Spin-Orbit Coupling and Gapped Magnetic Excitations in Iron-Based Superconductors

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"Correlated Electron Systems – Novel Developments"

Acknowledgements

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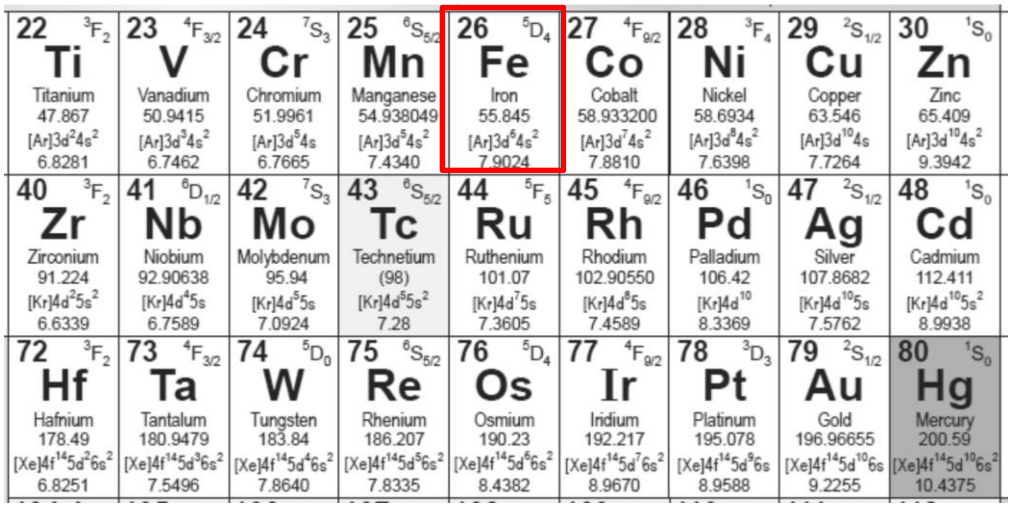
Outline

- **Introduction**
  - Why SOC, and how neutron scattering sees it
  - Gapped spin excitations
  - Previous results on $BaFe_{2-x}Co_xAs_2$
- **Results**
  1) $Sr_{1-x}Na_xFe_2As_2$
  2) $FeSe_{1-x}S_x$
- **Summary**

Why spin-orbit coupling (SOC)?

Fe is a only 3d metal…



22 $^3F_2$ Ti Titanium 47.867 [Ar]$3d^24s^2$ 6.8281	23 $^4F_{3/2}$ V Vanadium 50.9415 [Ar]$3d^34s^2$ 6.7462	24 $^7S_3$ Cr Chromium 51.9961 [Ar]$3d^54s$ 6.7665	25 $^6S_{5/2}$ Mn Manganese 54.938049 [Ar]$3d^54s^2$ 7.4340	26 $^5D_4$ Fe Iron 55.845 [Ar]$3d^64s^2$ 7.9024	27 $^4F_{9/2}$ Co Cobalt 58.933200 [Ar]$3d^74s^2$ 7.8810	28 $^3F_4$ Ni Nickel 58.6934 [Ar]$3d^84s^2$ 7.6398	29 $^2S_{1/2}$ Cu Copper 63.546 [Ar]$3d^{10}4s$ 7.7264	30 $^1S_0$ Zn Zinc 65.409 [Ar]$3d^{10}4s^2$ 9.3942
40 $^3F_2$ Zr Zirconium 91.224 [Kr]$4d^25s^2$ 6.6339	41 $^6D_{1/2}$ Nb Niobium 92.90638 [Kr]$4d^45s$ 6.7589	42 $^7S_3$ Mo Molybdenum 95.94 [Kr]$4d^55s$ 7.0924	43 $^6S_{5/2}$ Tc Technetium (98) [Kr]$4d^55s^2$ 7.28	44 $^5F_5$ Ru Ruthenium 101.07 [Kr]$4d^75s$ 7.3605	45 $^4F_{9/2}$ Rh Rhodium 102.90550 [Kr]$4d^85s$ 7.4589	46 $^1S_0$ Pd Palladium 106.42 [Kr]$4d^{10}$ 8.3369	47 $^2S_{1/2}$ Ag Silver 107.8682 [Kr]$4d^{10}5s$ 7.5762	48 $^1S_0$ Cd Cadmium 112.411 [Kr]$4d^{10}5s^2$ 8.9938
72 $^3F_2$ Hf Hafnium 178.49 [Xe]$4f^{14}5d^26s^2$ 6.8251	73 $^4F_{3/2}$ Ta Tantalum 180.9479 [Xe]$4f^{14}5d^36s^2$ 7.5496	74 $^5D_0$ W Tungsten 183.84 [Xe]$4f^{14}5d^46s^2$ 7.8640	75 $^6S_{5/2}$ Re Rhenium 186.207 [Xe]$4f^{14}5d^56s^2$ 7.8335	76 $^5D_4$ Os Osmium 190.23 [Xe]$4f^{14}5d^66s^2$ 8.4382	77 $^4F_{9/2}$ Ir Iridium 192.217 [Xe]$4f^{14}5d^76s^2$ 8.9670	78 $^3D_3$ Pt Platinum 195.078 [Xe]$4f^{14}5d^96s$ 8.9588	79 $^2S_{1/2}$ Au Gold 196.96655 [Xe]$4f^{14}5d^{10}6s$ 9.2255	80 $^1S_0$ Hg Mercury 200.59 [Xe]$4f^{14}5d^{10}6s^2$ 10.4375

$\lambda \sim 0.01$ eV

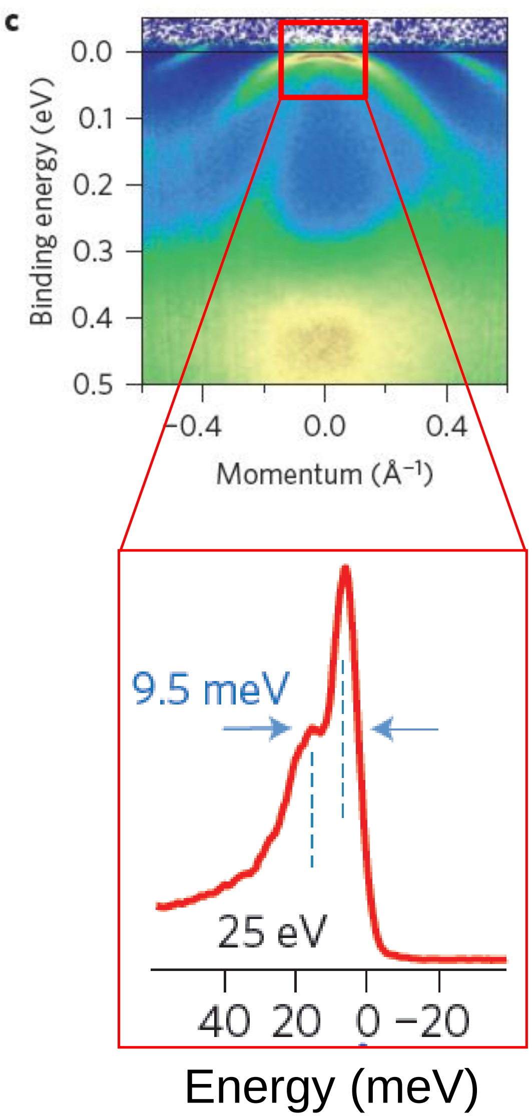
$\lambda \sim 0.1$ eV

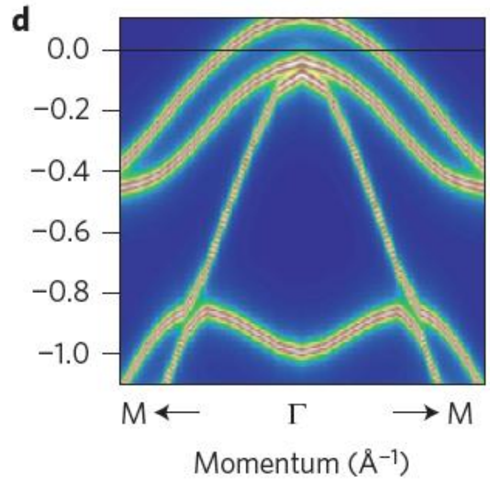
$\lambda \sim 1$ eV

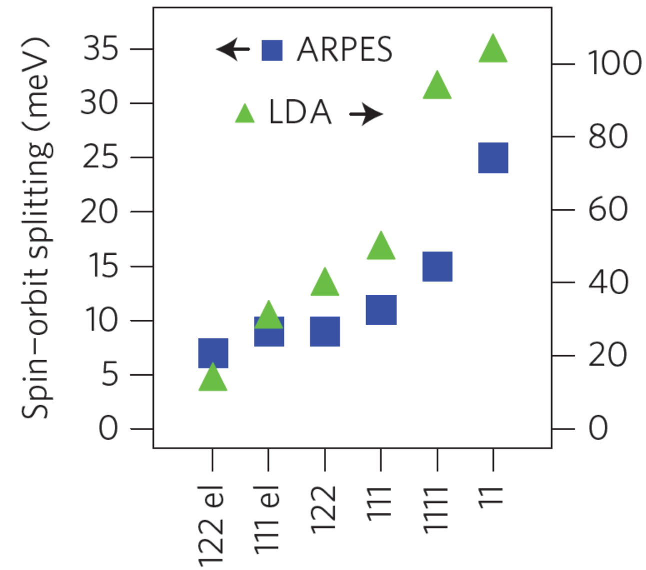
… on the other hand,

- multi-orbital
- orbital angular momentum not fully quenched
- **SOC comparable to other energies**

SOC revealed by ARPES







Borisenko *et al.*, *Nat. Phys.* (2016)

See also:
Watson *et al.*, *PRB* (2015)
Johnson *et al.*, *PRL* (2015)

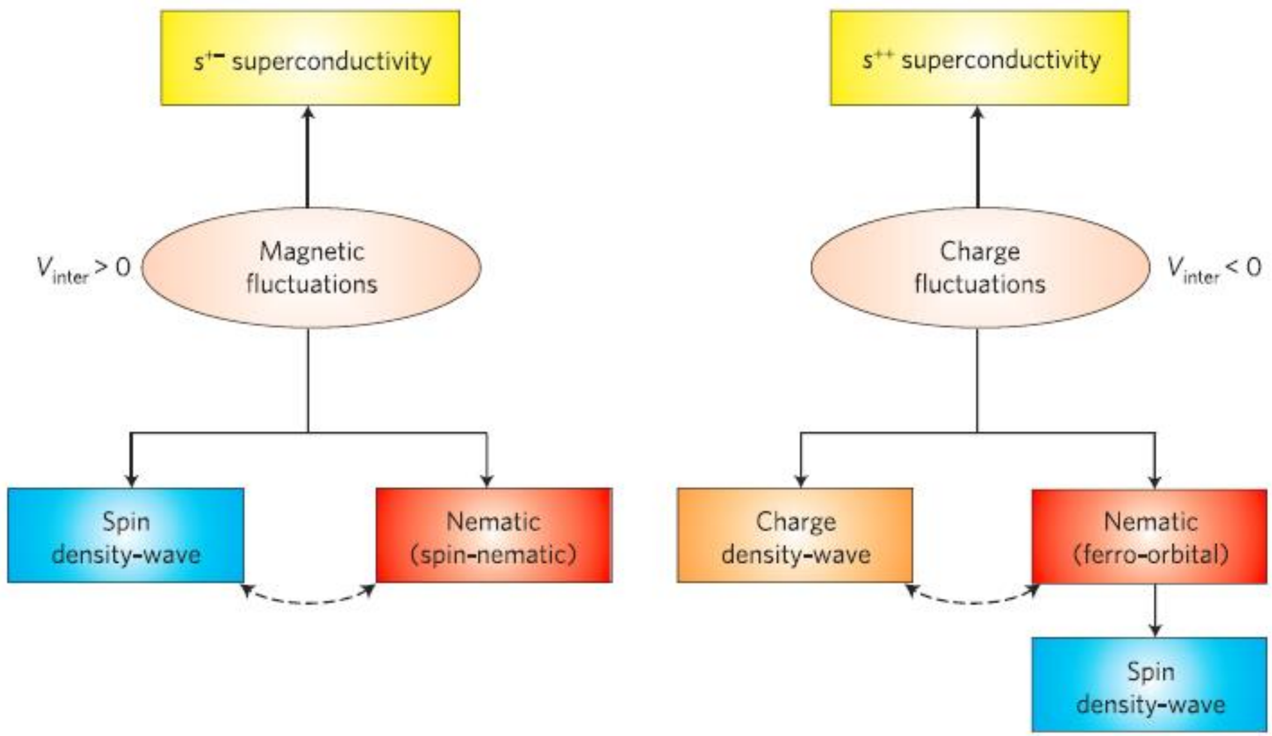
Zone-center splitting of *xz*/*yz* bands

Nematic order: spin or orbital?

nature physics
REVIEW ARTICLE
PUBLISHED ONLINE: 31 JANUARY 2014 | DOI: 10.1038/NPHYS2877

What drives nematic order in iron-based superconductors?

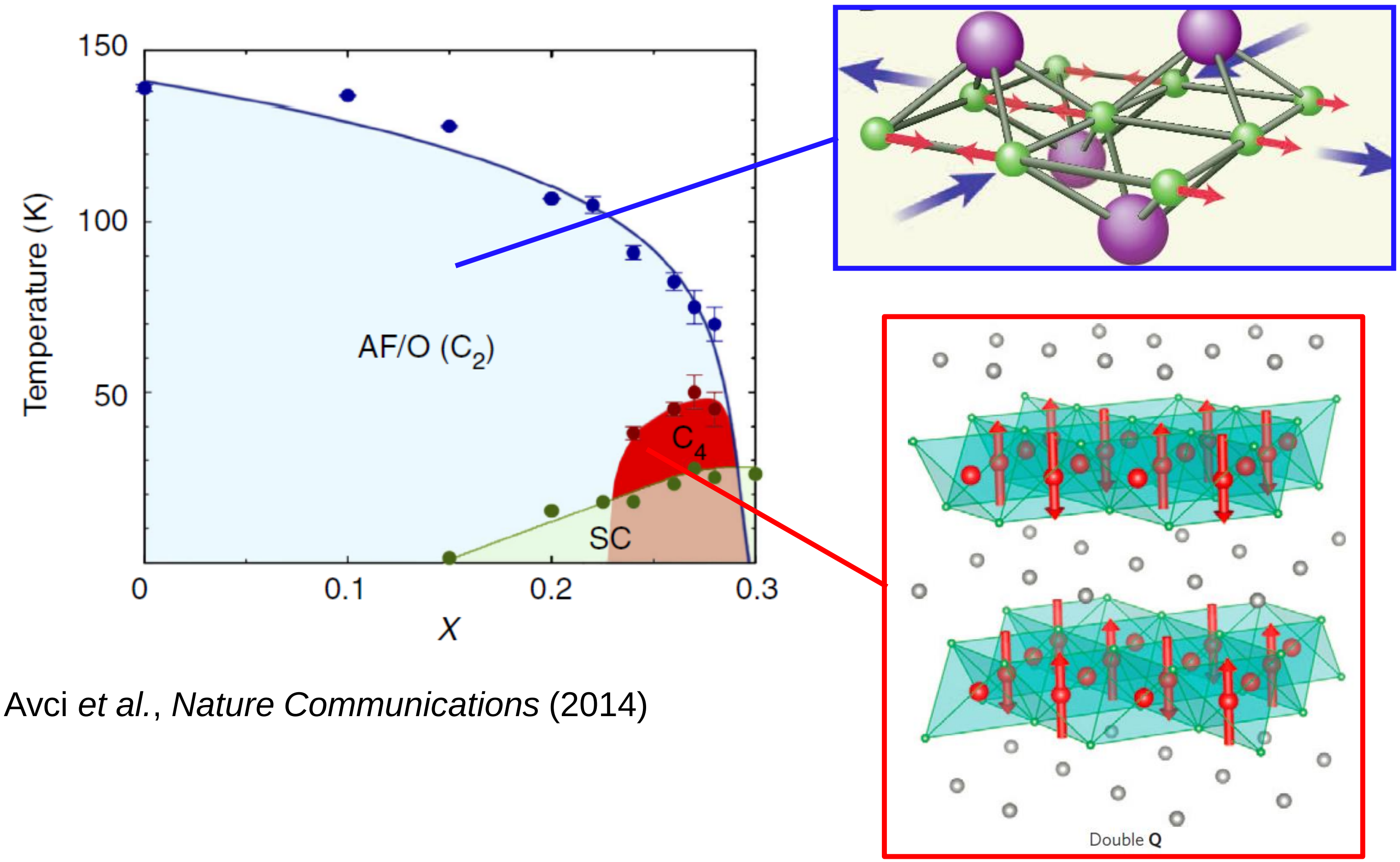
R. M. Fernandes[1*], A. V. Chubukov[2*] and J. Schmalian[3*]



Strong evidence for spin-nematicity

The C_4 magnetic phase in hole-doped pnictide

Spin reorientation: clear manifestation of SOC



Wang & Lee, Science (2011)

Avci *et al.*, *Nature Communications* (2014)

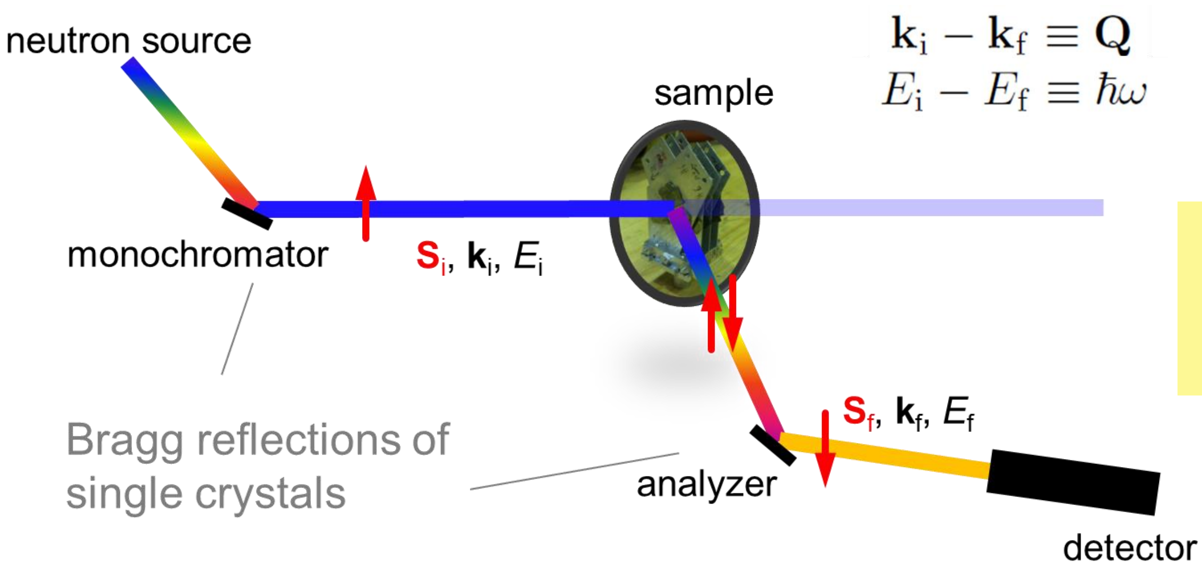
Allred *et al.*, *Nature Physics* (2016)

Neutron scattering sees SOC as anisotropy

Without SOC, the spin space is isolated and should retain its full rotational symmetry

➔ Pros: reveals SOC's influence on magnetism

➔ Cons: spin-polarized experiments are hard to do



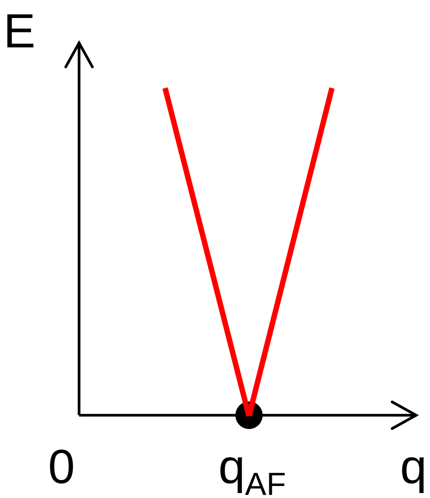
"Spin-flip scattering detects moments perpendicular to both **Q** and $\mathbf{S}_i$"

"Q + S_i" enables selective detection of spin orientations

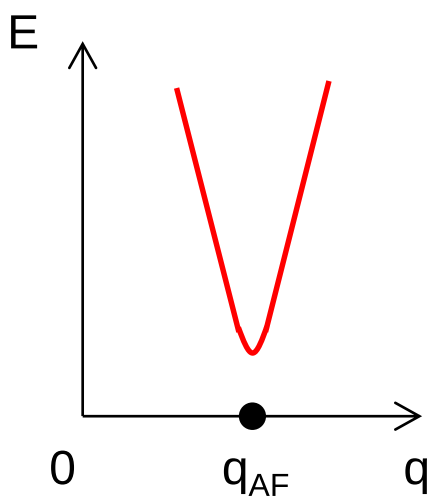
Gapped spin excitations

Three ways to have gapped spin excitations

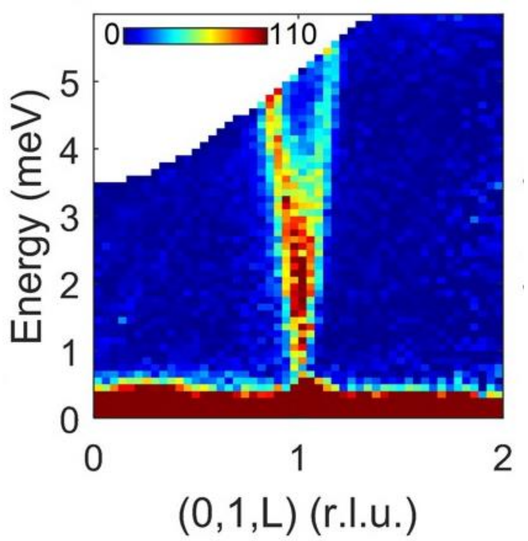
1. Magnetic order with no continuous symmetry to break (usually due to SOC)



Heisenberg antiferromagnet with Néel order



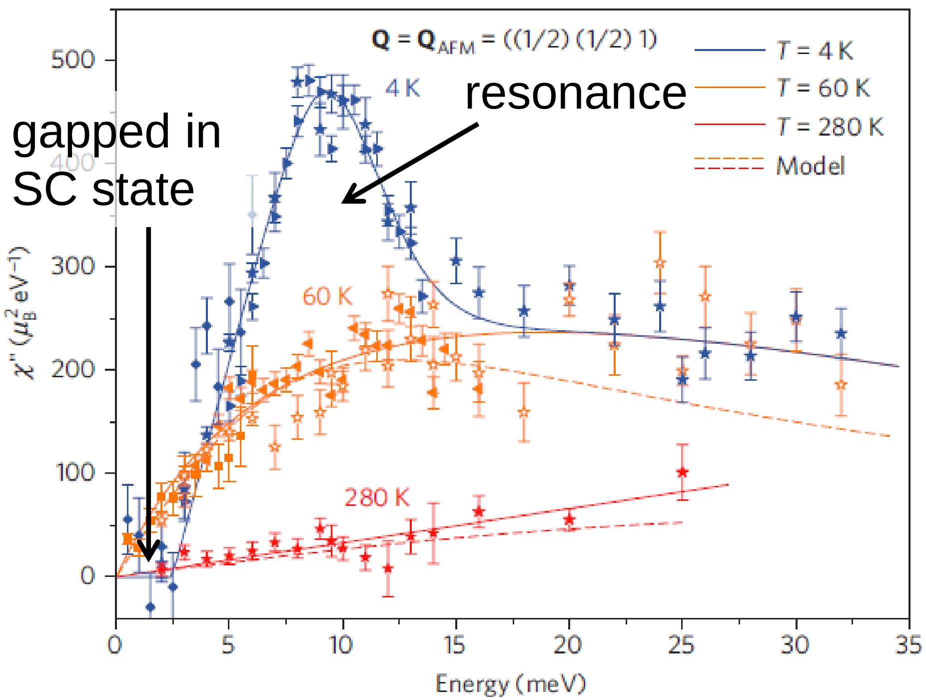
Without spin-rotation symmetry

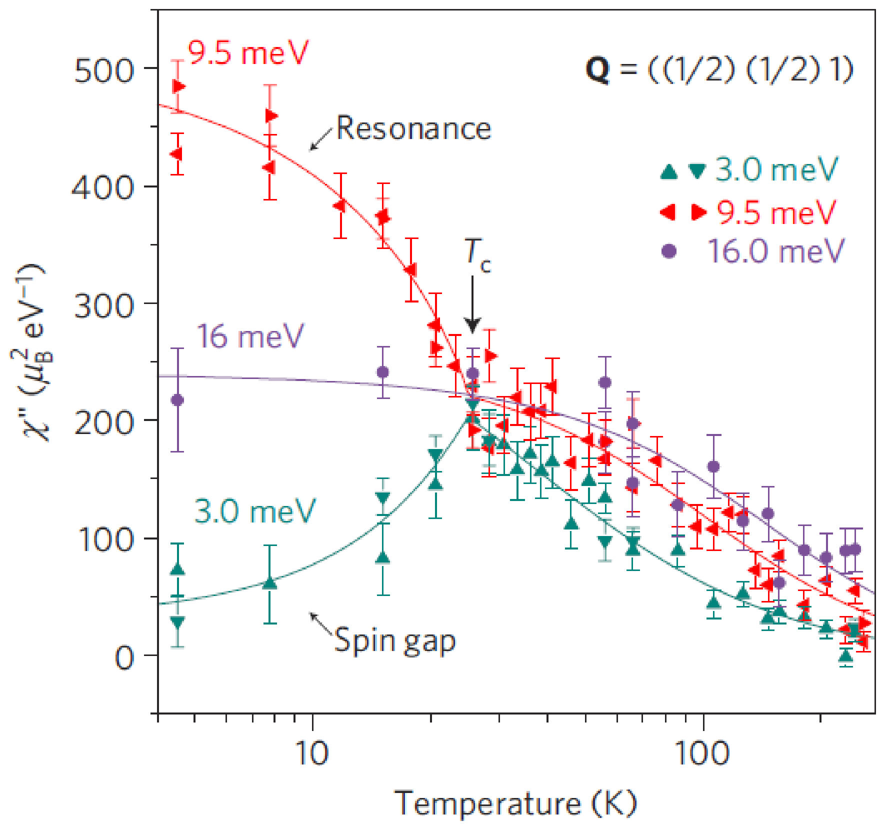


Spin waves in Cu_3TeO_6 (DM interactions in this case) arXiv:1711.00632

Three ways to have gapped spin excitations

2. Response from itinerant electrons, plus a gap at the Fermi level (*e.g.*, a superconductor)





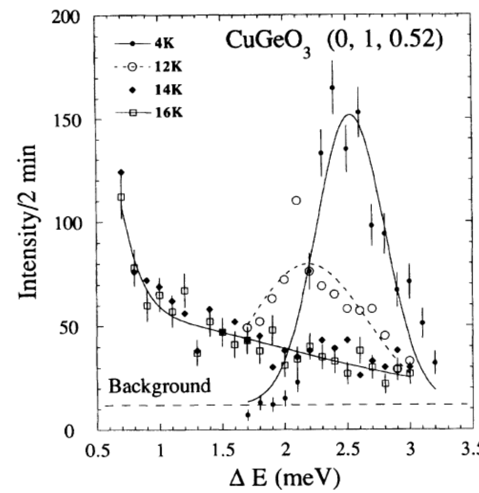
Inosov *et al.*, *Nat. Phys.* 6, 178 (2010)

Three ways to have gapped spin excitations

3. Valence-bond dimers

Majumdar & Ghosh (1969)

$$H = J \sum_i (\mathbf{S}_i + \mathbf{S}_{i+1} + \mathbf{S}_{i+2})^2$$

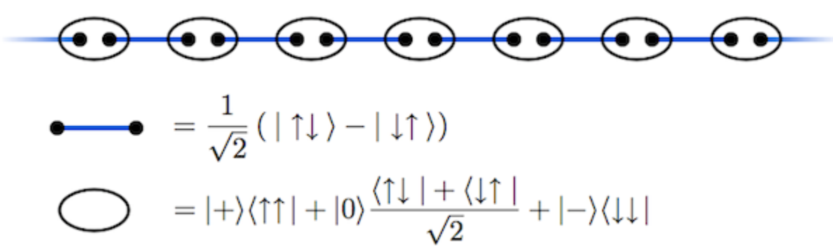


Spin-Peierls state

Nishi et al. (1994)

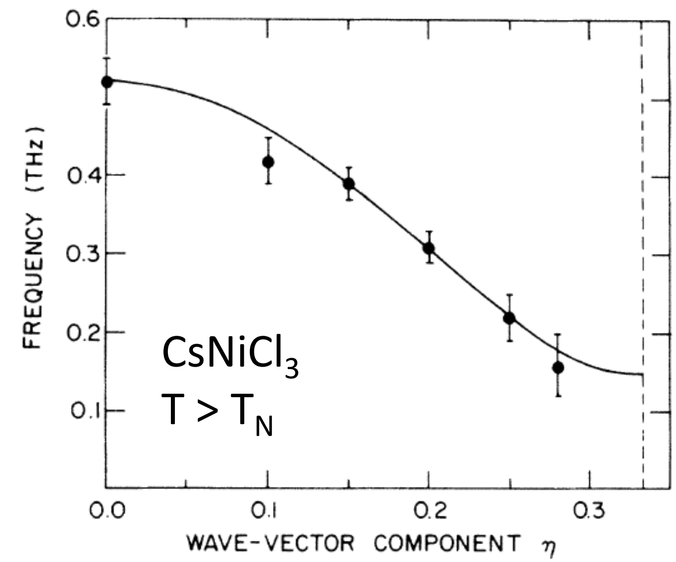
or, AKLT states (and QSLs)

$$H^{AKLT}_{[a,b]} = \sum_{x=a}^{b-1} [\frac{1}{3} + \frac{1}{2}\mathbf{S}_x \cdot \mathbf{S}_{x+1} + \frac{1}{6}(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2]$$



Haldane (1981)

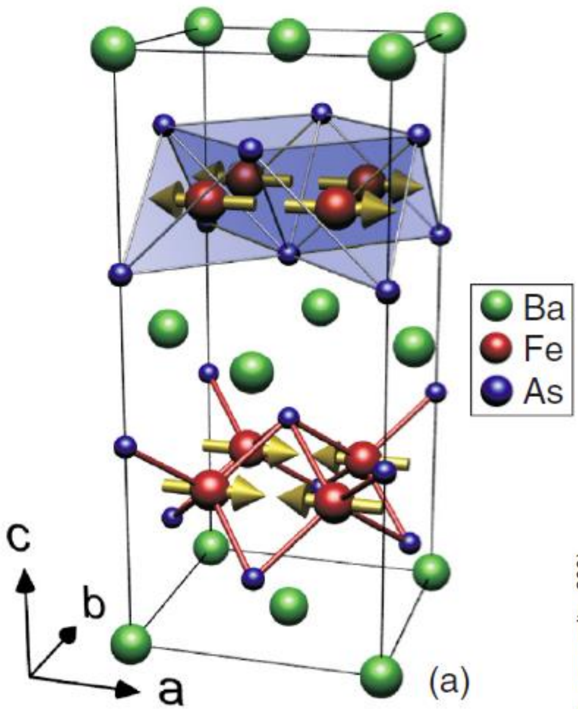
Affleck, Kennedy, Lieb & Tasaki (1987)

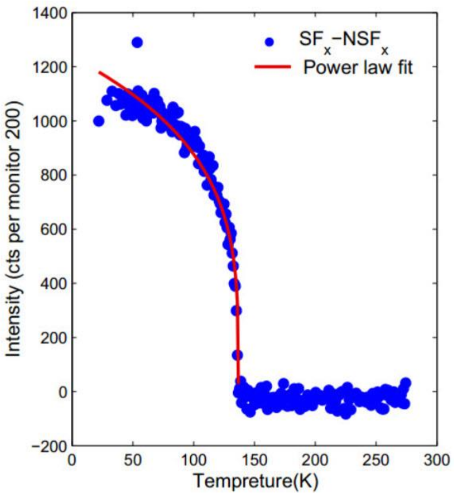


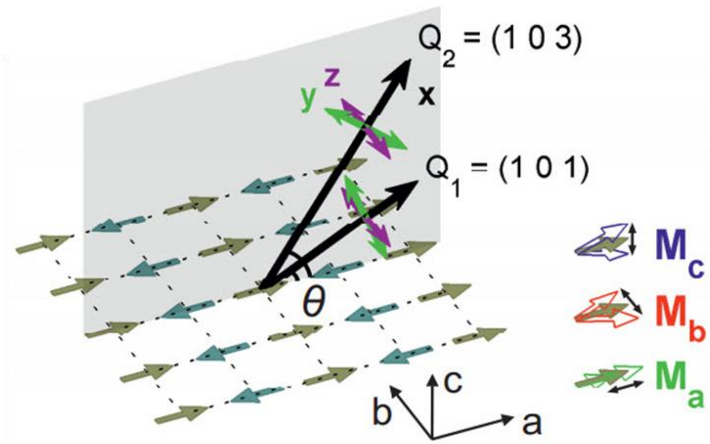
Buyer et al. (1986)

Previous results in $BaFe_{2-x}Co_xAs_2$

$BaFe_2As_2$

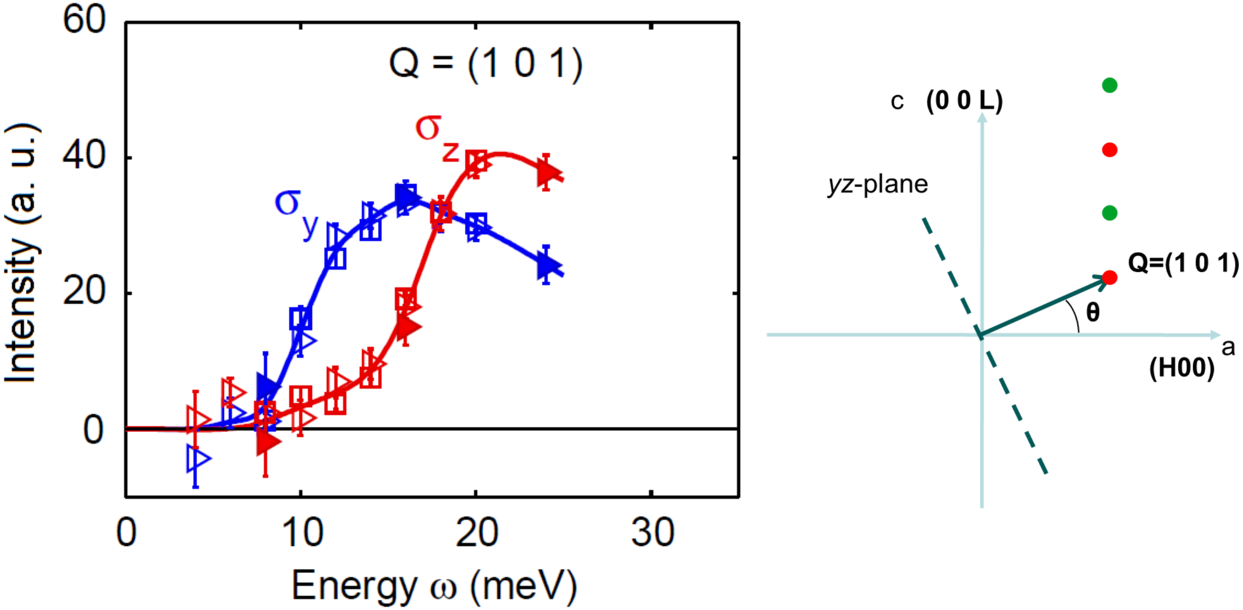






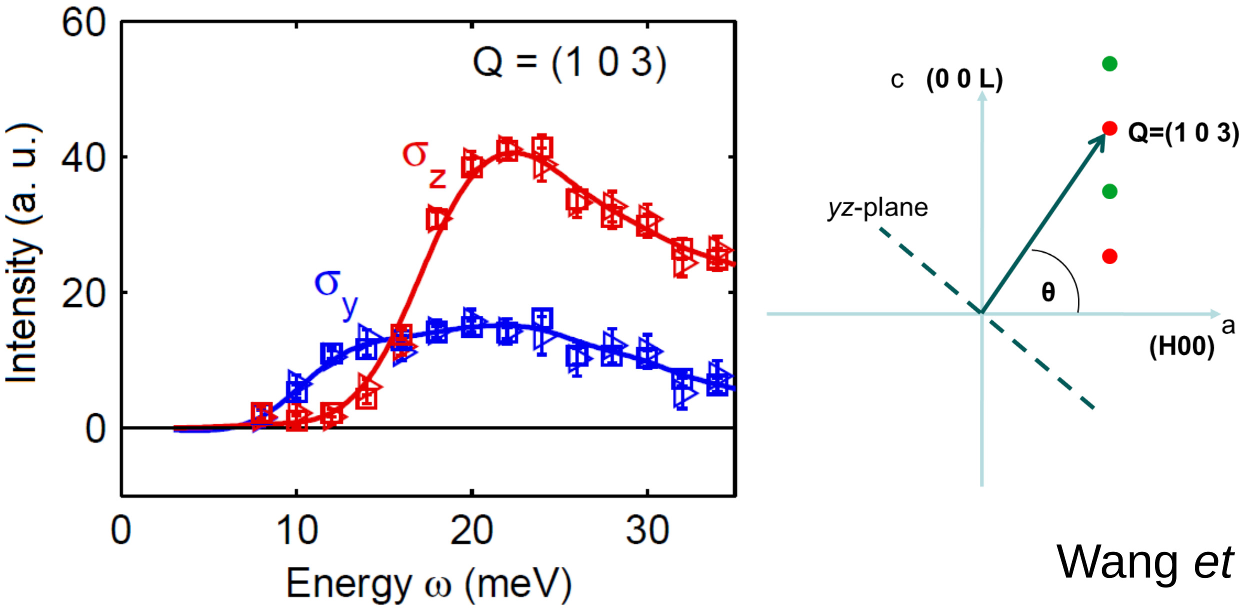
Work in collaboration with Pengcheng Dai’s group

Selective probe of different spin components



$$\sigma_y = 0.63M_a + 0.37M_c$$

$$\sigma_z = M_b$$



$$\sigma_y = 0.16M_a + 0.84M_c$$

$$\sigma_z = M_b$$

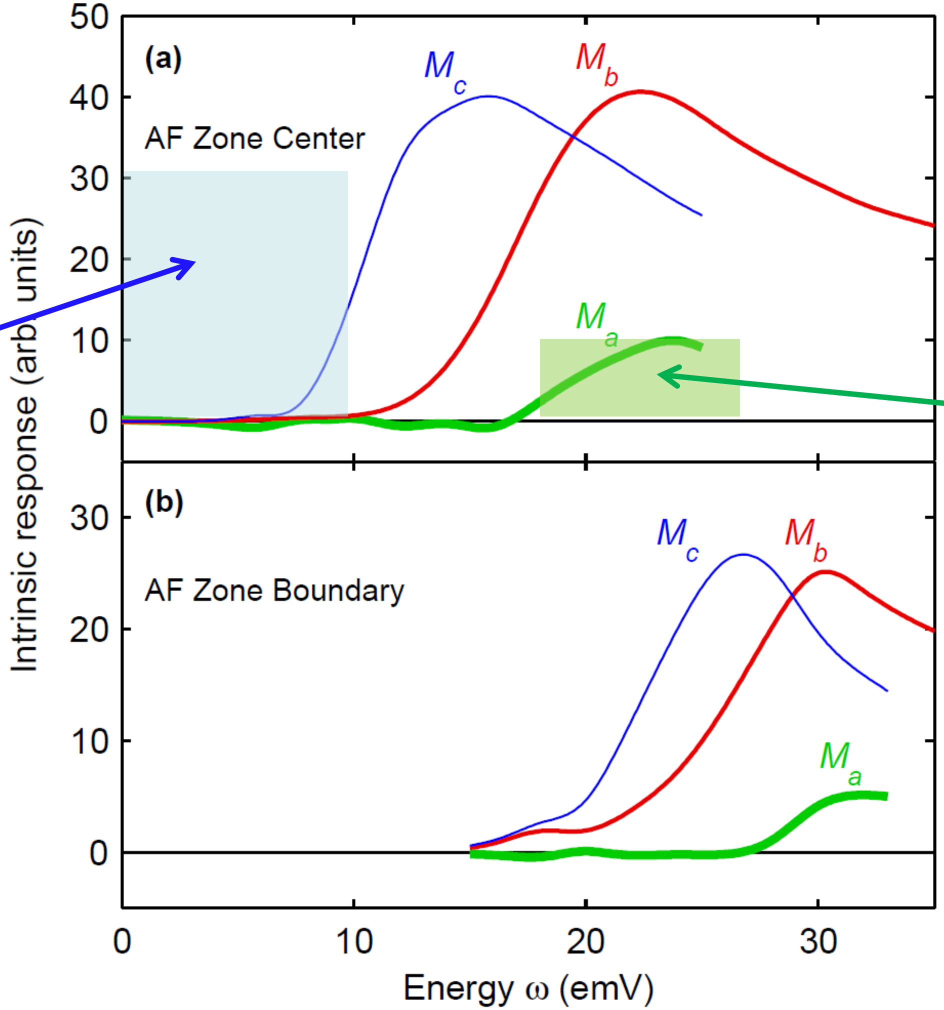
Wang *et al.*, *PRX* **3**, 041036 (2013)

Anisotropy gaps and longitudinal excitations

T = 4 K

Anisotropy gap

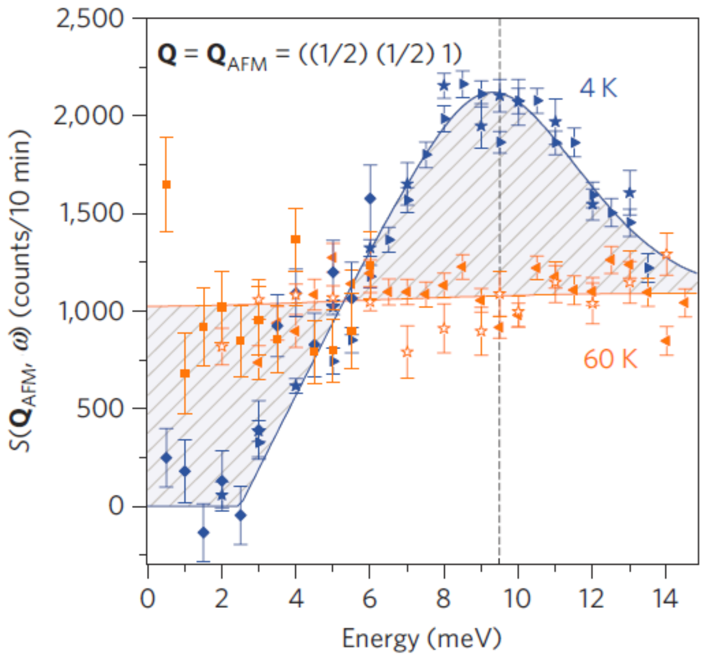
Confirming an earlier study by Qureshi *et al.* *PRB* ***86****, 060410(R) (2012)*

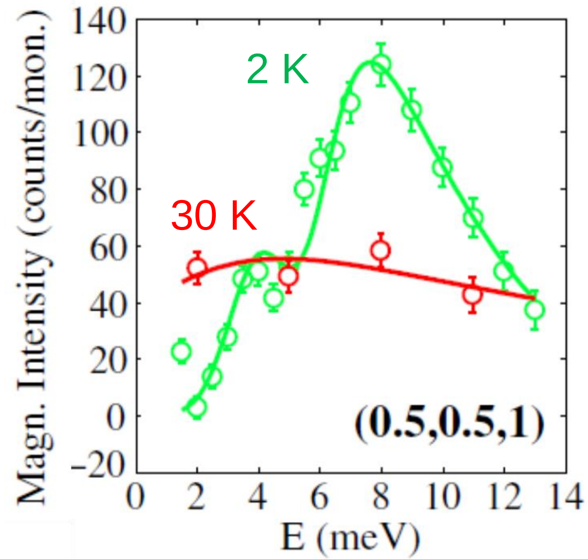


longitudinal excitations (attributed to itinerant magnetism back then)

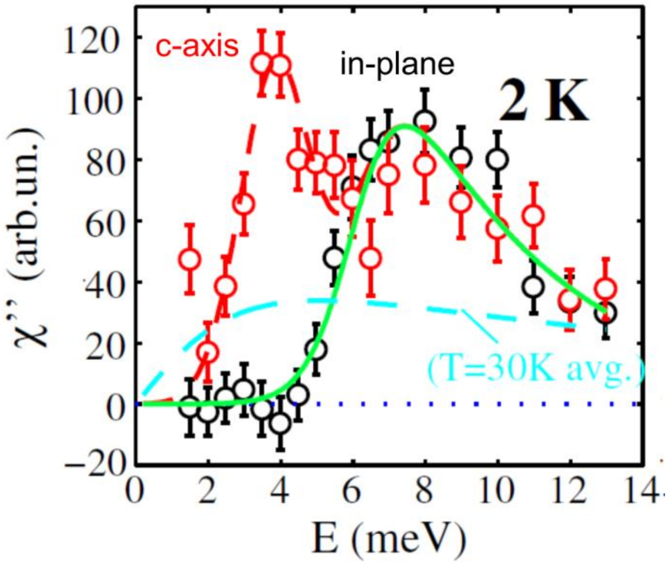
Wang *et al.*, *PRX* **3**, 041036 (2013)

Nearly optimally-doped $BaFe_{2-x}Co_xAs_2$





Unpolarized measurement, x = 0.15
Inosov *et al.*, *Nat. Phys.* 6, 178 (2010)



Spin-polarized measurement, x = 0.12
Distinct resonance in M_c
Steffens *et al.*, *PRL* 110, 137001 (2013)

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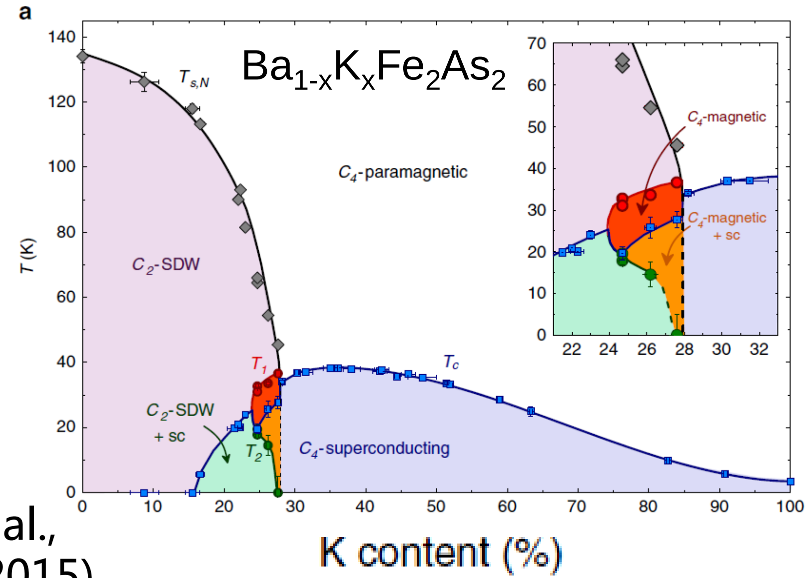
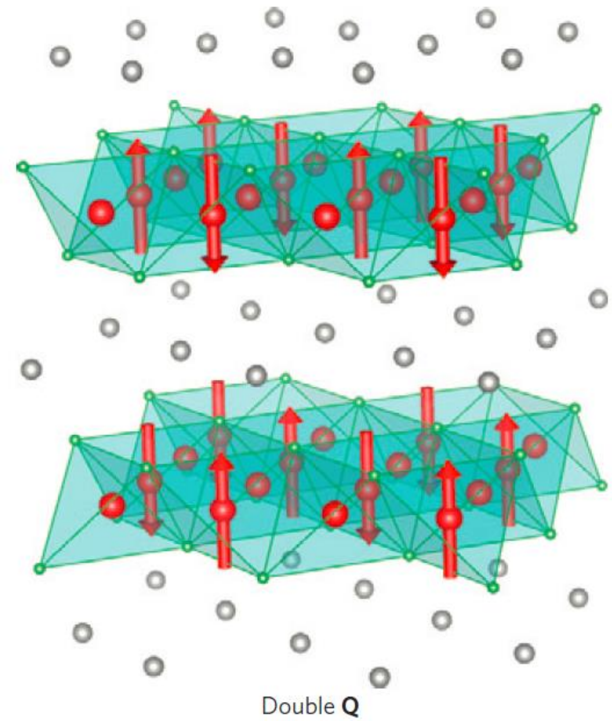
- ❑ **Summary**

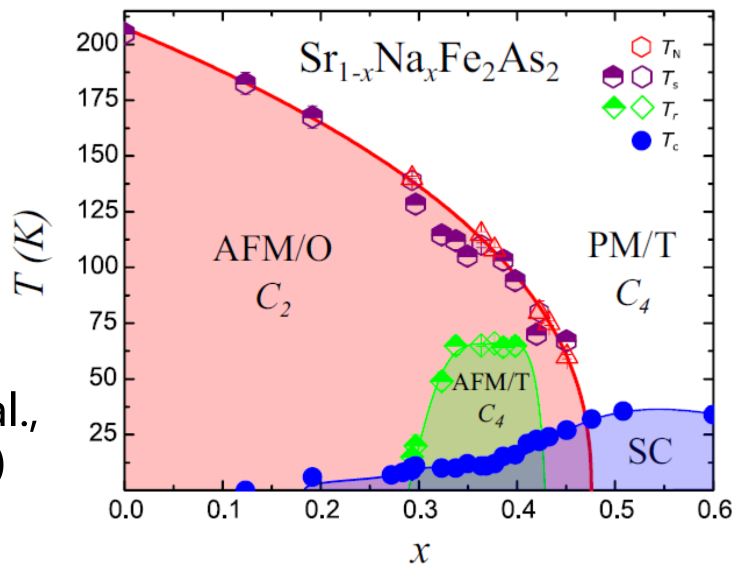
Reentrant C_4 magnetic phase



Boehmer et al., Nat. Phys. (2015)



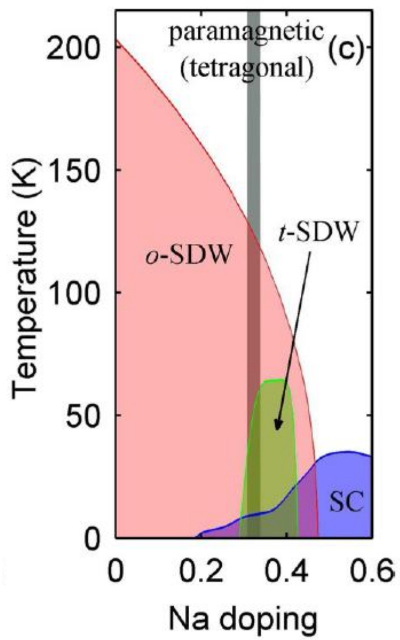
Allred et al., Nat. Phys. (2016)

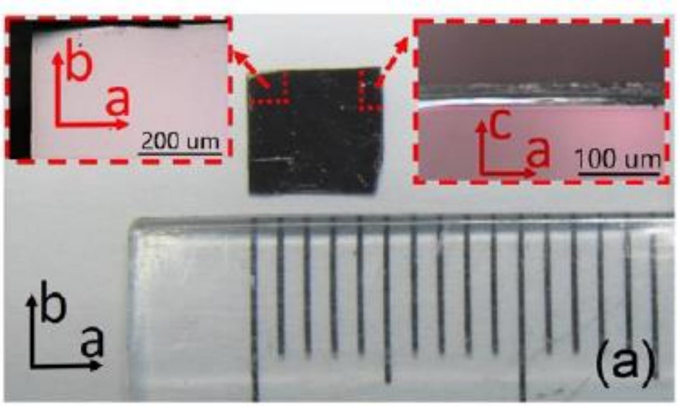


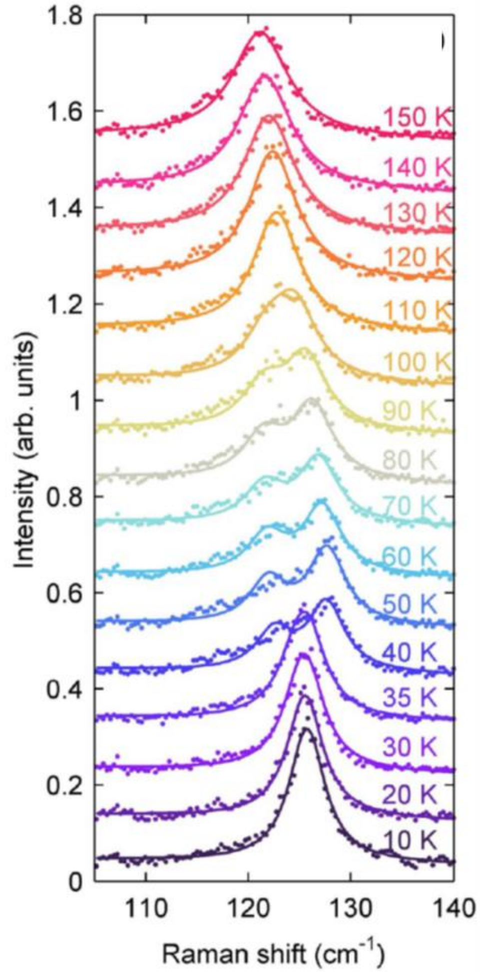
Taddei et al., PRB (2016)

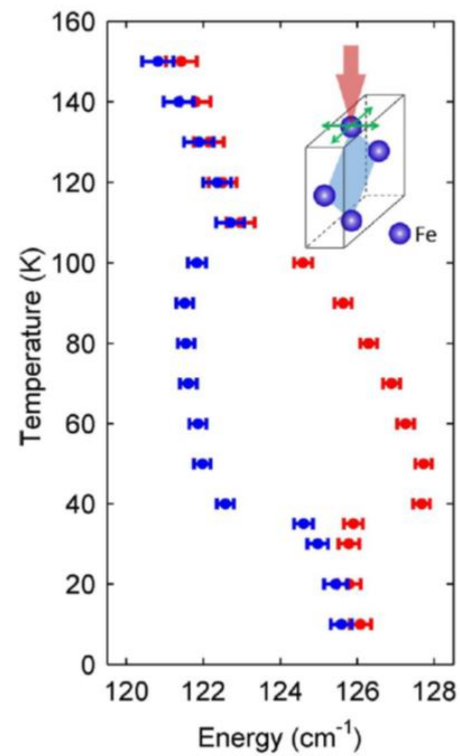
- Spin reorientation to the *c* axis
- Strong competition with SC

Raman spectroscopy: reentrant phase behavior



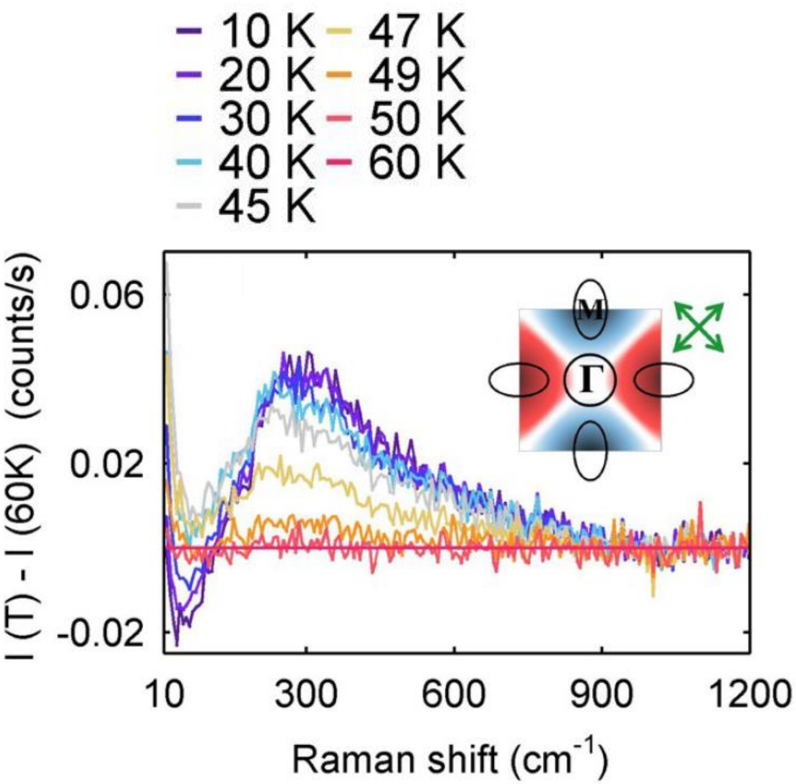


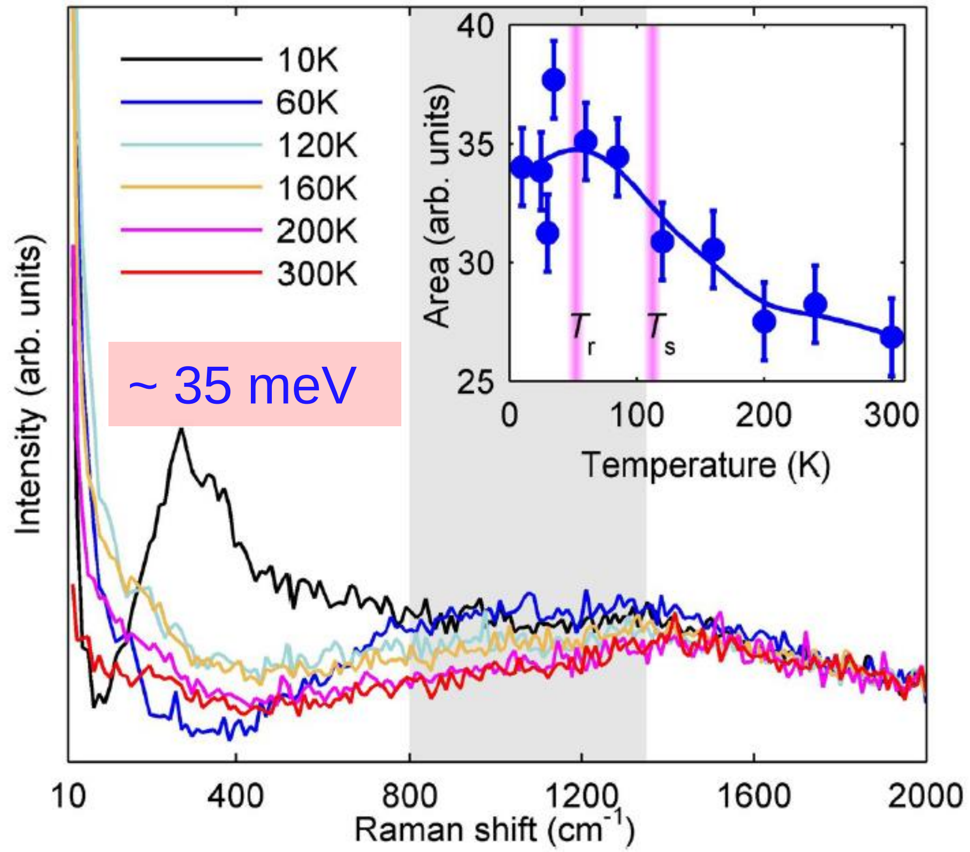




Yue *et al.*, *PRB* **96**, 180505(R) (2017)

Electronic Raman signals

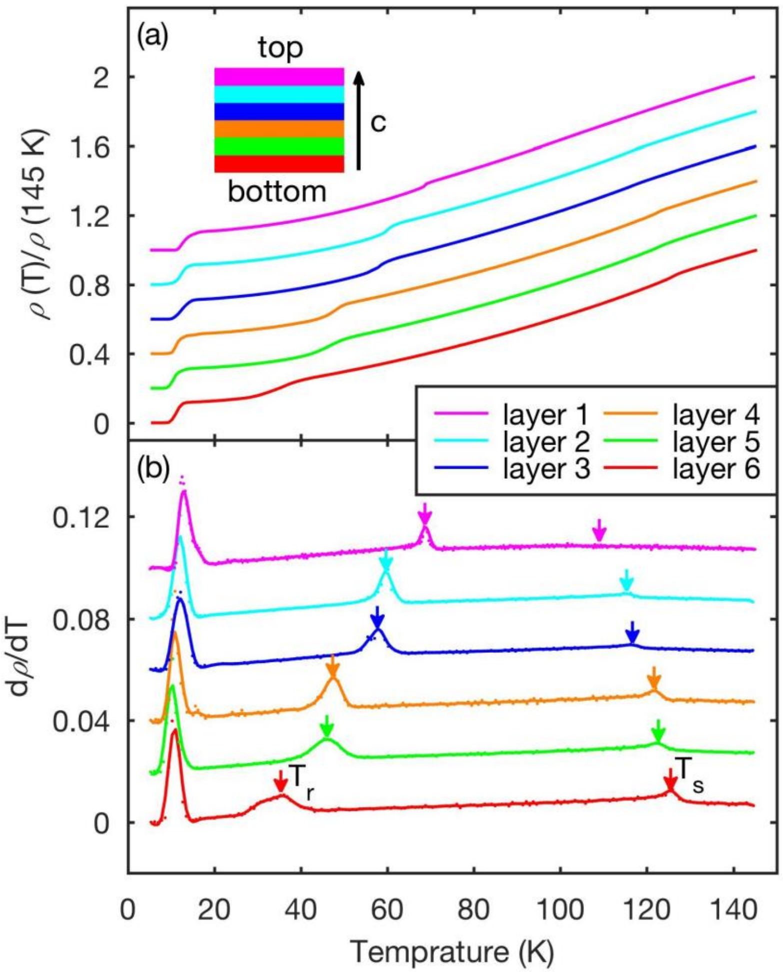


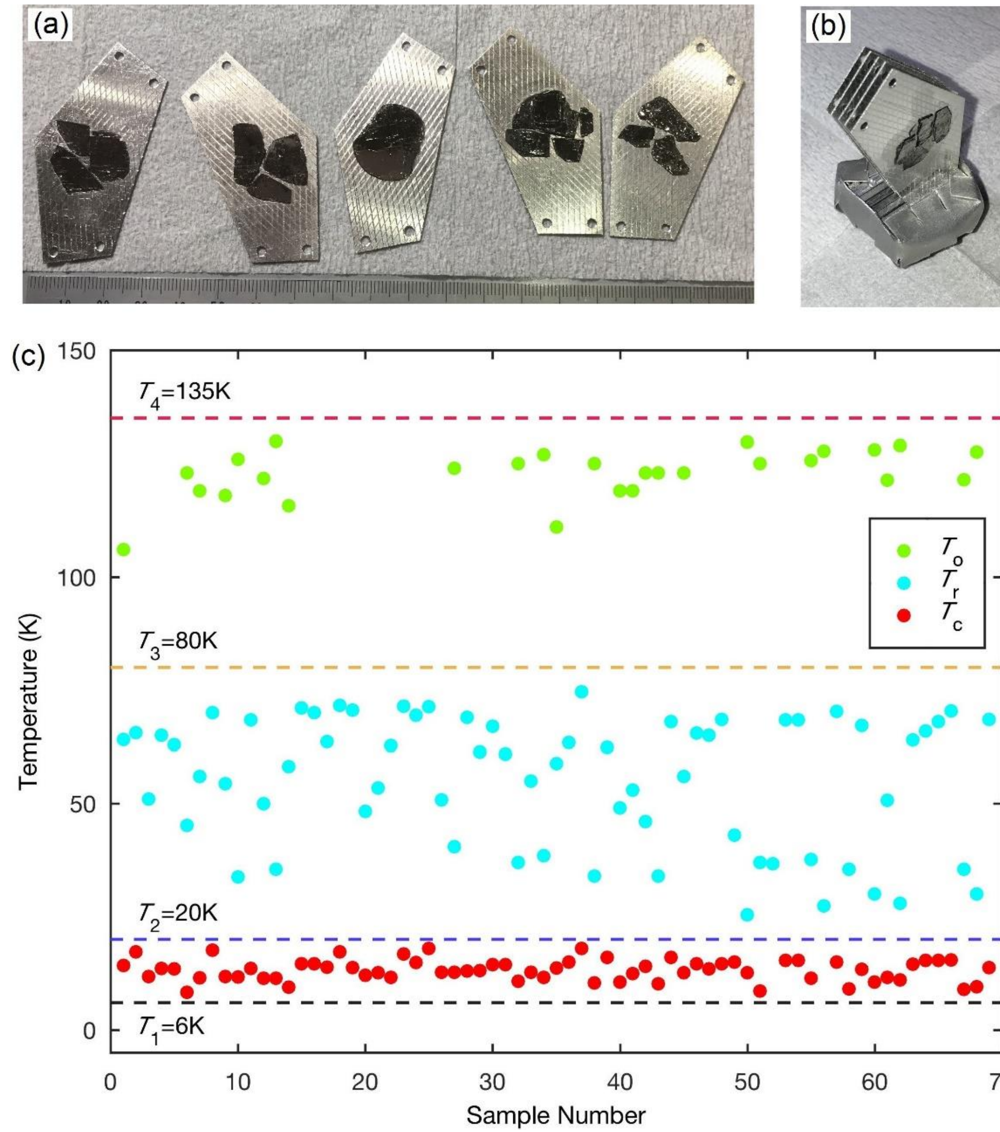


The C_2-C_4 phase transition involves a new and relatively small electronic energy scale ~35 meV: possibly related to SOC

Yue *et al.*, *PRB* **96**, 180505(R) (2017)

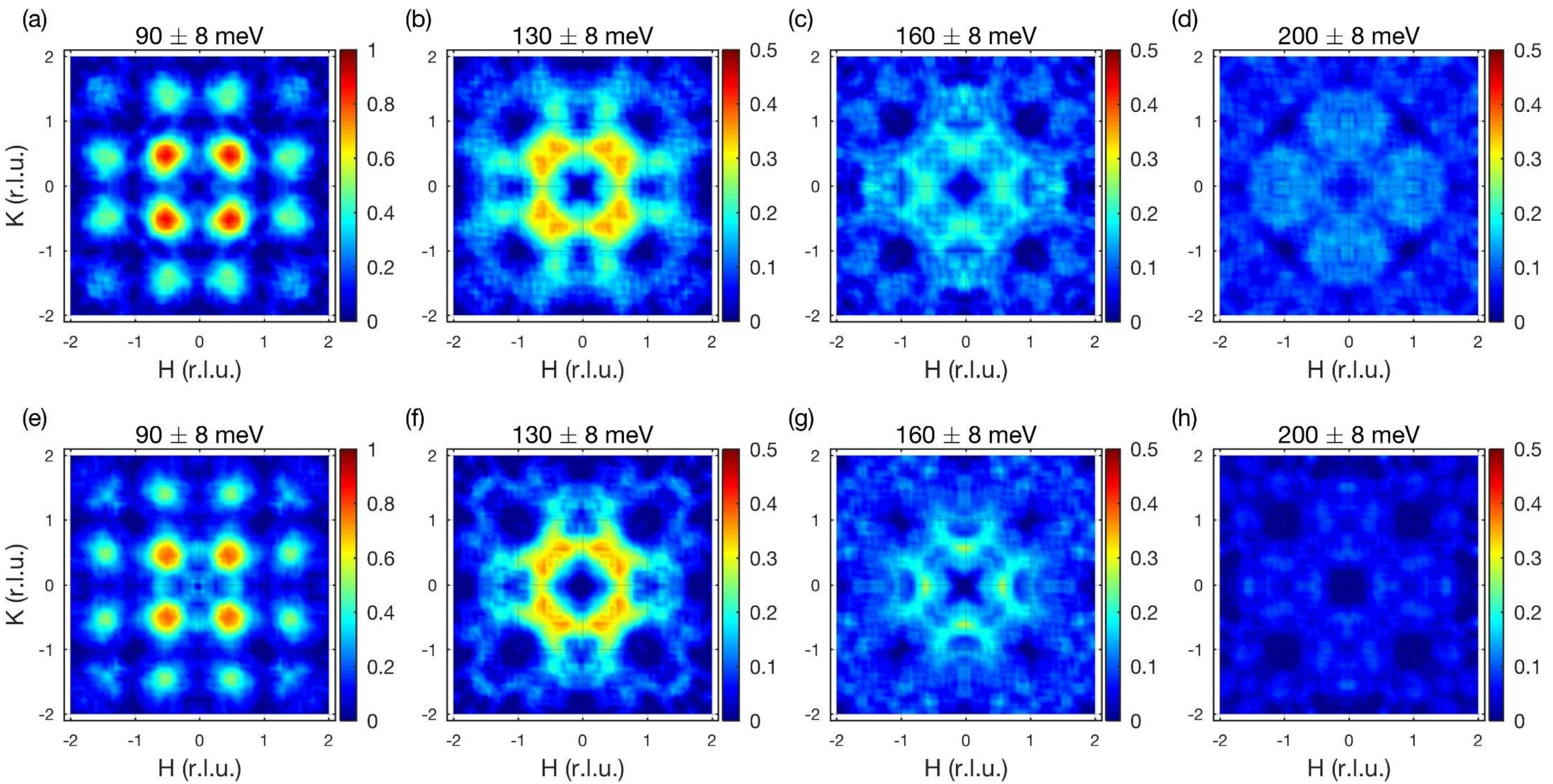
Inelastic neutron scattering – sample





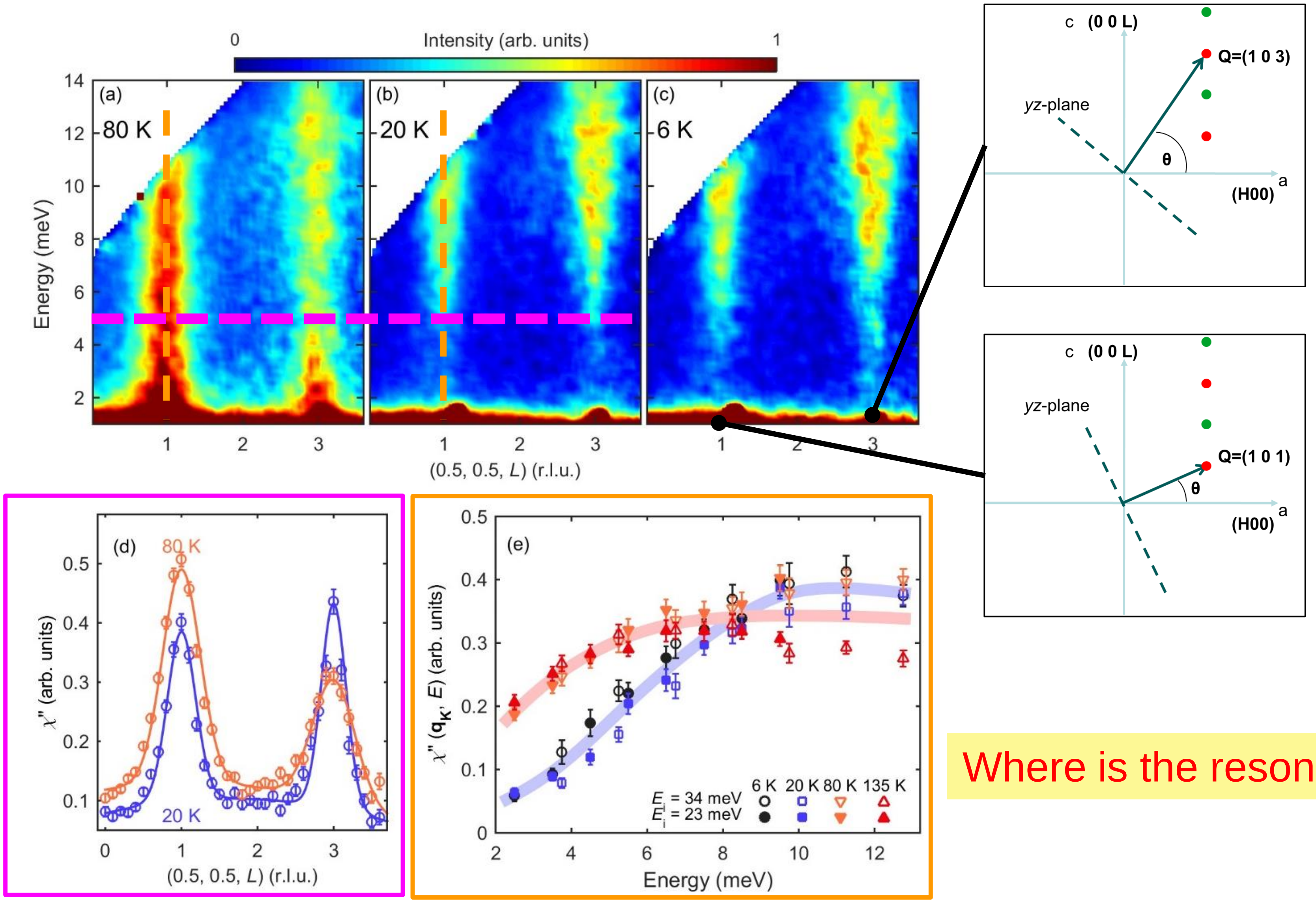
Similar high-energy excitations

C_4 magnetic phase



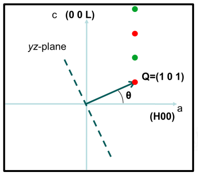
C_2 magnetic phase

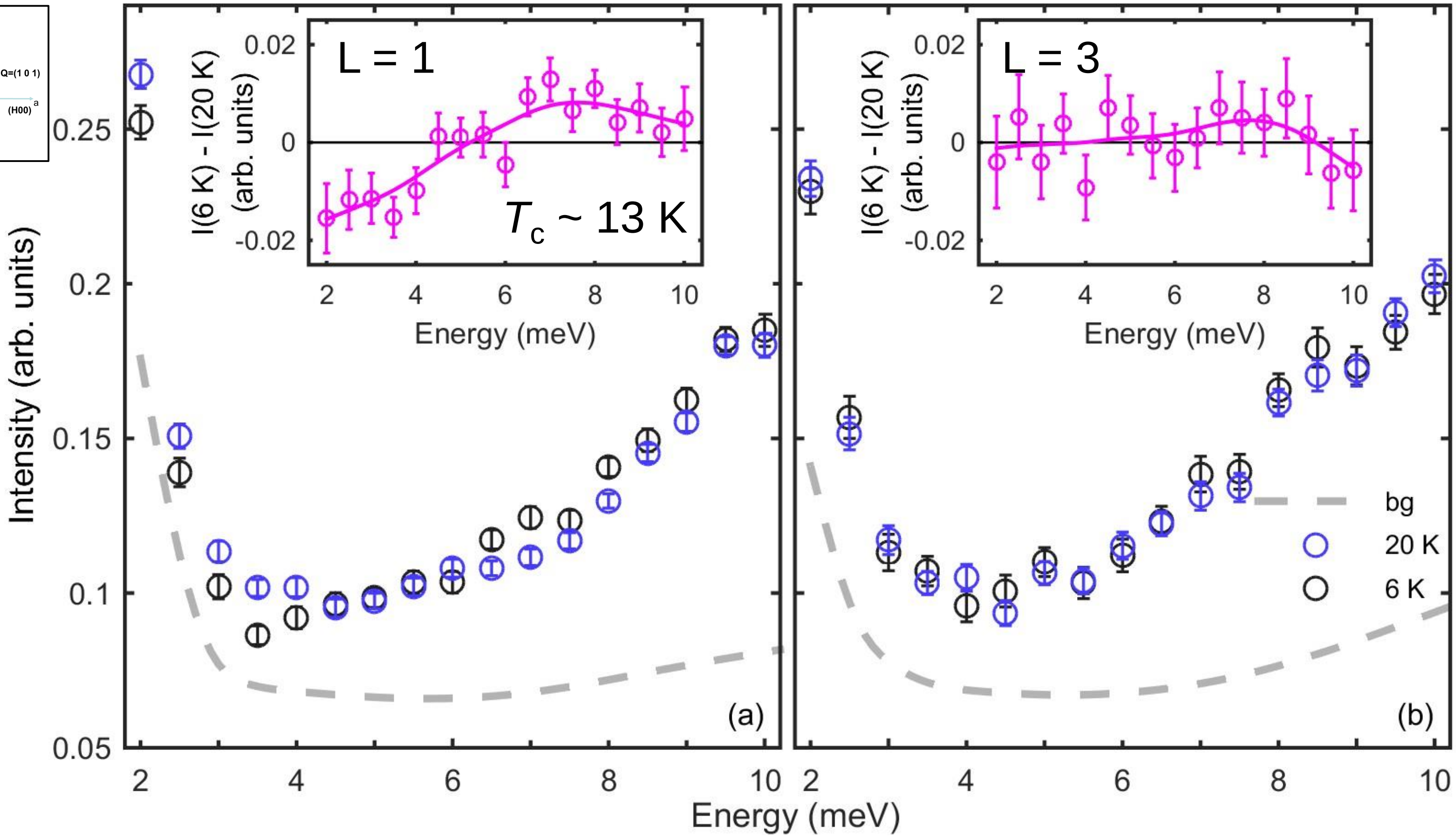
Gapped excitations for M_c in the C_4 phase

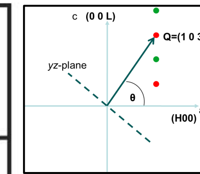


Where is the resonance??

Weak M_c resonance at ~7 meV!







- “Preferred” spin excitations: M_c!
- Naturally explains the competition between C_4 magnetic order and SC

Guo *et al.*, in preparation

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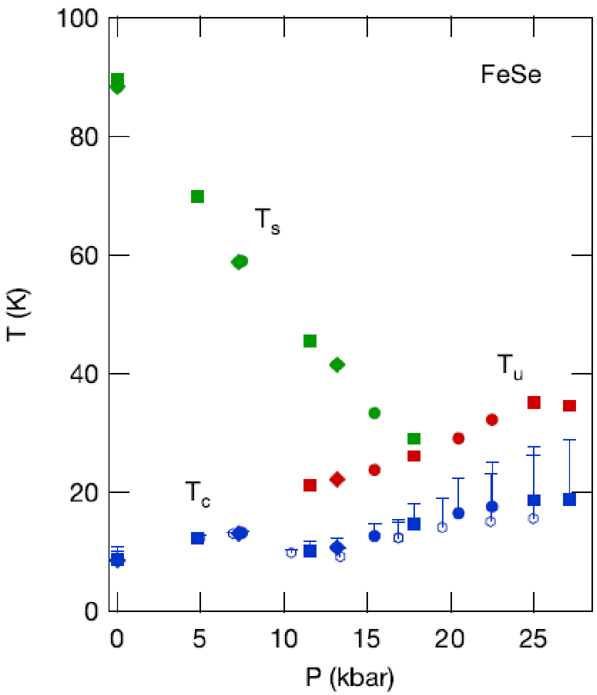
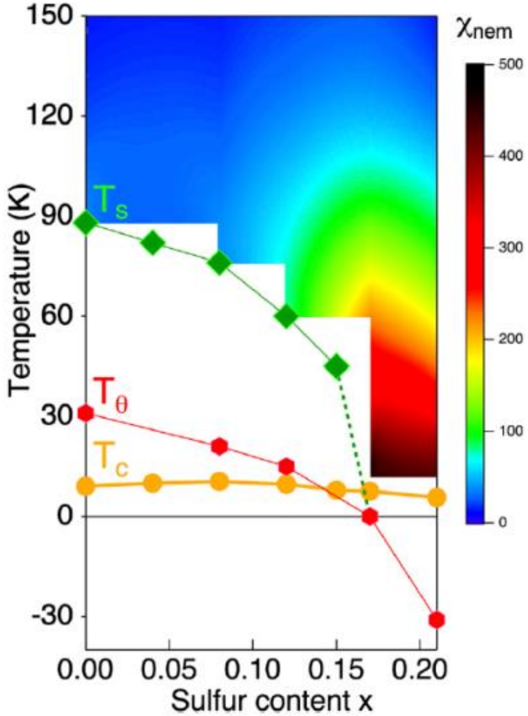
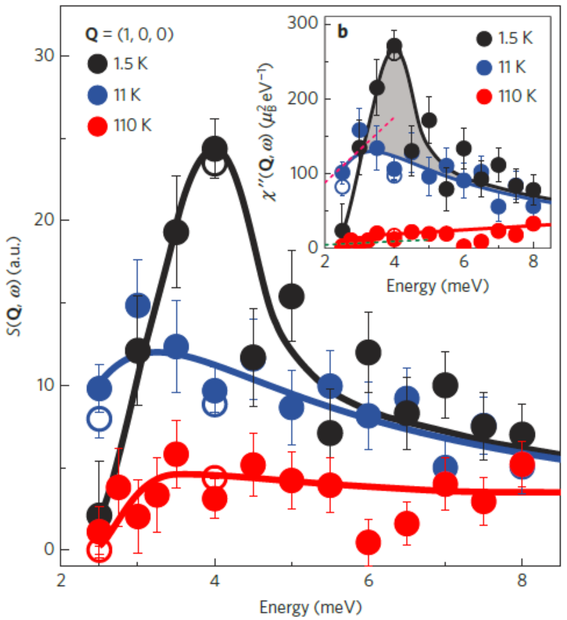
Magnetism and nematicity in $FeSe_{1-x}S_x$



Terashima *et al.*, *JPSJ* 84, 063701 (2015)



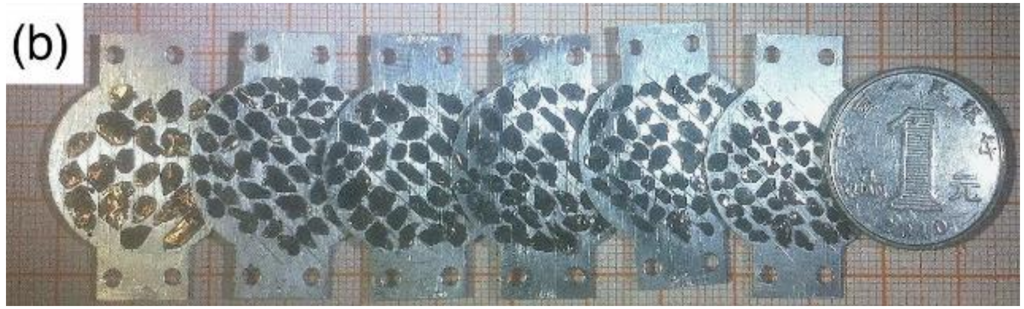
Hosoi *et al.*, *PNAS* 113, 8139 (2016)



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

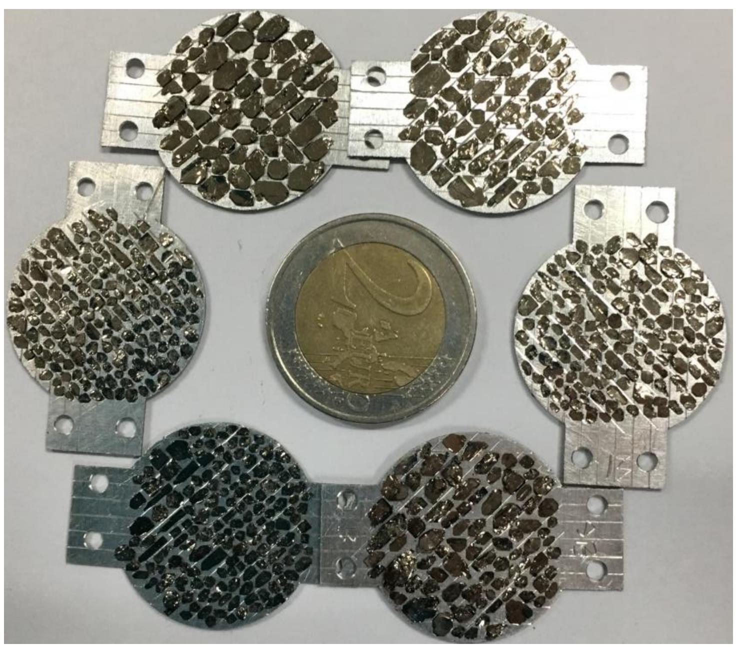
- Nematic but no magnetic order at ambient pressure
- Isovalent sulfur doping suppresses nematicity
- Plenty of stripe-AFM magnetic fluctuations

INS samples

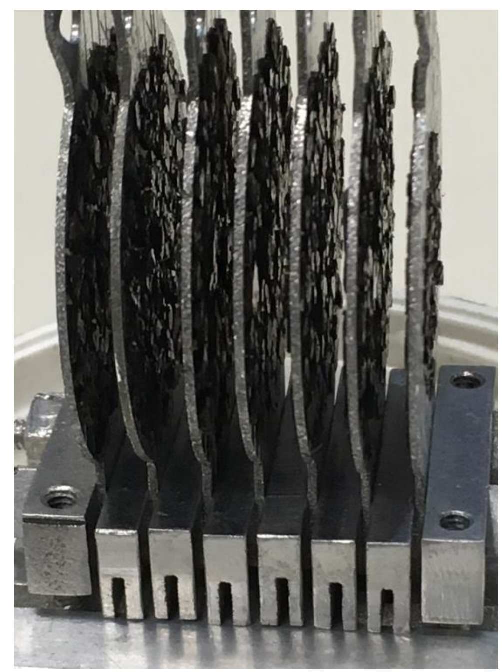


x = 0 **500 pcs**

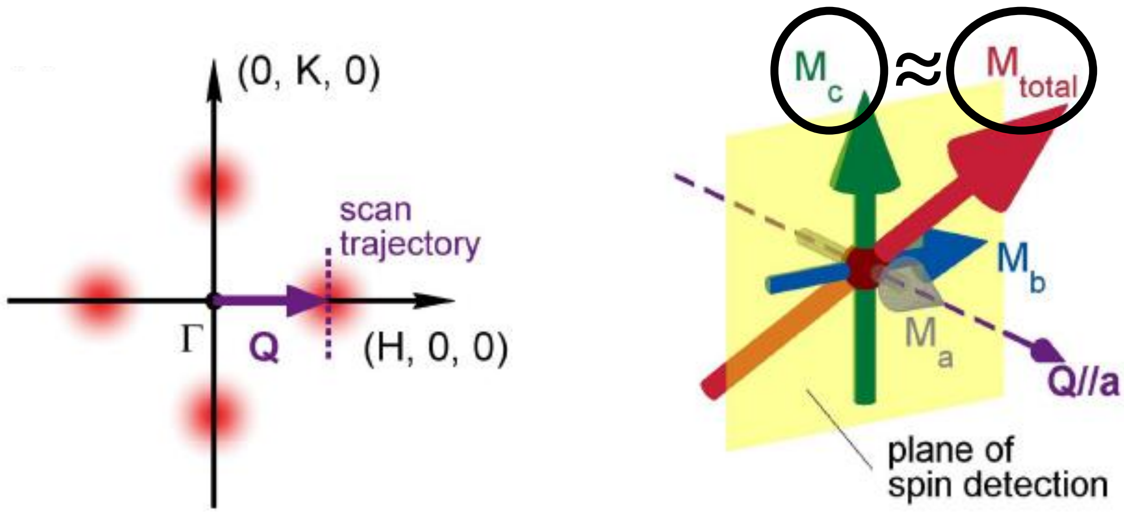
x = 0.07 **1300 pcs**

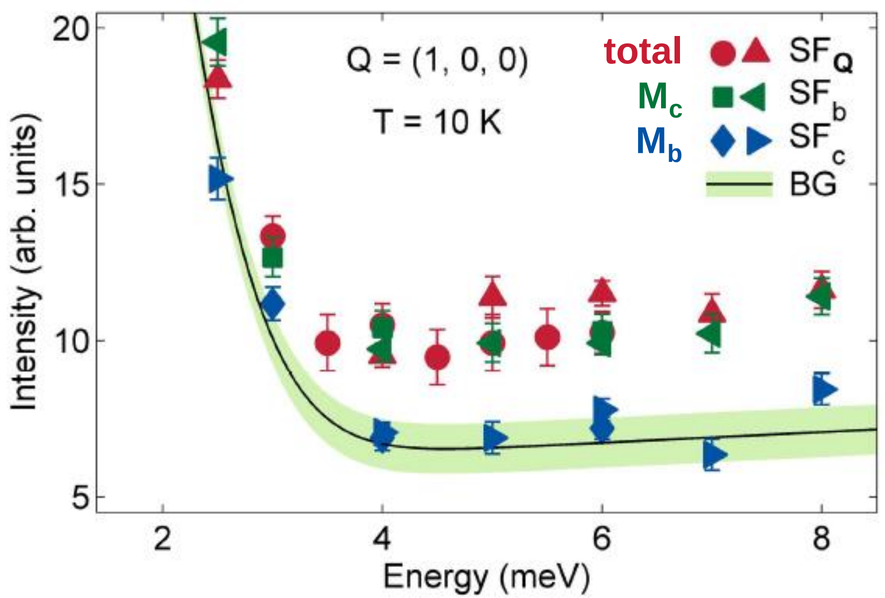


x = 0.11 **1500 pcs**



Highly anisotropic response in FeSe

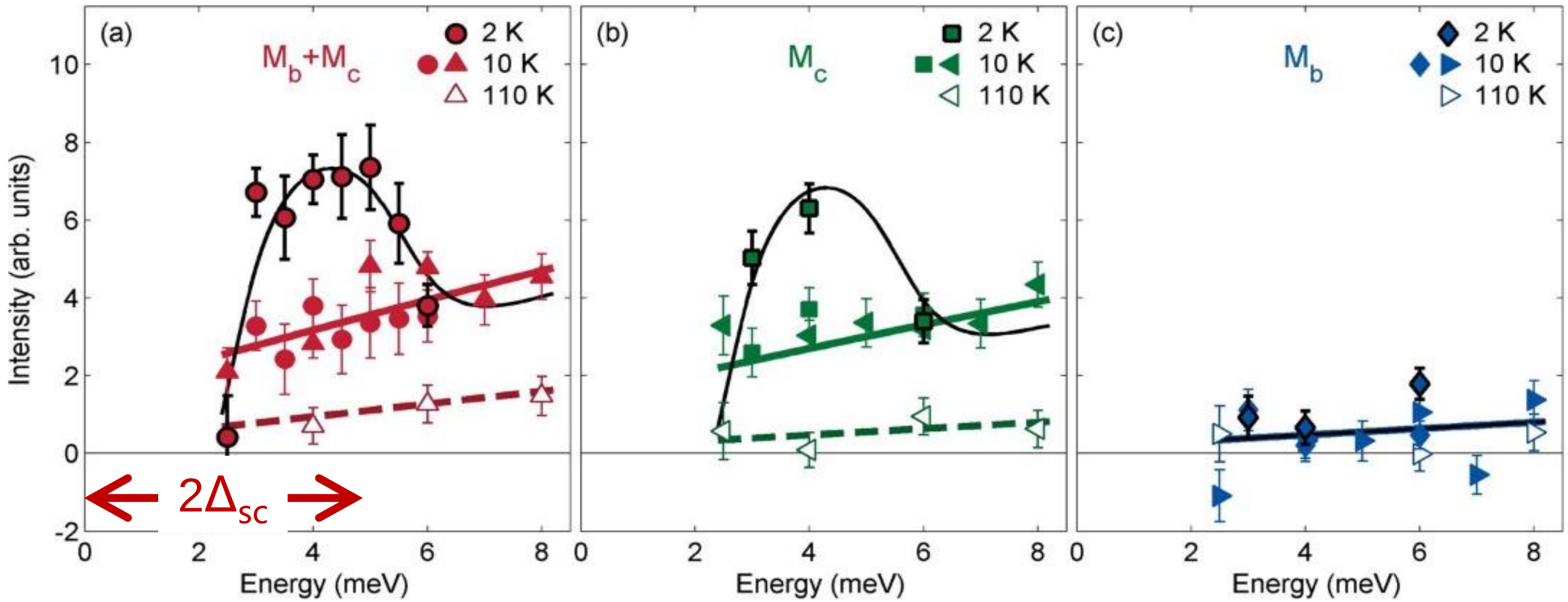




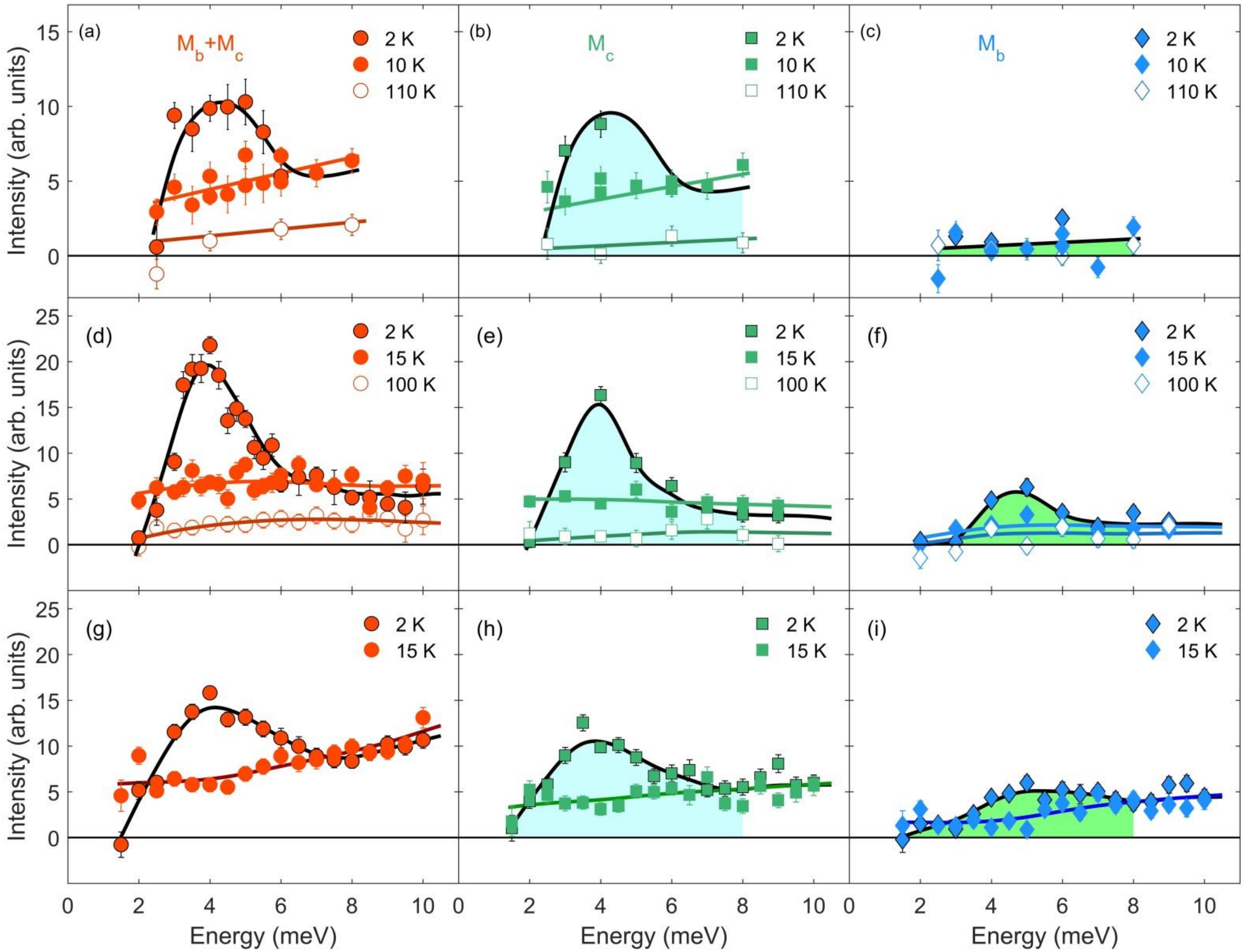
- Strong spin anisotropy
- Paramagnetic phase
- Signal at L = 0 is dominated by the *c*-axis response ($M_c : M_b \sim 7$)

Ma *et al.*, *PRX* **7**, 021025 (2017)

Highly anisotropic response in FeSe



Ma *et al.*, *PRX* **7**, 021025 (2017)

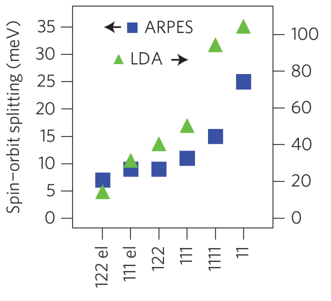


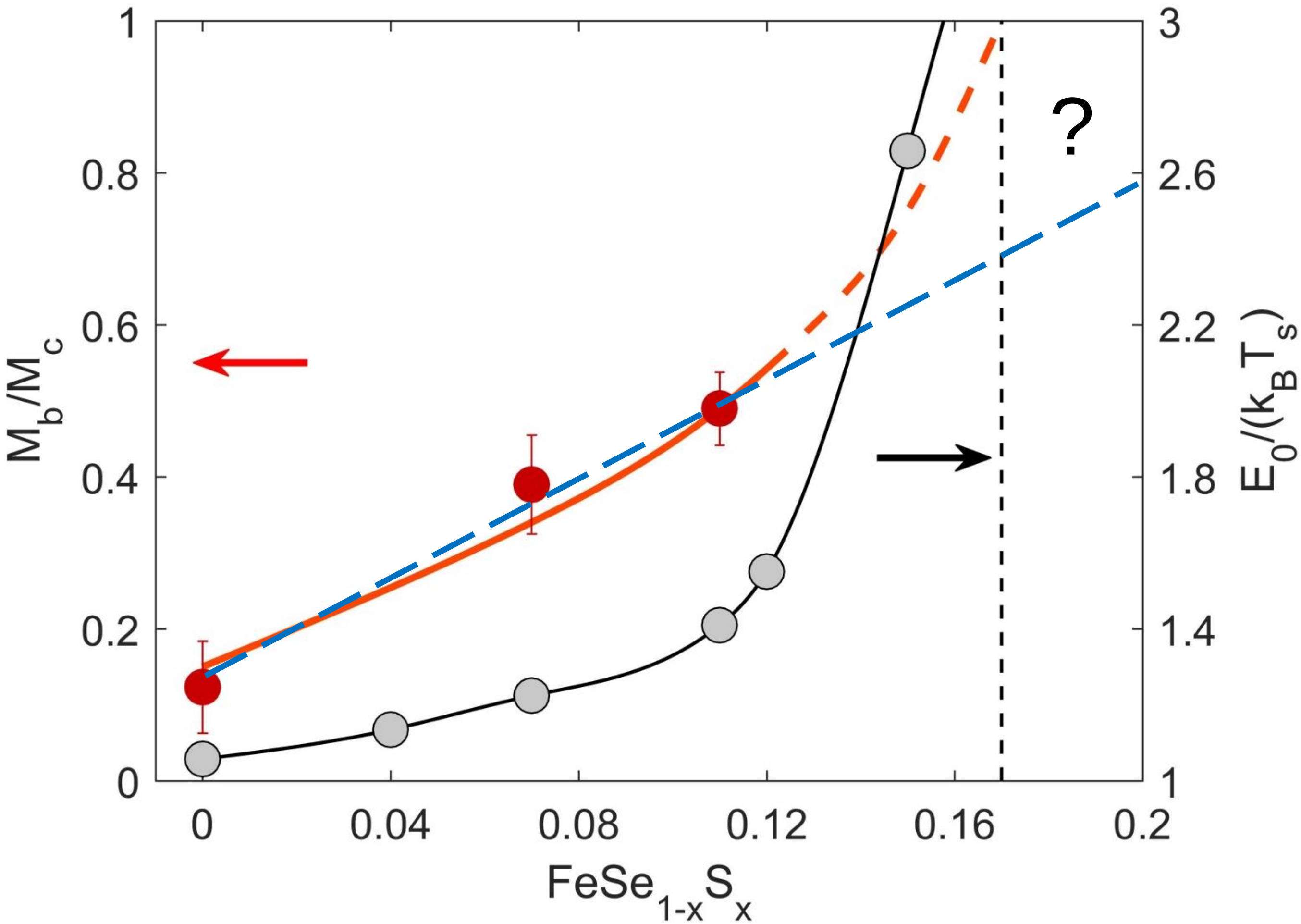
x = 0

x = 0.07
(twice stronger signal than FeSe)

x = 0.11

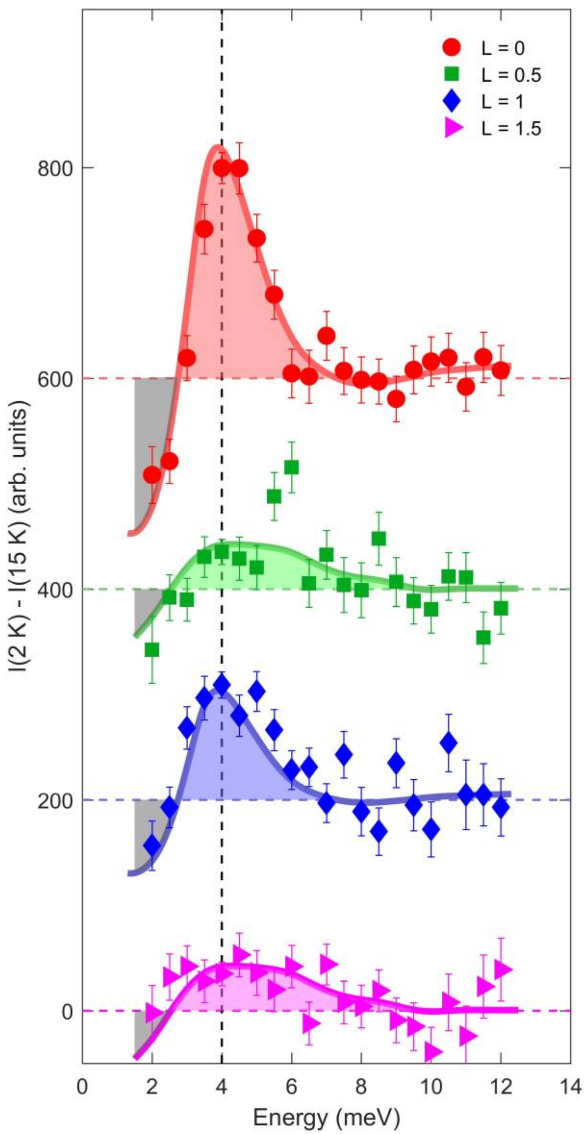
- Main resonance is *c*-axis-polarized
- Spin anisotropy decreases with sulfur doping
  → SOC related to ligand atom

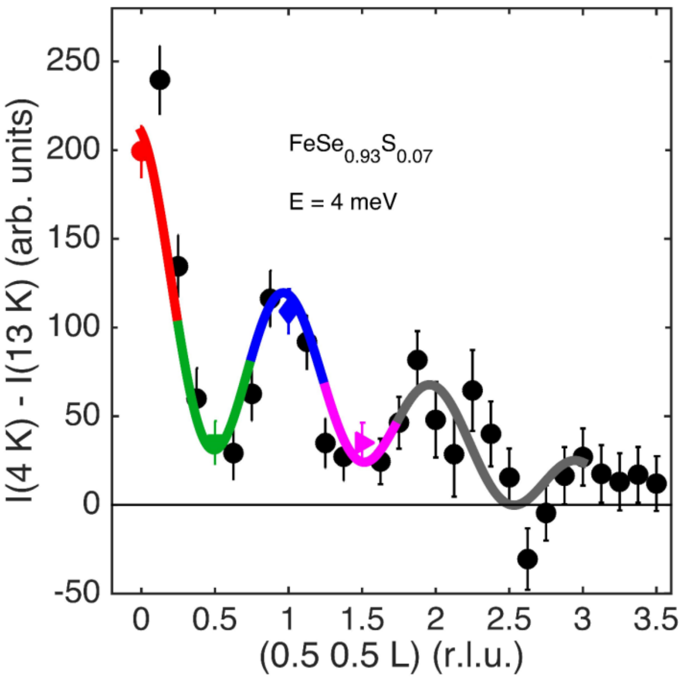


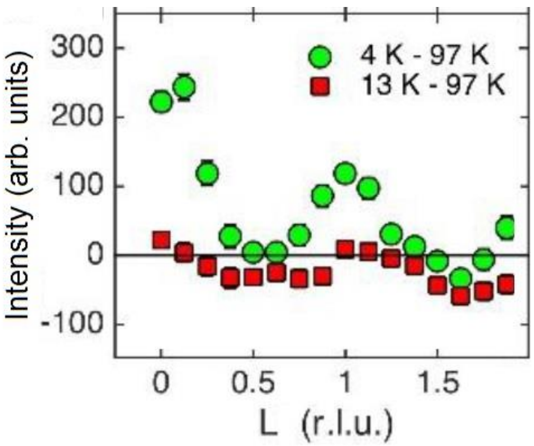


Ma *et al.*, in preparation

L (or q_c) dependence

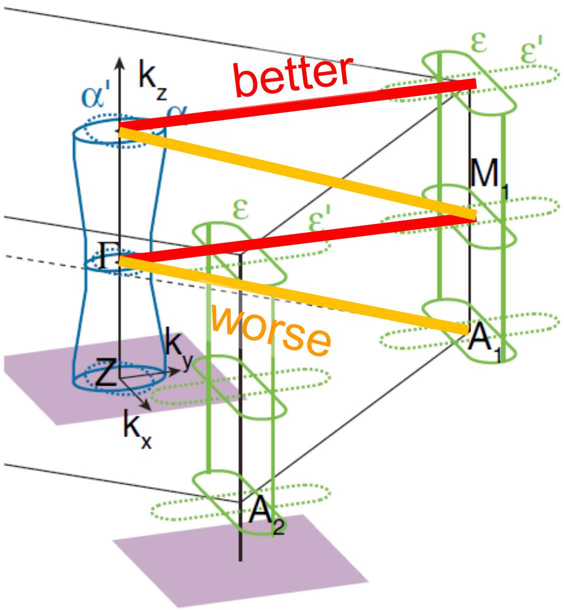


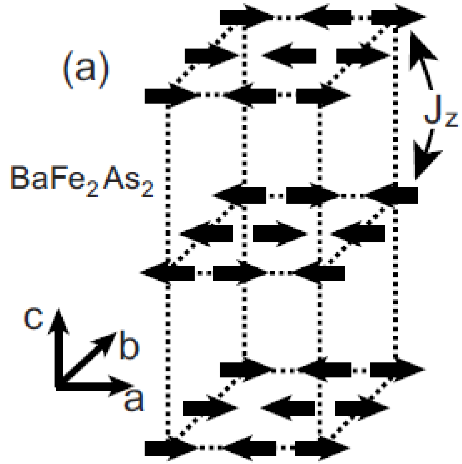


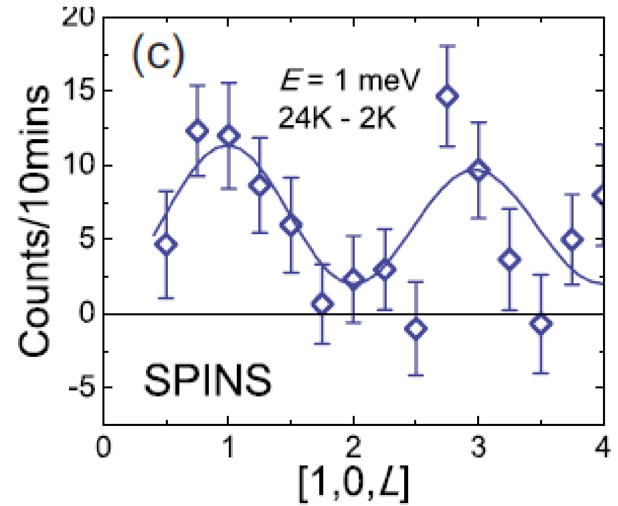


already in the normal state

k_z (or q_c) dependence



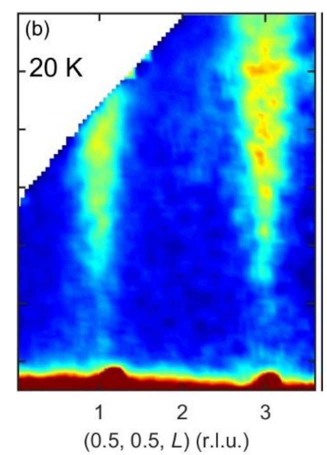




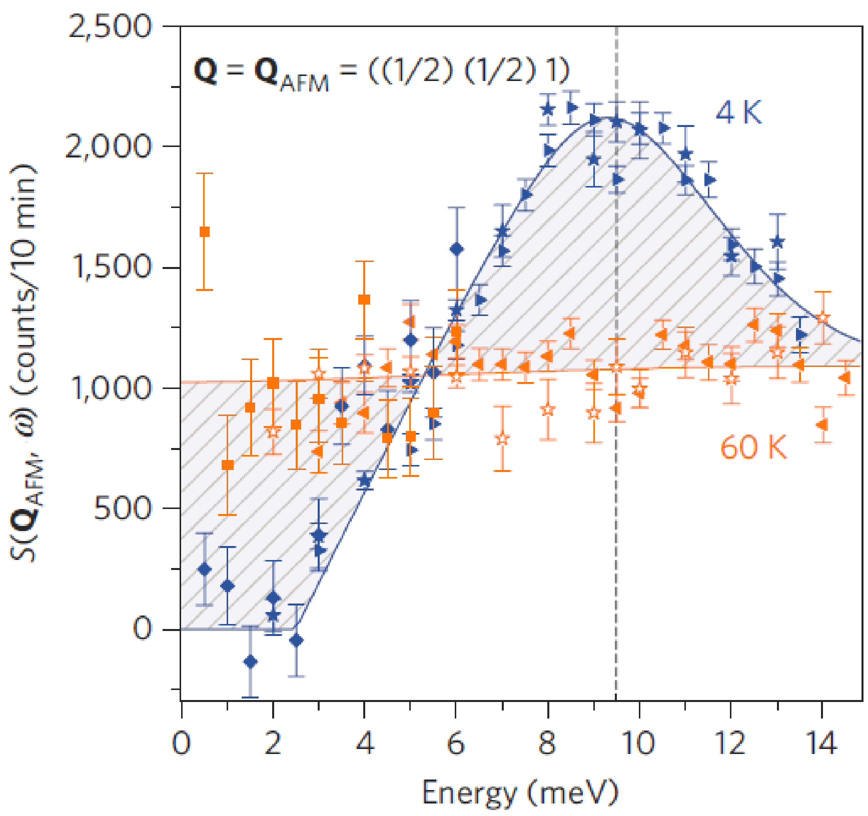
$BaFe_{1.9}Ni_{0.1}As_2$
Li et al., *PRB* (2009)

May correspond to k_z dependence seen by ARPES
Xu *et al.*, *PRL* (2016)
(also discussed in the talks on Wednesday by Borisenko & Watson)

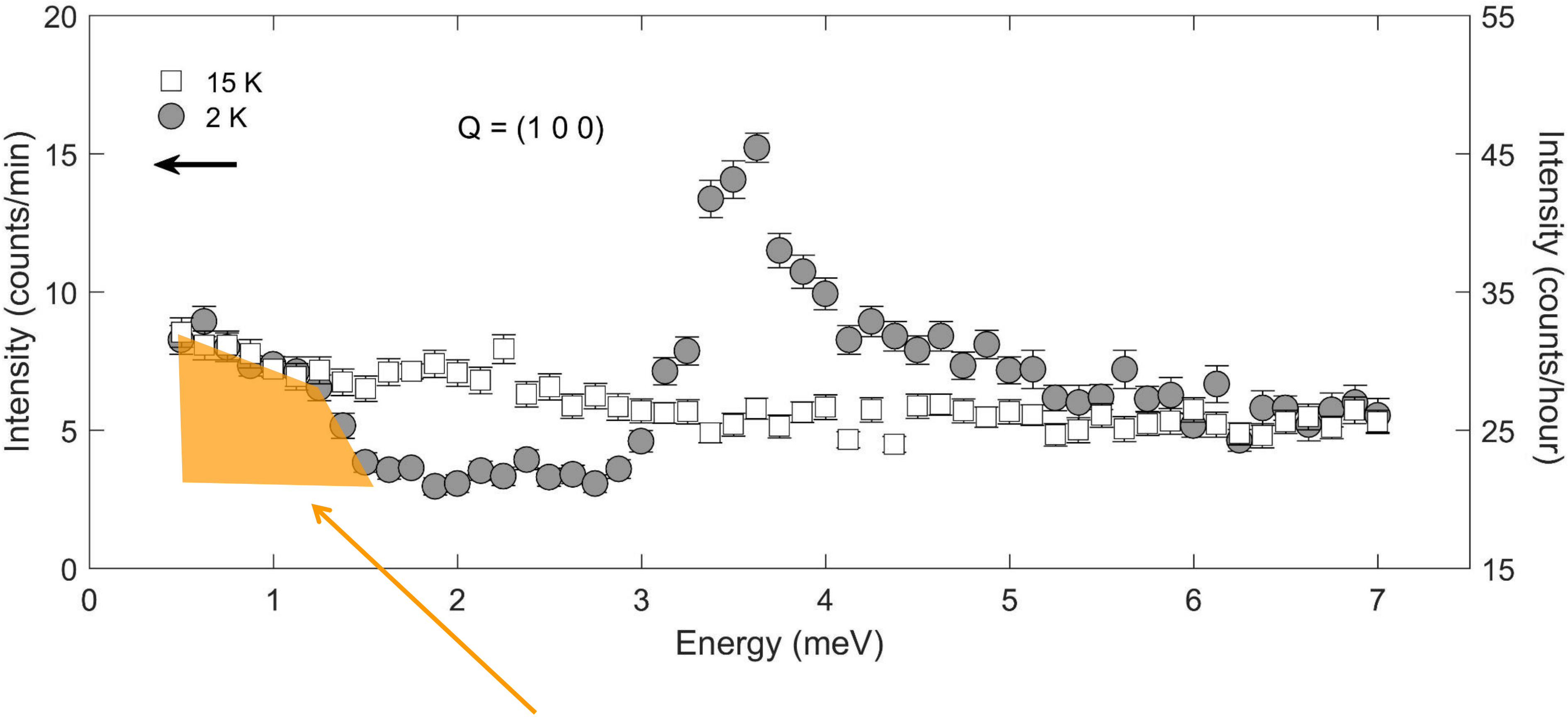
Opposite to the pnictides!



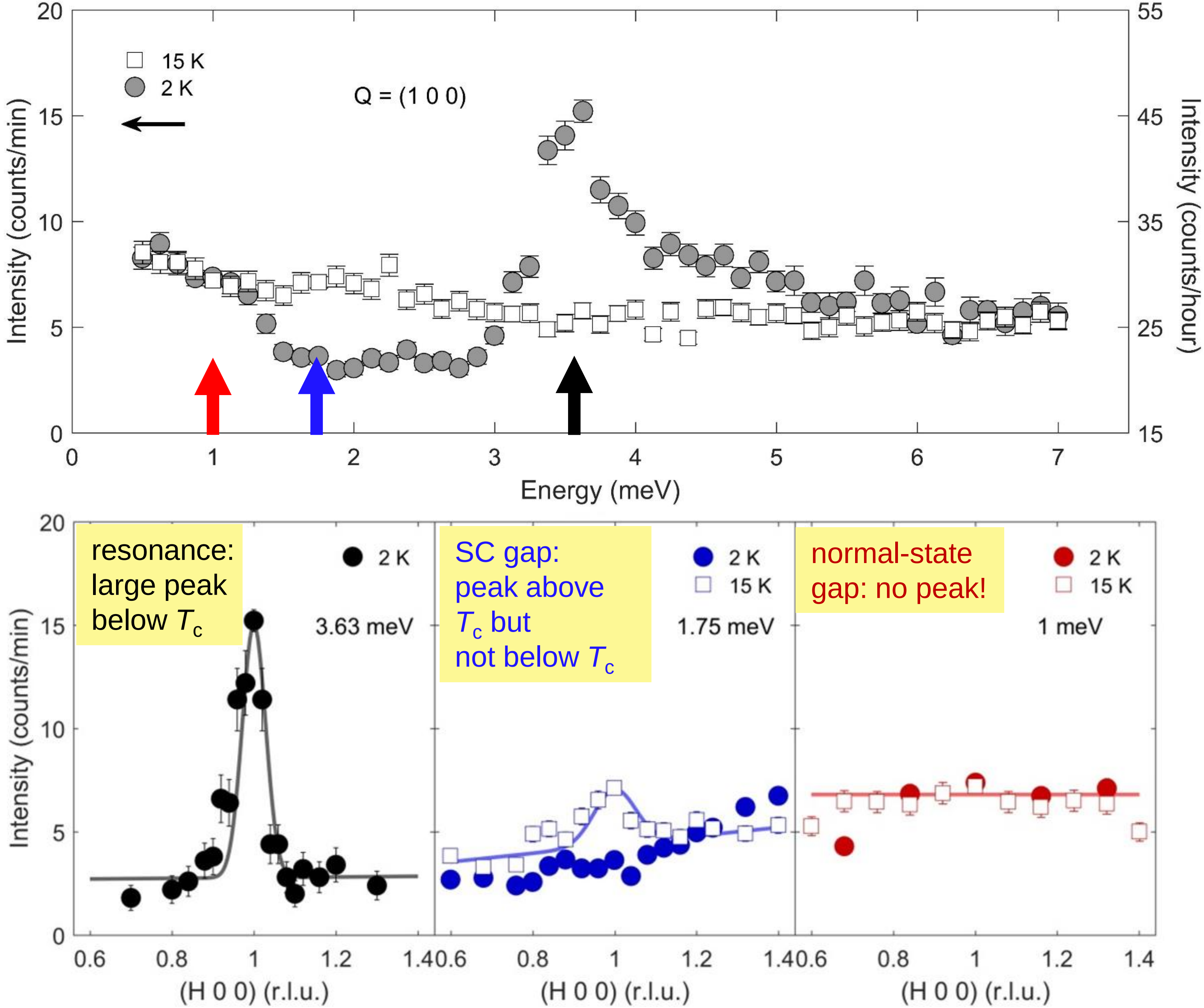
Most unexpected: a normal-state gap!

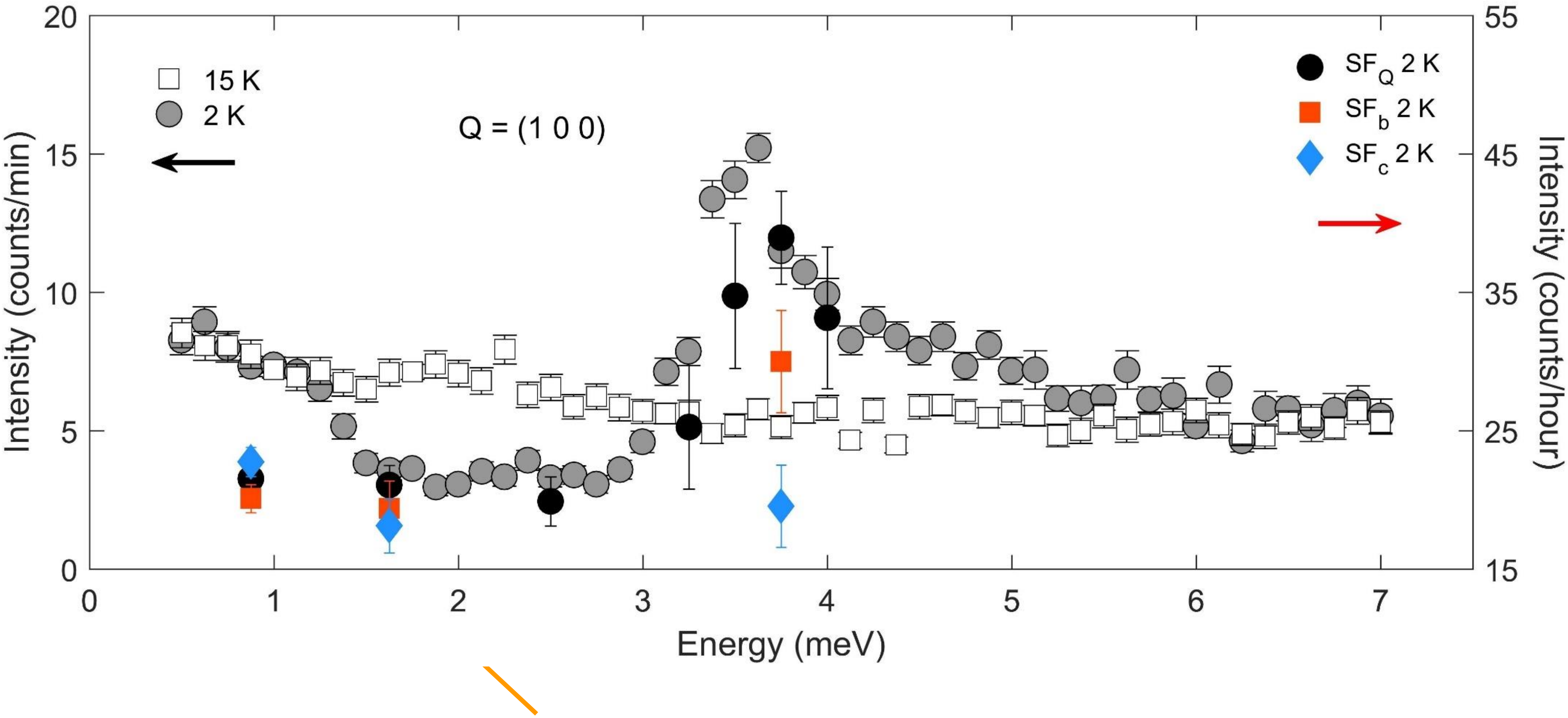


Inosov *et al.*, *Nat. Phys.* (2010)

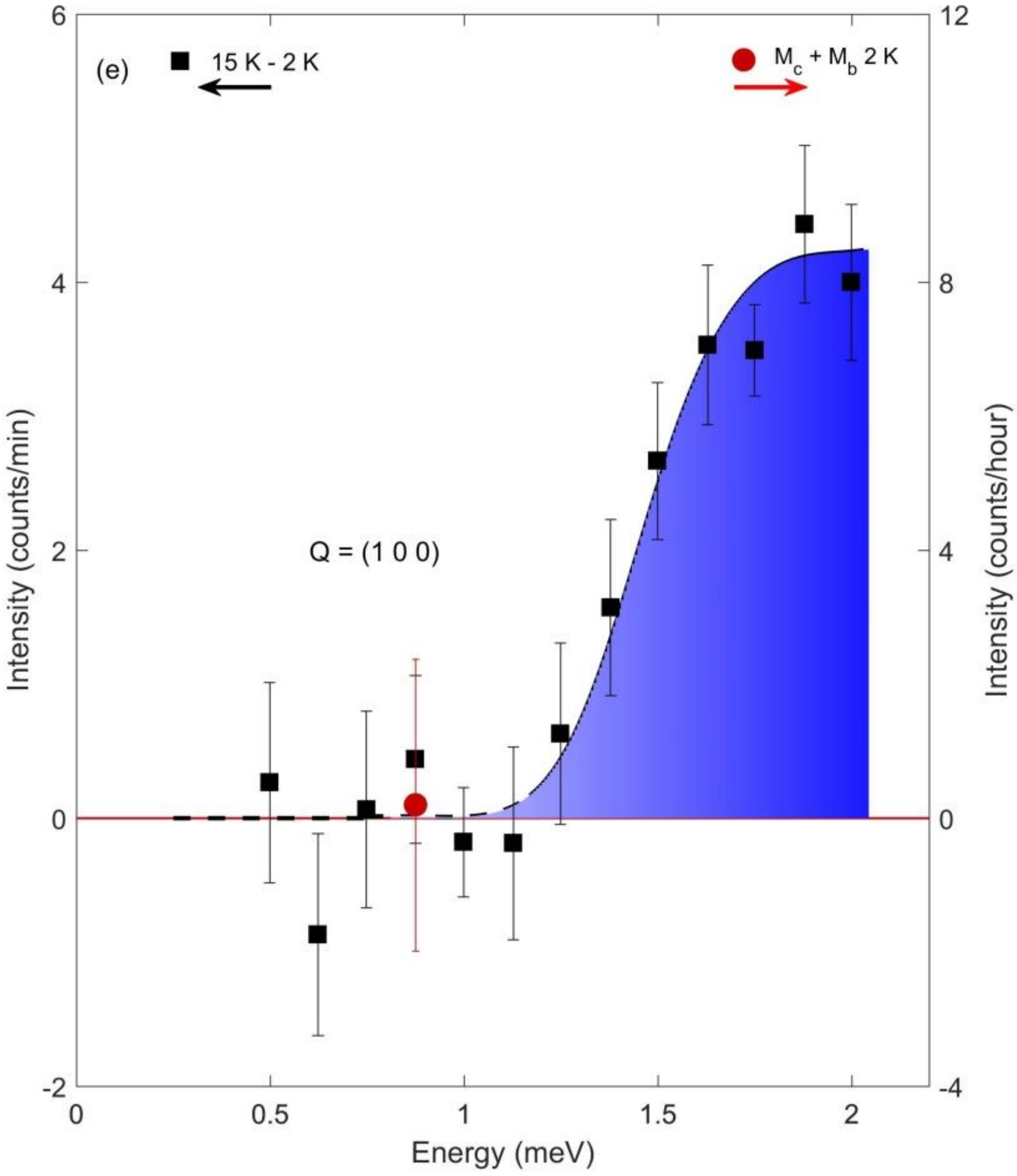


extra background scattering from the magnet we used


15 K
2 K
Q = (1 0 0)
Intensity (counts/min)
Intensity (counts/hour)
Energy (meV)
resonance:
large peak
below T_c
2 K
3.63 meV
SC gap:
peak above
T_c but
not below T_c
2 K
15 K
1.75 meV
normal-state
gap: no peak!
2 K
15 K
1 meV
(H 0 0) (r.l.u.)
(H 0 0) (r.l.u.)
(H 0 0) (r.l.u.)



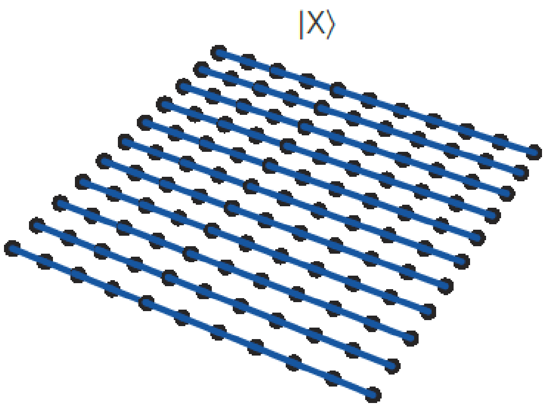
extra background scattering from the magnet we used



- **No magnetic order**
- **Not in the SC state (pseudogap? probably not)**
- **What does this mean? AKLT physics(?)**

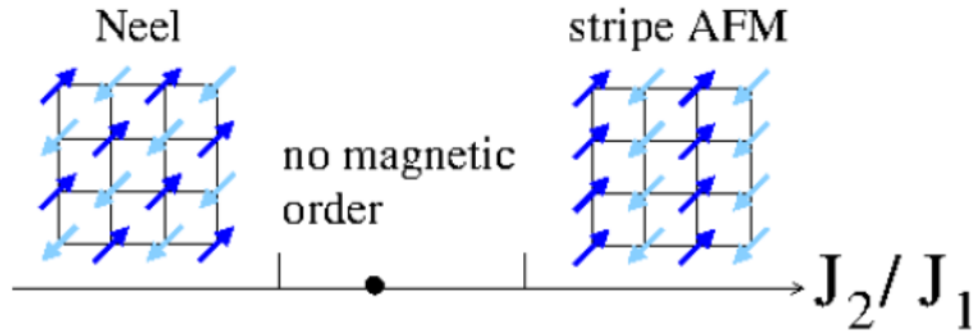
  … with itinerant electrons
  … with anisotropy

Ma *et al.*, in preparation

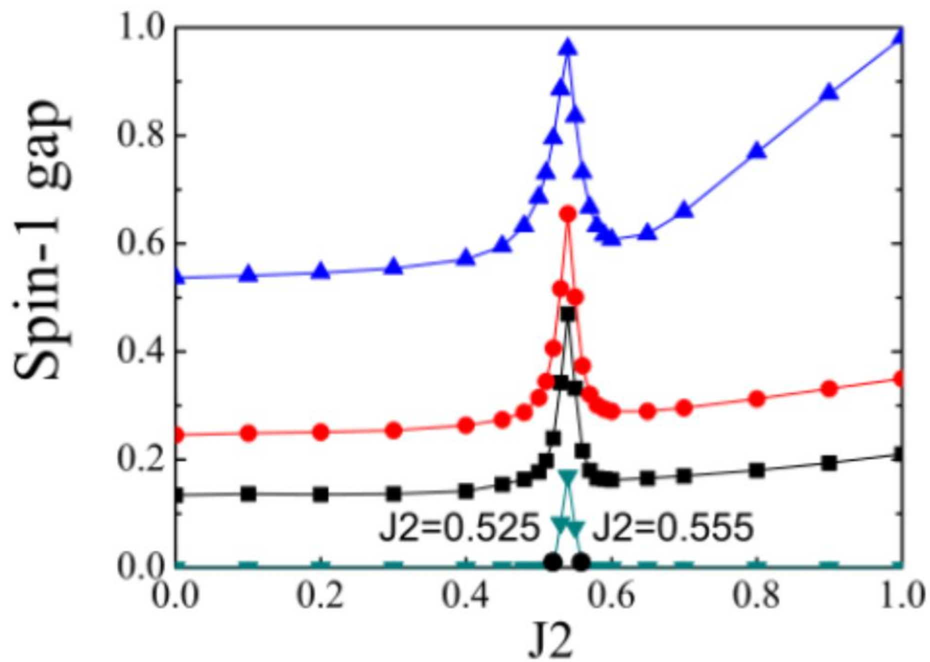


“Quantum paramagnet” scenario for nematicity
Wang, Kivelson & Lee, Nat. Phys. (2015)

Haldane’88
Read & Sachdev’89



Chandra & Doucot (1988)



DMRG for J_{1x}-J_{1y}-J_2 model, Jiang *et al.* (2009)

1. **Local + itinerant magnetism**

- The spin resonant mode (and its *L* dependence) can be understood from an itinerant point of view

- The normal-state gaps (anisotropy gap in $Sr_{1-x}Na_xFe_2As_2$, and possible AKLT gap in $FeSe_{1-x}S_x$) can be understood with local moments

- Hund's metal:
  Itinerant electrons = trigger, local moments = amplifier

2. **Near a stripe-AFM vs. AKLT quantum critical point?**

   - Longitudinal spin excitations in $BaFe_2As_2$
   (related discussions in Zhang & Hu, arXiv:1703.10721)

Summary

1. The $C_2 \rightarrow C_4$ magnetic transition is related to SOC.

2. Superconductivity “prefers” *c*-axis spin fluctuations. The C_4 magnetic phase competes with superconductivity by gapping out the preferred fluctuations.

3. SOC is prominent in $FeSe_{1-x}S_x$ and is mainly due to Se/S.

4. We observe a normal-state spin-1 gap in $FeSe_{1-x}S_x$, in support of AKLT physics as the origin for nematicity