2 band
- “antiphase” oscillation







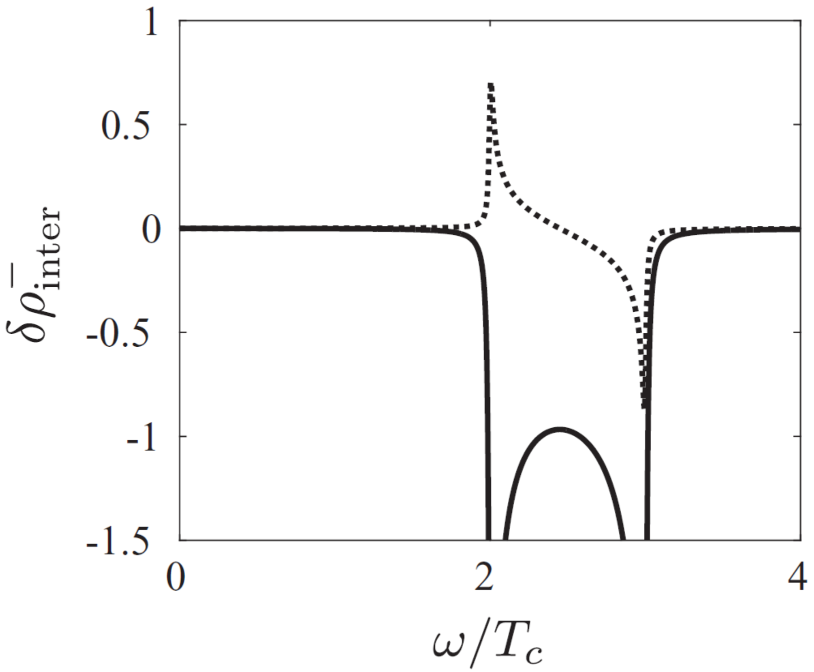
Sign change?!

Phase sensitive measurement

- HAEM procedure
- Consider:

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

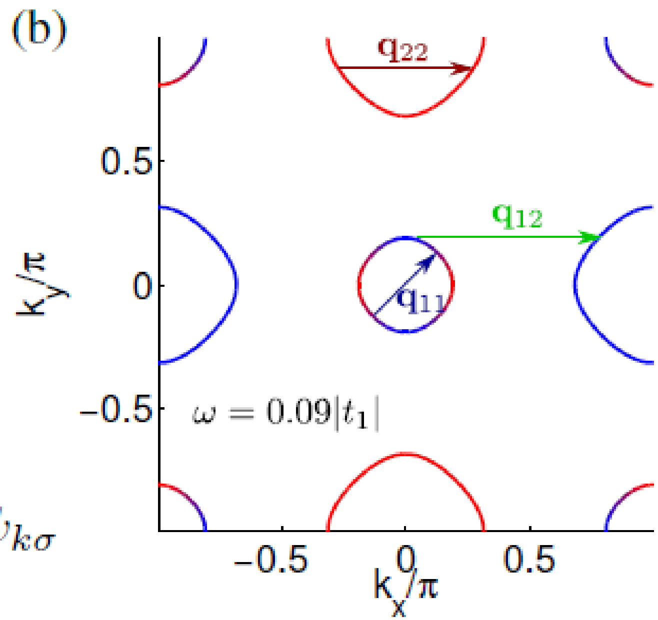
- s_{++}: sign change in signal
- s_{+-}: no sign change in signal



Hirschfeld et al., PRB **92**, 184513 (2015)

More realistic: 2 band model

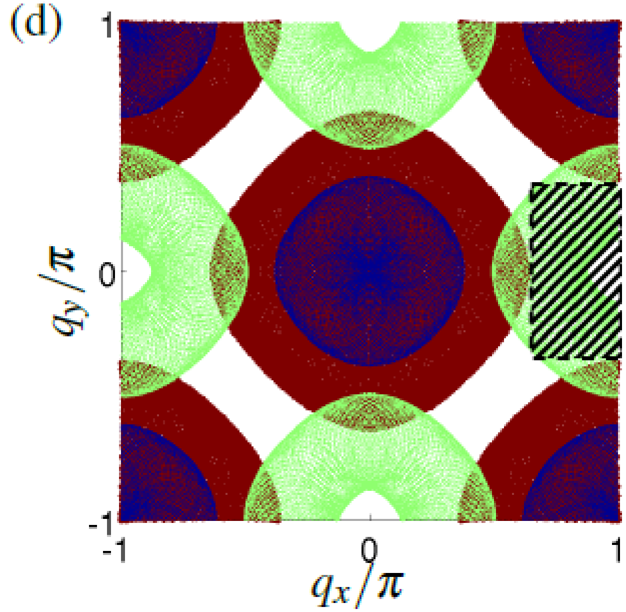
- Fermi surface



$$\mathcal{H}_0 = \sum_{k\sigma} \psi^\dagger_{k\sigma} \left[(\epsilon_+(k) - \mu)\tau_0 + \epsilon_-(k)\tau_3 + \epsilon_{xy}(k)\tau_1 \right] \psi_{k\sigma}$$

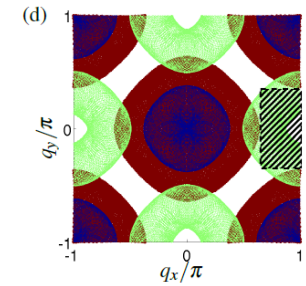
- JDOS for obtaining sign changing scattering vectors

$$\mathcal{H}_{\rm imp} = \sum_{\mu,\sigma=\pm} (V_{\rm imp} - \sigma J) c^\dagger_{i'\mu\sigma} c_{i'\mu\sigma}$$

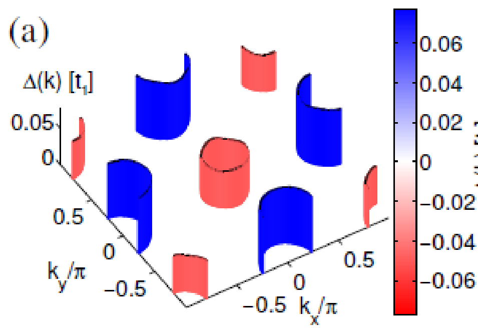


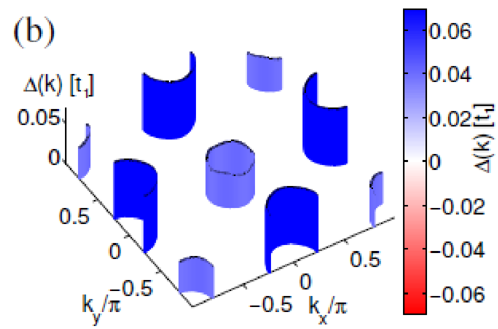
Martiny, Kreisel, Hirschfeld, Andersen, arXiv:1703.04891v1

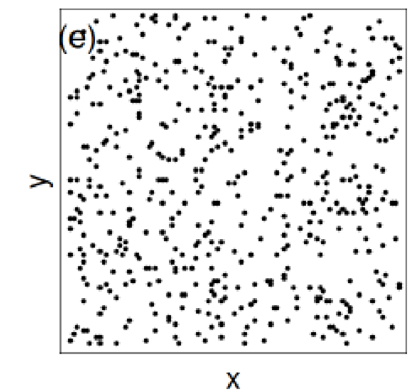
Results: possible ways to recover signal

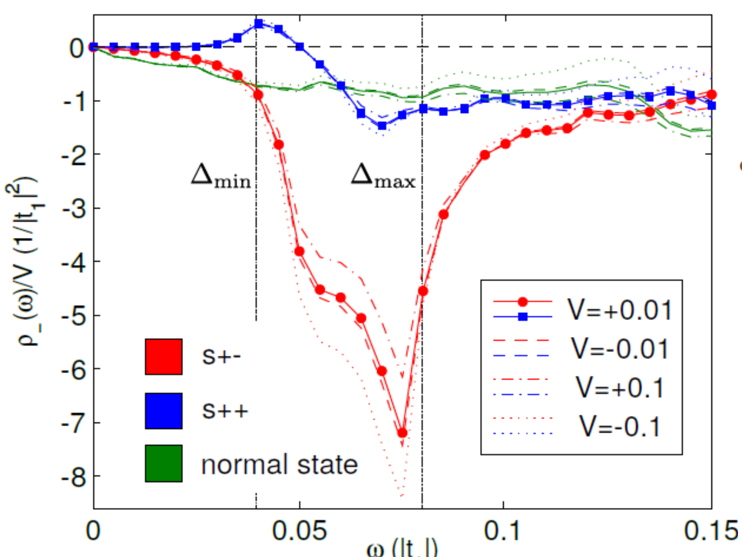


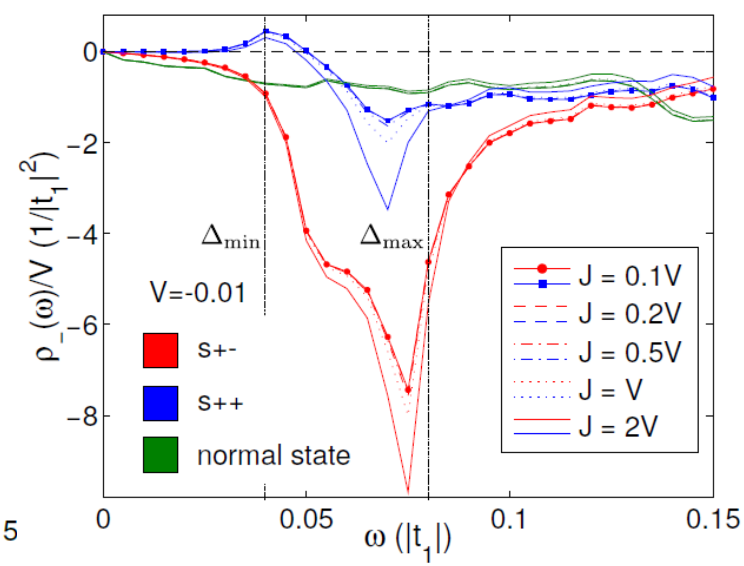
- Calculate antisymmetrized density response $\rho_{-}(\vec{q},\omega) = Re\{g(\vec{q},+\omega)\} - Re\{g(\vec{q},-\omega)\}$

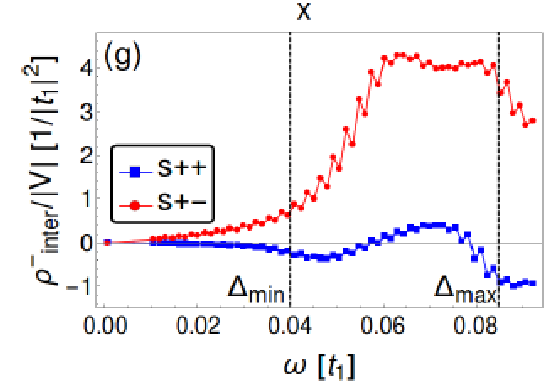












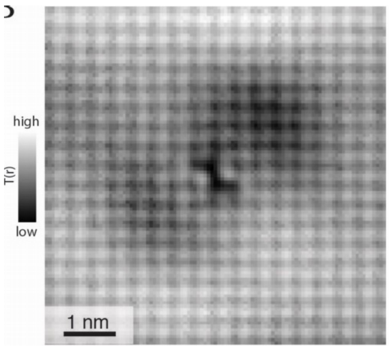
multiple impurities, dirty limit
→ Cherbychev BdG

Single impurity (centered!) → robust against impurity potential

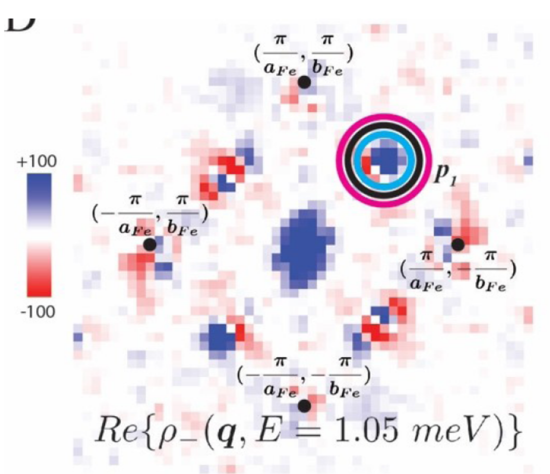
Measurement+modelling

- Problem: shift theorem in FT → single impurity (centered)

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



- separate interband scattering contributions



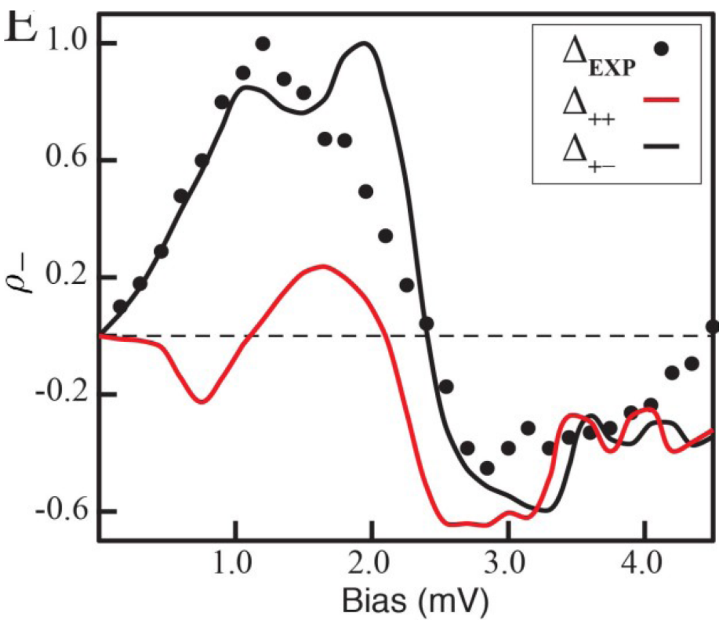
- Theory:
  use measured gap
  +electronic structure

$$G_{\mathbf{k},\mathbf{k'}}(\omega) = G^0_{\mathbf{k}-\mathbf{k'}}(\omega) + G^0_{\mathbf{k}}(\omega)T(\omega)G^0_{\mathbf{k'}}(\omega)$$

$$T(\omega) = \left[1 - V_{imp}G_0(\omega)\right]^{-1}V_{imp}$$

$$\delta N(\mathbf{q},\omega) = \frac{1}{\pi}Tr\{Im\sum_{\mathbf{k}} G^0_{\mathbf{k}}(\omega)T(\omega)G^0_{\mathbf{k}+\mathbf{q}}(\omega)\}$$

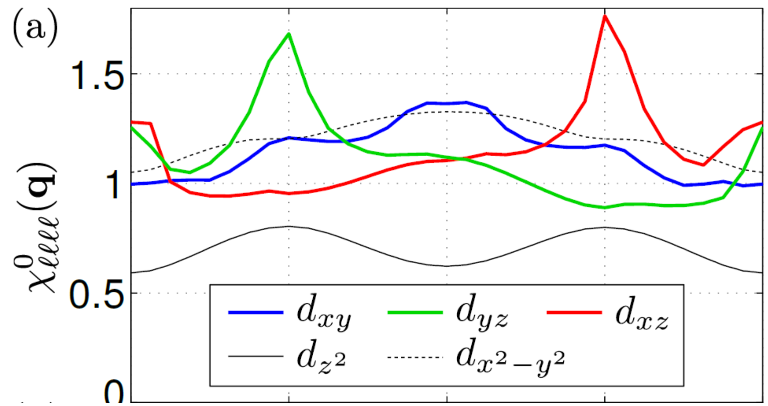
$$\rho(\omega) = \sum'_{\mathbf{q}} \delta N(\mathbf{q},\omega)$$



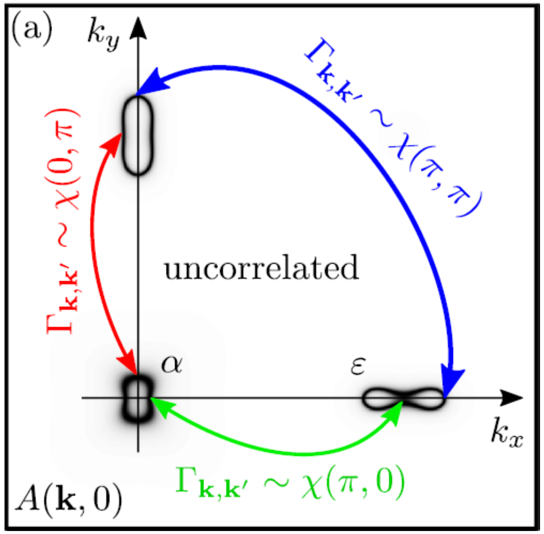
→ no sign change in signal, thus GAP changes sign

Pairing from spin-fluctuation theory?

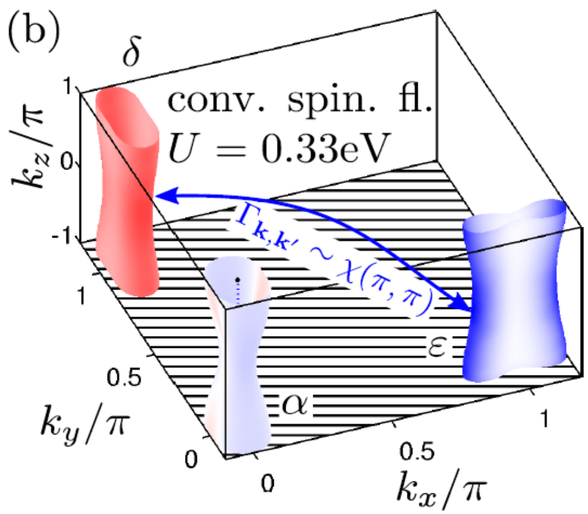
- Susceptibility

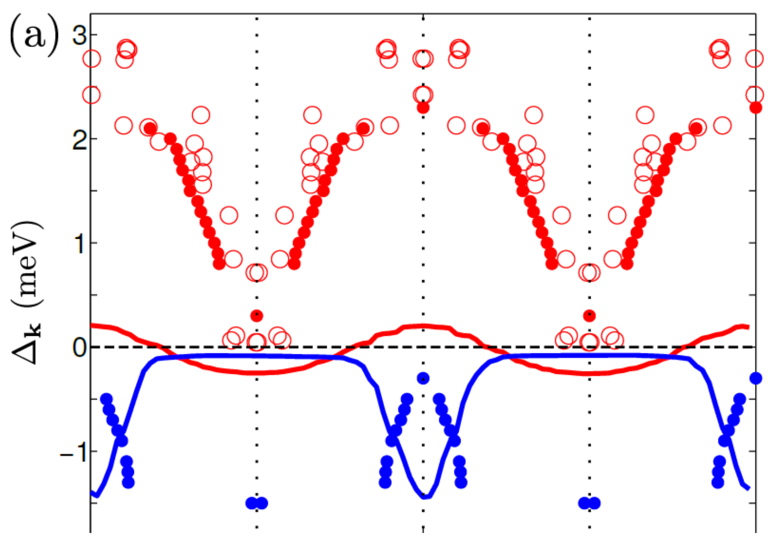


- Pairing glue



- Solution of BCS equation





Does not work!
→ "in-phase" anisotropy
→ Small anisotropy on Gamma pocket!

What is missing?

- Interactions (standard)
- Electronic structure (measured)
- Pairing mechanism?

$$H = H_0 + U \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + U' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$
$$+ J \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c^\dagger_{i\ell\sigma} c^\dagger_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma}$$
$$+ J' \sum_{i,\ell'\neq\ell} c^\dagger_{i\ell\uparrow} c^\dagger_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow},$$

$$\chi^0_{\ell_1\ell_2\ell_3\ell_4}(q) = -\sum_{k,\mu\nu} M^{\mu\nu}_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{q}) G^\mu(k+q) G^\nu(k)$$

$$\Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}') = \left[\frac{3}{2}\bar{U}^s \chi_1^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^s + \frac{1}{2}\bar{U}^s - \frac{1}{2}\bar{U}^c \chi_0^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^c + \frac{1}{2}\bar{U}^c\right]_{\ell_1\ell_2\ell_3\ell_4}$$

$$\Gamma_{\nu\mu}(\mathbf{k},\mathbf{k}') = \mathrm{Re} \sum_{\ell_1\ell_2\ell_3\ell_4} a_\nu^{\ell_1,*}(\mathbf{k}) a_\nu^{\ell_4,*}(-\mathbf{k}) \times \Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}')\, a_\mu^{\ell_2}(\mathbf{k}') a_\mu^{\ell_3}(-\mathbf{k}')$$

Fermi liquid description

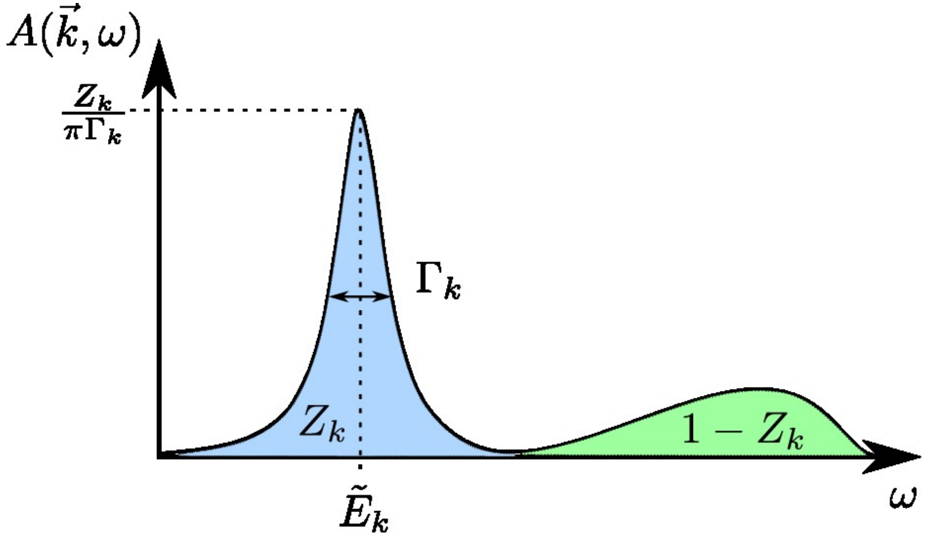
- Coherent electronic states

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

$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G(\vec{k},\omega)$$

- Dressed electronic states

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



Relevant for Fe based SC:

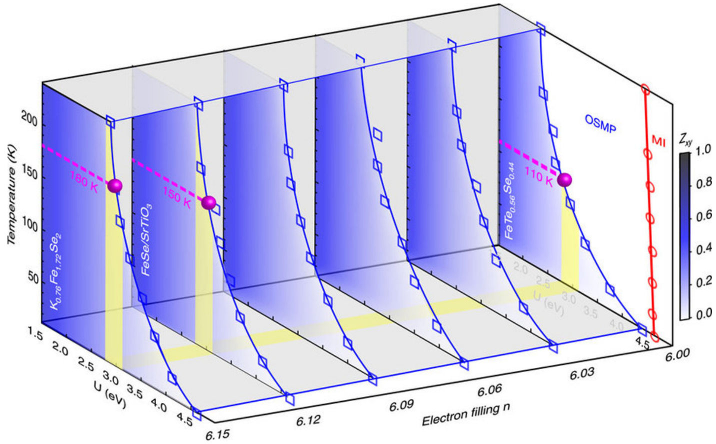
Yin, Haule, Kotliar, Nat. Mat. **10**, 932-935 (2011)
de' Medici, Giovannetti, Capone. Phys. Rev. Lett. **112**, 177001 (2014)
M. Aichhorn, et al., Phys. Rev. B **82**, 064504 (2010)
Liu et al., Phys. Rev. B **92**, 235138 (2015)
Yi et al., Nat. Comm. **6**, 7777 (2015)
...

Orbital selective physics

- States in some orbitals more decoherent than others

  Strong renormalizations of the d_{xy} orbital

  Yi et al., Nat. Comm. **6**, 7777 (2015)



- Spectroscopic probes struggle to detect d_{xy} orbital states

- FeSe: quasiparticle weights for d_{xz} and d_{yz} orbital distinct in nematic phase

$$G_{ab}(\boldsymbol{k},\omega) = Z_{ab} G^0_{ab}(\boldsymbol{k},\omega)$$

$$c_a \to \sqrt{Z_a} c_a \qquad\qquad Z_{ab} = \sqrt{Z_a}\sqrt{Z_b}$$

geometric mean of quasiparticle weights

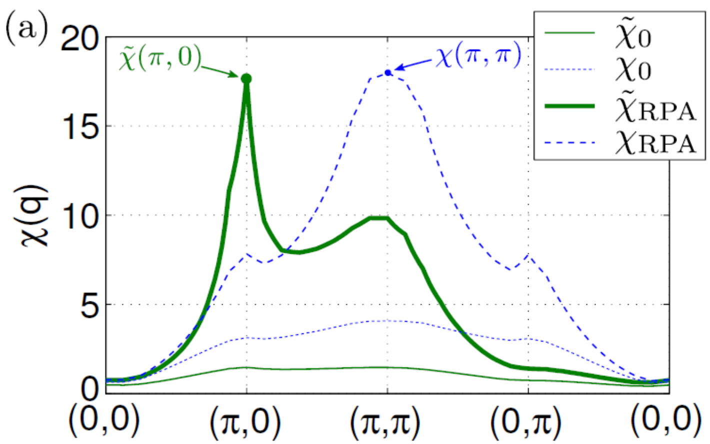
Spin-fluctuation theory

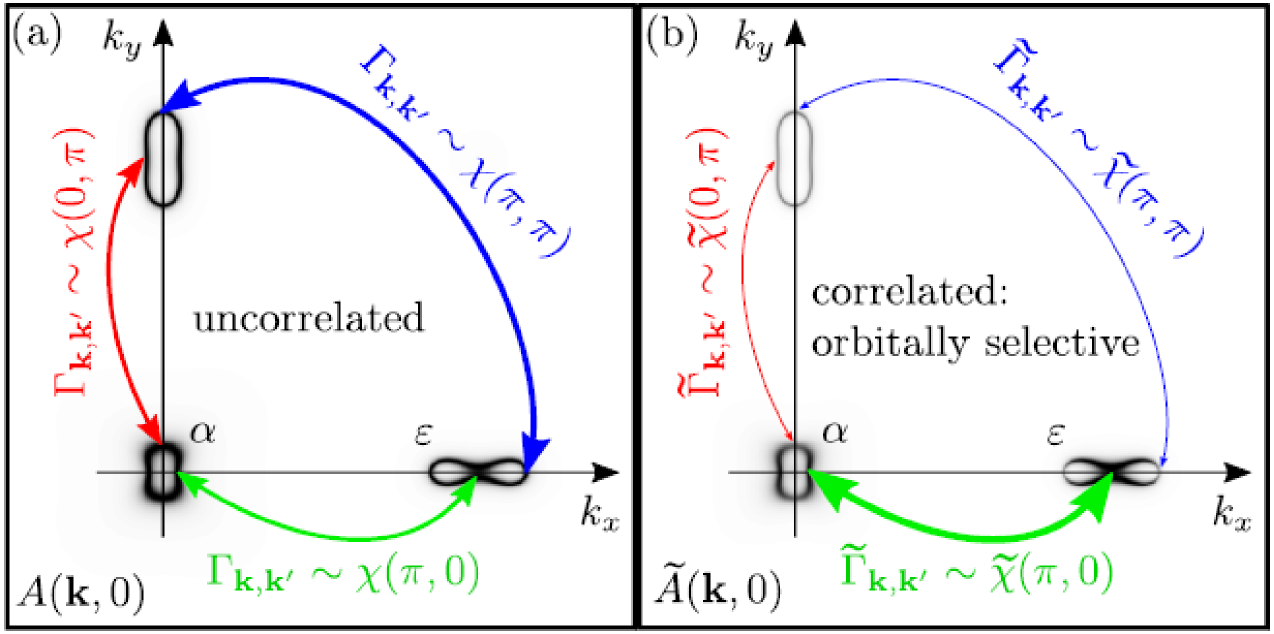
- "dressed susceptibility"

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

- Dressed pairing interaction

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

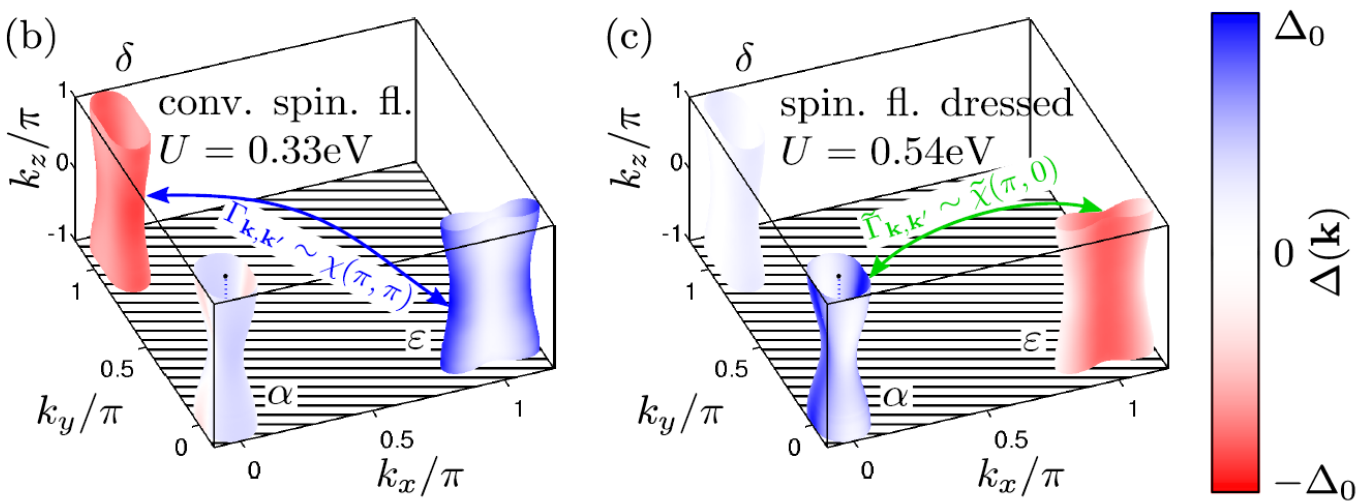




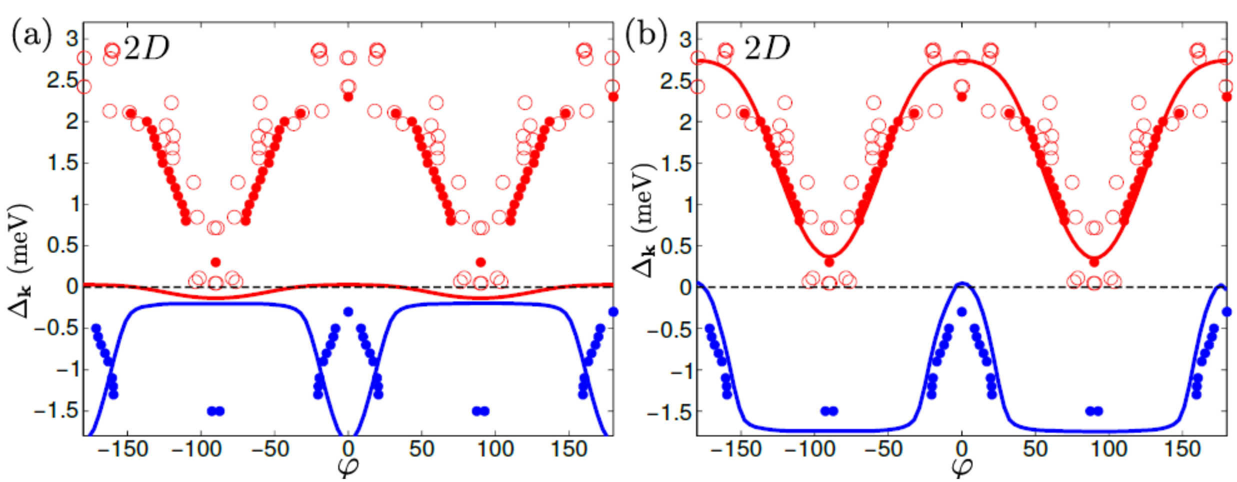
Dominant pairing in d_{yz} orbital channel
→ orbital selective pairing

Pairing and gap structure

uncorrelated correlated



$$c_a \to \sqrt{Z_a}\, c_a$$



Fit parameters, so far no microscopic calculation
But: same trends found in microscopic calculations

$$(d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2})$$

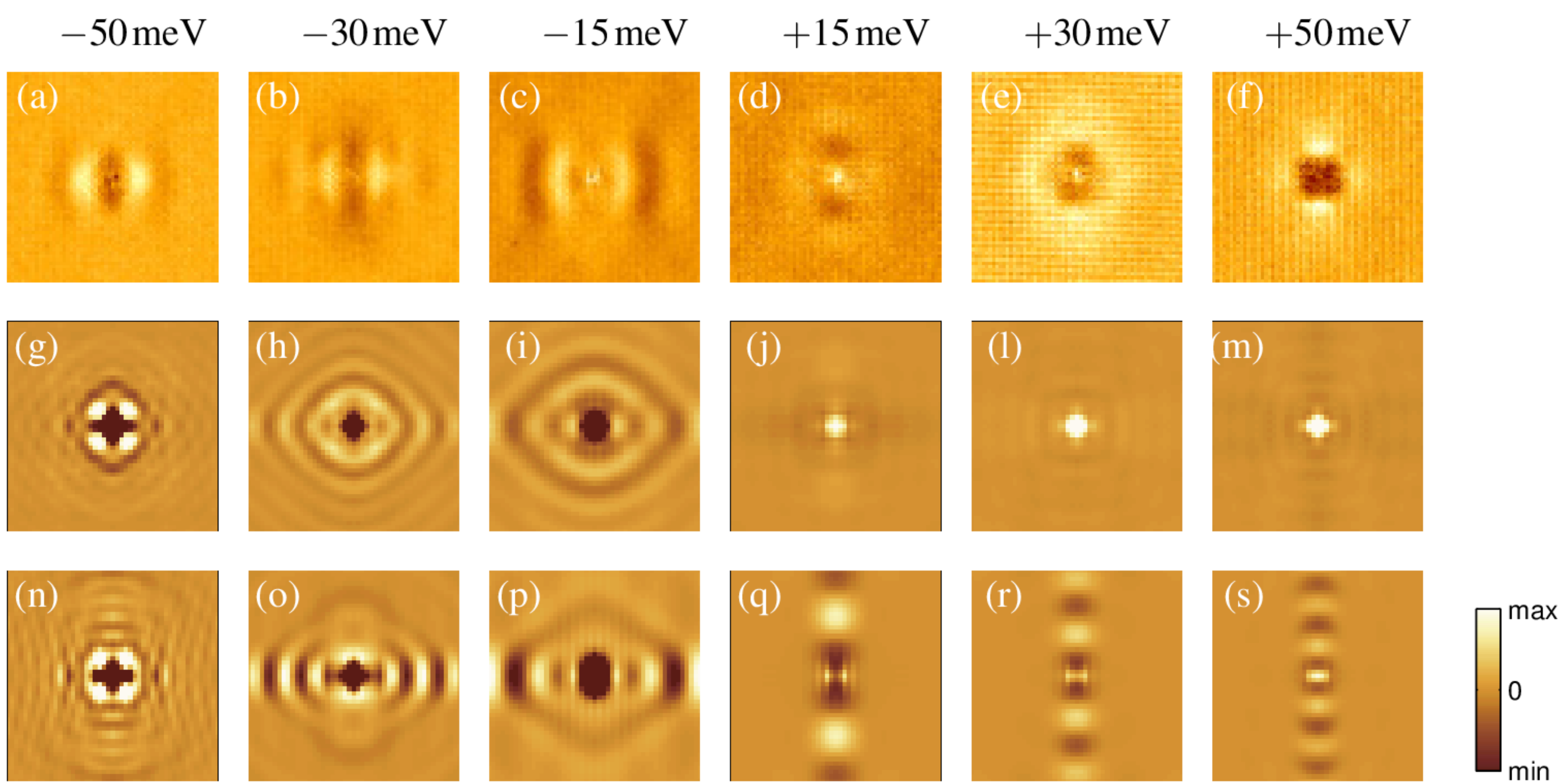
$$\{\sqrt{Z_l}\} = [0.2715, 0.9717, 0.4048, 0.9236, 0.5916]$$

Fermi liquid theory

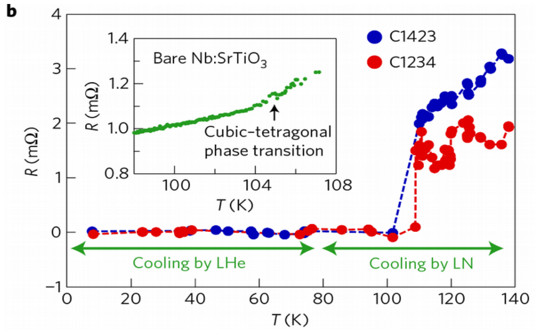
- Predictions for other experiments: electronic dimer close to impurity

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

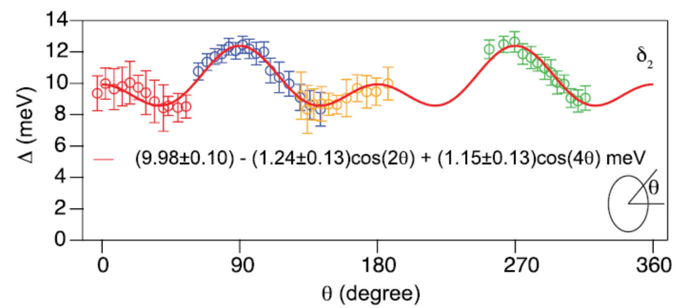
Kasahara et al., Proc. Natl. Acad. Sci. USA **46**, 16309 (2014)



Other systems: FeSe monolayer

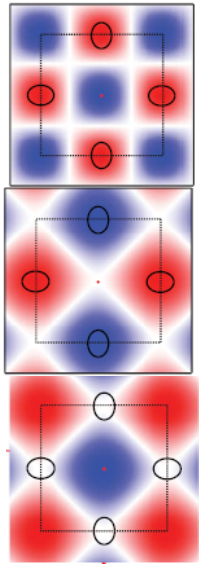


Ge et al. Nat. Mater. **14**, 285 (2015)

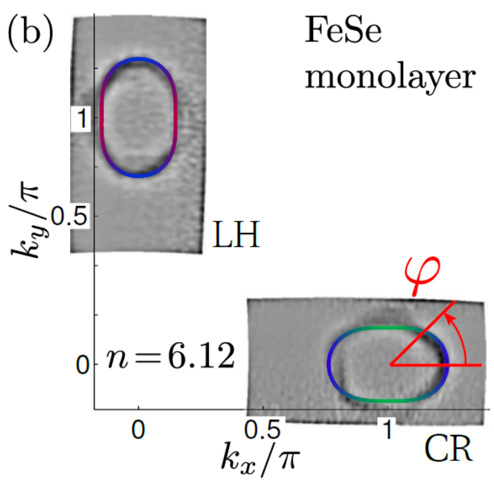


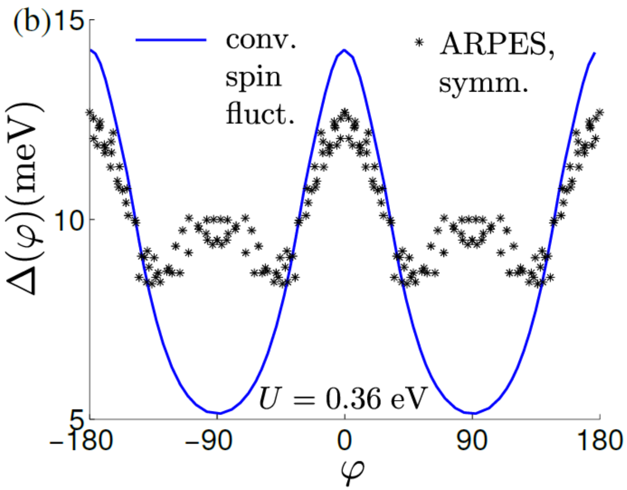
Zhang, et al., Phys. Rev. Lett. **117**, 117001 (2016)

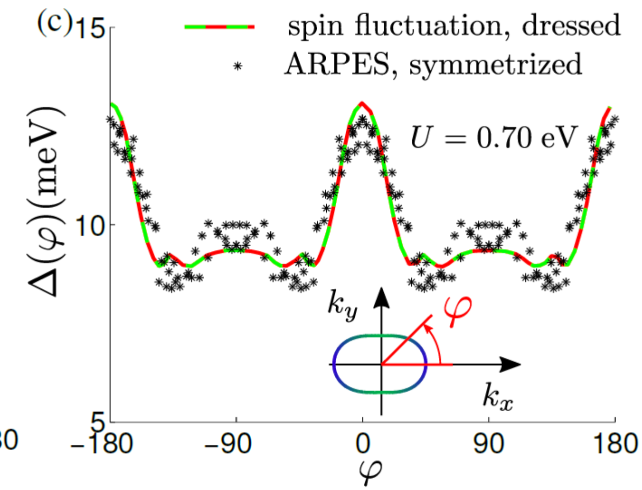
No explanation of the two maxima structure by conventional approaches



- Same model, but: 2D, no orbital order, rigid shift







$$\{\sqrt{Z_l}\} = [0.4273, 0.8000, 0.9826, 0.9826, 0.700]$$

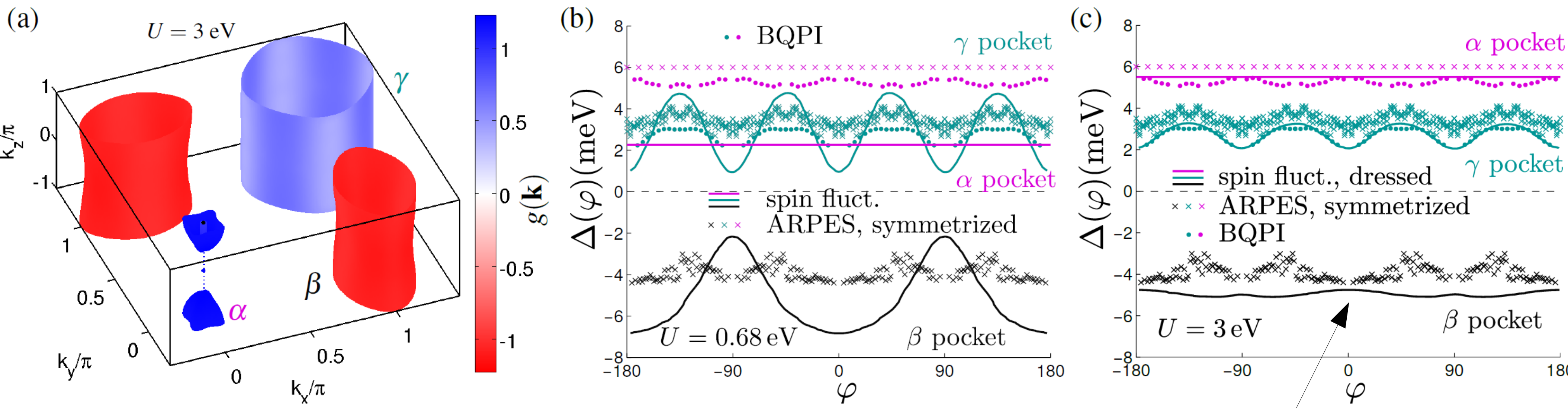
$$(d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2})$$

LiFeAs

- Large gap on the α pocket

Compare: Y. Wang et al. Phys. Rev. B **88**, 174516 (2013)

dressed Green function



$$\{\sqrt{Z_l}\} = [0.5493, 0.969, 0.5952, 0.5952, 0.9267]$$
$$(d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2})$$

"antiphase variation" of gap does not come out spot on

Borisenko et al. Symmetry **4**, 251 (2012)

Conclusions

- Many interesting and open questions remain in the field of high-T_c superconductivity
- FeSe is extremely interesting due to nematicity and orbital selective pairing due to strong correlations
- A modified spin-fluctuation approach allows for quantitative description of gap functions and other observables

$$G_{ab}(\boldsymbol{k}, \omega) = Z_{ab} G^0_{ab}(\boldsymbol{k}, \omega)$$

- HAEM procedure as alternative method to deduce the relative phase of the order parameter

Acknowledgements

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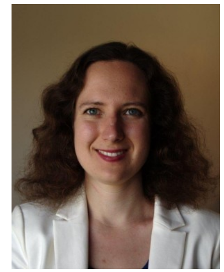
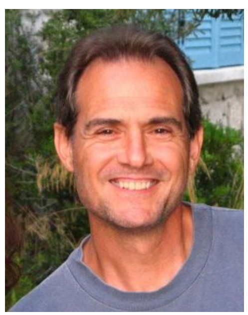
Valentin Taufour



Anna E. Böhmer

Paul C. Canfield

Shantanu Mukherjee



Peter J. Hirschfeld

Brian M. Andersen

Johannes H. J. Martiny

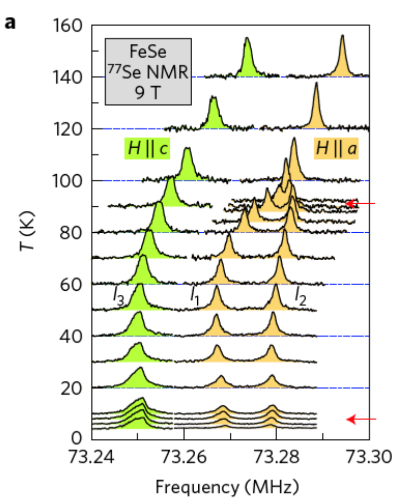
Peter O. Sprau, Andrey Kostin, Andreas Kreisel, Anna E. Böhmer, Valentin Taufour, Paul C. Canfield, Shantanu Mukherjee, Peter J. Hirschfeld, Brian M. Andersen, J.C. Séamus Davis
arXiv:1611.02134
Discovery of Orbital-Selective Cooper Pairing in FeSe

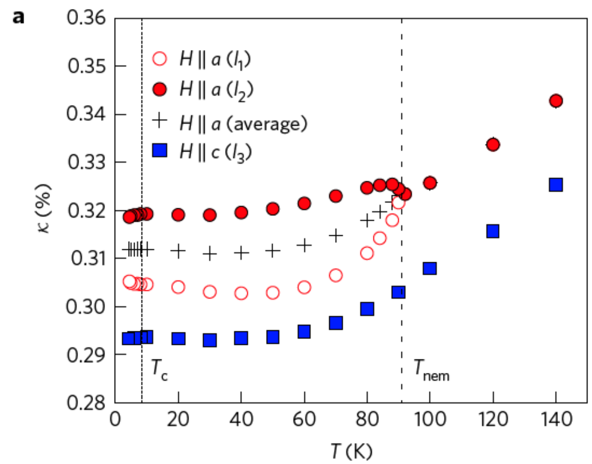
A. Kreisel, Brian M. Andersen, Peter O. Sprau, Andrey Kostin, J.C. Séamus Davis, P. J. Hirschfeld
arXiv:1611.02643
Orbital selective pairing and gap structures of iron-based superconductors

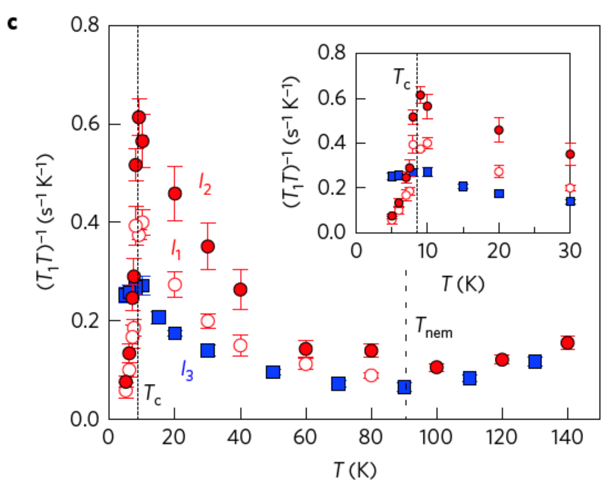
Johannes H. J. Martiny, Andreas Kreisel, P. J. Hirschfeld, Brian M. Andersen
arXiv:1703.04891
Robustness of Quasiparticle Interference Test for Sign-changing Gaps in Multiband Superconductors

NMR: Knight shift, 1/T1T

orbital order visible in Knight shift

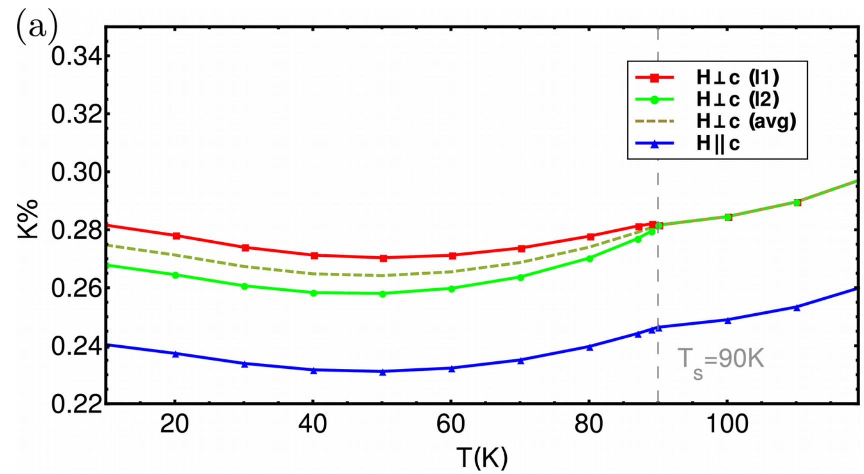


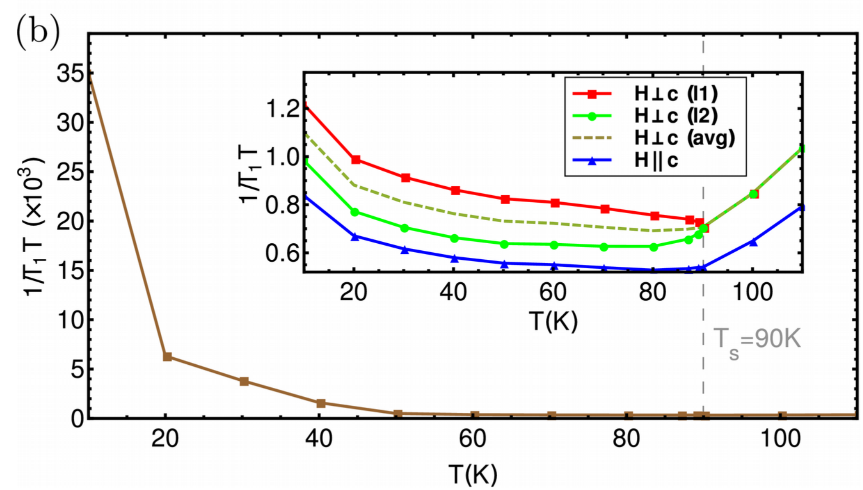




Baek, *et al.* Nature Materials **14**, 210 (2015)

no enhanced low-energy spin fluctuations visible in NMR

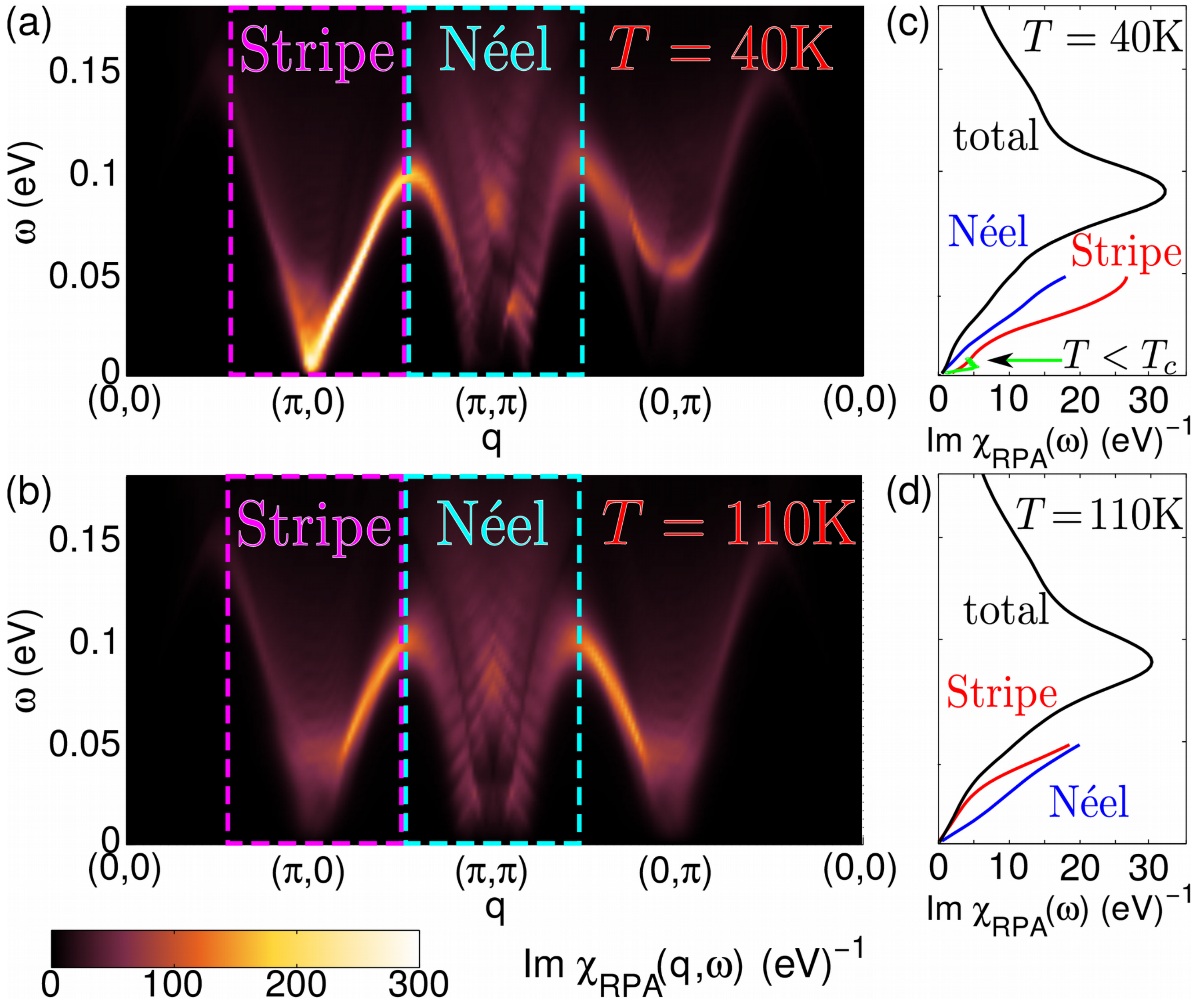




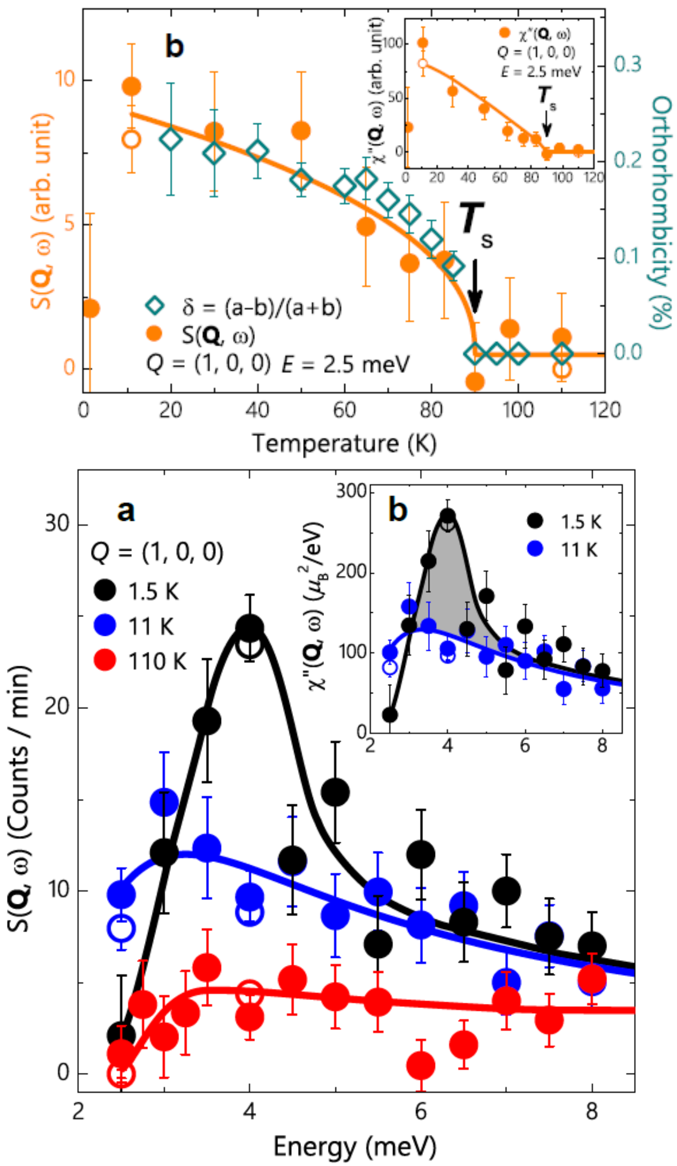
$$\frac{1}{T_1 T} = \lim_{\omega_0 \to 0} \frac{\gamma_N^2}{2N} k_B \sum_{\mathbf{q}\alpha\beta} |A_{hf}^{\alpha\beta}(\mathbf{q})|^2 \frac{\mathrm{Im}\{\chi_{\mathrm{RPA}}^{\alpha\beta}(\mathbf{q}, \omega_0)\}}{\hbar\omega_0}$$

Spin fluctuations at higher energies

- FeSe: close to magnetic instability (tune interactions accordingly)
- transfer from Néel fluctuations to Stripe fluctuations on lowering temperature
- spin resonance at low energies from transfer of spectral weight in the superconducting state



Inelastic neutron scattering



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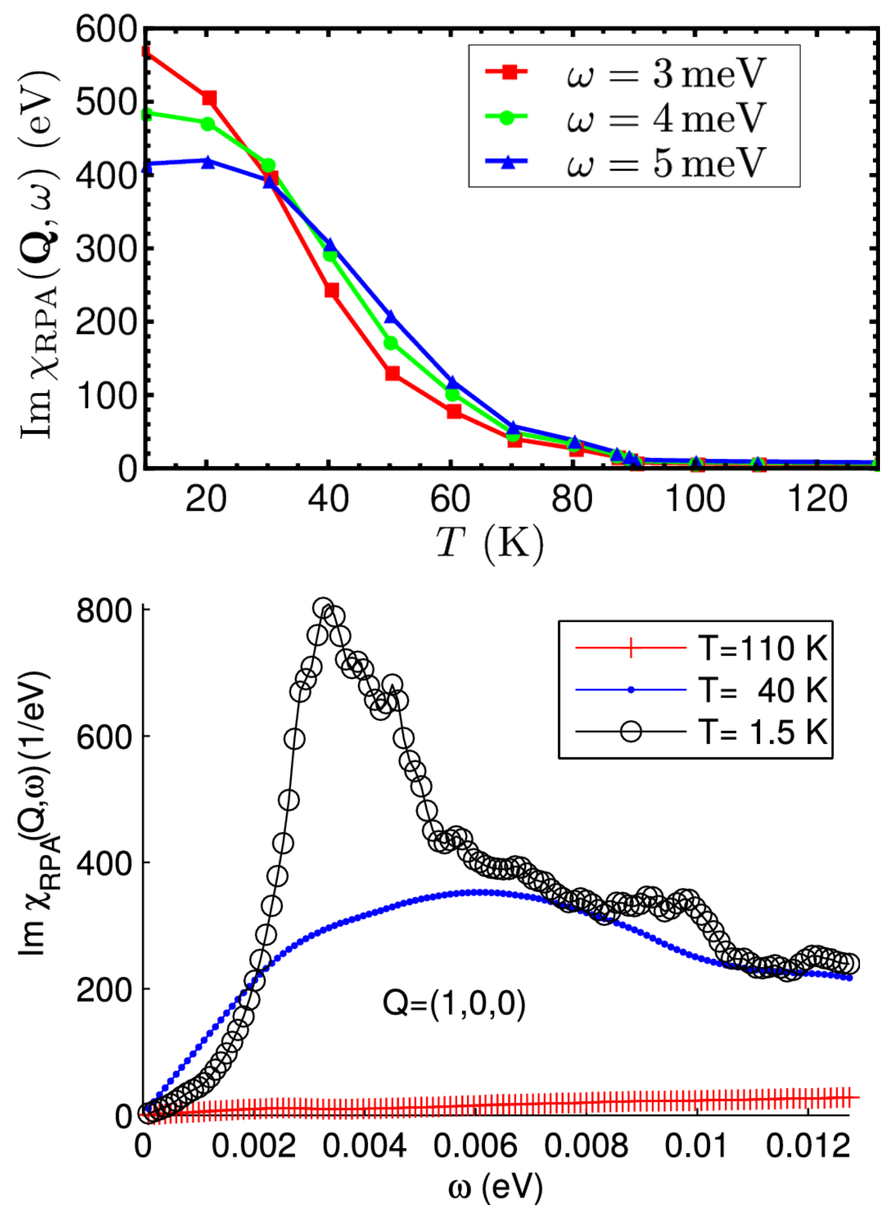
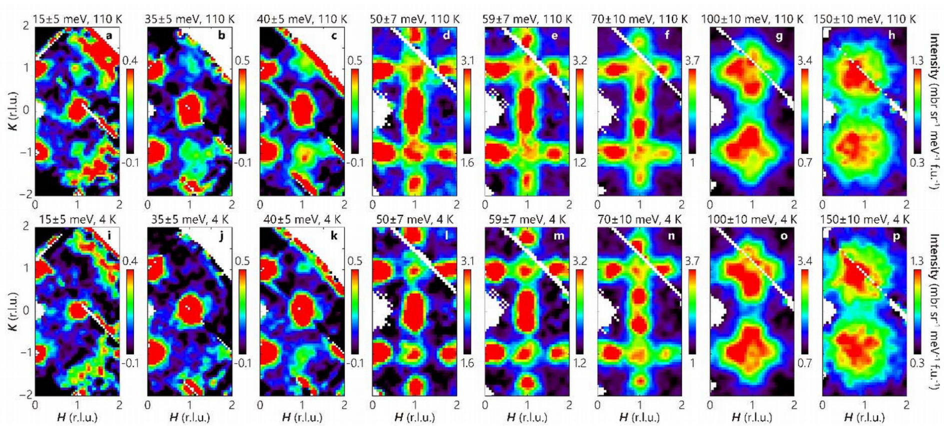
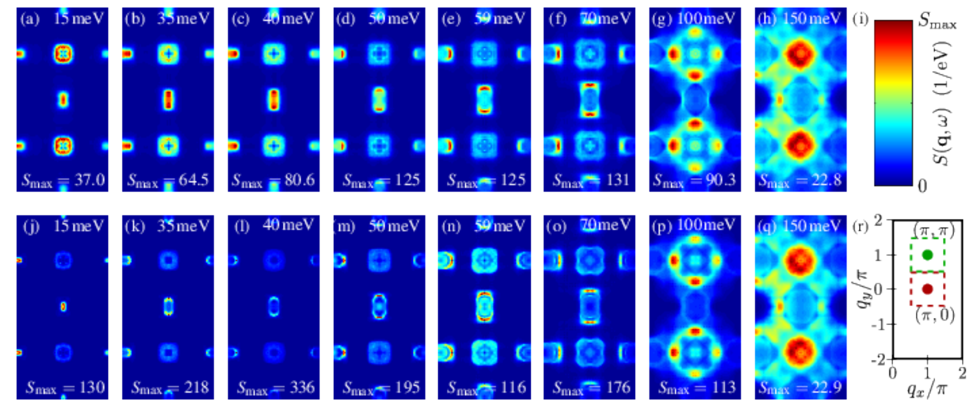
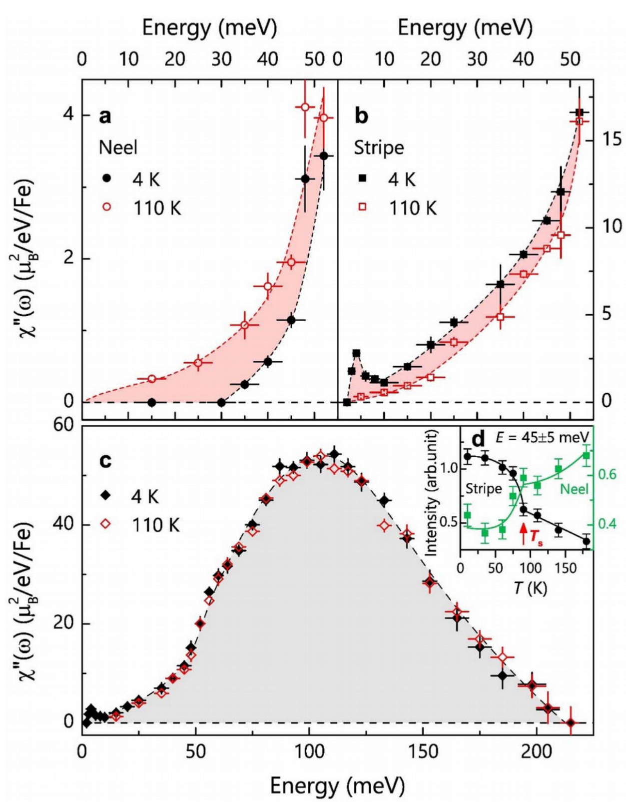


Inelastic neutron scattering







Q. Wang, *et al*, arXiv:1511.02485 (2015)