Superconductivity and spin excitations in orbitally ordered FeSe

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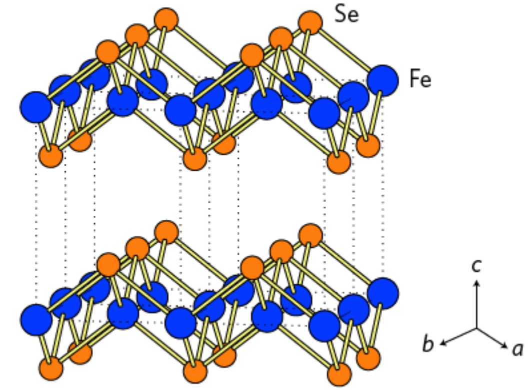
Phys. Rev. Lett. **115**, 026402 (2015)
Phys. Rev. B **92**, 224515 (2015)

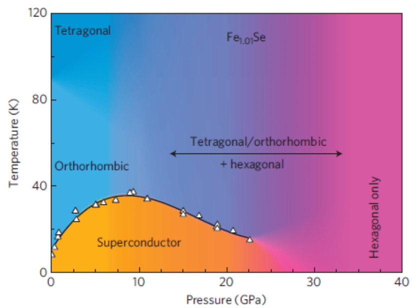
Motivation: FeSe



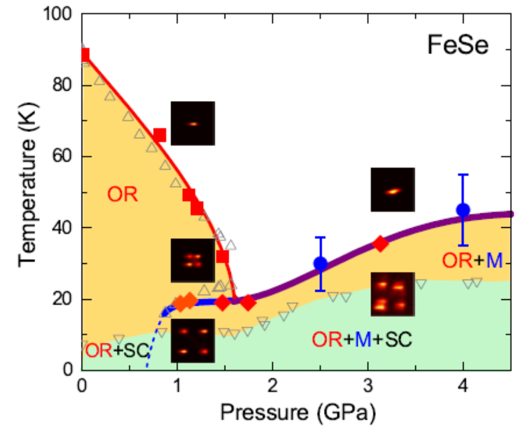
- FeSe
  - simplest compound
  - superconducting without doping
- interesting properties
  - non-magnetic
  - nematic phase
    possibility to study origin of nematicity without presence of magnetic order

Motivation: FeSe

- pressure experiments



Medvedev et al. (2010)
enhancement of Tc up to 37K

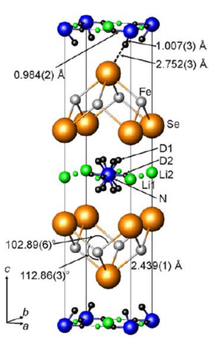


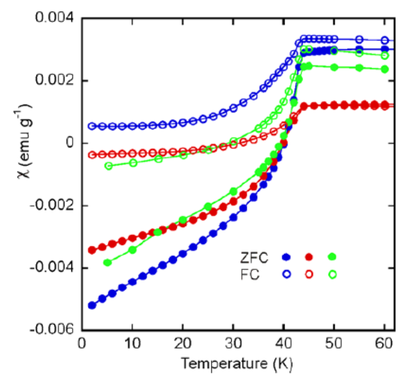
onset of magnetism under pressure

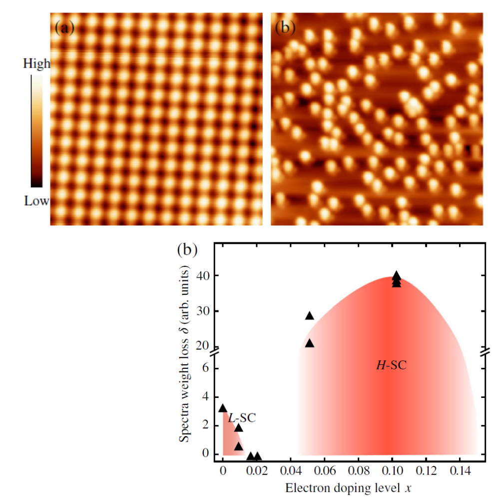
K. Kothapalli et al. arXiv:1603.04135 (2016)

- intercalation

Burrard-Lucas et al. 2012
Tc → 43K molecular intercalation

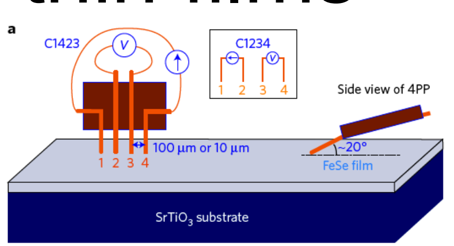


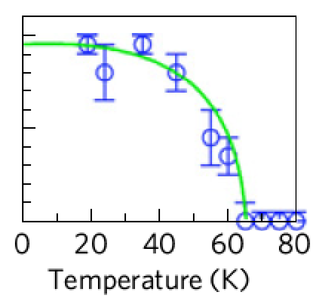




Can-Li Song, et al. Phys. Rev. Lett. **116**, 157001 (2016)

- thin films



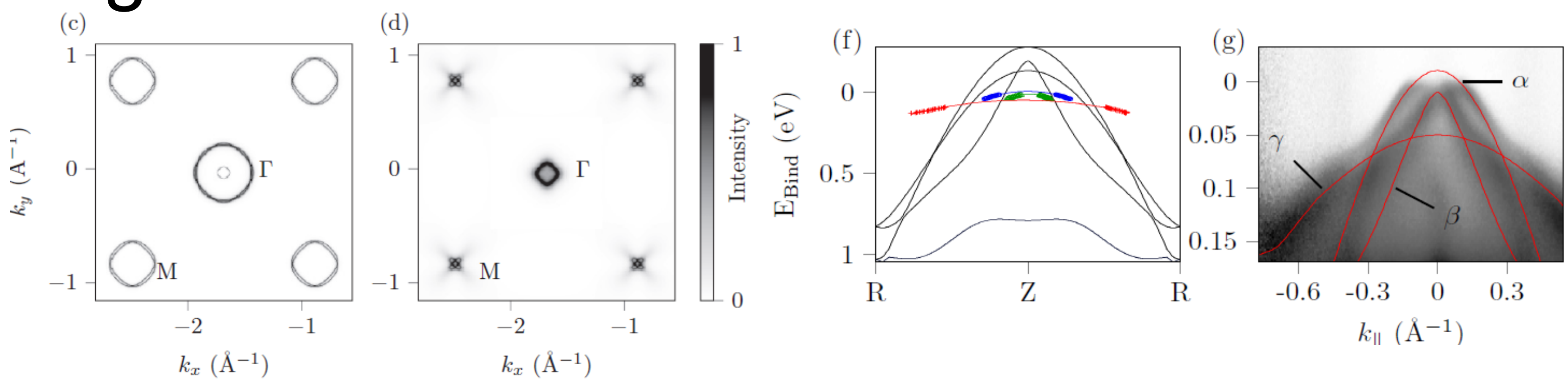


ARPES gap Tc → 65K
He et al., Nature Materials 12, 605–610 (2013)

Transport on monolayer: Tc ~ 100K
Ge et al. Nat. Mater. **14**, 285 (2015)

FeSe

- ARPES: unusual band renormalization, no agreement to DFT



Maletz, *et al.* PRB **89**, 220506(R) (2014)

- pragmatic approach TB engineering
  - shifts of tight binding parameters
  - orbital order
    - site centered orbital order
    - bond centered orbital order

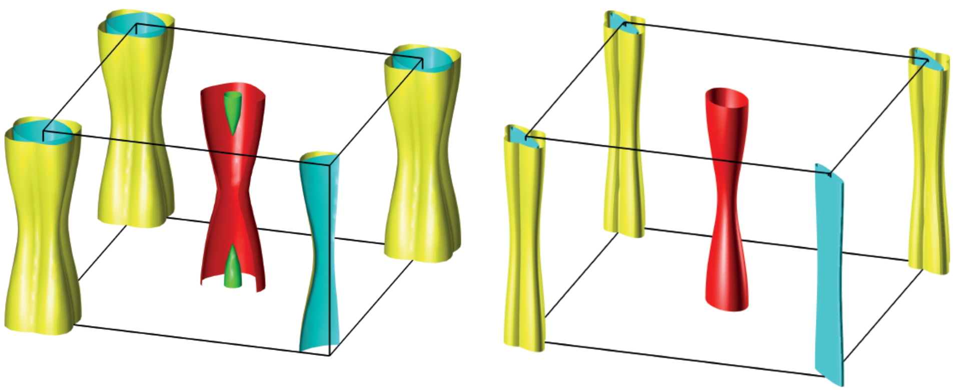
$$H = H_{\mathrm{TB}} + H_{\mathrm{OO}},$$

$$H_{\mathrm{TB}} = \sum_{\mathbf{k},\mu,\nu,\sigma} t_{\mu\nu}(\mathbf{k}) c^{\dagger}_{\mu\sigma}(\mathbf{k}) c_{\nu\sigma}(\mathbf{k}),$$

$$H_{\mathrm{OO}} = \Delta_s(T) \sum_{\mathbf{k}\sigma} [n_{xz\sigma}(\mathbf{k}) - n_{yz\sigma}(\mathbf{k})].$$

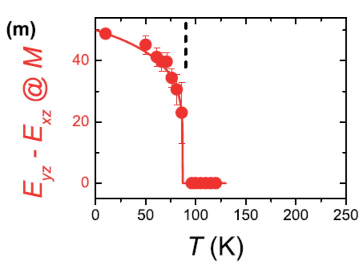
FeSe: tight binding model

- ARPES

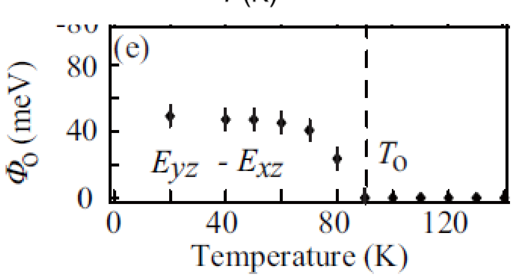


T>T_S T<T_S

Watson *et al.*, PRB **91**, 155106 (2015); no color code

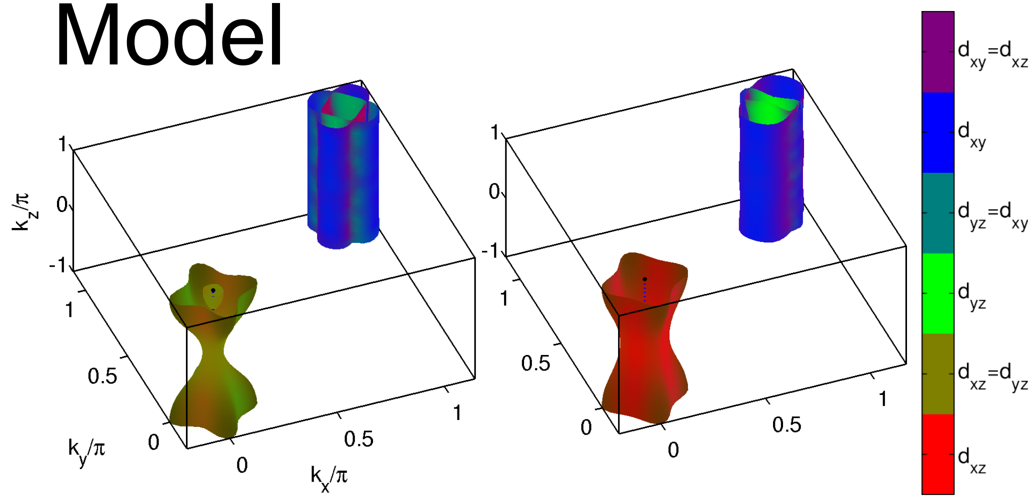


orbital order: 50 meV
T_S=87K

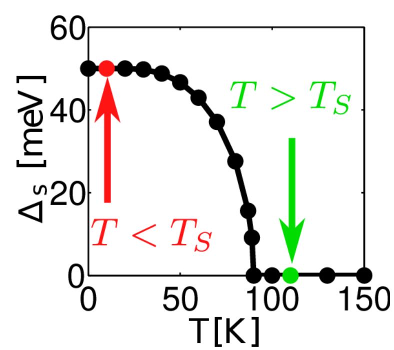


Shimojima, *et al.* PRB **90**, 121111(R) (2014)

Model



T>T_S T<T_S



10-orbital model based on:

Eschrig *et. al*, Phys Rev B, **80**, 104503 (2009)

+shift of hoppings
+inclusion of orbital order

$$H_{OO} = \Delta_b g(t) \sum_{\mathbf{k}\sigma} (\cos k_x - \cos k_y)[n_{xz\sigma}(\mathbf{k}) + n_{yz\sigma}(\mathbf{k})]$$

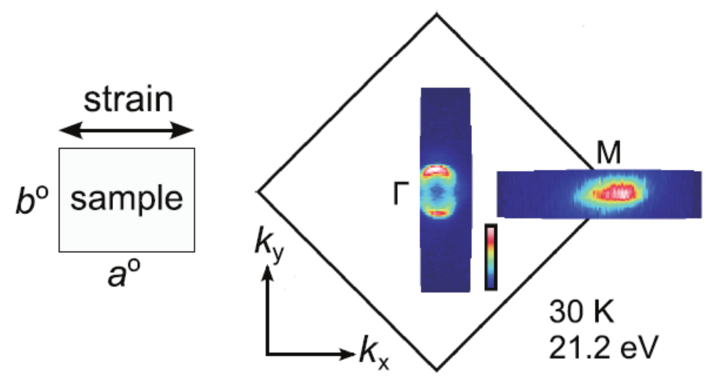
$$+ \Delta_s g(t) \sum_{\mathbf{k}\sigma} [n_{xz\sigma}(\mathbf{k}) - n_{yz\sigma}(\mathbf{k})].$$

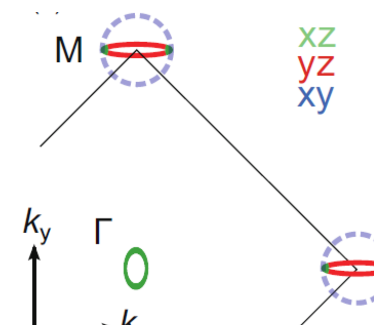
FeSe: tight binding model

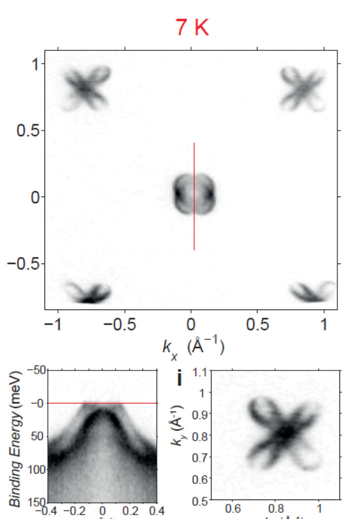
- orbital order
  - bond centered OO
  - site centered OO
- sign changing orbital splitting

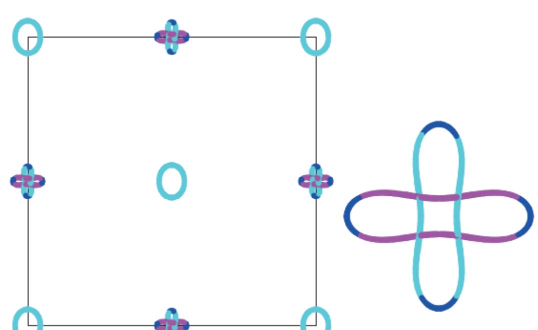
$$H_{OO} = \Delta_b g(t) \sum_{\mathbf{k}\sigma} (\cos k_x - \cos k_y)[n_{xz\sigma}(\mathbf{k}) + n_{yz\sigma}(\mathbf{k})] + \Delta_s g(t) \sum_{\mathbf{k}\sigma} [n_{xz\sigma}(\mathbf{k}) - n_{yz\sigma}(\mathbf{k})].$$

ARPES on detwinned samples
Suzuki et al., Phys. Rev. B **92**, 205117 (2015)







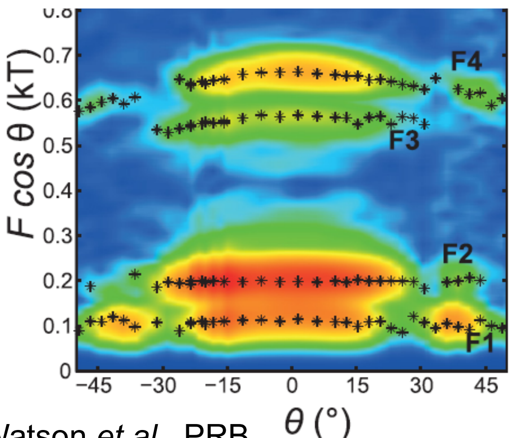


Unidirectional bond order:
Watson et al., arXiv:1603.04545 (2016)

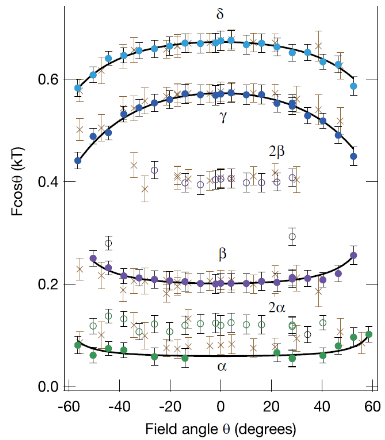
$$h = \Delta_S (n'_{yz} - n'_{xz}) \cos(k_x)$$

FeSe: tight binding model

- Quantum oscillations

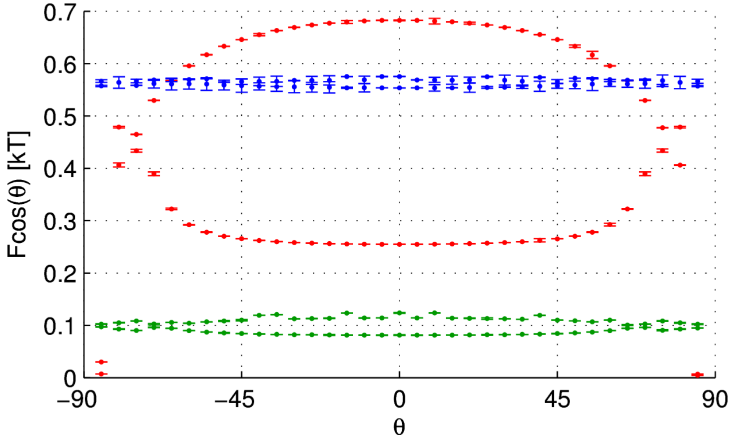


Watson *et al.*, PRB **91**, 155106 (2015)



Terashima, *et al.* PRB **90**, 144517 (2014)

Model

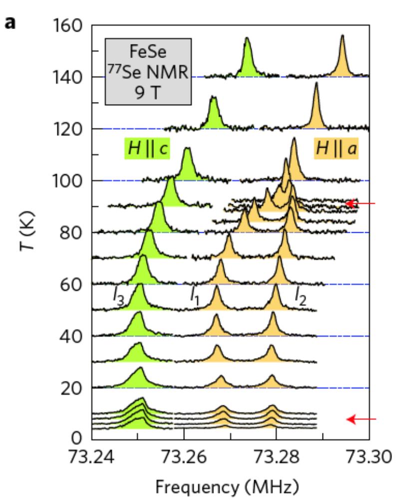


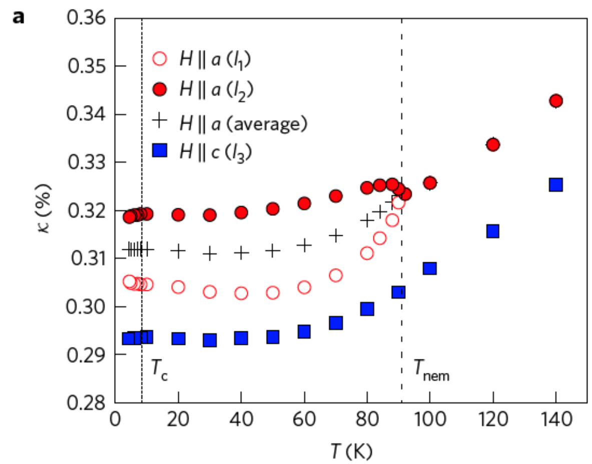
Daniel Guterding: https://github.com/danielguterding/dhva

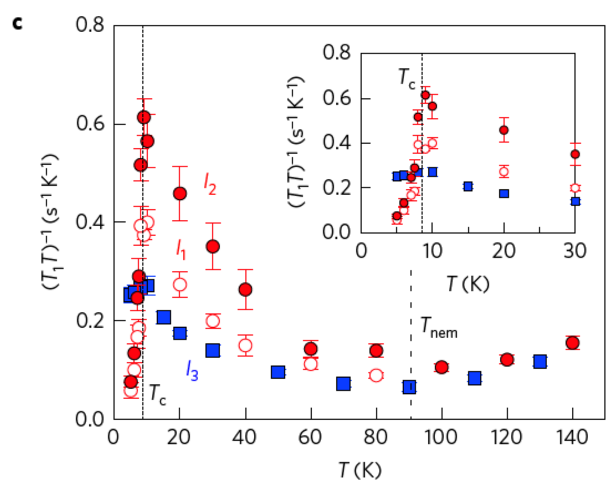
- **Question:** Can model electronic structure account for various other experimental results?
  - NMR: no spin-fluctuations until very low T — Baek, *et al.* Nature Materials **14**, 210 (2015)
  - Neutron diffraction: Stripe fluctuations at intermediate energies, Neutron resonance in SC state — Rahn *et al.* PRB (2015); Wang *et al.*, Nature Materials **15**, 159 (2016)
  - Scanning tunnelling microscopy: V-shaped DOS — Kasahara *et al.* (2014); Song *et al.*, Science **332**, 1410 (2011)
  - ...

NMR: Knight shift, 1/T1T

orbital order visible in Knight shift

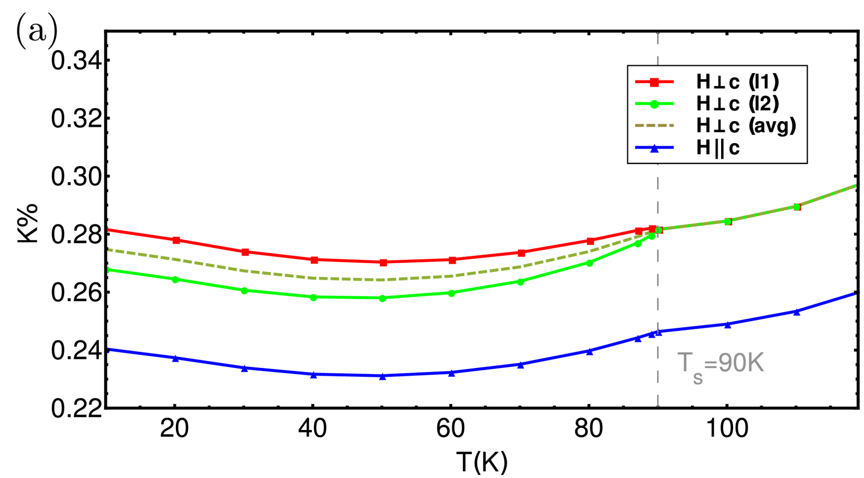


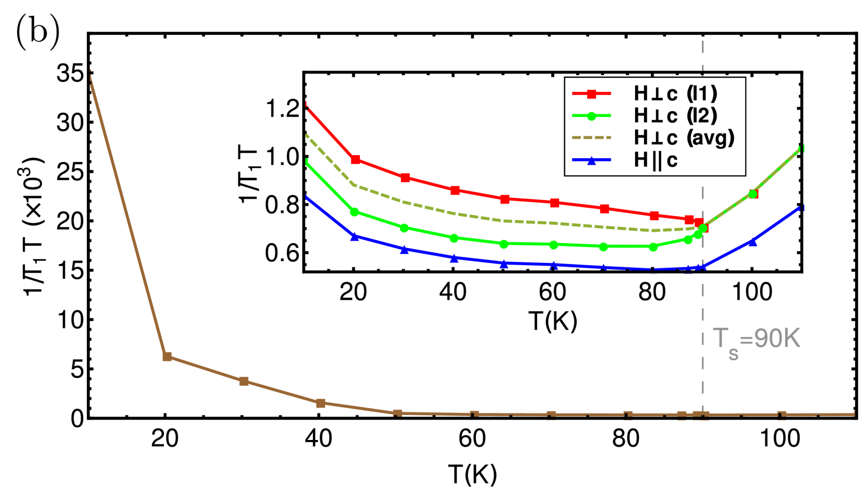




Baek, *et al.* Nature Materials **14**, 210 (2015)

no enhanced low-energy spin fluctuations visible in NMR

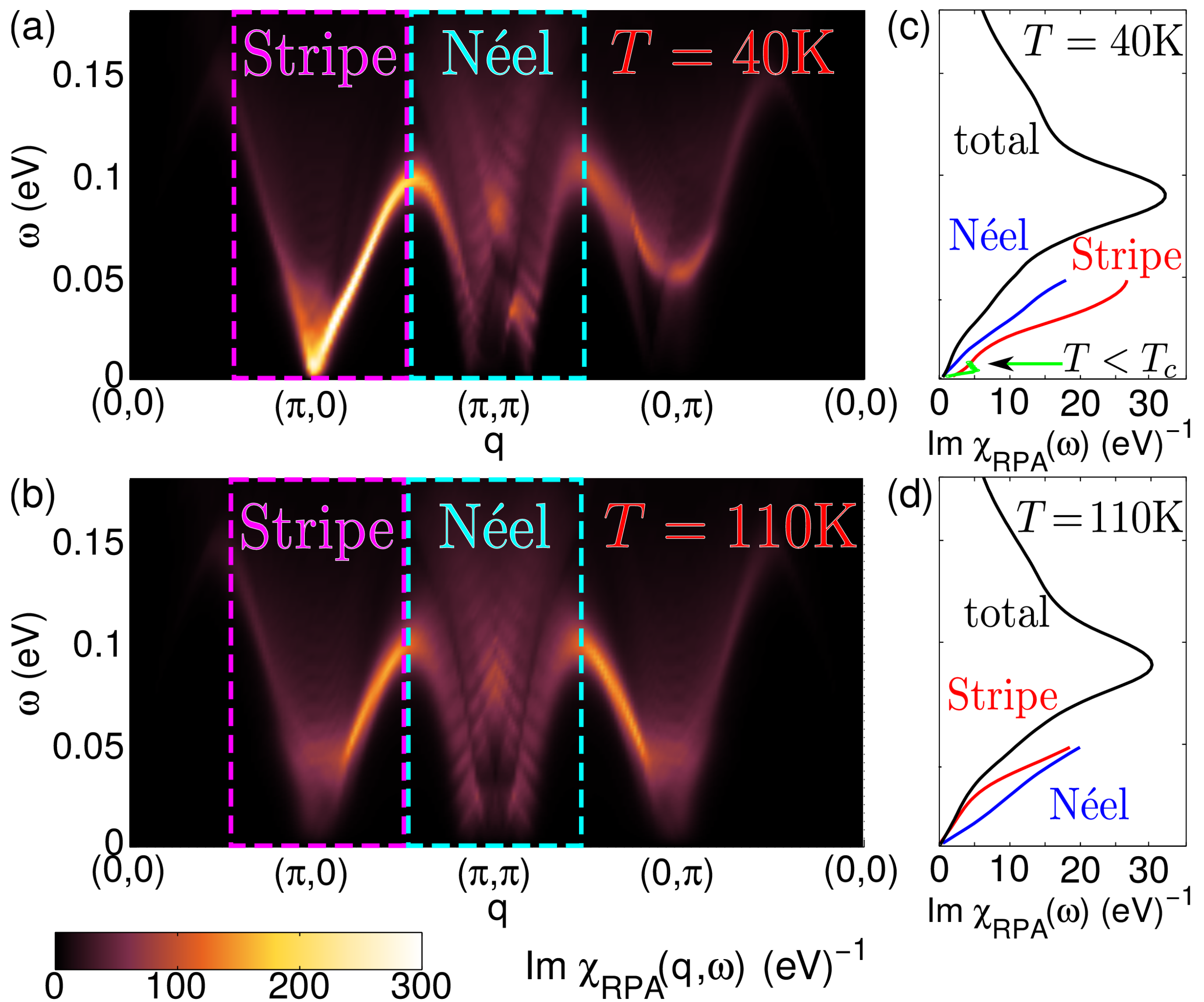




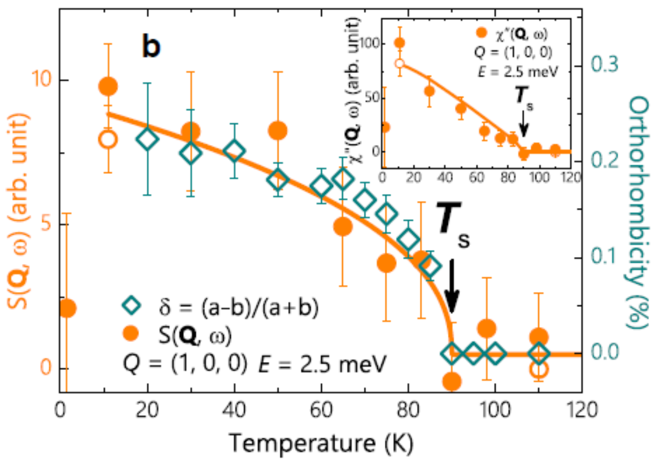
$$\frac{1}{T_1T} = \lim_{\omega_0\to 0} \frac{\gamma_N^2}{2N} k_B \sum_{\mathbf{q}\alpha\beta} |A_{hf}^{\alpha\beta}(\mathbf{q})|^2 \frac{\mathrm{Im}\{\chi_{\mathrm{RPA}}^{\alpha\beta}(\mathbf{q},\omega_0)\}}{\hbar\omega_0}$$

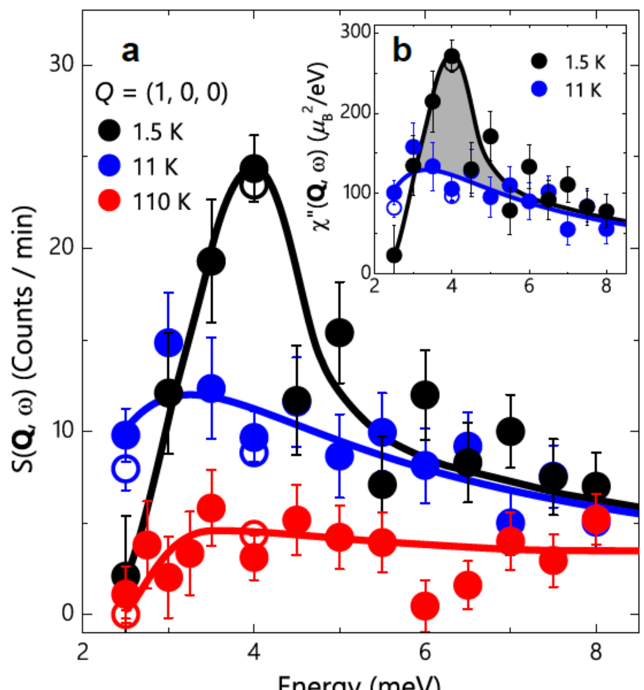
Spin fluctuations at higher energies

- 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

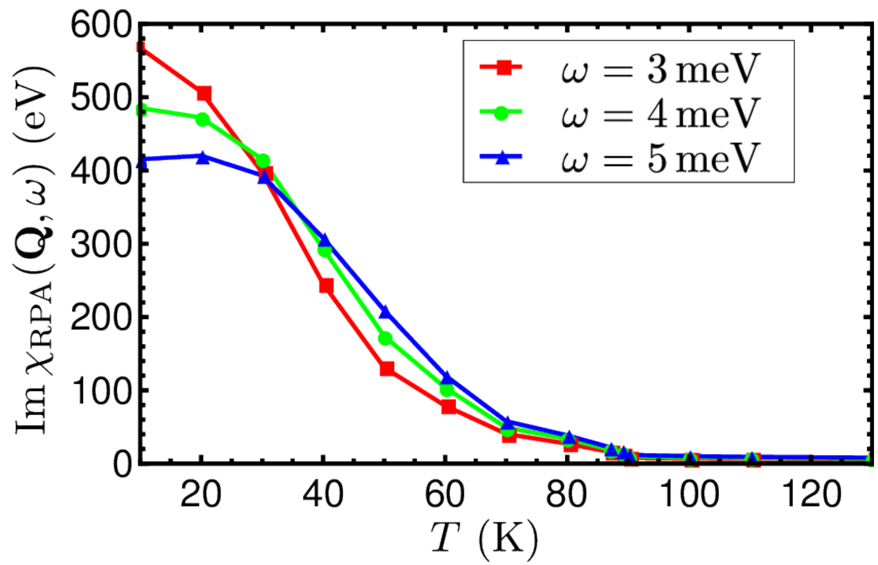


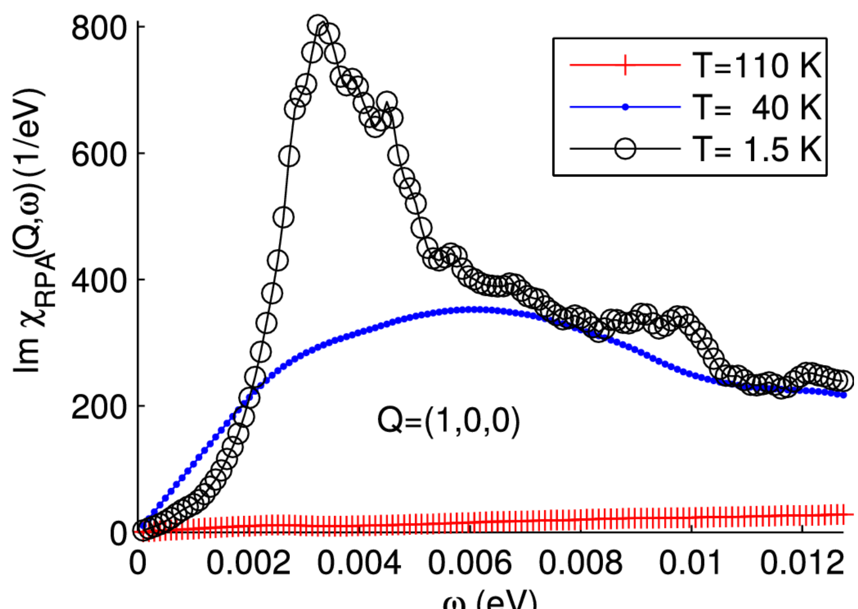
Inelastic neutron scattering



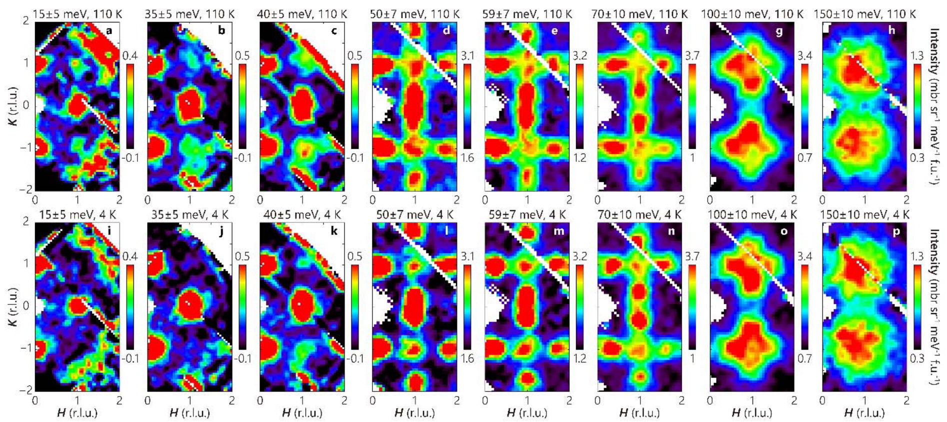


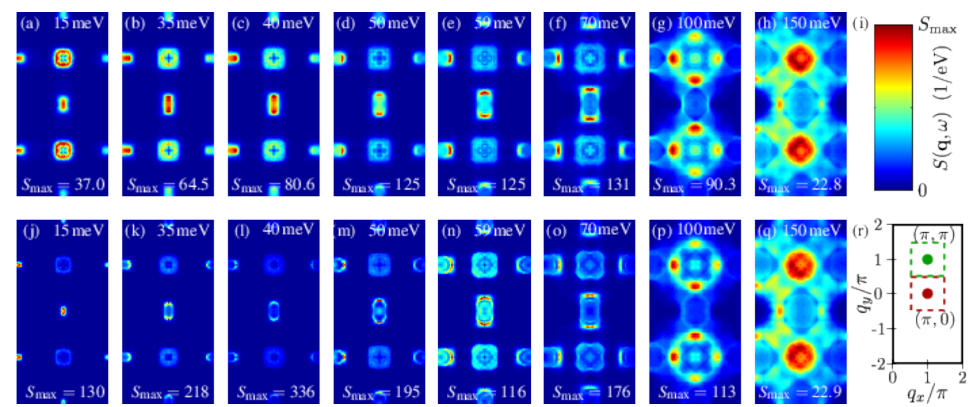
Wang *et al.*, Nature Materials **15**, 159 (2016)

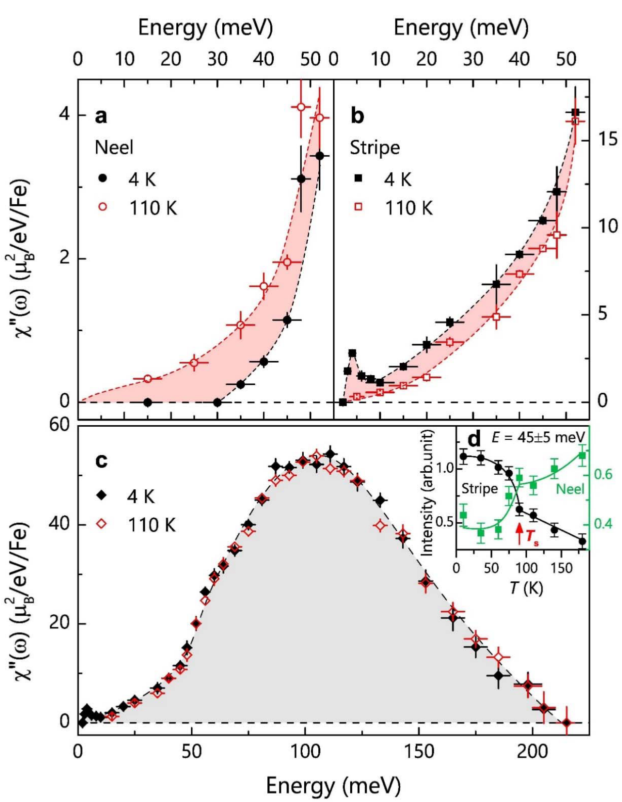




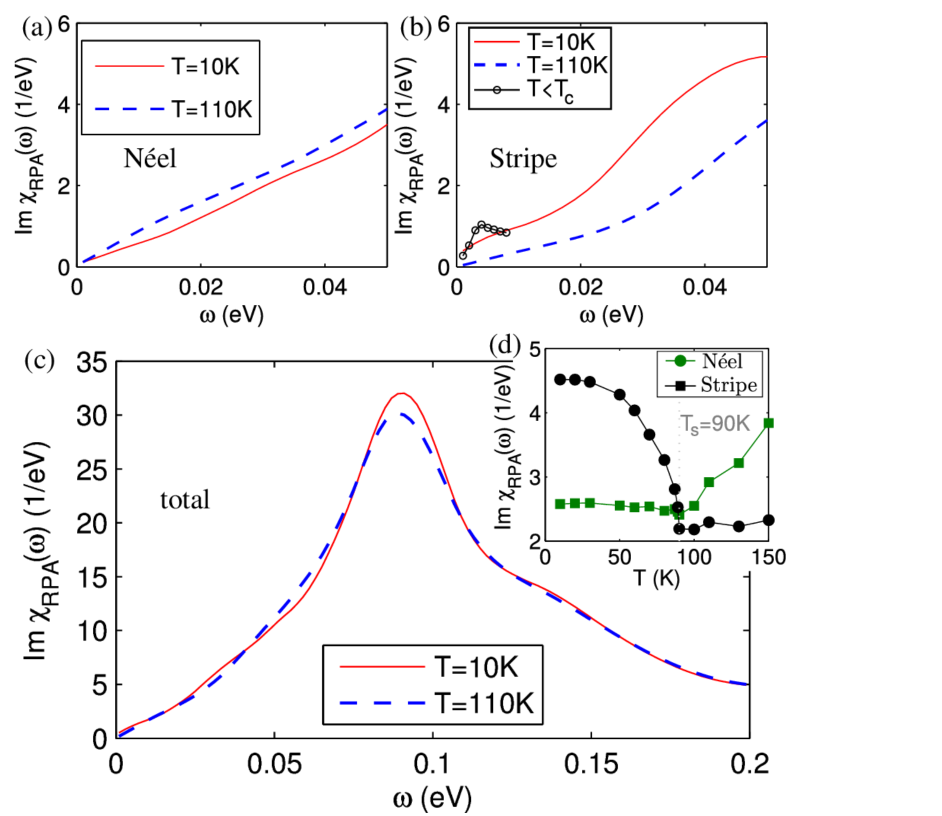
Inelastic neutron scattering







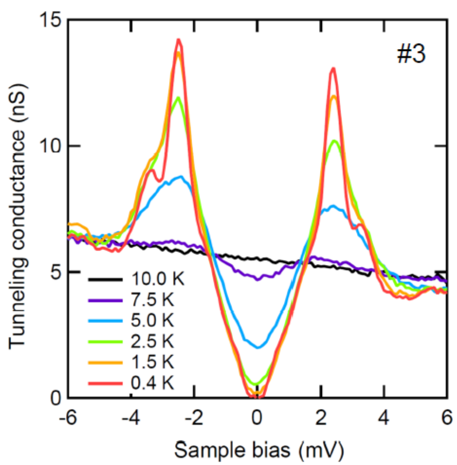
Q. Wang, *et al*, arXiv:1511.02485 (2015)



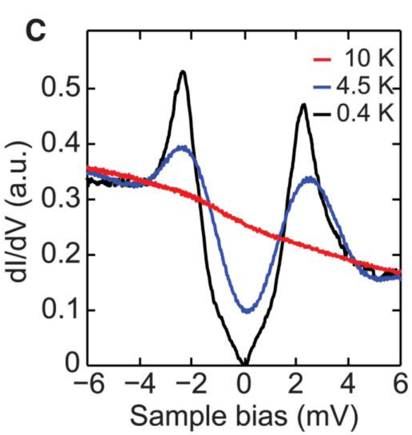
Superconducting order parameter

- spin-fluctuation driven superconductivity

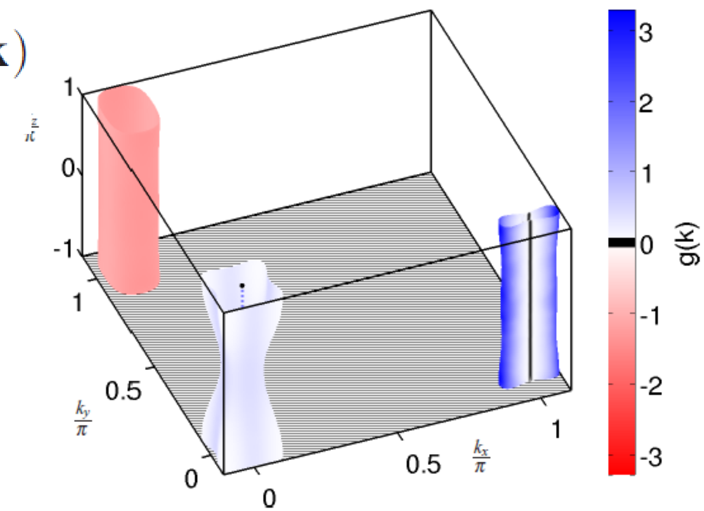
$$-\frac{1}{V_G}\sum_j \int_{\mathrm{FS}_j} dS' \Gamma(\mathbf{k},\ \mathbf{k}')\frac{g_\alpha(\mathbf{k}')}{|v_{\mathrm{F}j}(\mathbf{k}')|} = \lambda_\alpha g_\alpha(\mathbf{k})$$

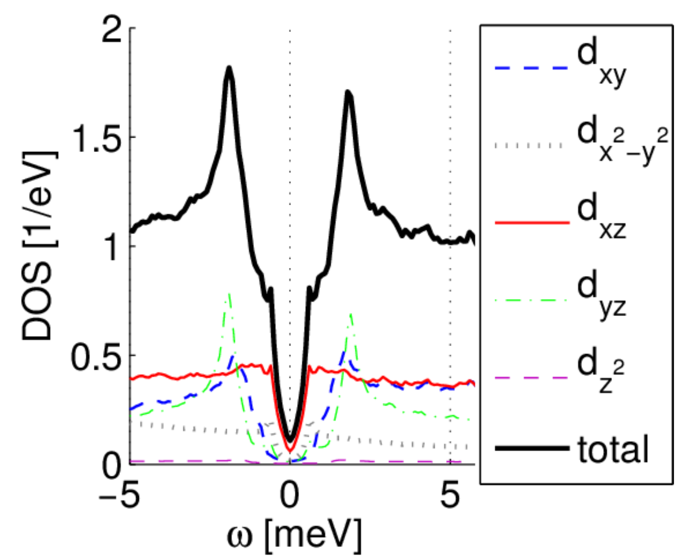


STM on FeSe:
Kasahara *et al*. (2014)



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





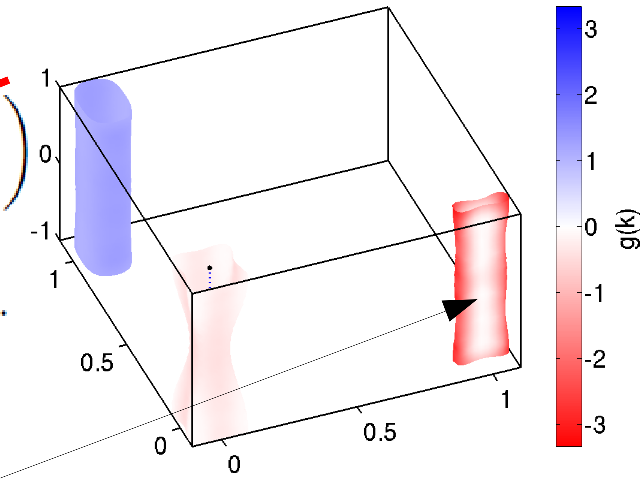
sign changing nodal gap structure

Further probes of the order parameter?

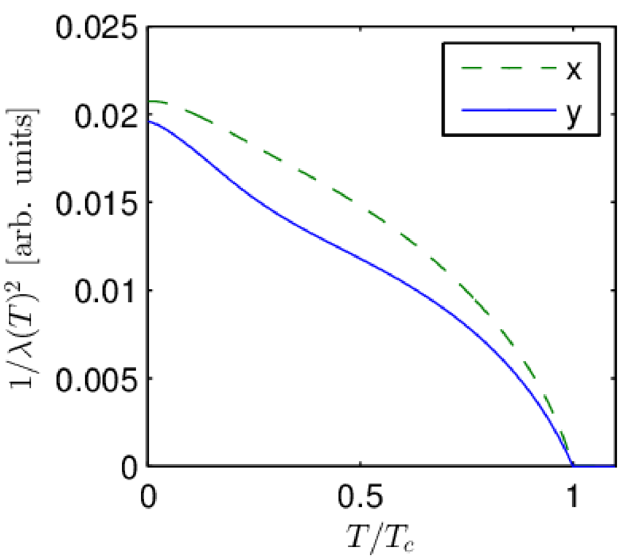
Magnetic field penetration depth

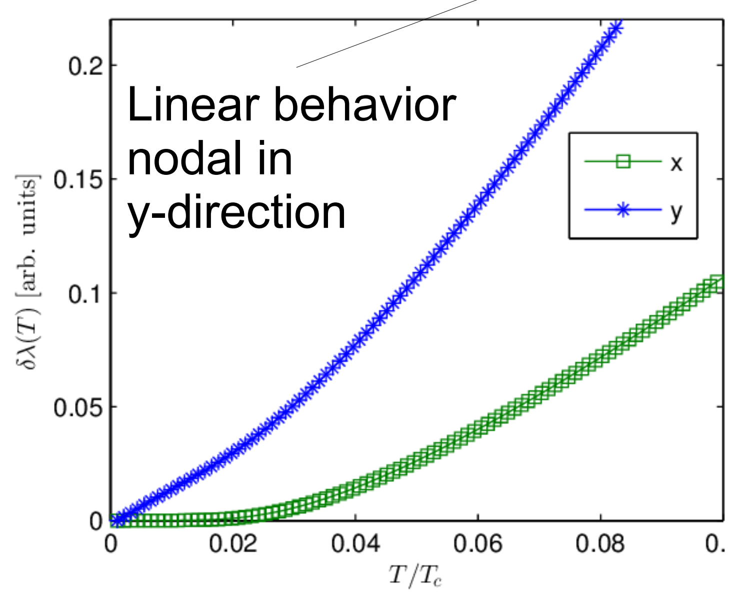
Fermi velocity (sensitive to nodes)

$$\frac{1}{\lambda_{\nu,i}^2} = \frac{4\pi e^2}{c^2\hbar^2}\sum_{\mathbf{k}} \frac{d\xi_\nu(\mathbf{k})}{dk_i}\left(\frac{d\xi_\nu(\mathbf{k})}{dk_i}|\Delta_\mathbf{k}|^2 - \cancel{\frac{d|\Delta_\mathbf{k}|}{dk_i}|\Delta_\mathbf{k}|\xi_\nu(\mathbf{k})}\right) \times \frac{1}{E_{\nu,\mathbf{k}}^2}\left(\frac{1}{E_{\nu,\mathbf{k}}}\tanh\left(\frac{E_{\nu,\mathbf{k}}}{2k_BT}\right) - \frac{1}{2k_BT}\mathrm{sech}\left(\frac{E_{\nu,\mathbf{k}}}{2k_BT}\right)^2\right).$$



superfluid density tensor

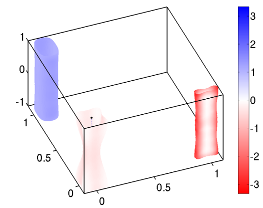


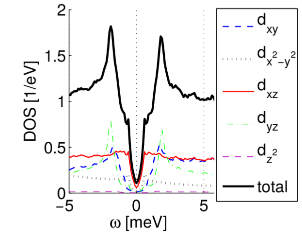


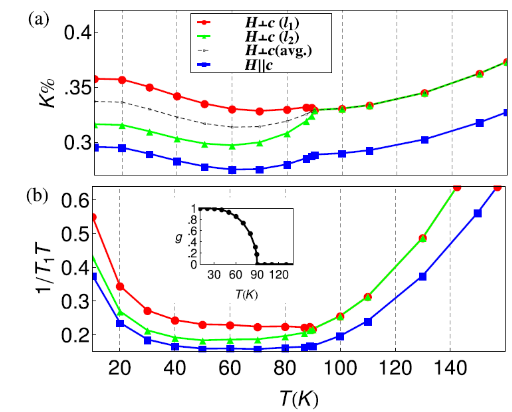
“full gap” in
x-direction ~T^3

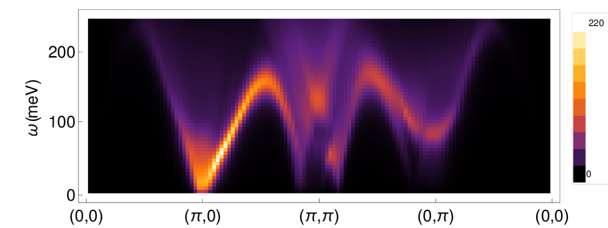
Summary

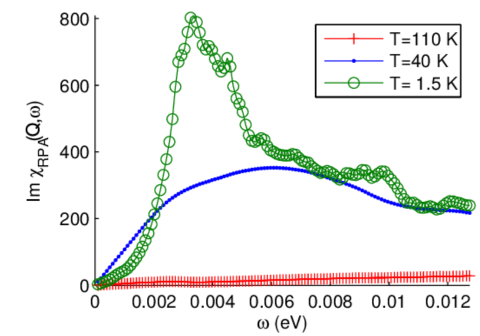
- model electronic structure for FeSe consistent with ARPES and quantum oscillations
- further experimental findings consistent with
  - spin-fluctuation driven superconductivity
  - absence of magnetic order, but nematic order (orbital order, origin not explained yet)
- Predictions:
  - linear T-dependence in magnetic penetration depth
  - impurity bound states: possible to model with given electronic structure







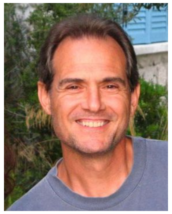




S. Mukherjee, AK, P. J. Hirschfeld, Brian M. Andersen, Phys. Rev. Lett. **115**, 026402 (2015)

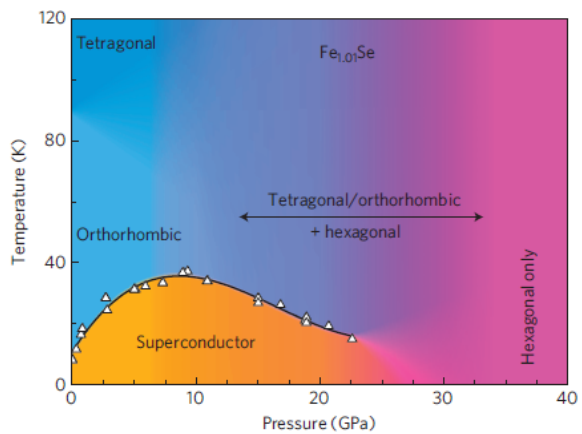
AK, S. Mukherjee, P. J. Hirschfeld, Brian M. Andersen Phys. Rev. B **92**, 224515 (2015)

Acknowledgements:

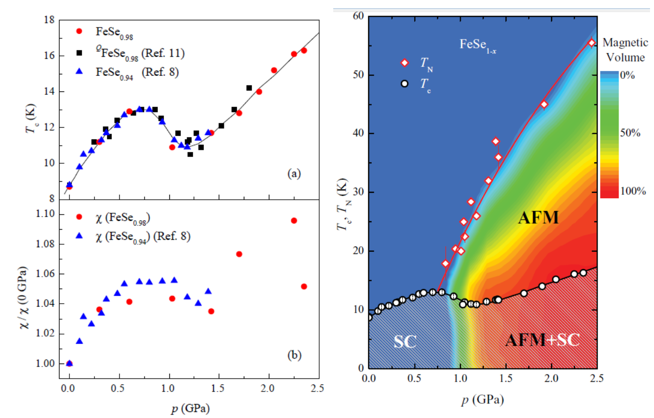


Spin fluctuations under pressure

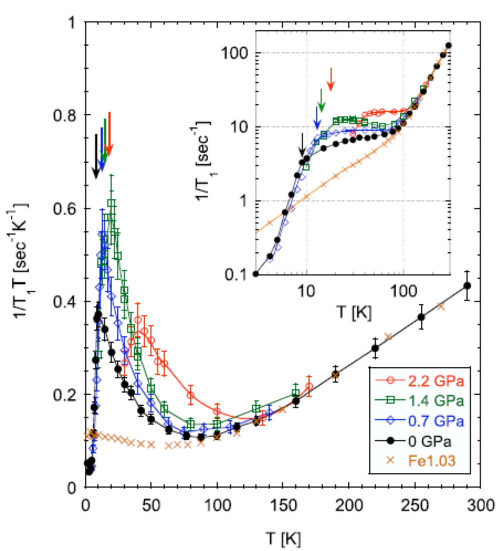
- Close to magnetic instability: pressure experiments



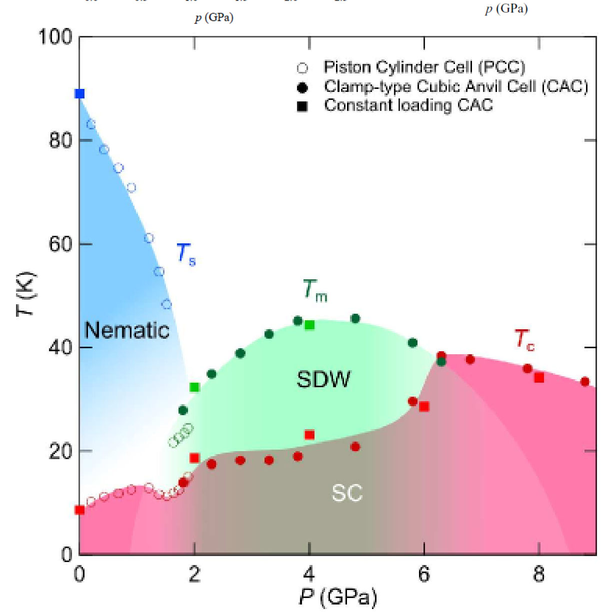
Medvedev et al. (2010)



Bendele *et al.* 2012: magnetic state at low pressure

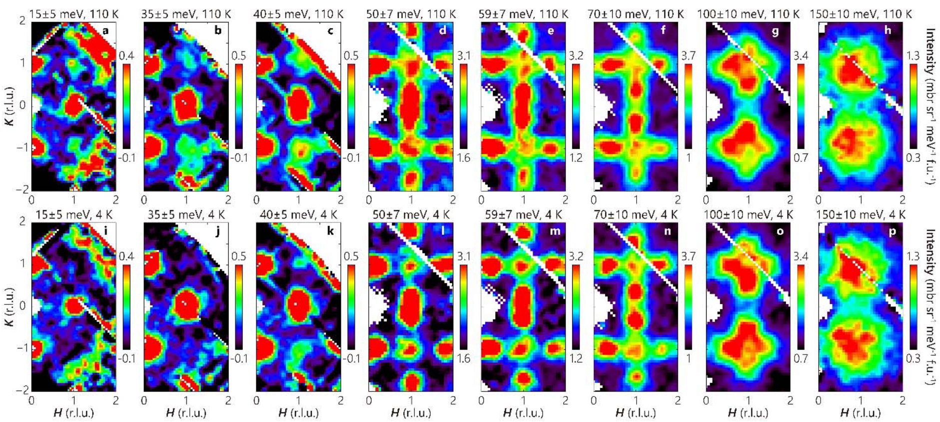


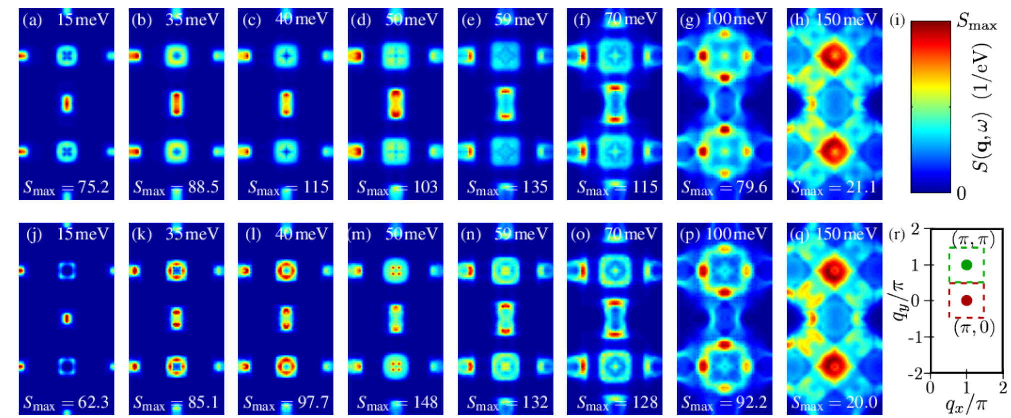
enhanced spin fluctuations Imai, Cava PRL (2009)

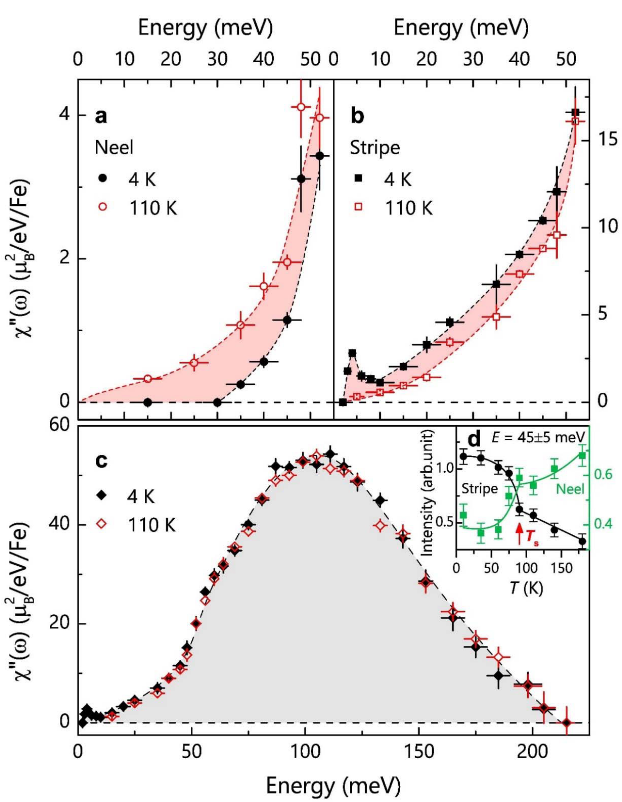


J.P. Sun, et al., arXiv:1512.06951 (2016)

INS: stripe orbital order







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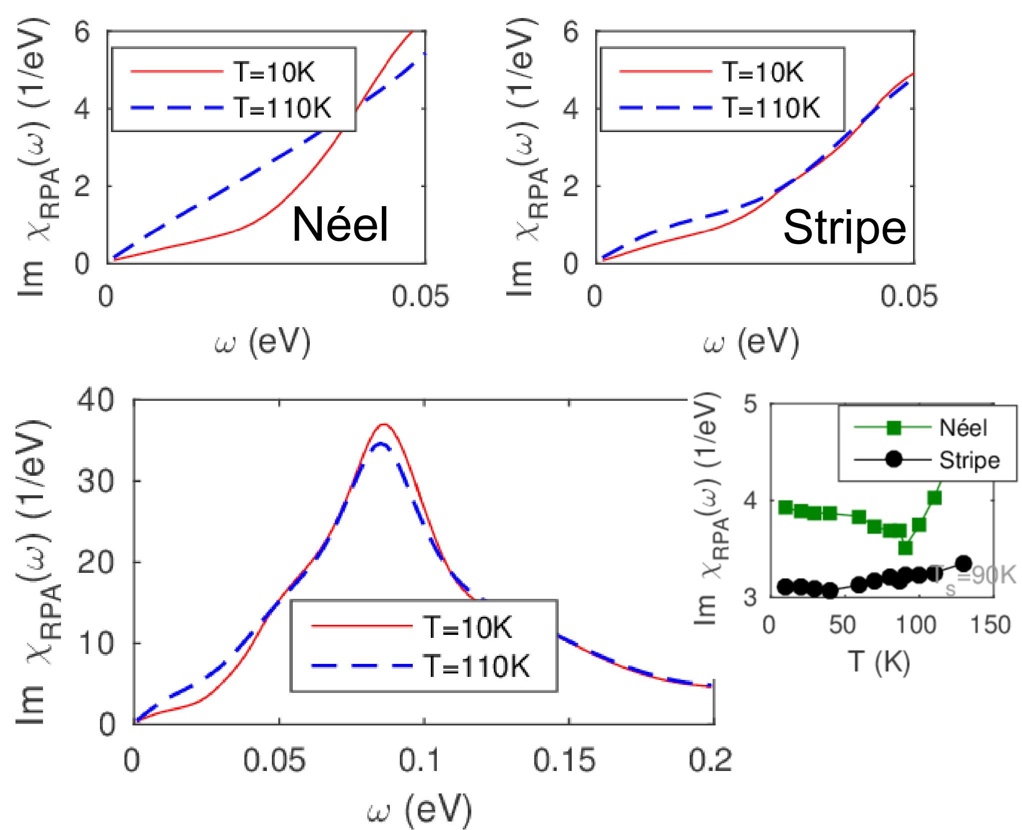

Superconducting order parameter: stripe OO

- spin-fluctuation driven superconductivity

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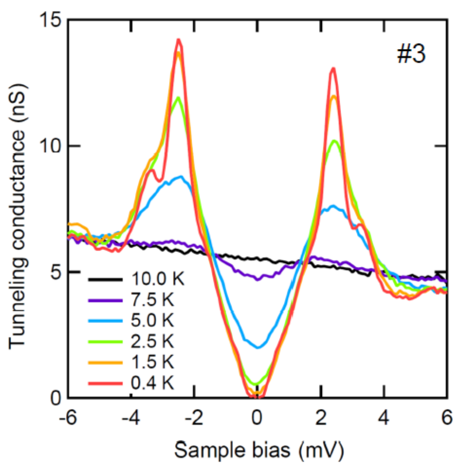
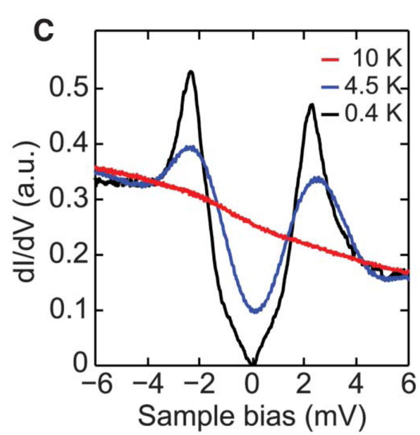
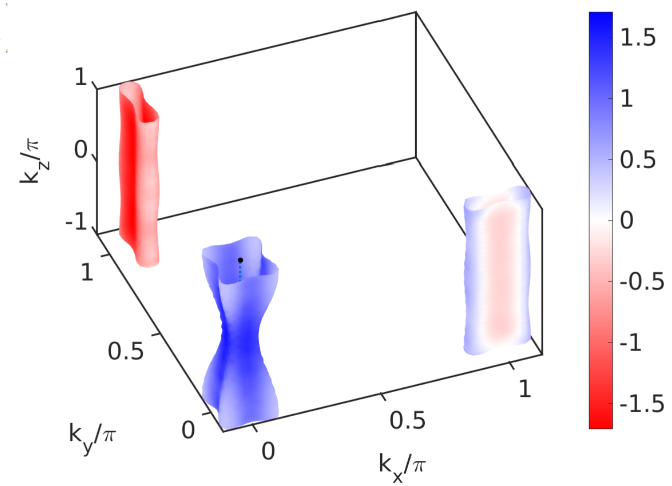


STM on FeSe:
Kasahara *et al*. (2014)



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



sign changing nodal gap structure