Orbital-Selective Pairing and Gap Structures of Iron-Based Superconductors

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

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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

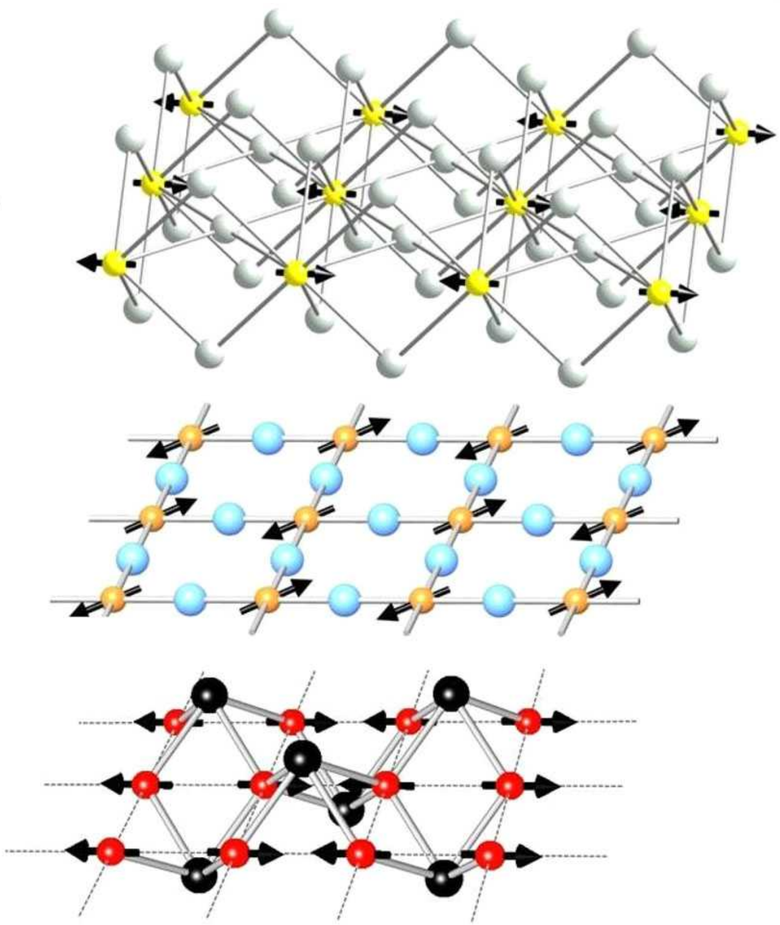
Unconventional superconductivity

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

CeIn$_3$

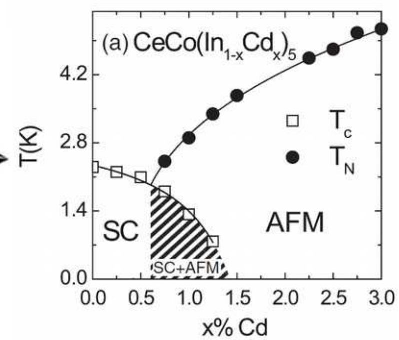
CuO$_2$

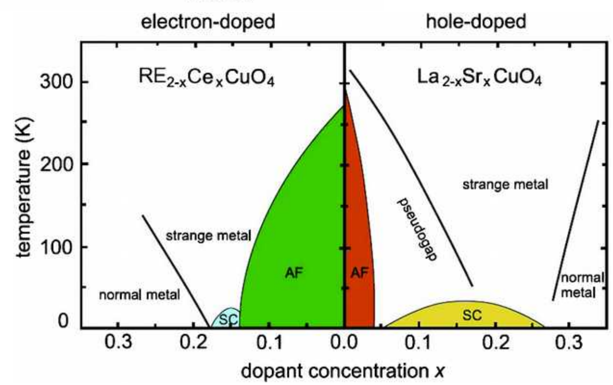
FeAs

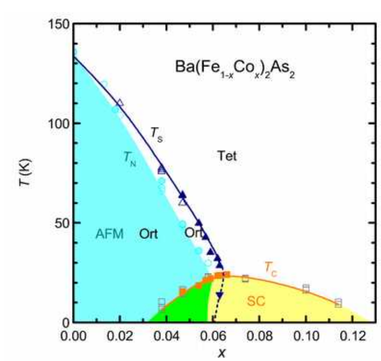


D. J. Scalapino
Rev. Mod. Phys. **84**, 1383 (2012)

Phase diagram: close proximity of antiferromagnetism and superconductivity





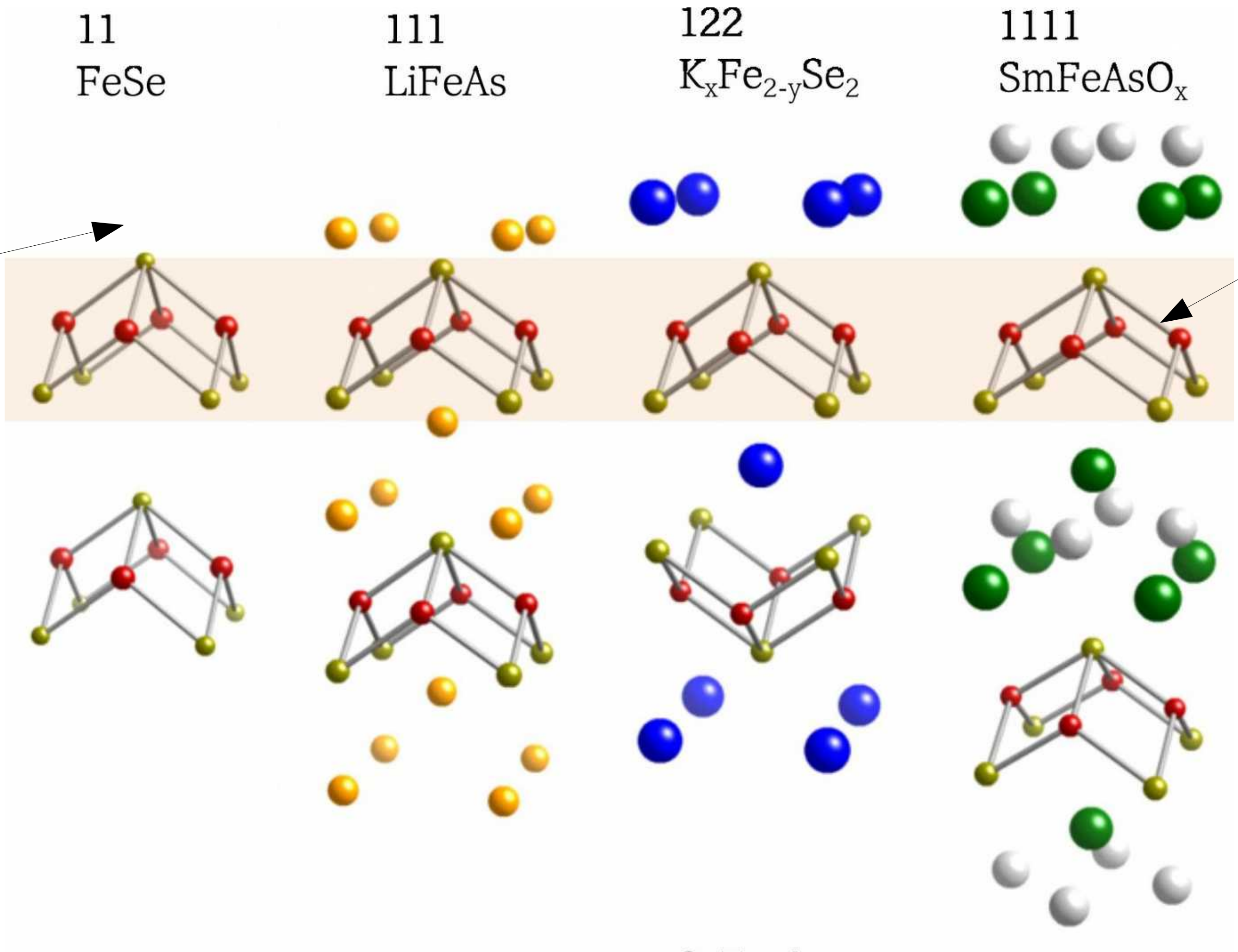


other interesting phases:
charge density wave
C4 symmetric magnetic phases
Nematic phase

Similarities in physical mechanisms?

Fe based superconductors

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

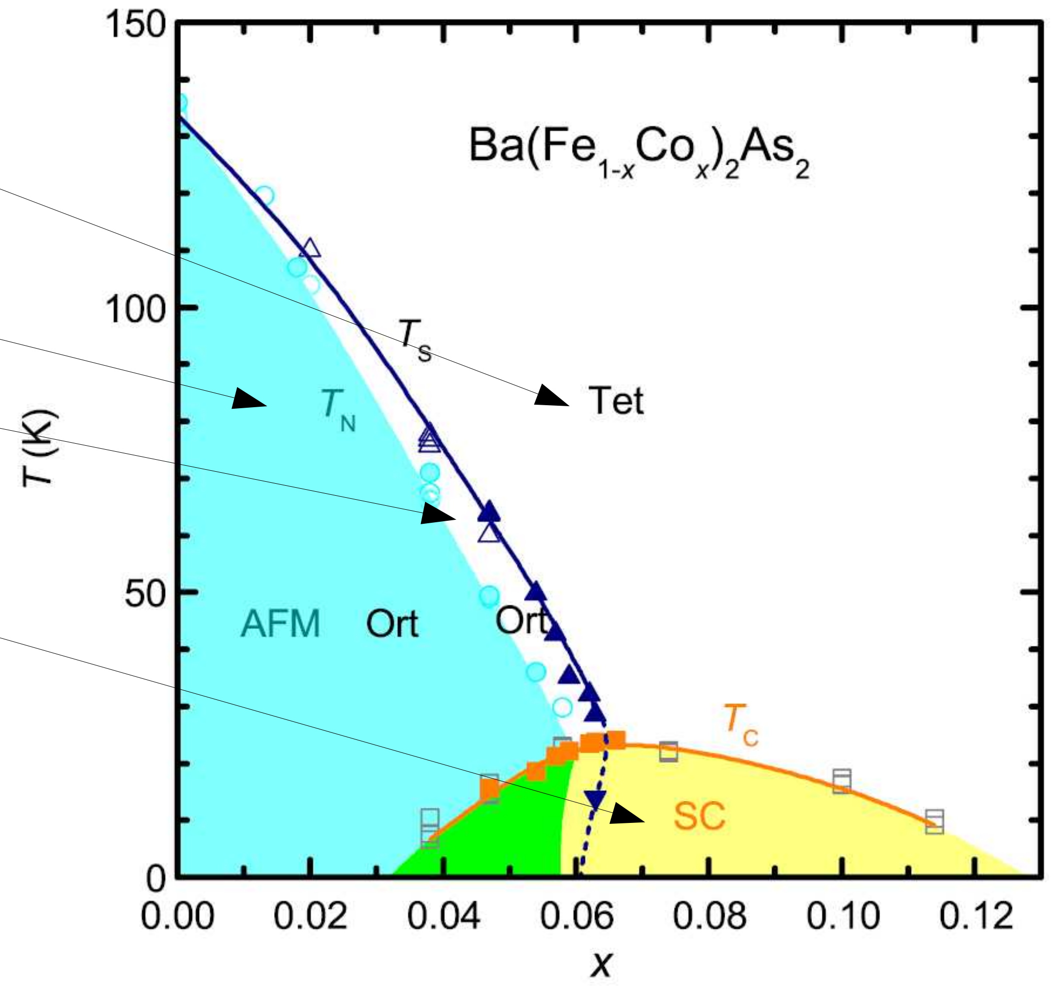


common layer: states at the Fermi level

surface termination:
Se (FeSe)
Li (LiFeAs)

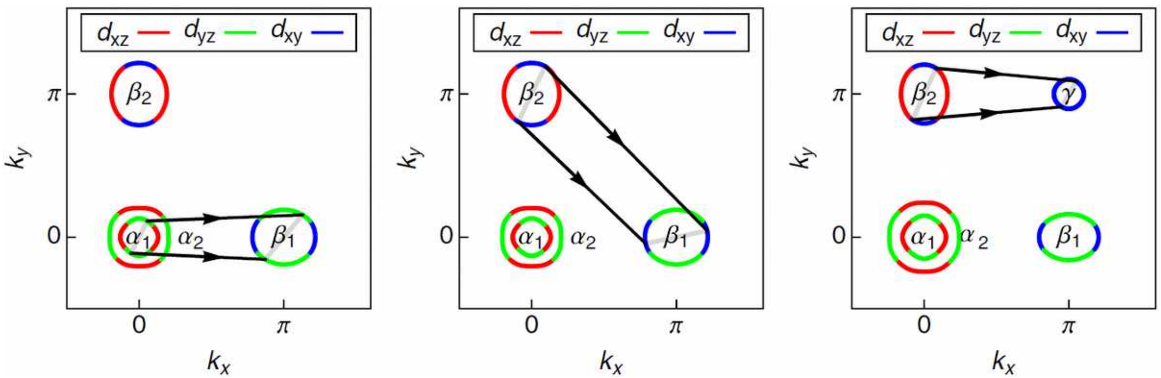
Fe based superconductors

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

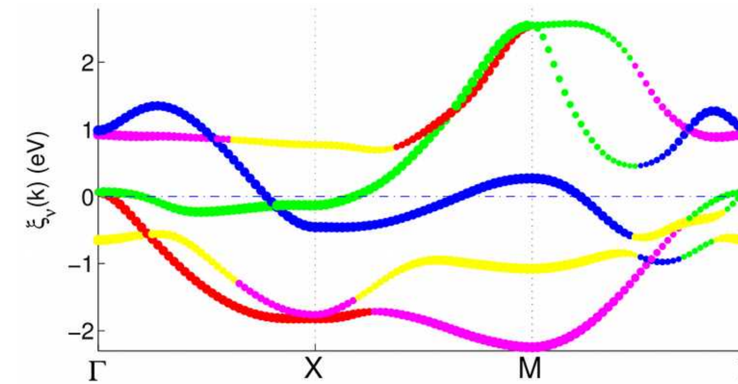


Band structure / Magnetism

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

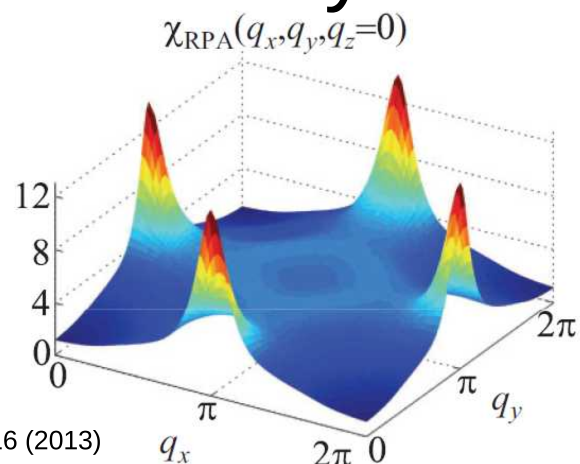


D. J. Scalapino Rev. Mod. Phys. **84**, 1383 (2012)

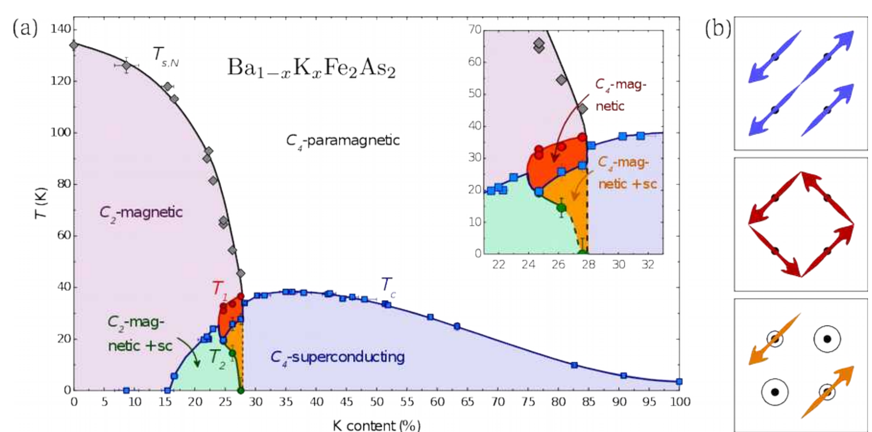


Chi et al., PRB **94**, 134515 (2016) [LiFeAs]

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



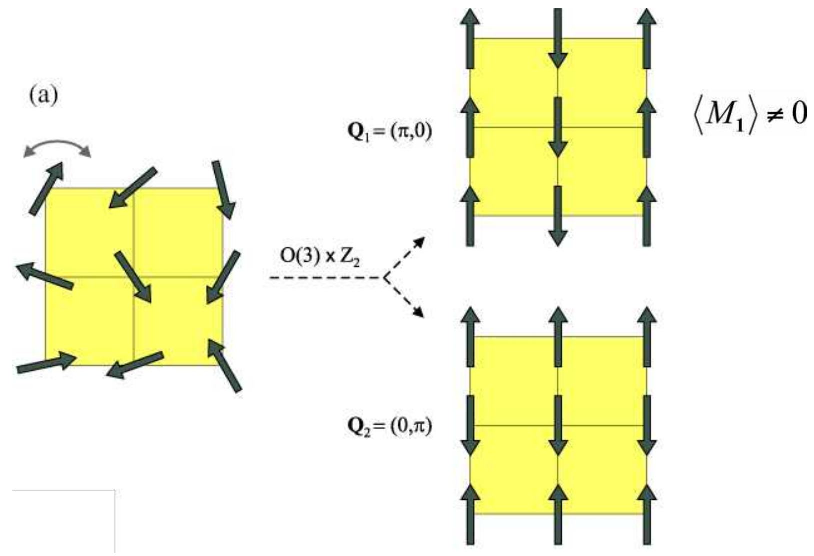
Wang, et al., PRB **88**, 174516 (2013)

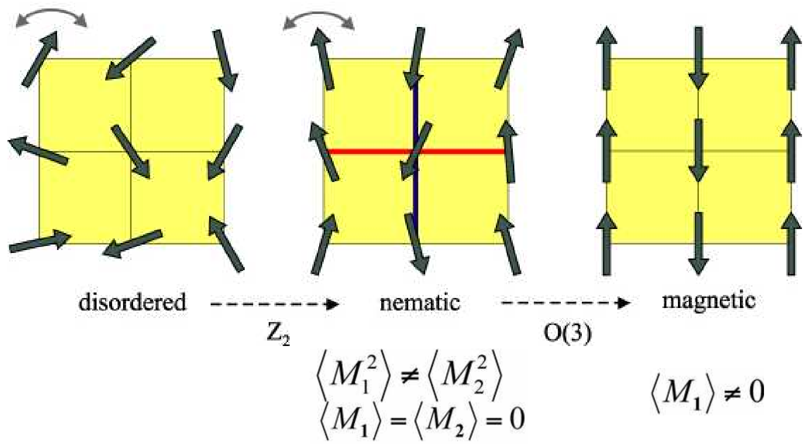


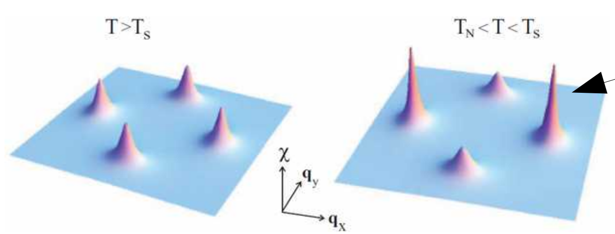
Böhmer, et al., Nat. Commun. **6**, 7911 (2015)
Gastiasoro, Andersen, PRB **92**, 140506 (2015)

Nematicity

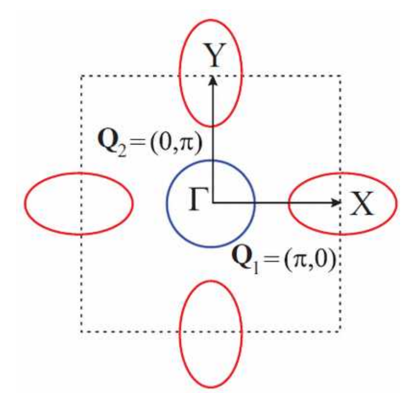
- Magnetic ordering
- Nematic state







Magnetic fluctuations stronger in x-direction
Tetragonal symmetry breaking



Itinerant approach to nematic state

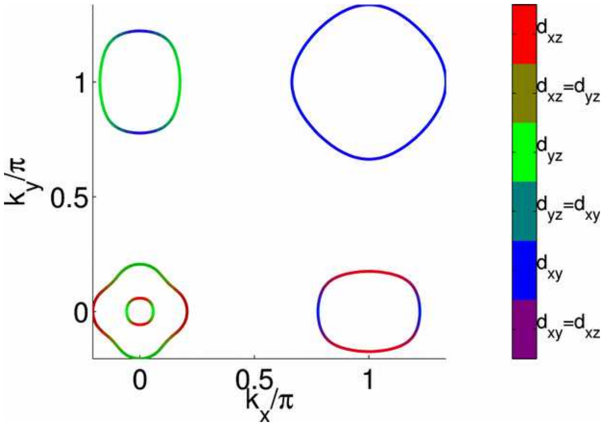
$$\chi_{\mathrm{nem}} \sim \chi_{\mathrm{mag}}^2$$

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

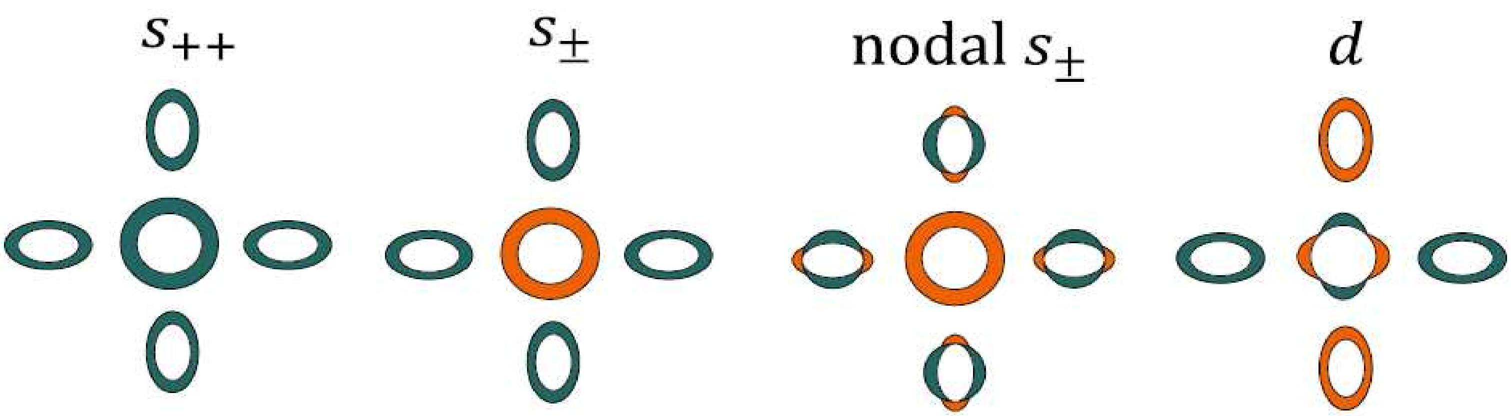
Fernandes, et al., PRB **85**, 024534 (2012)

Superconductivity: gap structure

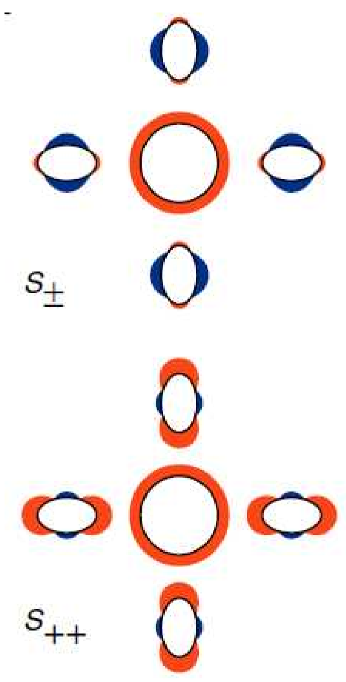
- Fermi surface



- Possible order parameters



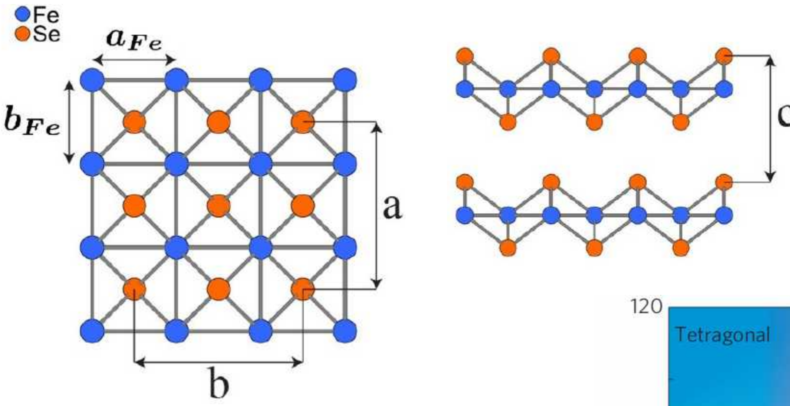
Hirschfeld, Korshunov, Mazin
Rep. Prog. Phys. **74** 124508 (2011)



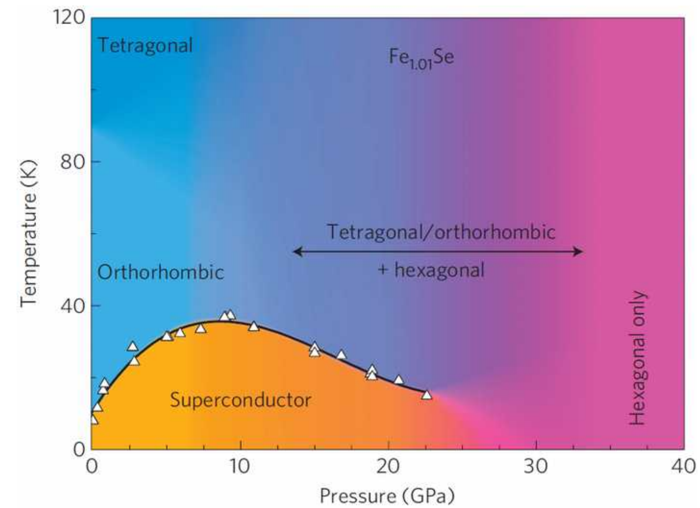
Mizukami, et al.
Nat. Commun. **5**, 5657 (2014)

FeSe: Why interesting?

- 11 compound

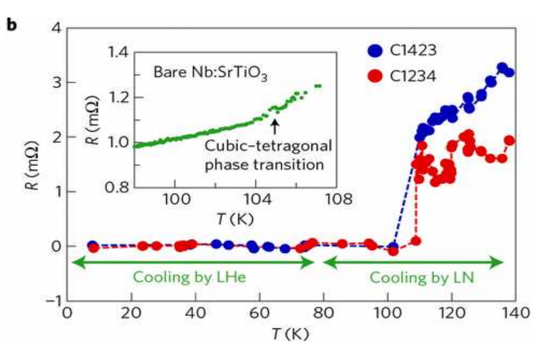


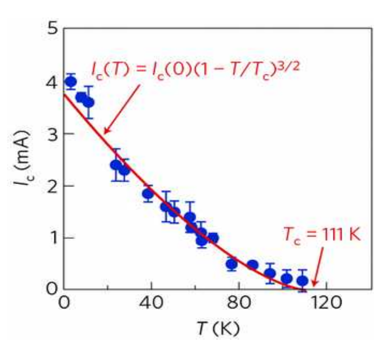
- Tc 8K, under pressure ~40K

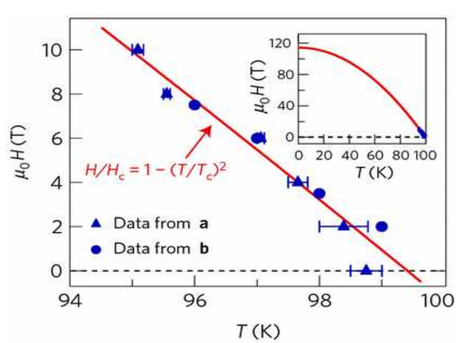


Medvedev, et al. Nat. Mater. **8**, 630 (2009)

- Tc 100K (single layer) transport measurement





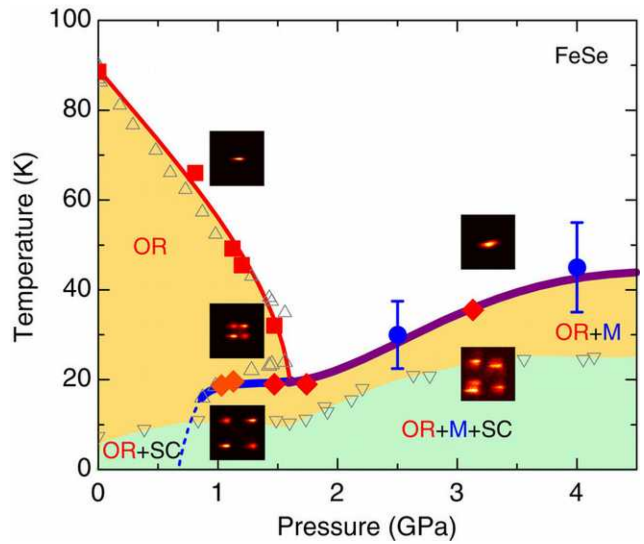


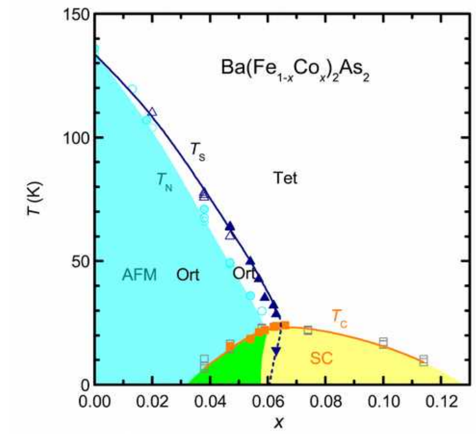
Ge et al. Nat. Mater. **14**, 285 (2015)

FeSe: Why interesting?

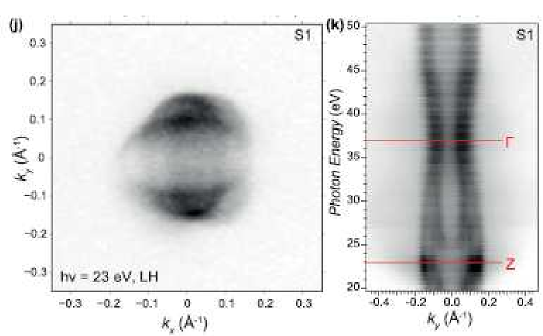
- nematic phase
  no magnetism
  (p=0)

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

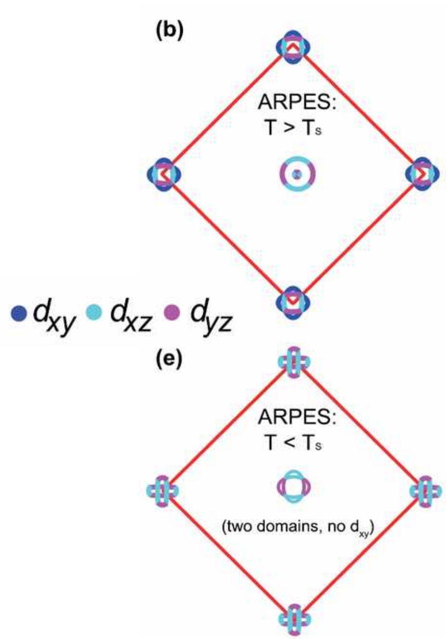




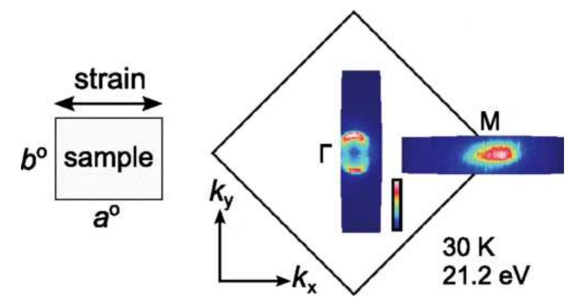
- ARPES
  measured band structure
  tiny Fermi surface
  (far from ab initio results)



Measured
orbital
splitting



detwinned ARPES



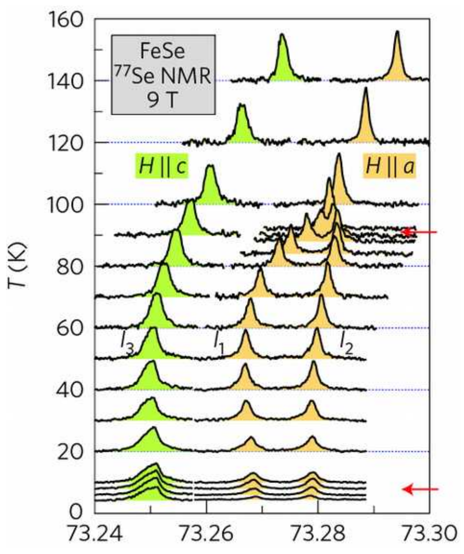
Watson, et al., PRB 94, 201107(R) (2016)
Watson, et al., PRB 90, 121111(R) (2014)
Suzuki, et al., PRB 92, 205117 (2015)
Maletz, et al., PRB 89, 220506(R) (2014)
Fedorov, et al., Sci. Rep. 6, 36834 (2016)

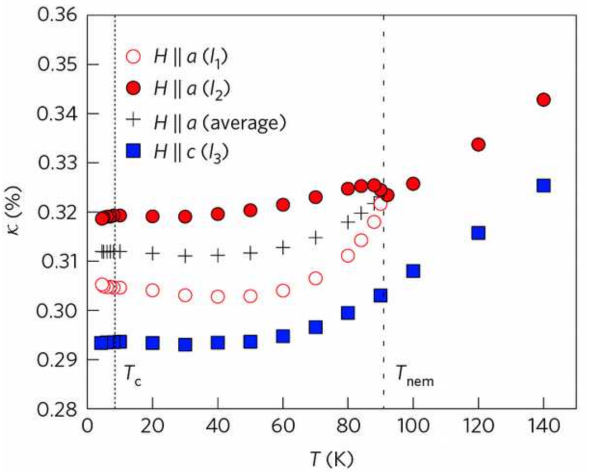
FeSe

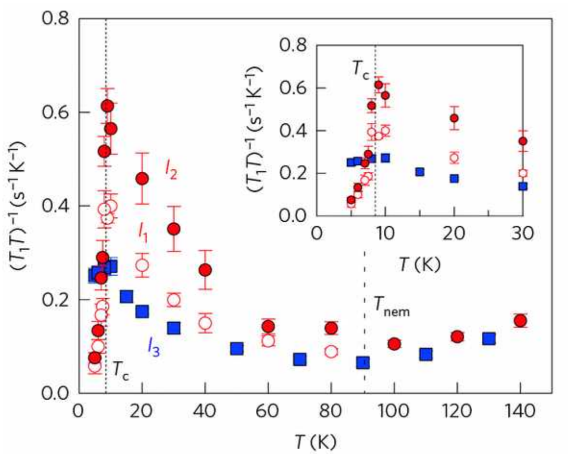
- Origin of nematic order
  - Orbital order
    Baek et al., Nat. Mat. **14**, 210 (2015)
    Yamakawa, Onari, Kontani, Phys. Rev. X **6**, 021032 (2016)
  - Quantum paramagnet
    Wang, Kivelson, Lee, Nat. Phys. **11**, 959 (2015)
  - Spin ferroquadrupolar / antiferroquadrupolar order
    Wang, Hu,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

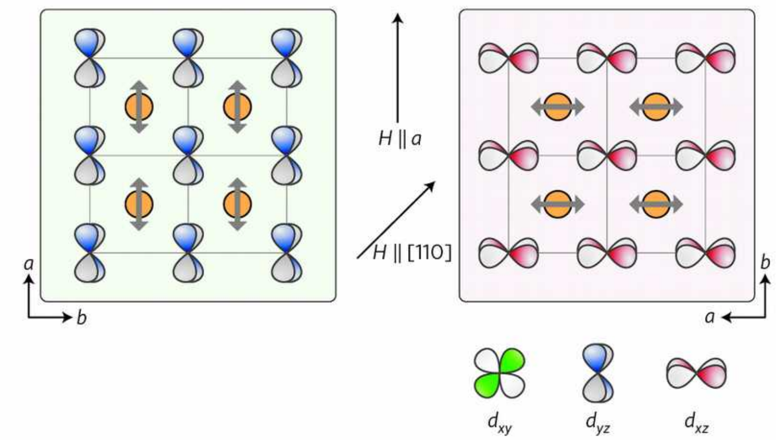
Nematic order

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







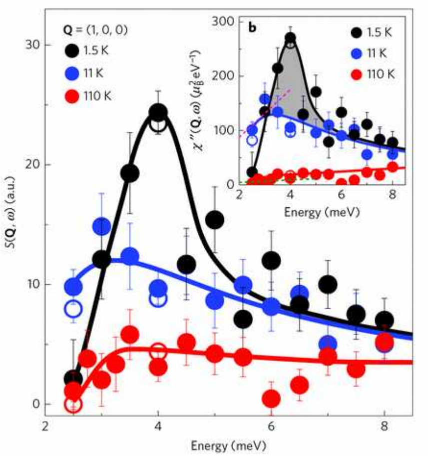


→ not caused by lattice distortion
→ evidence for orbital order (ferro)

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

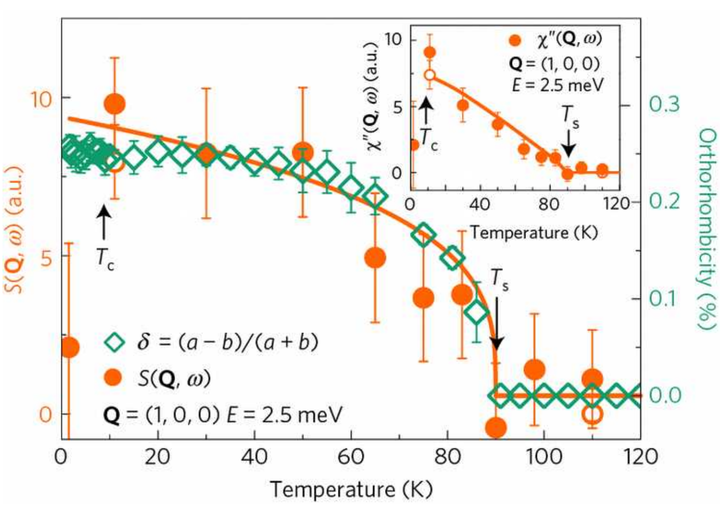
Spin excitations and magnetism

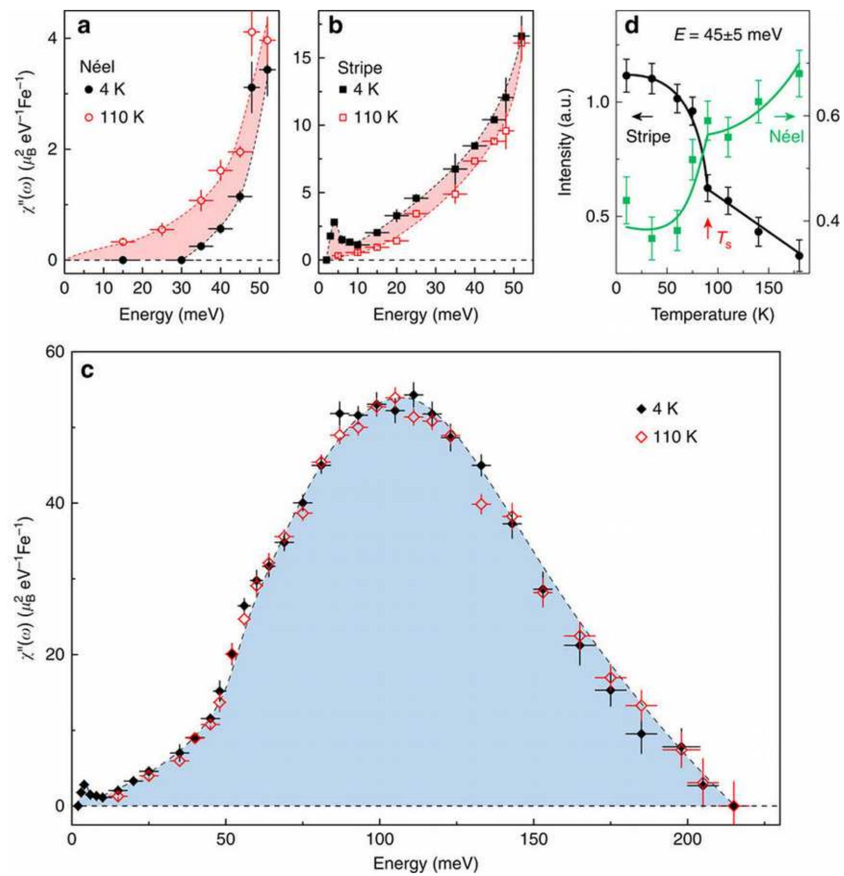
- Competition between stripe and Néel fluctuations



"spin resonance" at (pi,0)

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

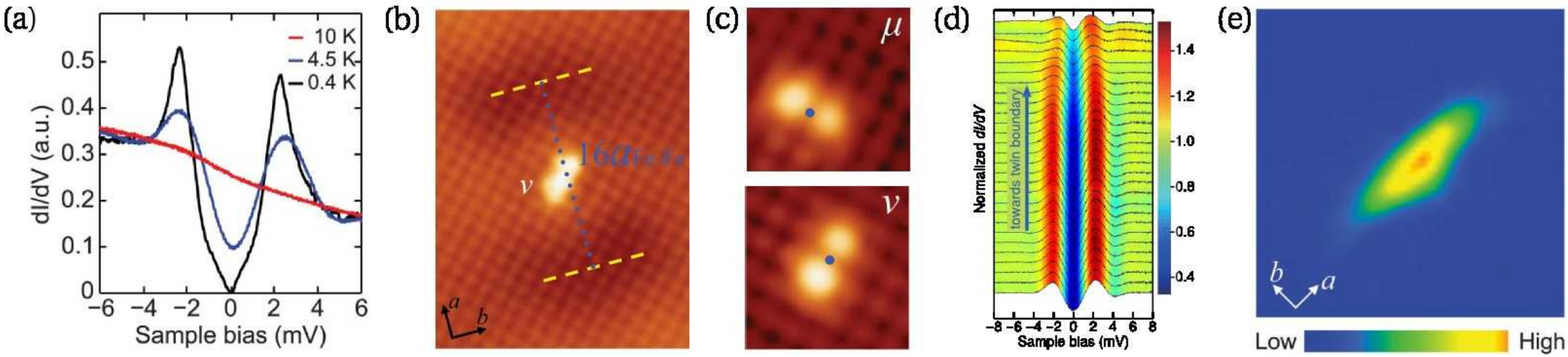




Wang et al., Nat. Commun. **7**, 12182 (2016)

Superconducting gap structure

- consequences: nodal gapstructure, anisotropy



Song et al. PRL 109, 137004 (2012)

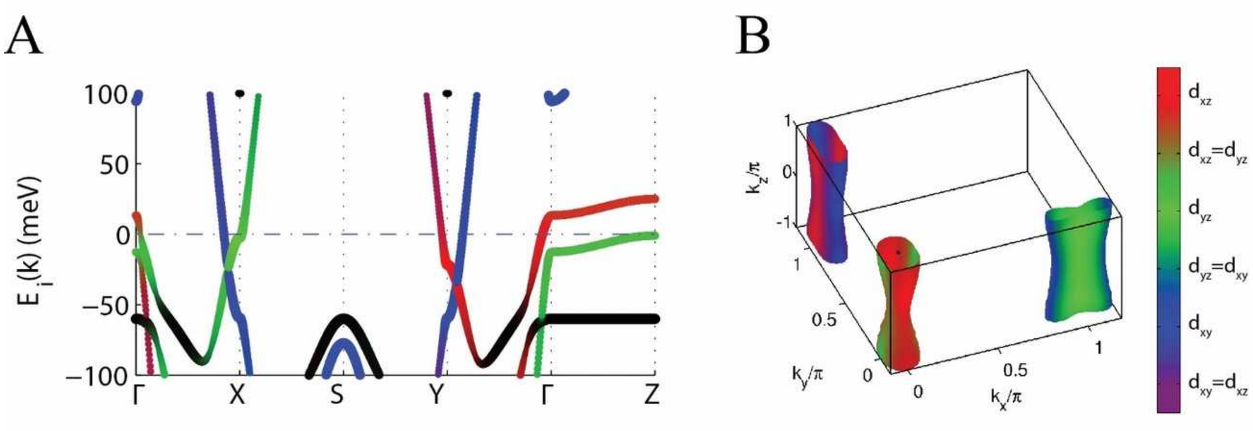
Song et al. Science 332, 1410 (2011)

Modelling

- Band structure:
  measured spectral function

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

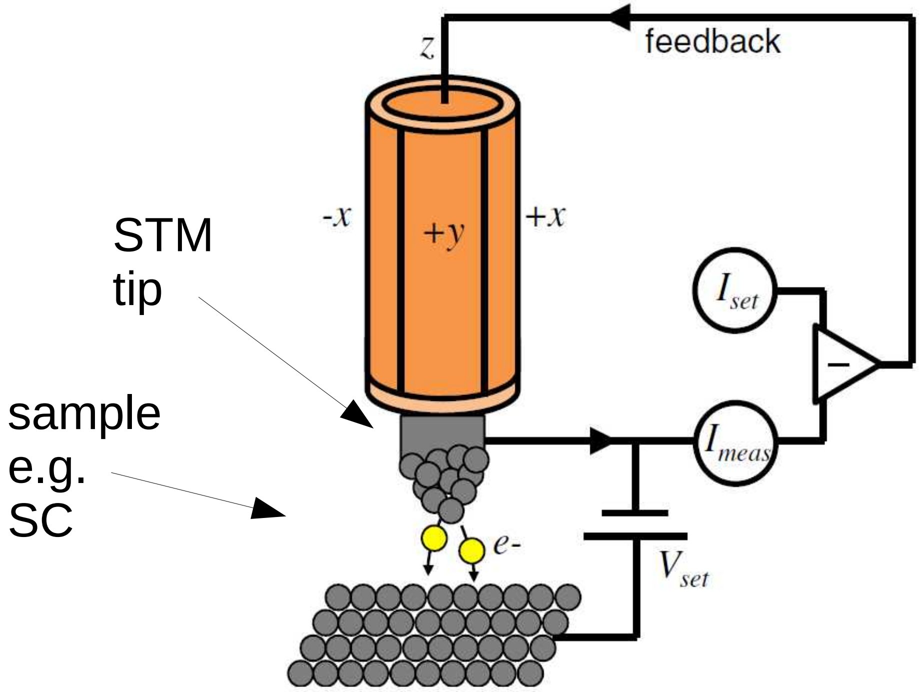
$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G(\vec{k},\omega)$$



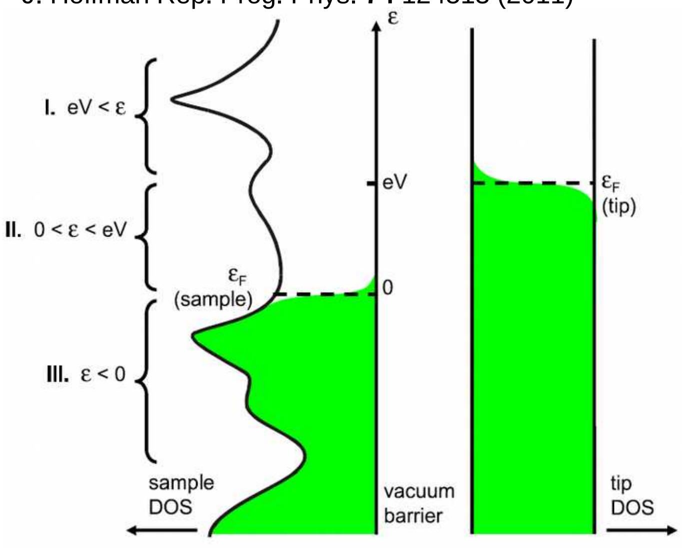
- ARPES
- Quantum oscillations
- Scanning tunnelling microscopy

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



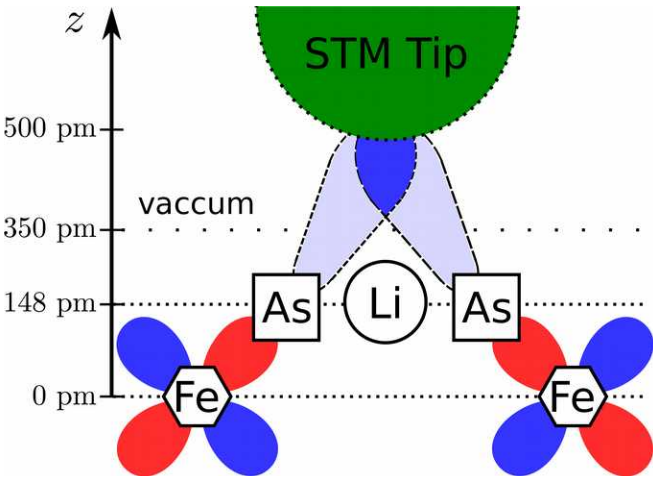
J. Hoffman Rep. Prog. Phys. **74** 124513 (2011)



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

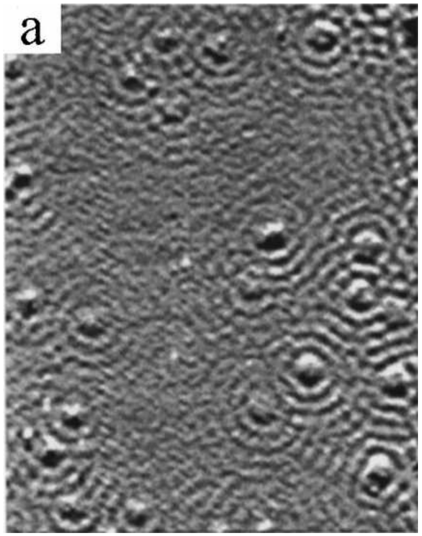


A. Kreisel, et al., Phys. Rev. B **94**, 224518 (2016)

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

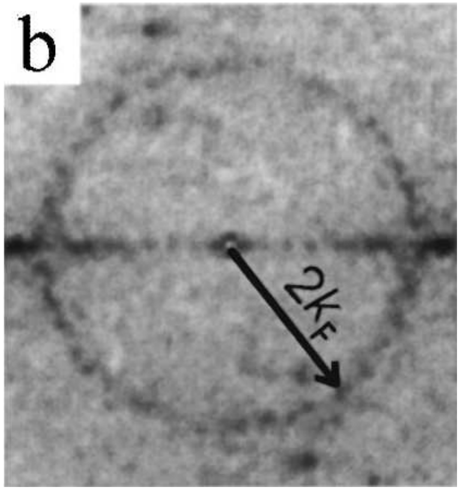
Quasiparticle Interference (QPI)

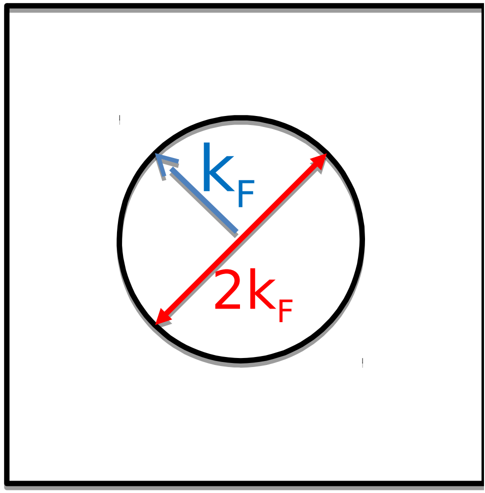
- STM on normal metal (Cu)
  - impurities
  - Friedel oscillations



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

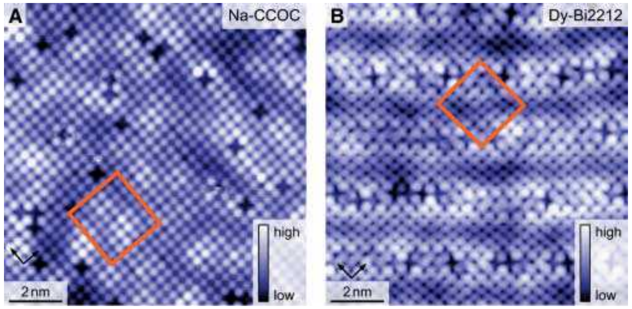
- Fourier transform of conductance map
  - mapping of constant energy contour



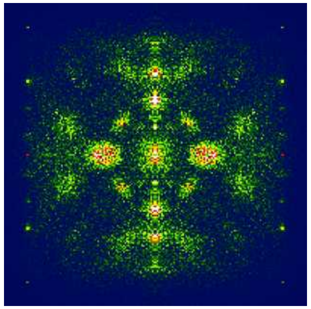


QPI in superconductors

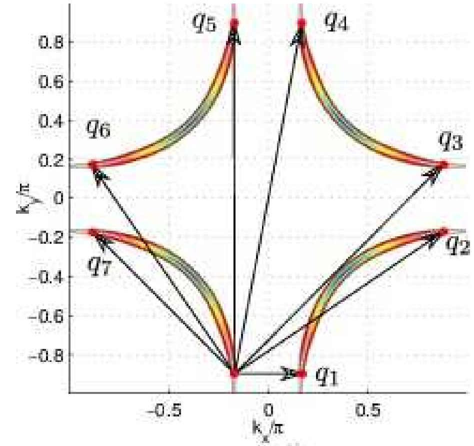
- Fourier transform of differential conductance maps

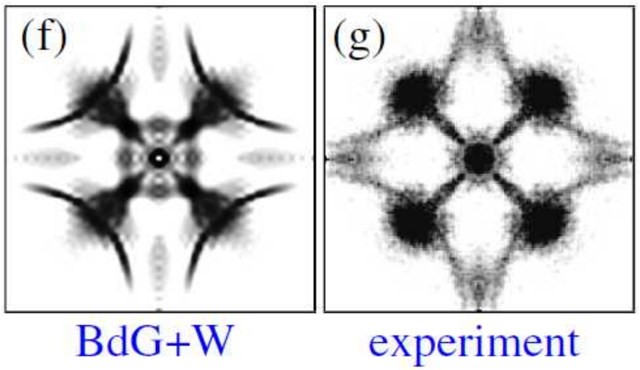


FT



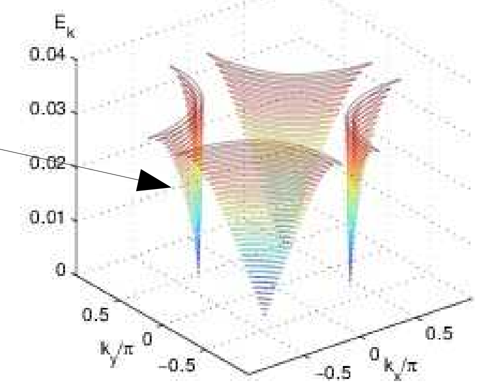
K Fujita et al. Science **344**, 612 (2014)





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

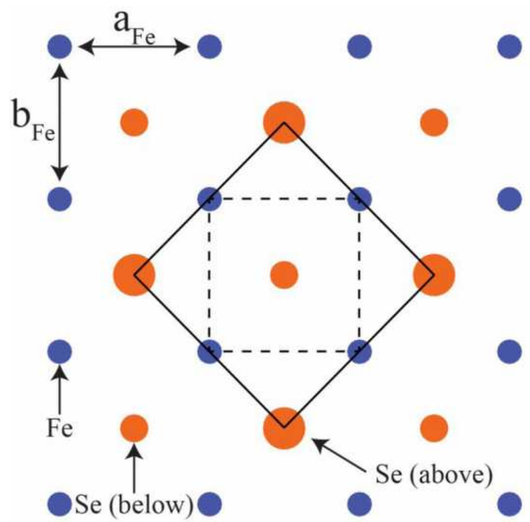
$$E_{\mathrm{k}} = \pm\sqrt{\epsilon_{\mathrm{k}}^2 + \Delta_{\mathrm{k}}^2}$$



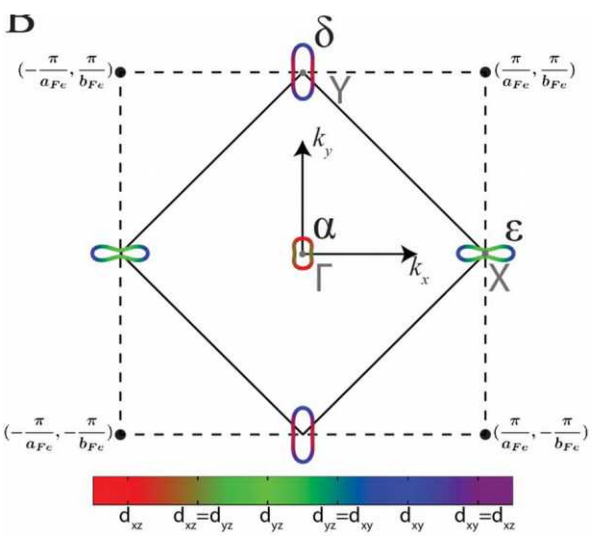
Trace back Fermi surface+measure superconducting gap function

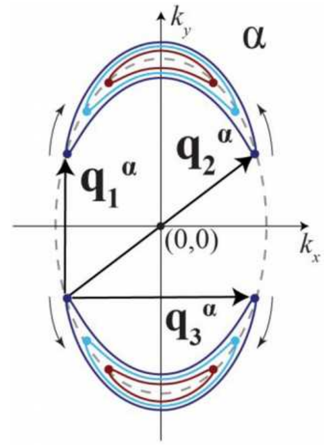
octet model: 7 scattering vectors between regions of high DOS

FeSe BQPI



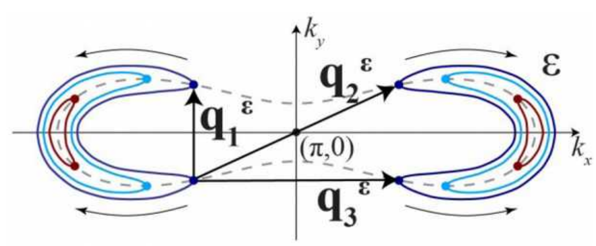
Coordinate system,
expected Fermi surface

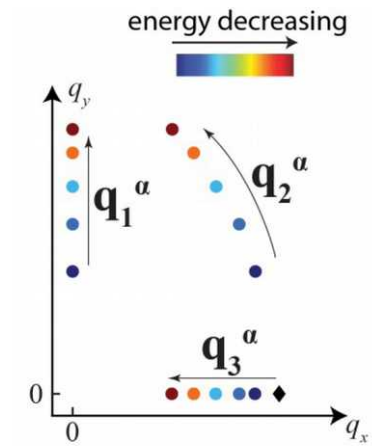




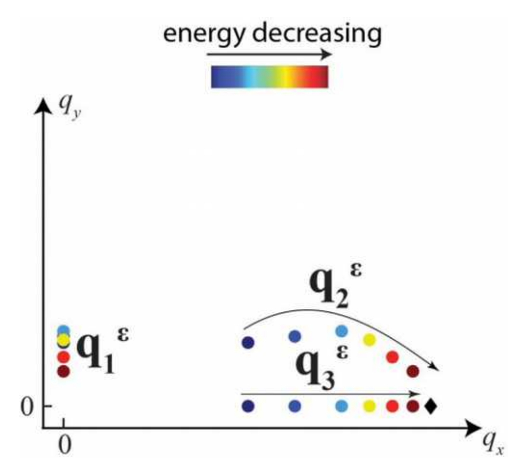
CEC: constant
energy contour
Expected
scattering vectors

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

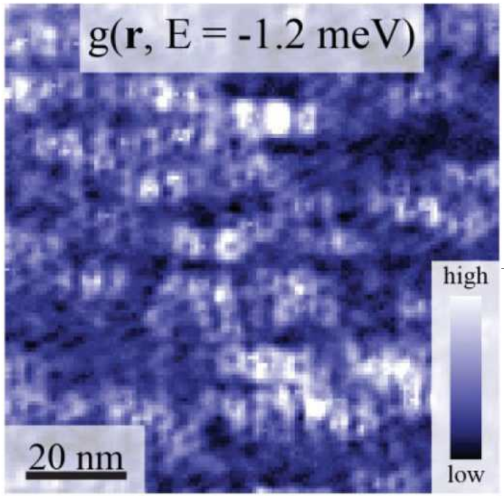




Dispersion of QPI peaks
q(E) → k(E) → E(k)



FeSe measurement



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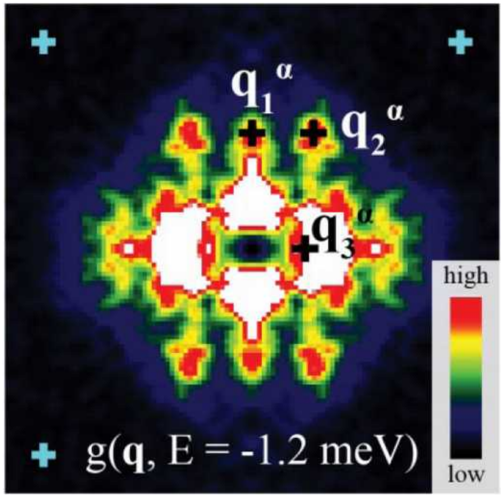
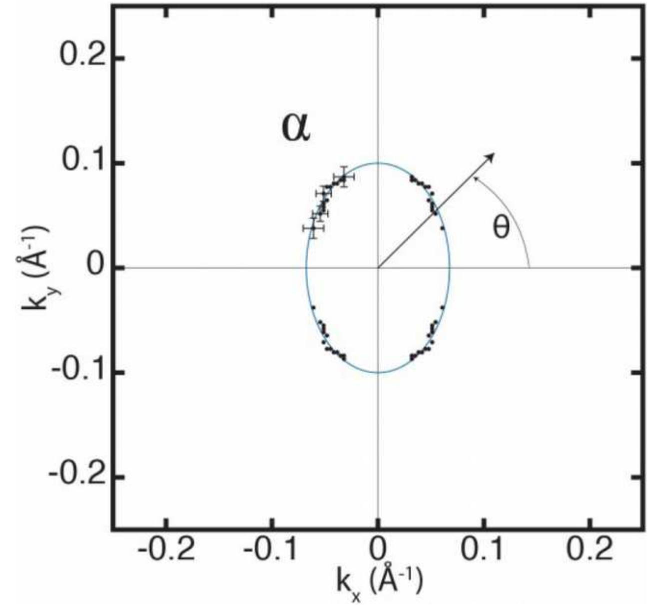
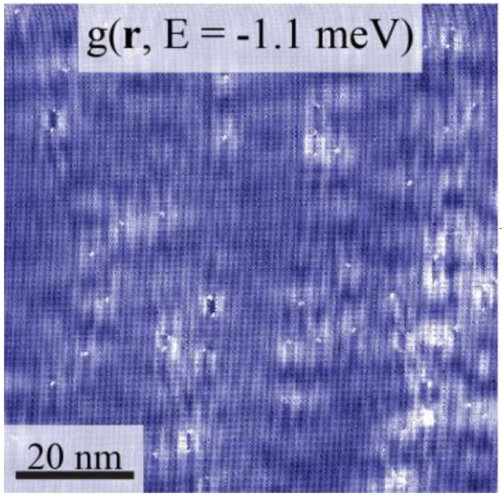


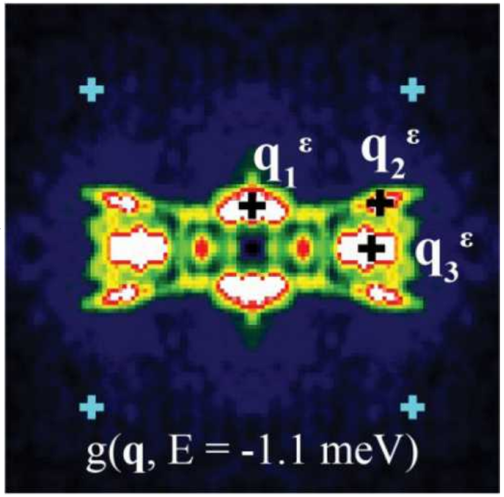


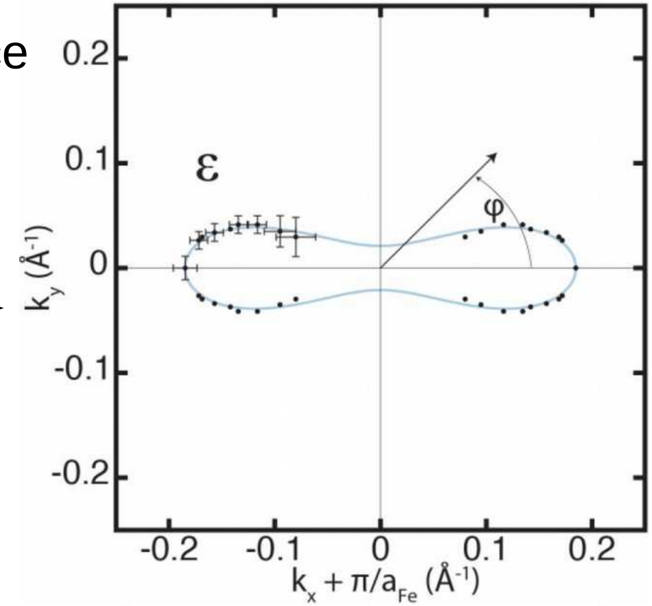
Conductance maps

Trace back Fermi surface



FT





Band structure modelling

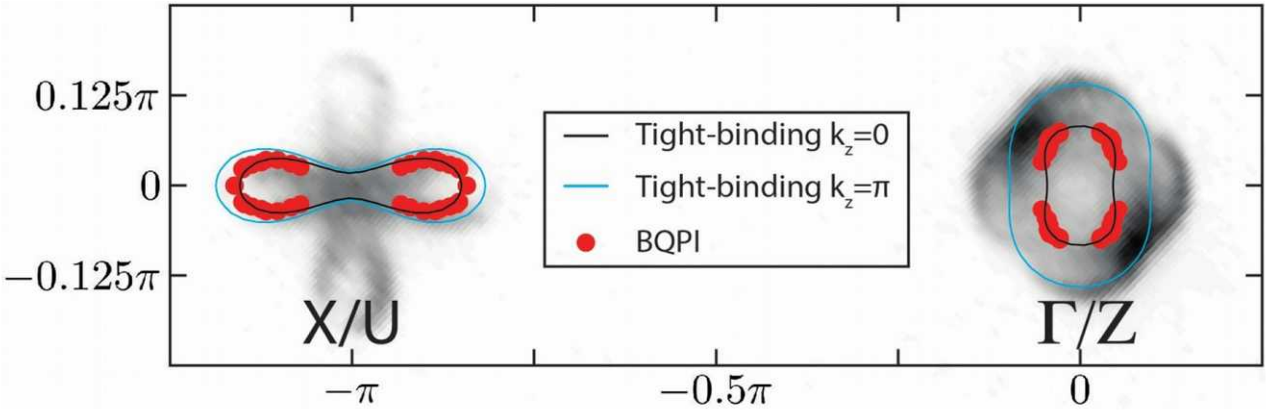
- Tight binding model $H_N = H_0 + H_{OO} + H_{SOC}$

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

site+bond centered orbital order

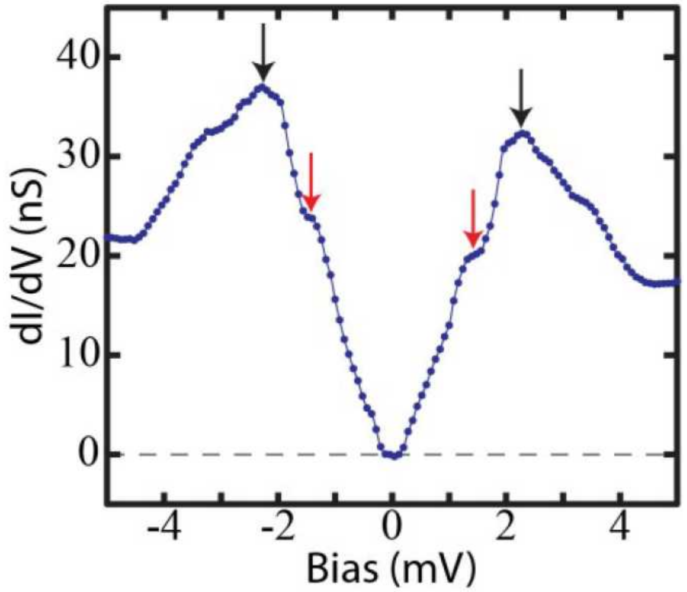
$$H_{SOC} = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

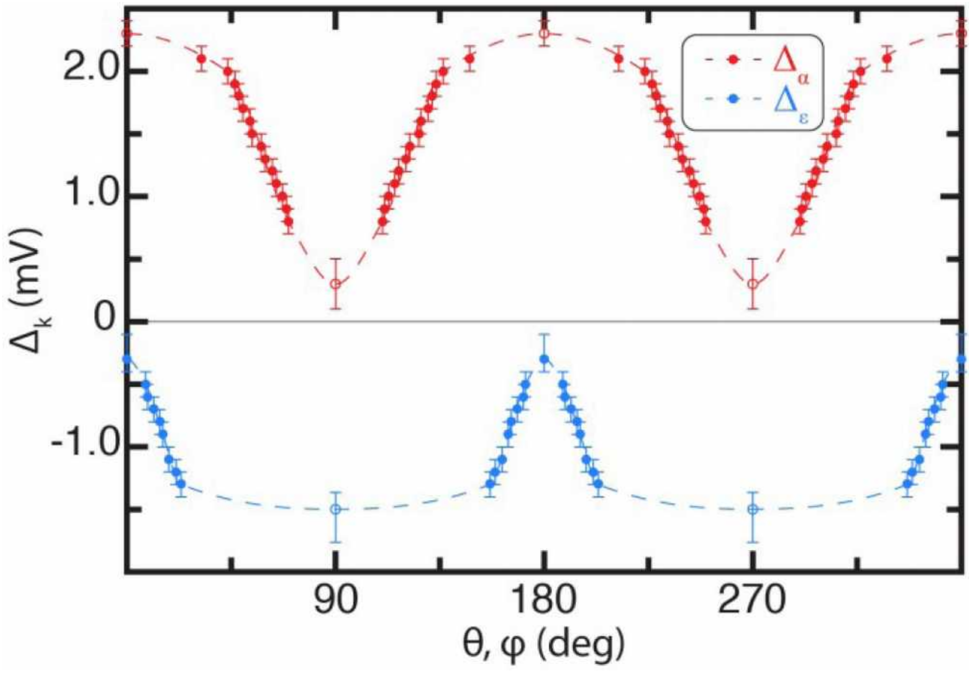
needed for consistent splitting at Gamma

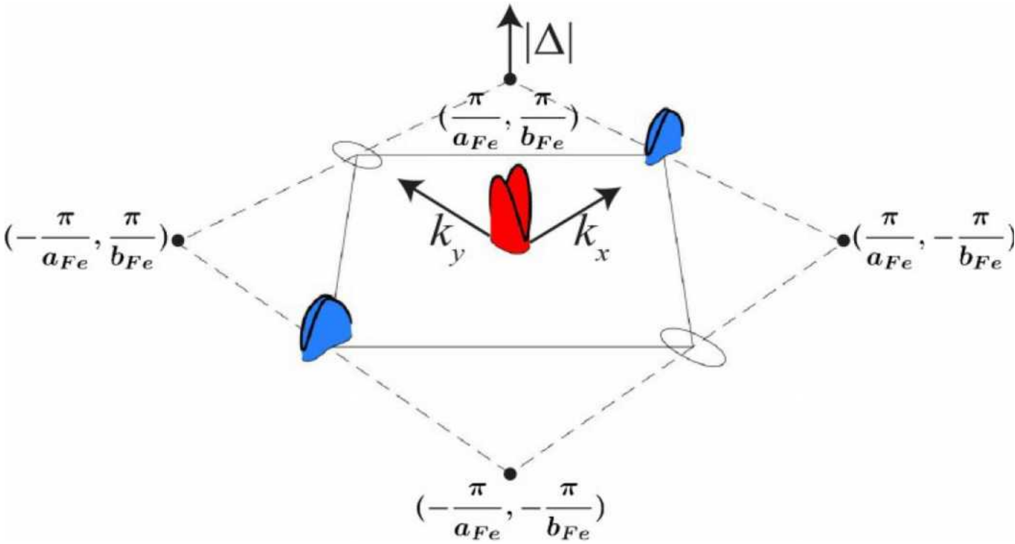


Superconducting gap

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







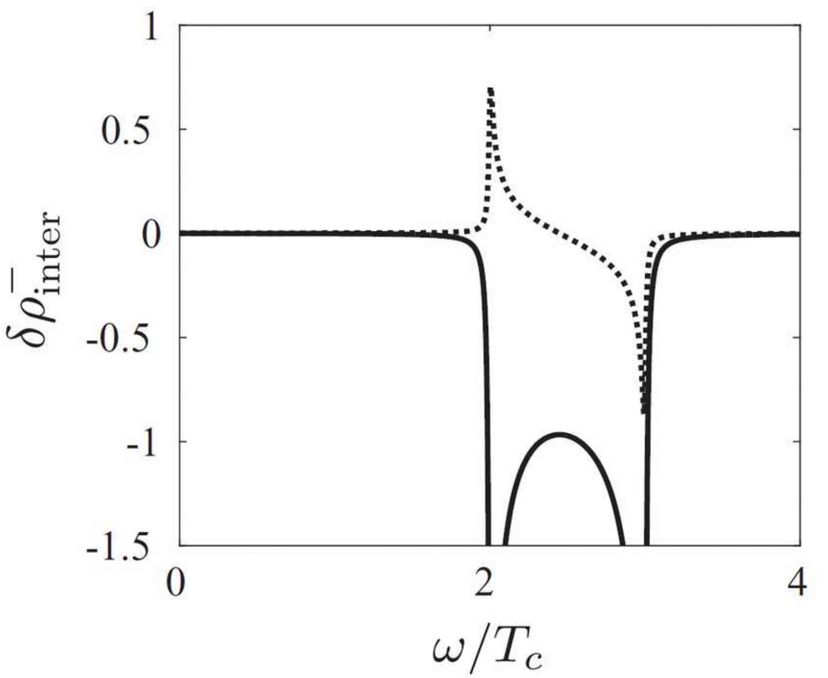
Sign change?!

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

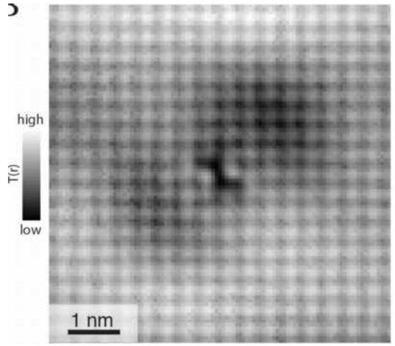


Hirschfeld et al., PRB **92**, 184513 (2015)

Measurement+modelling

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

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



- Theory:
  use measured gap
  +electronic structure

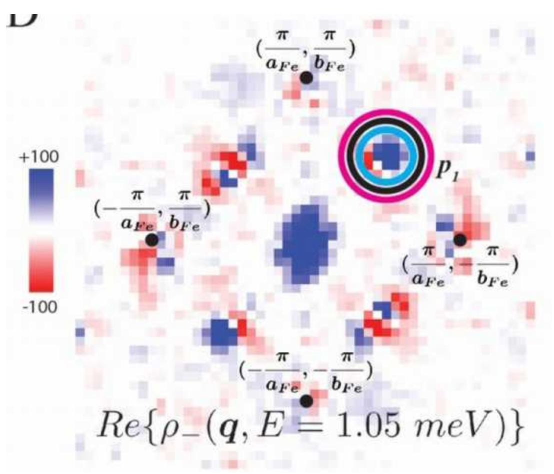
$$G_{k,k'}(\omega) = G^0_{k-k'}(\omega) + G^0_k(\omega)T(\omega)G^0_{k'}(\omega)$$

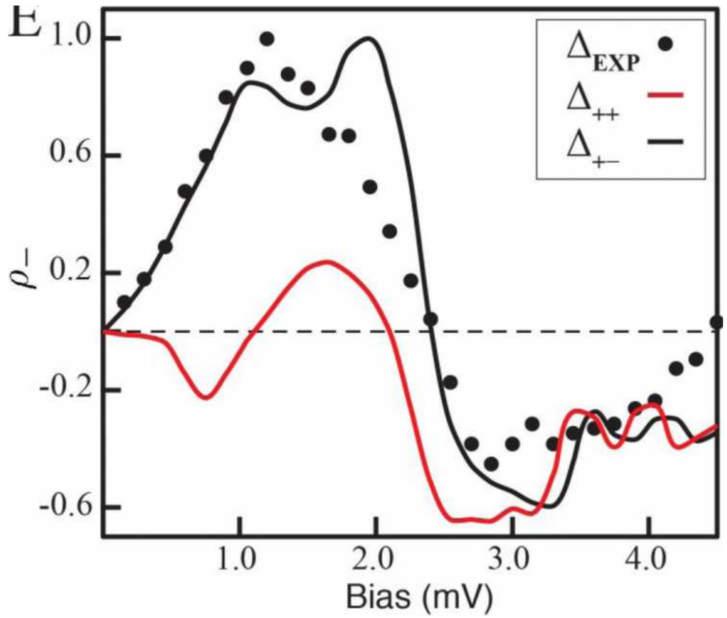
$$T(\omega) = \left[1 - V_{imp}G_0(\omega)\right]^{-1}V_{imp}$$

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

$$\rho(\omega) = \sum_q' \delta N(\boldsymbol{q},\omega)$$

- separate interband scattering contributions

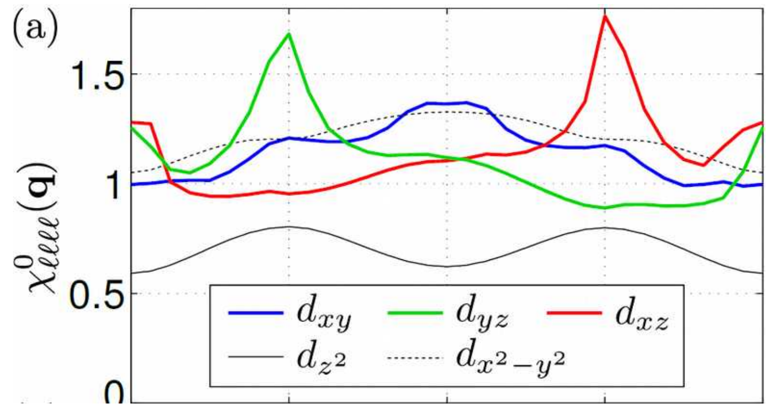




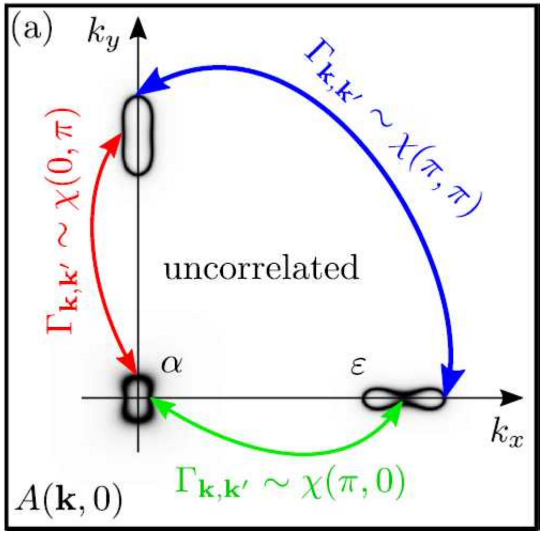
→ no sign change in signal, thus GAP changes sign

Pairing from spin-fluctuation theory?

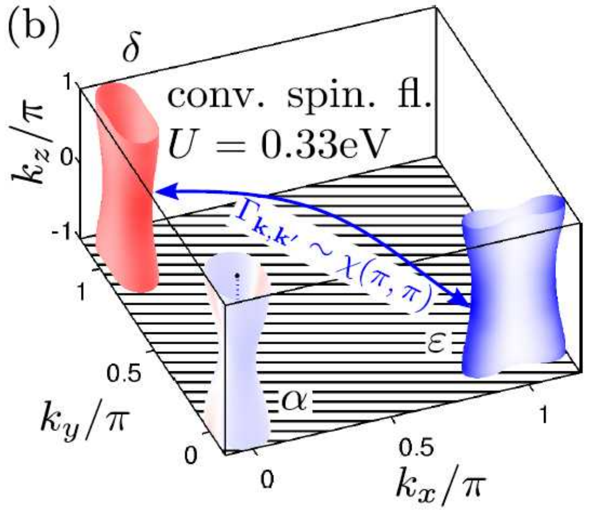
- Susceptibility

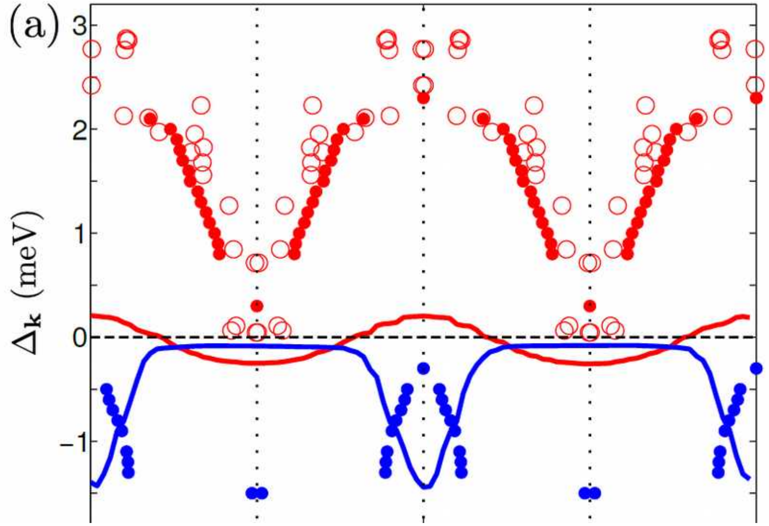


- Pairing glue



- 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?

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

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

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

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

Fermi liquid description

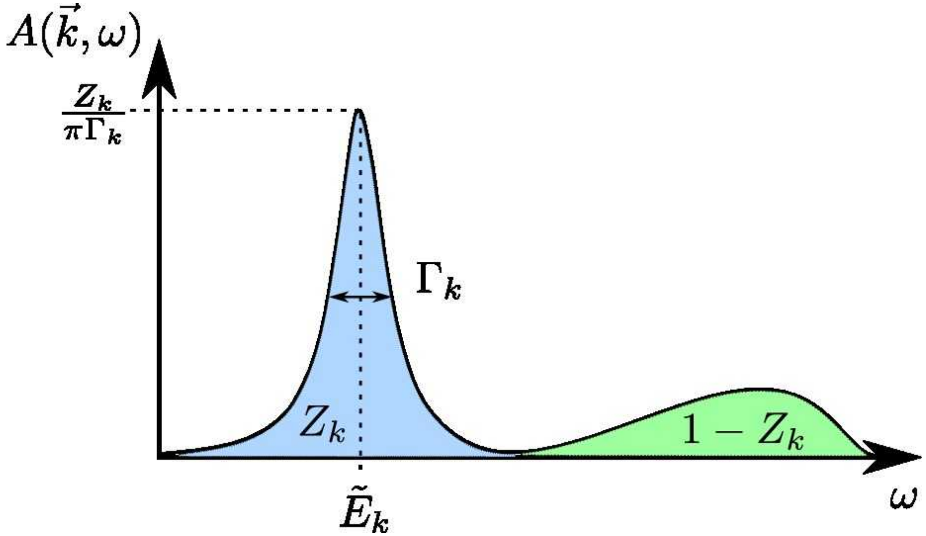
- Coherent electronic states

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

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

- Dressed electronic states

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



Relevant for Fe based SC:

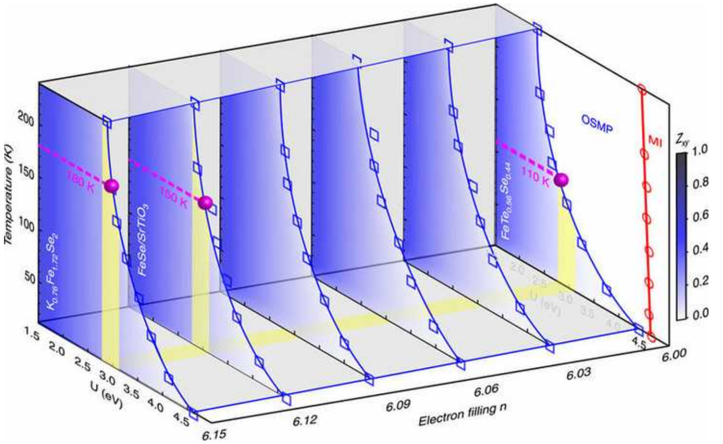
Yin, Haule, Kotliar, Nat. Mat. 10, 932-935 (2011)
de' Medici, Giovannetti, Capone. Phys. Rev. Lett. 112, 177001 (2014)
M. Aichhorn, et al., Phys. Rev. B 82, 064504 (2010)
Liu et al., Phys. Rev. B 92, 235138 (2015)
Yi et al., Nat. Comm. 6, 7777 (2015)
...

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

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

$$c_a \rightarrow \sqrt{Z_a}c_a$$

$$Z_{ab} = \sqrt{Z_a}\sqrt{Z_b}$$

geometric mean of quasiparticle weights

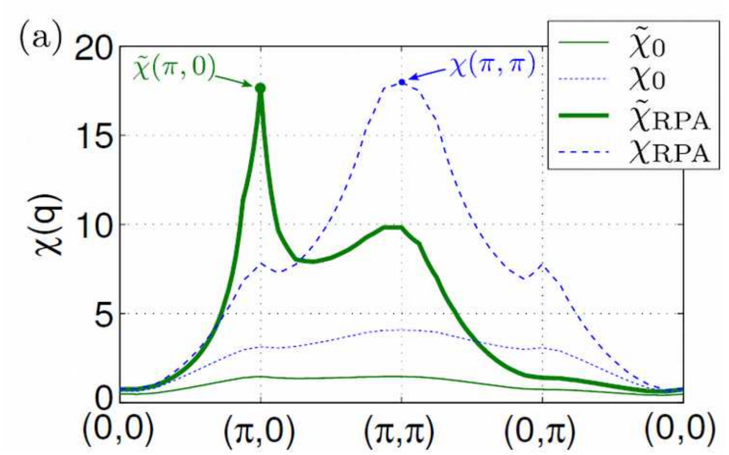
Spin-fluctuation theory

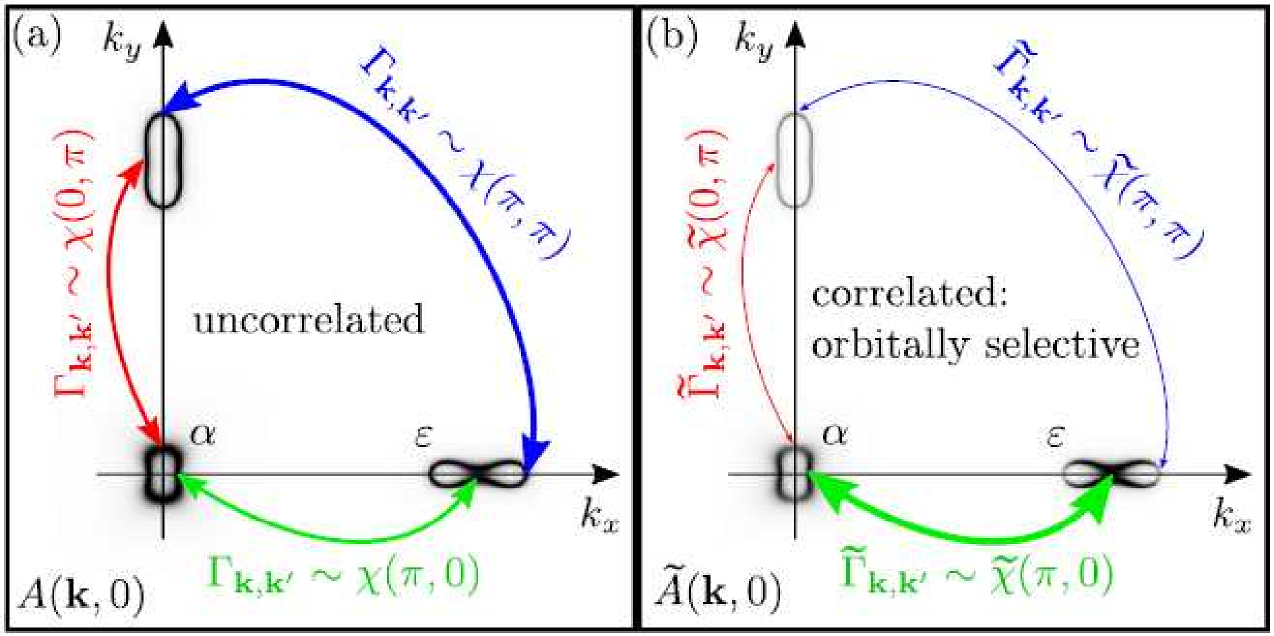
- "dressed susceptibility"

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

- Dressed pairing interaction

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

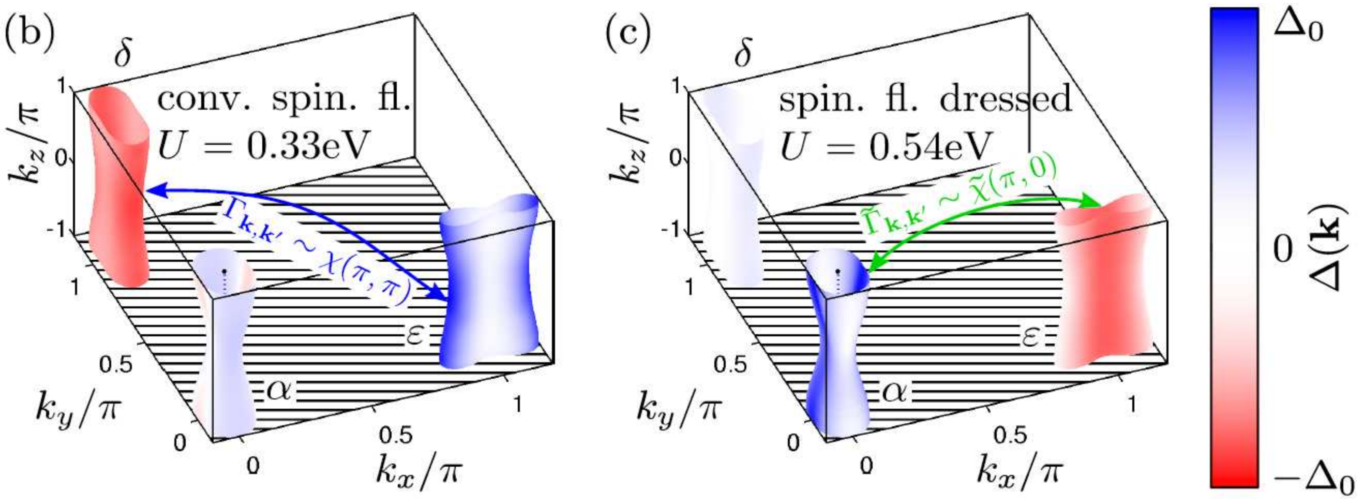


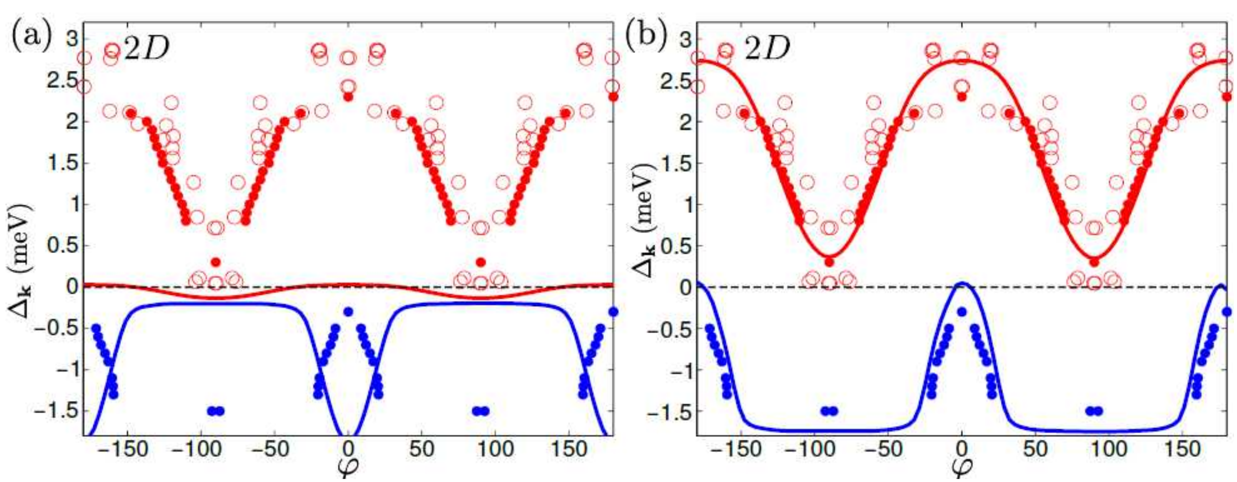


Dominant pairing in d_yz orbital channel
→ orbital selective pairing

Pairing and gap structure

uncorrelated correlated





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

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

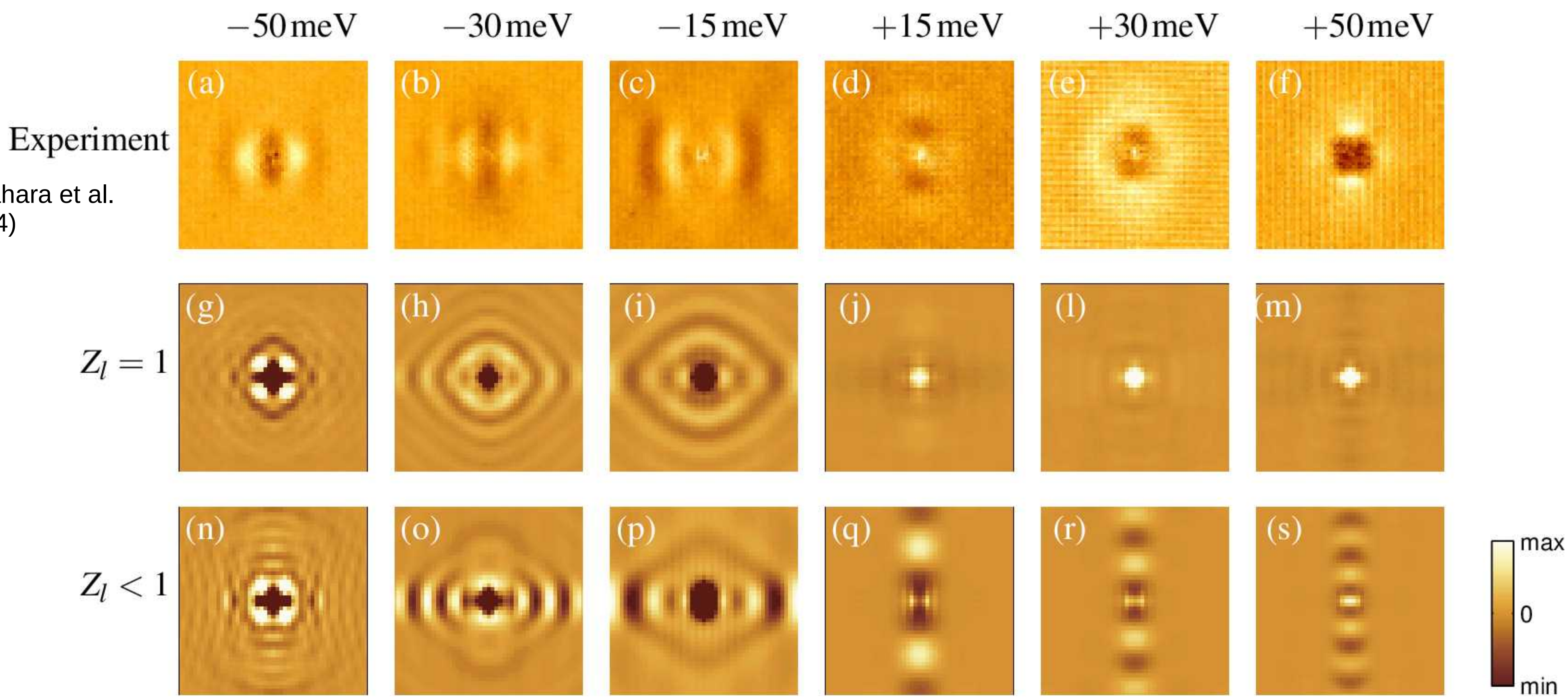
$$\{\sqrt{Z_l}\} = [0.2715, 0.9717, 0.4048, 0.9236, 0.5916]$$

Fermi liquid theory

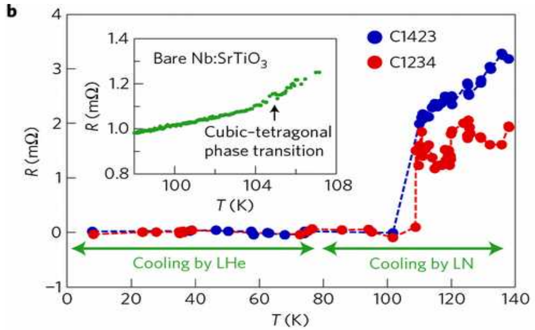
- Predictions for other experiments: electronic dimer close to impurity

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

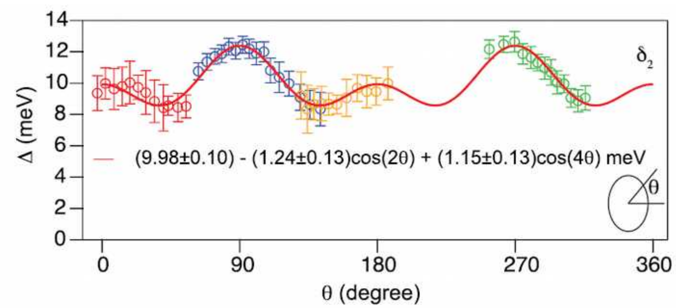
Kasahara et al. (2014)



Other systems: FeSe monolayer

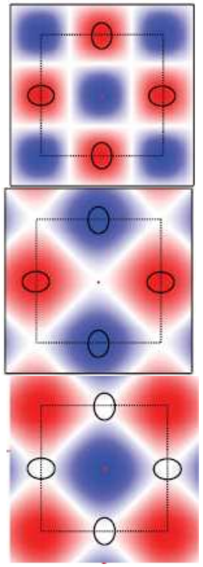


Ge et al. Nat. Mater. **14**, 285 (2015)

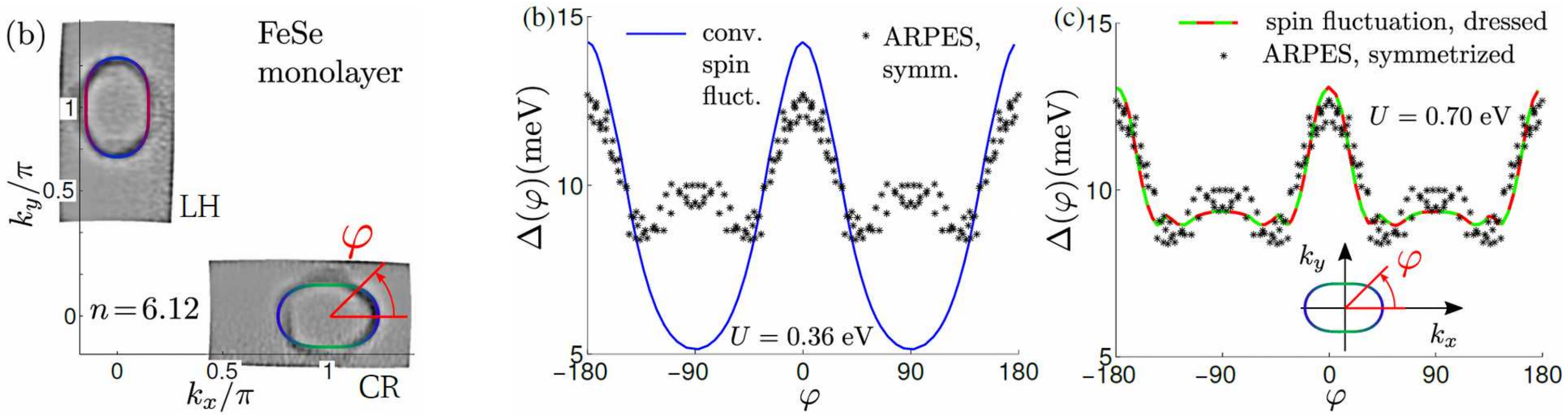


Zhang, et al., Phys. Rev. Lett. **117**, 117001 (2016)

No explanation of the two maxima structure by conventional approaches



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



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

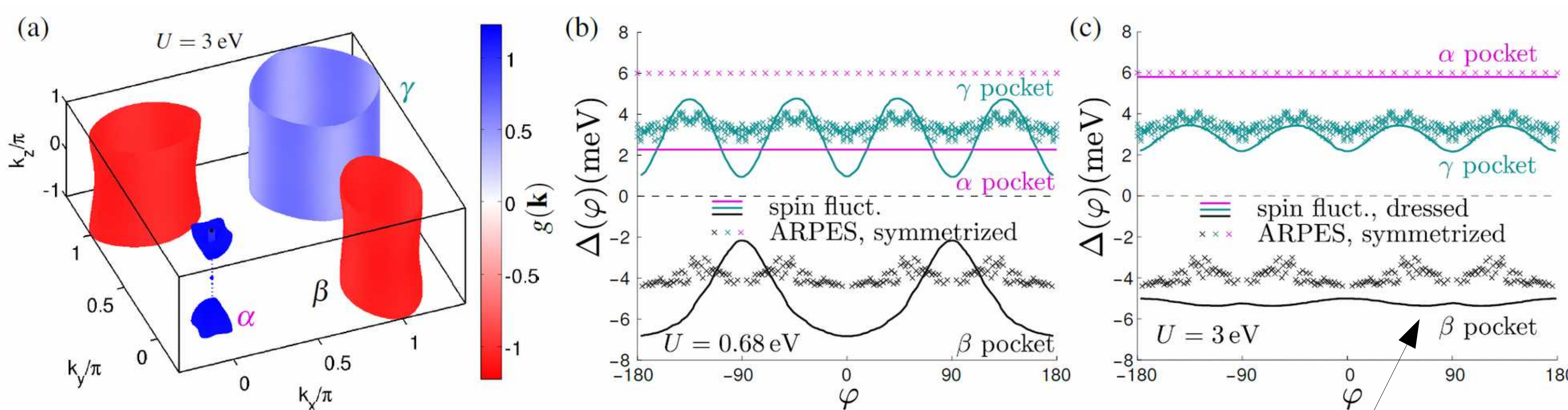
$$(d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2})$$

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-Tc 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

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

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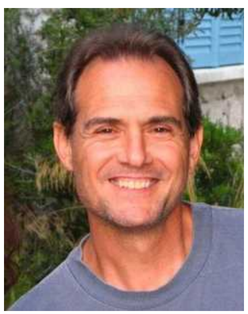

Peter J. Hirschfeld

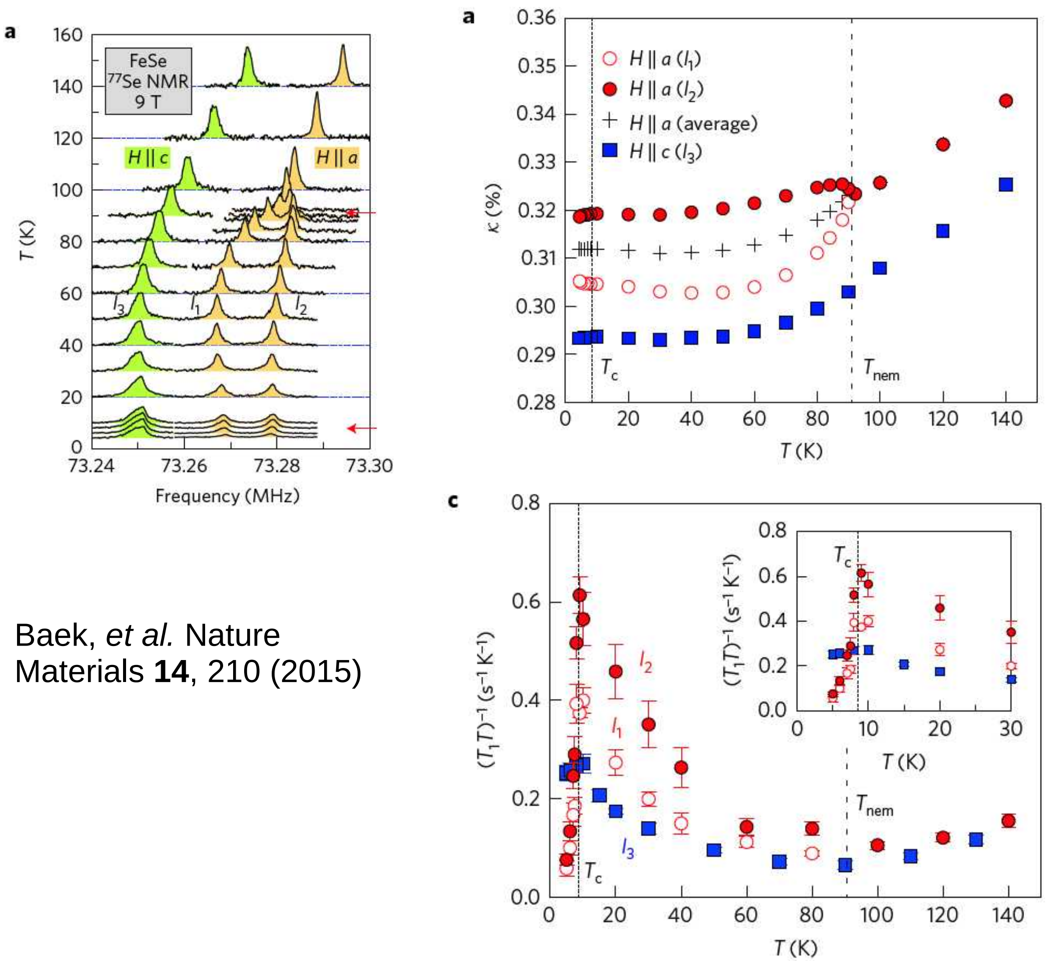

Brian M. Andersen

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

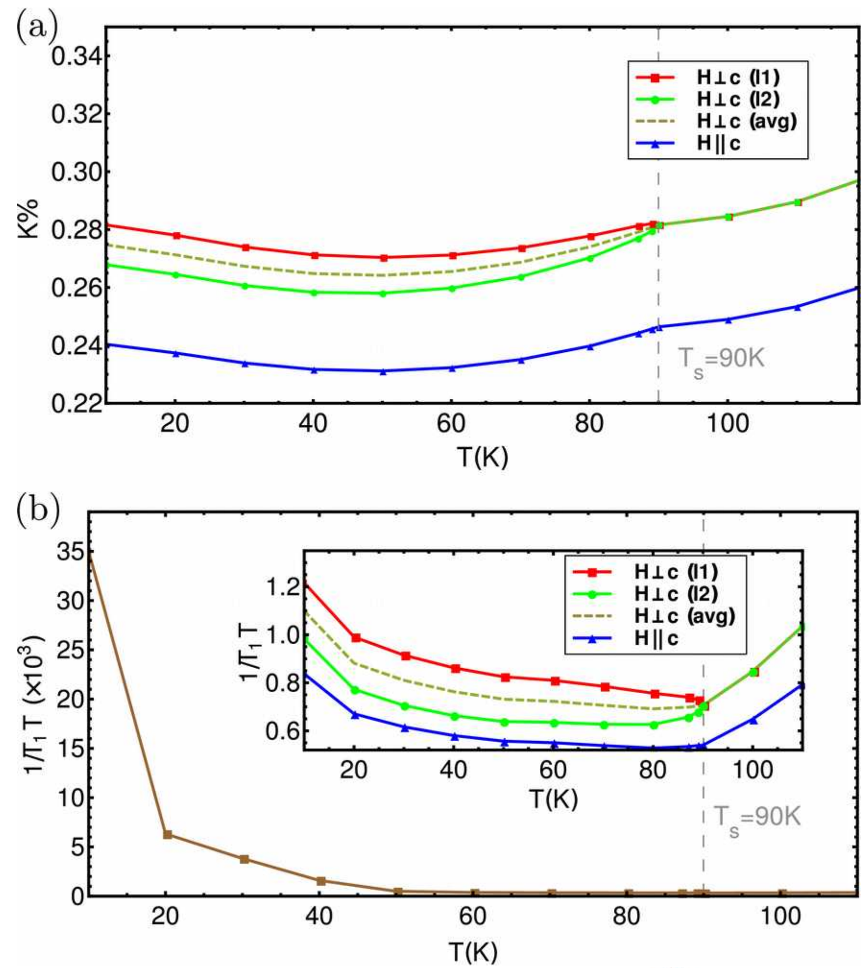
NMR: Knight shift, 1/T1T

orbital order visible in Knight shift



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

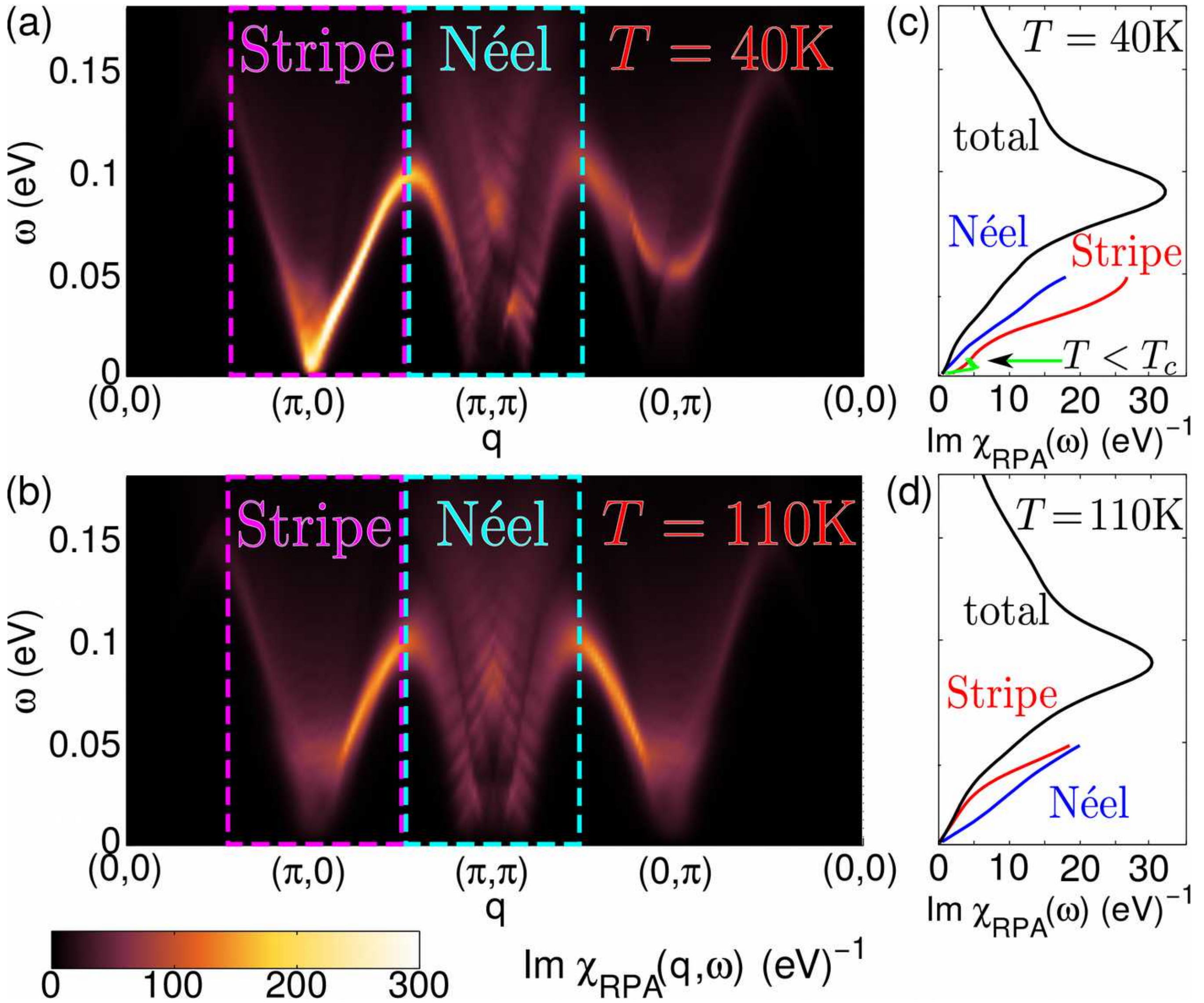
no enhanced low-energy spin fluctuations visible in NMR



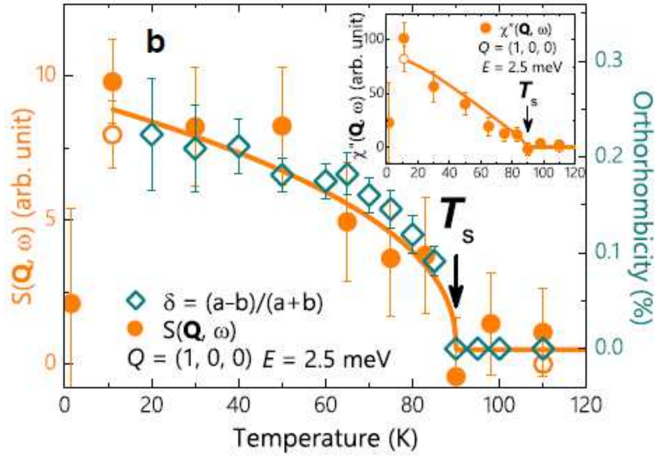
$$\frac{1}{T_1 T} = \lim_{\omega_0 \to 0} \frac{\gamma_N^2}{2N} k_B \sum_{\mathbf{q}\alpha\beta} |A_{hf}^{\alpha\beta}(\mathbf{q})|^2 \, \frac{\mathrm{Im}\{\chi_{\mathrm{RPA}}^{\alpha\beta}(\mathbf{q}, \omega_0)\}}{\hbar\omega_0}$$

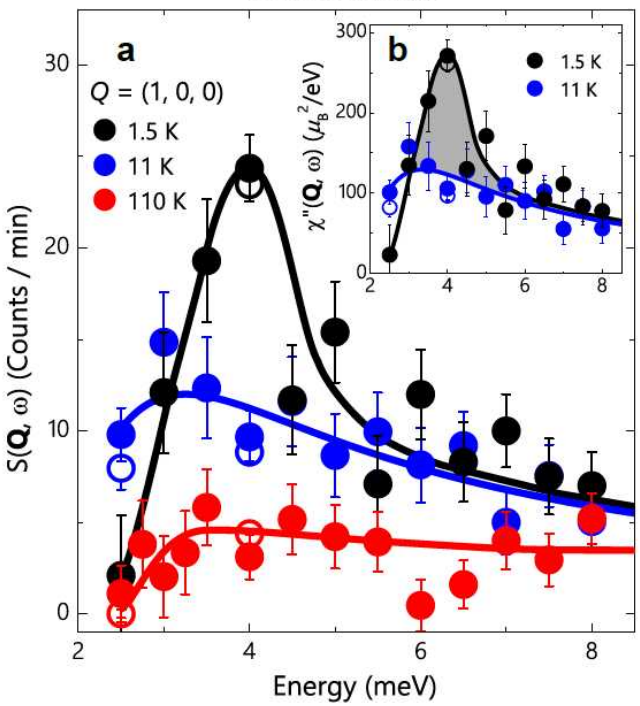
Spin fluctuations at higher energies

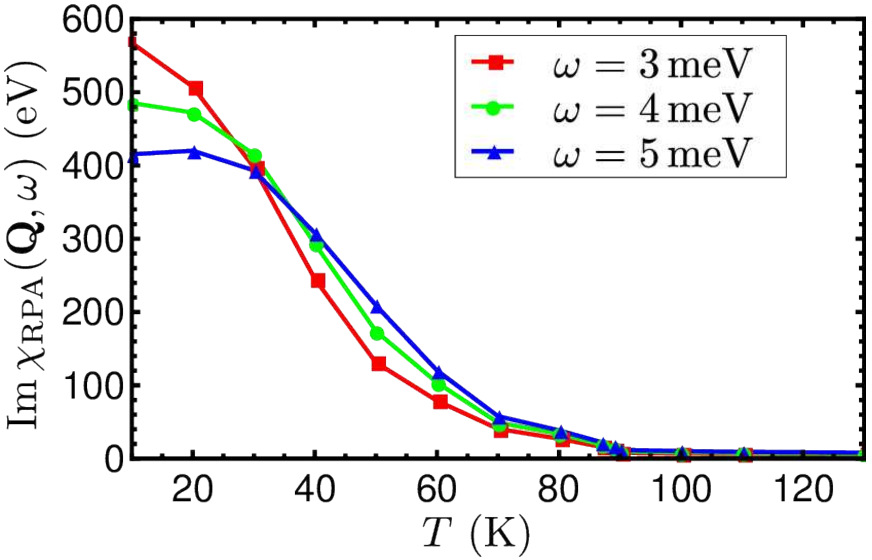
- FeSe: close to magnetic instability (tune interactions accordingly)
- transfer from Néel fluctuations to Stripe fluctuations on lowering temperature
- spin resonance at low energies from transfer of spectral weight in the superconducting state

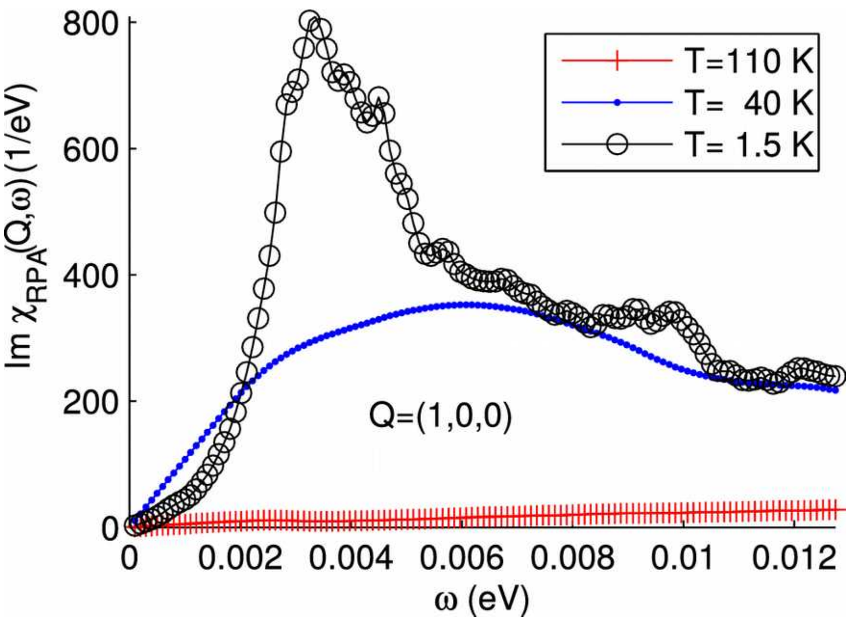


Inelastic neutron scattering



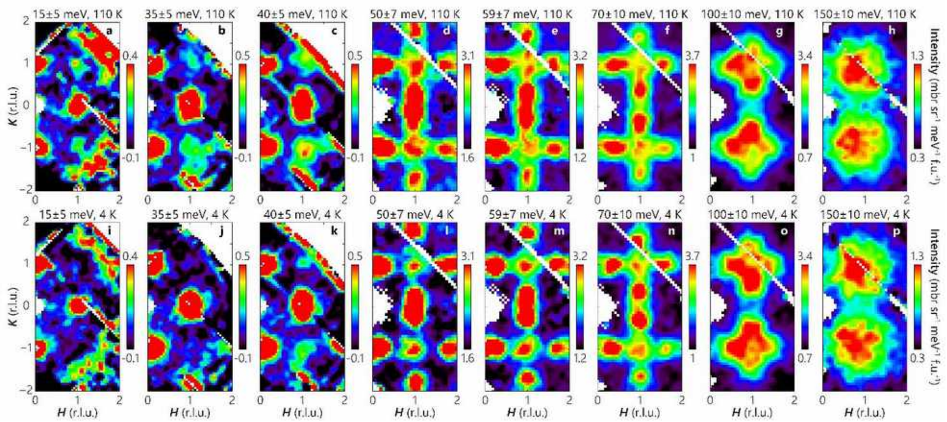


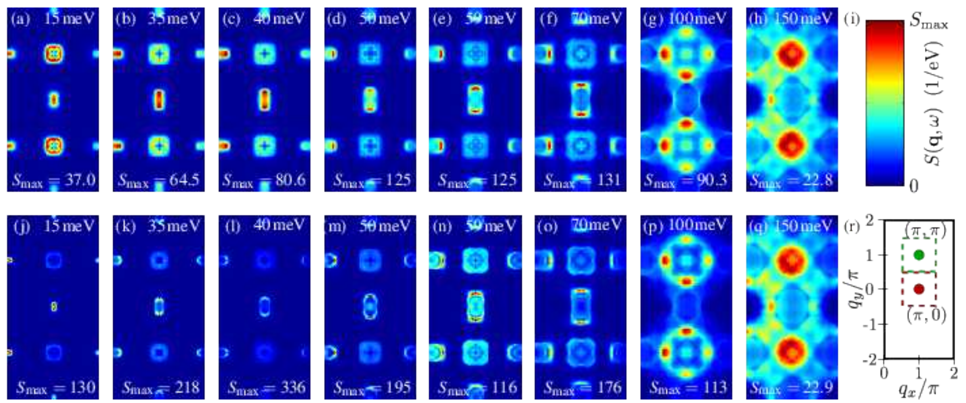


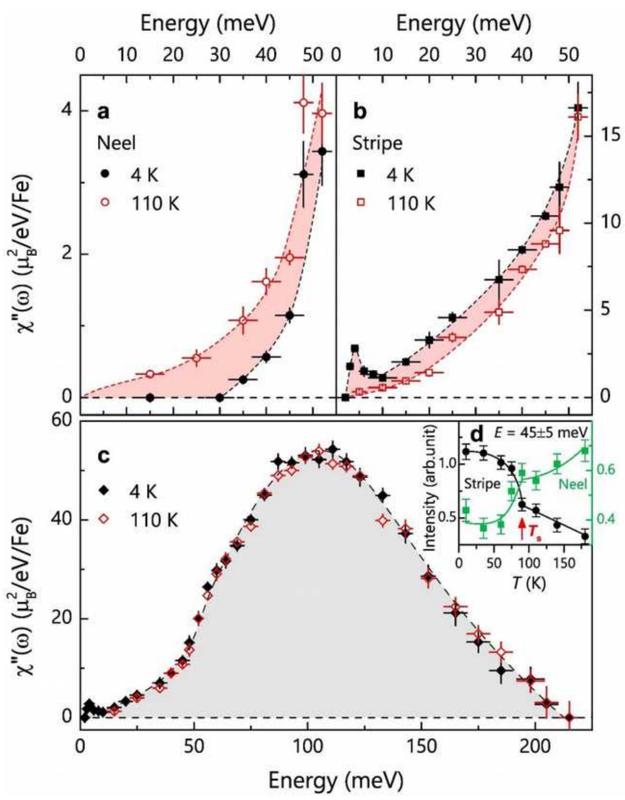


Wang *et al.,* Nature Materials **15**, 159 (2016)

Inelastic neutron scattering







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