Polarized inelastic neutron scattering: application to unconventional superconductors

Sr_2RuO_4 / $BaFe_{1.88}Co_{0.12}As_2$

НИЦ «Курчатовский институт» Петербургский институт ядерной физики

Спектрина

Markus Braden

Universität zu Köln

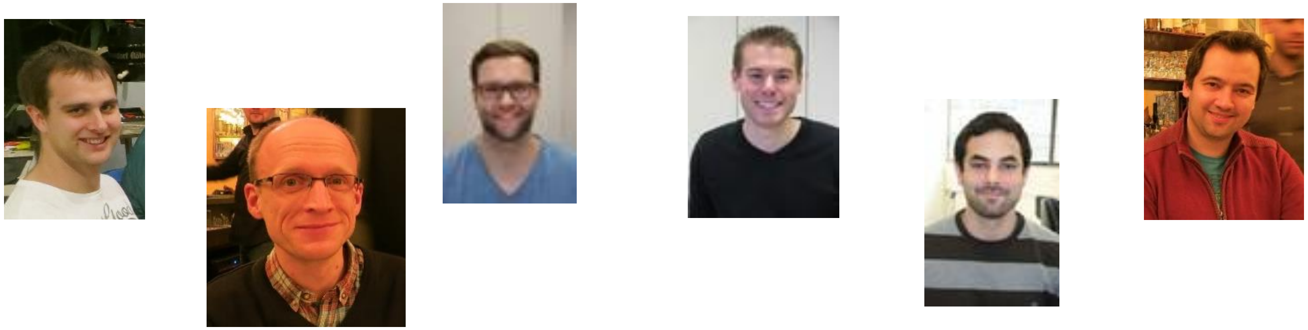
CRC 1238
Control and Dynamics
of Quantum Materials

5th Workshop on Inelastic Neutron Scattering "Spectrina – 2020"

11–12 November 2020 Gatchina, NRC KI PNPI

Collaboration

St. Kunkemöller, Kevin Jenni, Florian Waßer, Navid Qureshi, Dmitry Gorkov   Universität zu Köln



CRC 1238
Control and Dynamics of Quantum Materials

- Paul Steffens, Jiri Kulda, K. Schmalzl   Institut Laue Langevin

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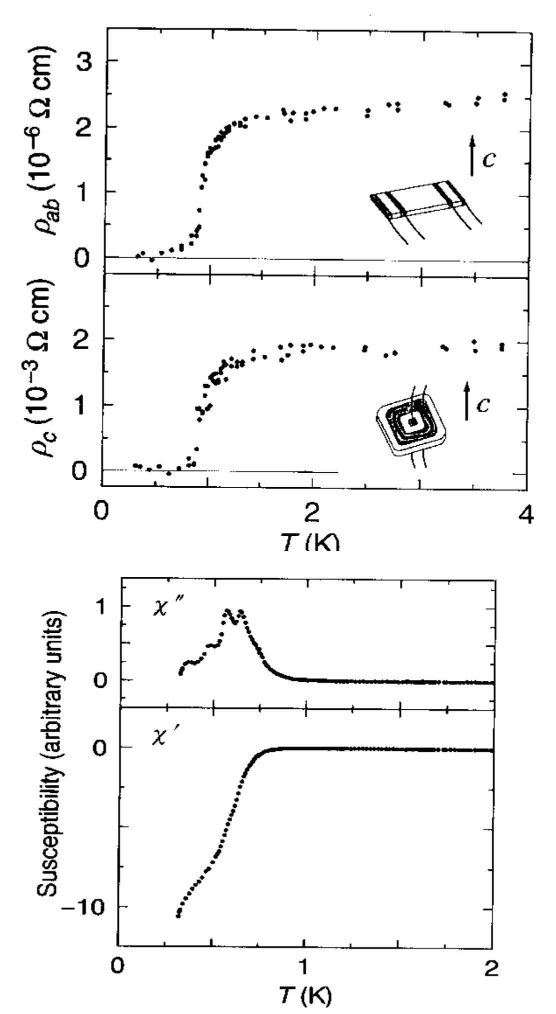
Outline

- Fermi surface sheets and associated magnetic excitations in Sr_2RuO_4
- Quasiferromagnetic excitations in Sr_2RuO_4

- Anisotropy of magnetic order in $BaFe_2As_2$
- Anisotropy of spin-resonance modes in optimum Co doped $BaFe_2As_2$

- Conclusions

26 years of superconductivity in Sr_2RuO_4

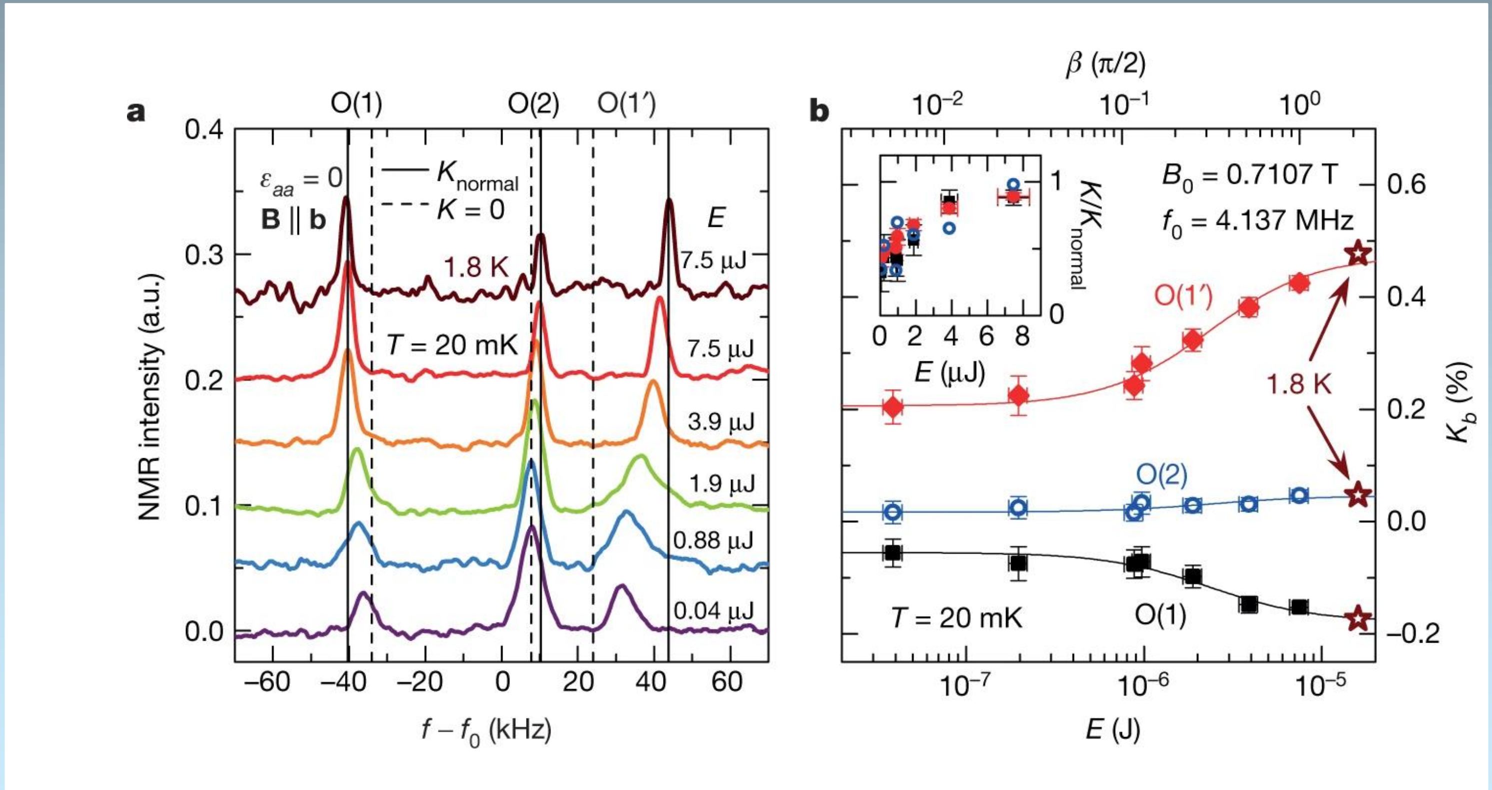


Y. Maeno *et al.*,
Nature 1994

Knight shift experiments on Sr_2RuO_4

Constraints on the superconducting order parameter in Sr_2RuO_4 from oxygen-17 nuclear magnetic resonance

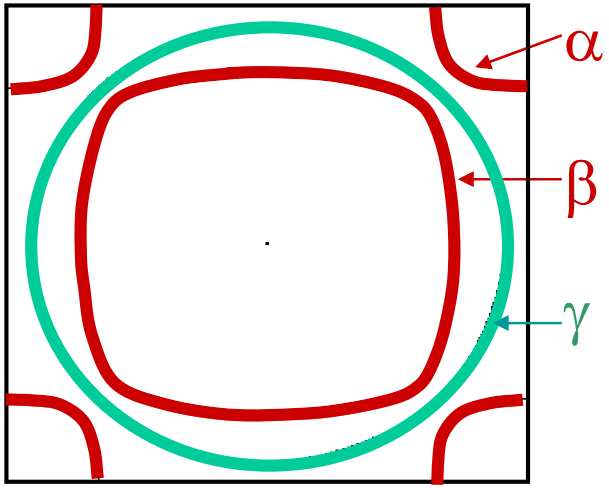
A. Pustogow[1,8]*, Yongkang Luo[1,2,8]*, A. Chronister[1], Y.-S. Su[1], D. A. Sokolov[3], F. Jerzembeck[3], A. P. Mackenzie[3,4], C. W. Hicks[3],
N. Kikugawa[5], S. Raghu[6], E. D. Bauer[7] & S. E. Brown[1]*



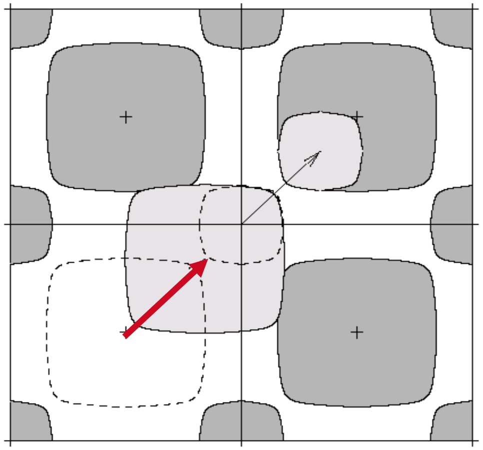
Pustogow *et al.*, Nature **574**, 72 (2019)

confirmed by: K. Ishida et al., J.Ph.Soc.Jpn **89**, 034712 (2020).

Fermi-surface nesting



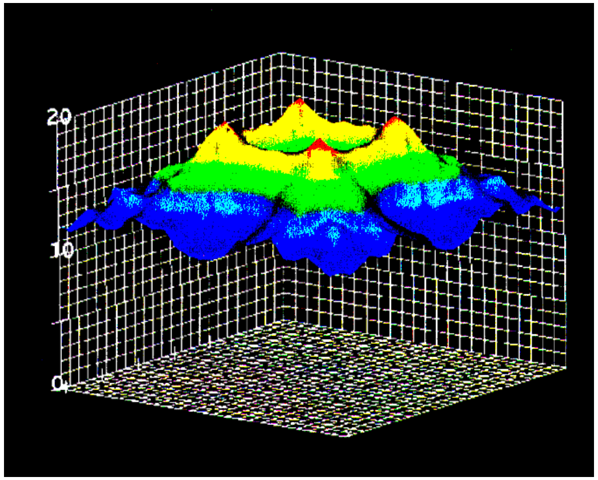
nesting : α/β-Fermi surface



dynamic susceptibility (RPA)

$$\chi_0(q,\omega) = (g\mu_B)^2 \sum_{k,i,j} \frac{M^{i,j}_{k;(k+q)}[f(\varepsilon_{k,i}) - f(\varepsilon_{(k+q),j})]}{\varepsilon_{(k+q),j} - \varepsilon_{q,i} - \hbar\omega + i0^+}$$

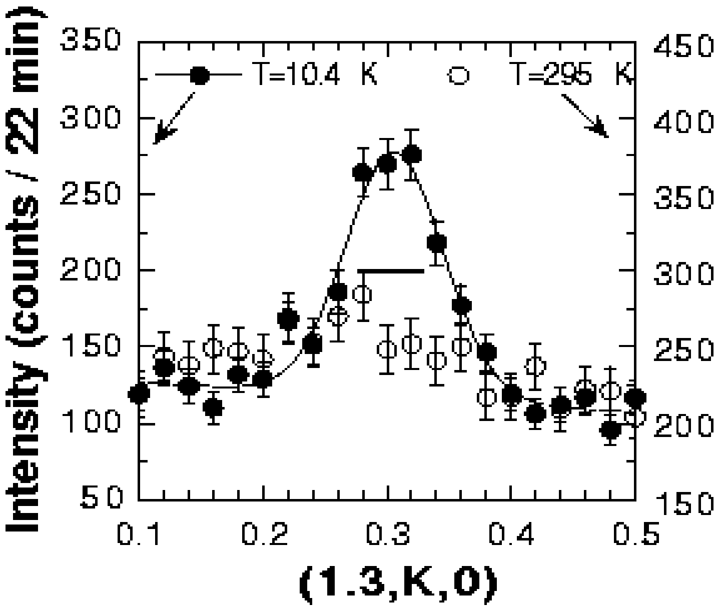
$$\chi(q) = \frac{\chi_0(q)}{1 - I(q)\chi_0(q)}$$



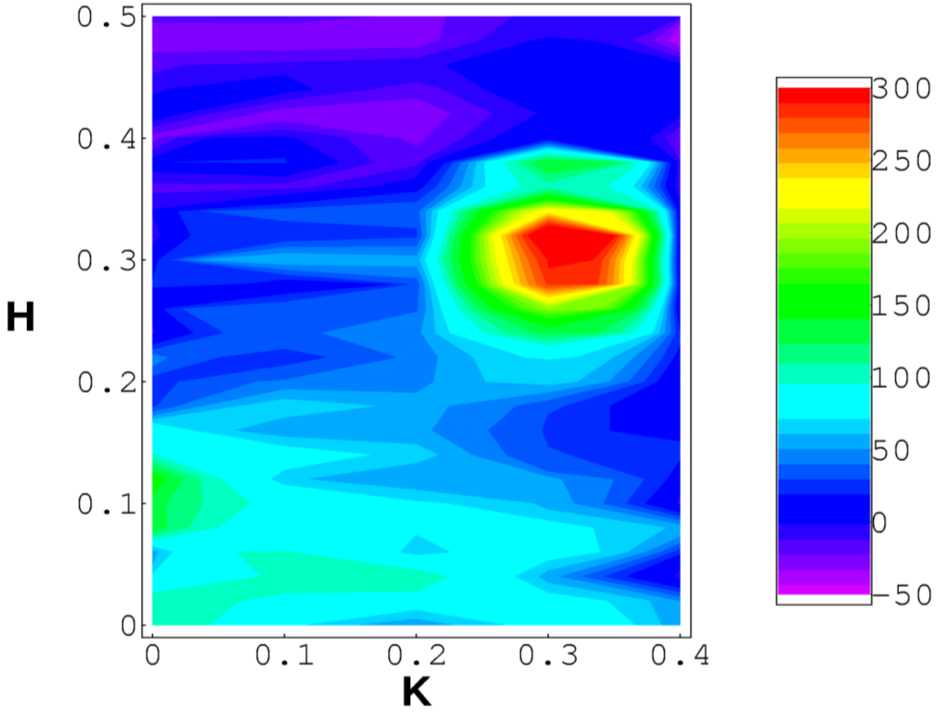
Mazin and Singh , PRL (1999)

inelastic neutron scattering

$$\frac{d^2\sigma}{d\Omega d\omega} = r_0^2 \cdot \frac{2F^2(Q)}{\pi(g\mu_B)^2} \cdot \frac{\chi''(Q,\omega)}{1-\exp(-\frac{h\omega}{kt})}$$



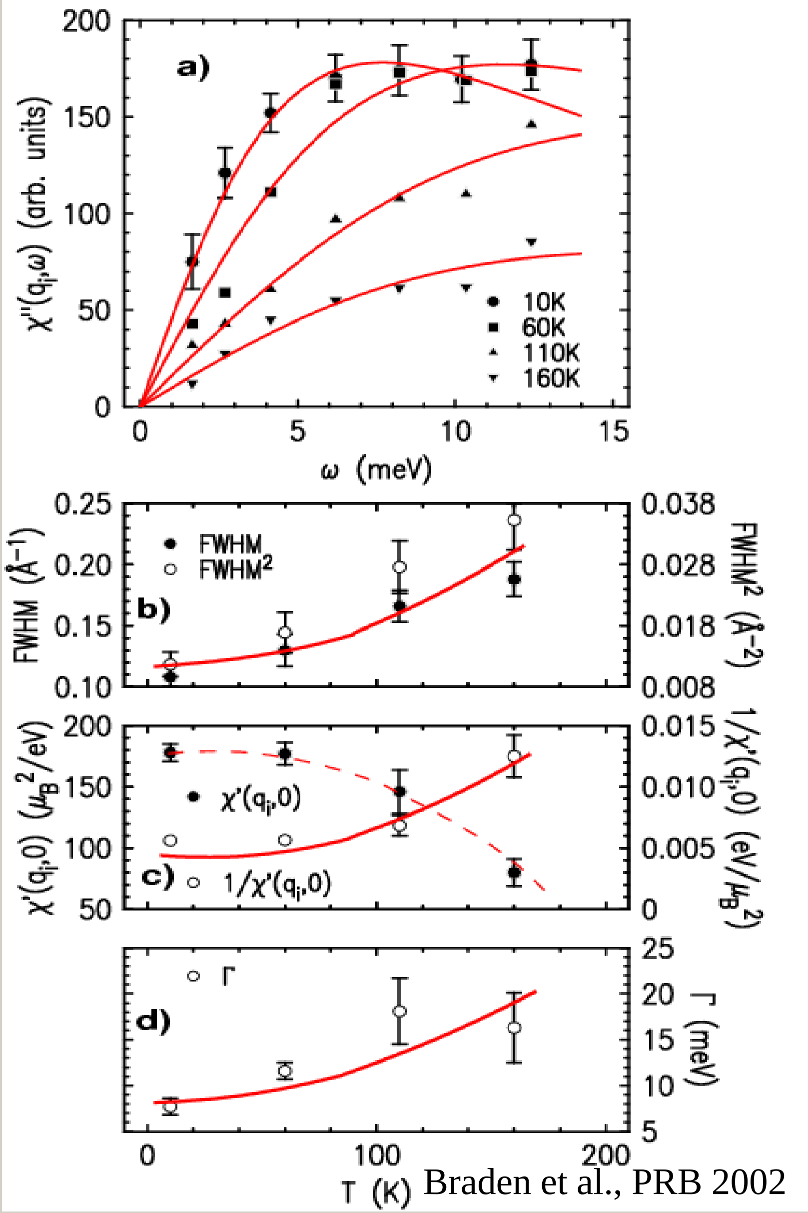
Y. Sidis et al., Phys. Rev. Lett. 83, 3320 (1999).



Braden et al., PRB66, 064522 2002; PRL92, 097402, 2004.

see also:
F. Servant, B. Fak, S. Raymond, J. P. Brison, P. Lejay, and J. Flouquet, Phys. Rev. B 65, 184511 (2002).
K. Iida, M. Kofu, N. Katayama, J. Lee, R. Kajimoto, Y. Inamura, M. Nakamura, M. Arai, Y. Yoshida, M. Fujita, K. Yamada, and S.-H. Lee, Phys. Rev. B 84, 060402(R) (2011). . . .

energy and temperature dependency



Braden et al., PRB 2002

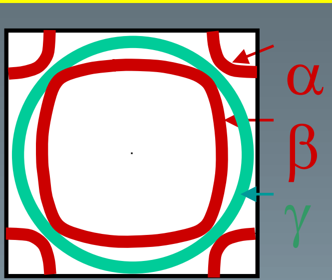
$$\chi''(q_i,\omega) = \chi'(q_i,0)\cdot\frac{\Gamma\cdot\omega}{\Gamma^2+\omega^2}$$

- $\chi'(q_0,0)$ and Γ and FWHM
  vary as function of T
- all indicate a close instability !

SDW order appears for 2.5% Ti doping
or in $Sr_{2-x}Ca_xRuO_4$
M. Braden et al., PRL 88, 2002.
S. Kunkemöller et al., PRB 89, 045119 (2014).
J.P. Carlo et al., nature mat. 11, 323 (2012).

➔ Sr_2RuO_4 is close to QCP

Active bands ? ? ?



2D bands are active
Ferromagnetic fluctuations

1D bands are active
Nesting is essential

Baskaran, G., Physica B 224, 490 (1996).

Rice, T. M. and M. Sigrist,
J. Phys.: Condens. Matter 7, L643 (1995).
…
J.W. Huo, T. M. Rice, and F.-C. Zhang, Phys. Rev. Lett. 110, 167003 (2013).

triplet superconductivity
chiral p-wave
mediated through quasi-ferromagnetic fluctuations

S. Raghu, A. Kapitulnik, and S. A. Kivelson, Phys. Rev. Lett. 105, 136401 (2010).

S Raghu, Suk Bum Chung and Samuel Lederer,
J. PhysConference Series 449 (2013) 012031

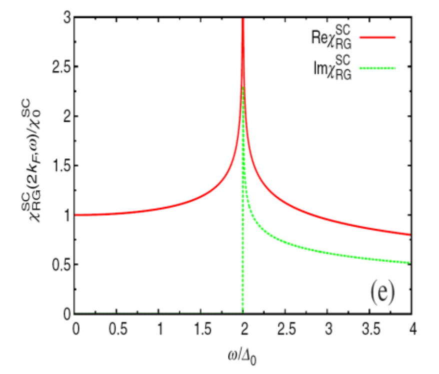
…

superconductivity in Sr_2RuO_4
resembles more closely the quasi-one dimensional organic superconductors

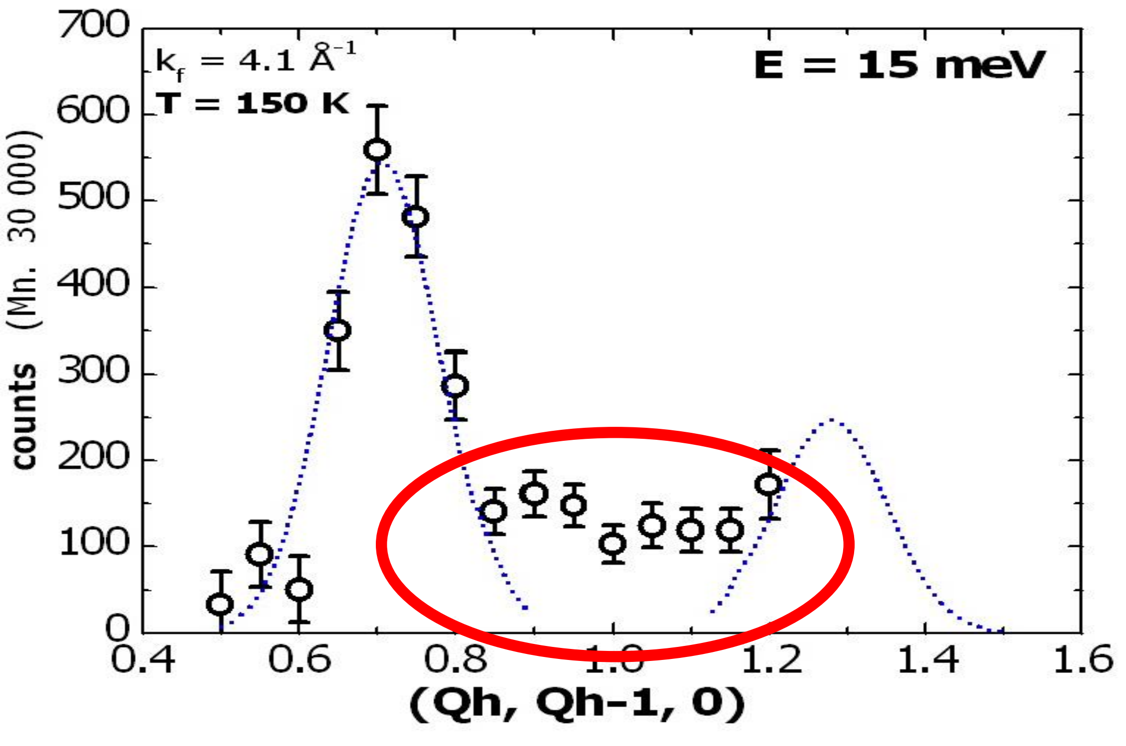
- S. Kivelson et al., npj QM **5**, 43 (2020) **near degeneracy $d_{x^2-y^2}$ and nodal $g_{xy(x^2-y^2)}$**
- H. S. Røising et al., Phys. Rev. Research 1, 033108 (2019): ***d*-wave and helical orders**
- Astrid T. Romer & Brian M. Andersen arXiv2001.11265; Romer et al. PRL 123, 247001 (2019)
- R. Sharma et al. PNAS (2020) **117** 5222

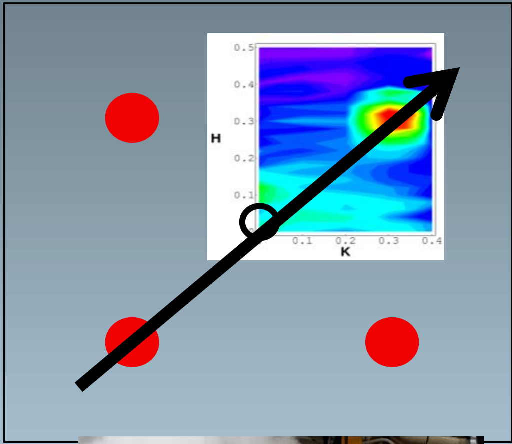
⬄ S. Kunkemöller et al., PRL **118,** 147002 (2017)

Role of ferromagnetic fluctuations?



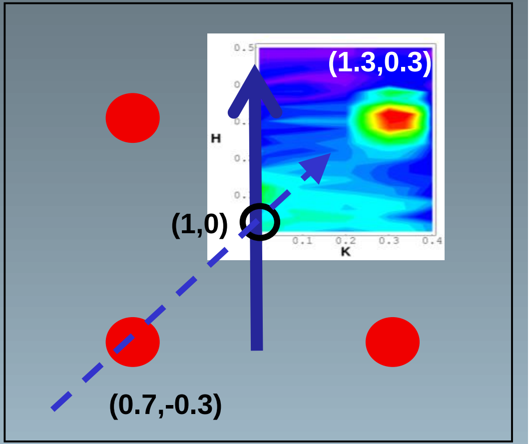
polarized neutrons (IN20 at ILL)



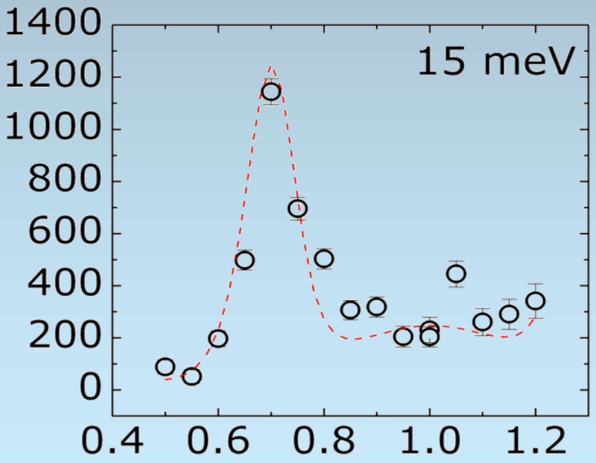


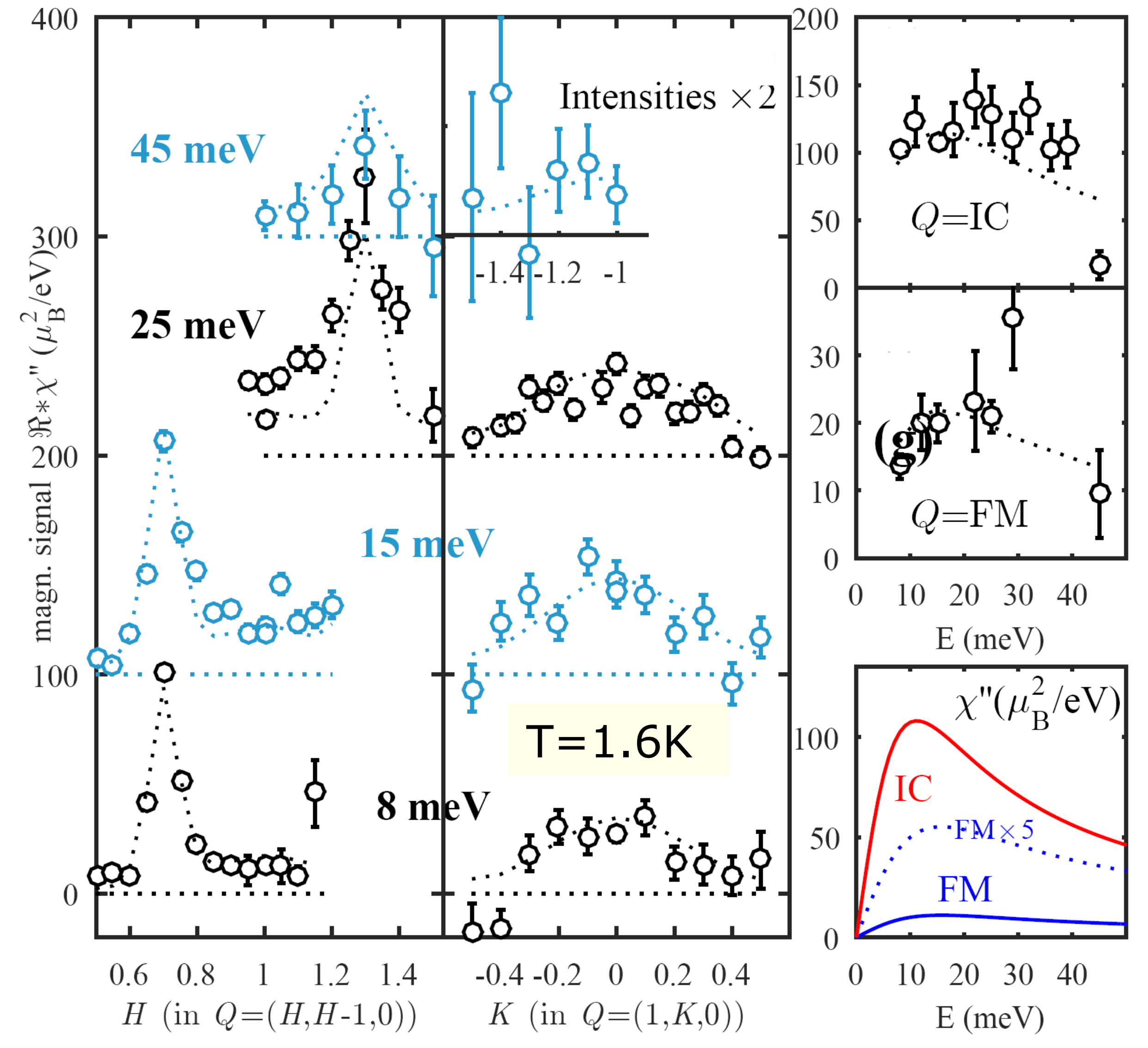
- first clear INS evidence for a – still weak - quasi-ferromagnetic contribution !

ferromagnetic fluctuations in Sr_2RuO_4



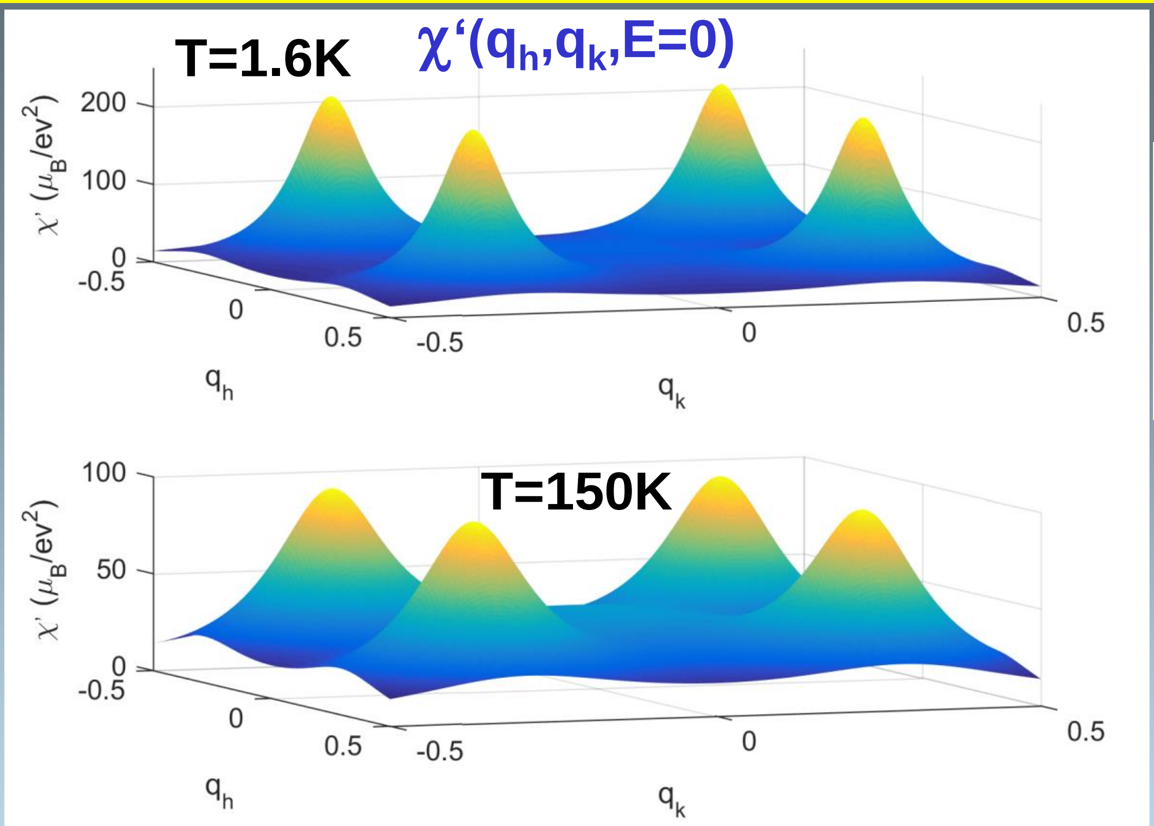
diagonal





there is a weak FM component persisting at low T

fitting all data simultaneously



total spectrum : two contributions

a) nesting signal

b) centered low-q response

➔ 6 parameters

$$\chi''(q,\omega) = \chi_{fm}''(q,\omega) + \chi_{inc}''(q,\omega)$$

$$\chi_{fm,inc}''(q,\omega) = \chi_{fm,inc}'(q,0)\cdot\frac{\Gamma_{fm,inc}(q)\cdot\omega}{\Gamma_{fm,inc}(q)^2+\omega^2}$$

$$\Gamma_{inc}(q) = \Gamma_{inc}\left(1+\xi^2(q-q_{inc})^2\right) \qquad \Gamma_{fm}(q) = \Gamma_{fm}$$

$$\chi_{inc}'(q,0) = \frac{\chi_{inc}'}{1+\xi^2(q-q_{inc})^2} \qquad \chi_{fm}'(q,0) = \chi_{fm}'\cdot e^{-\left(\frac{(q-q_{fm,inc})^2}{W^2}4\cdot\ln(2)\right)}$$

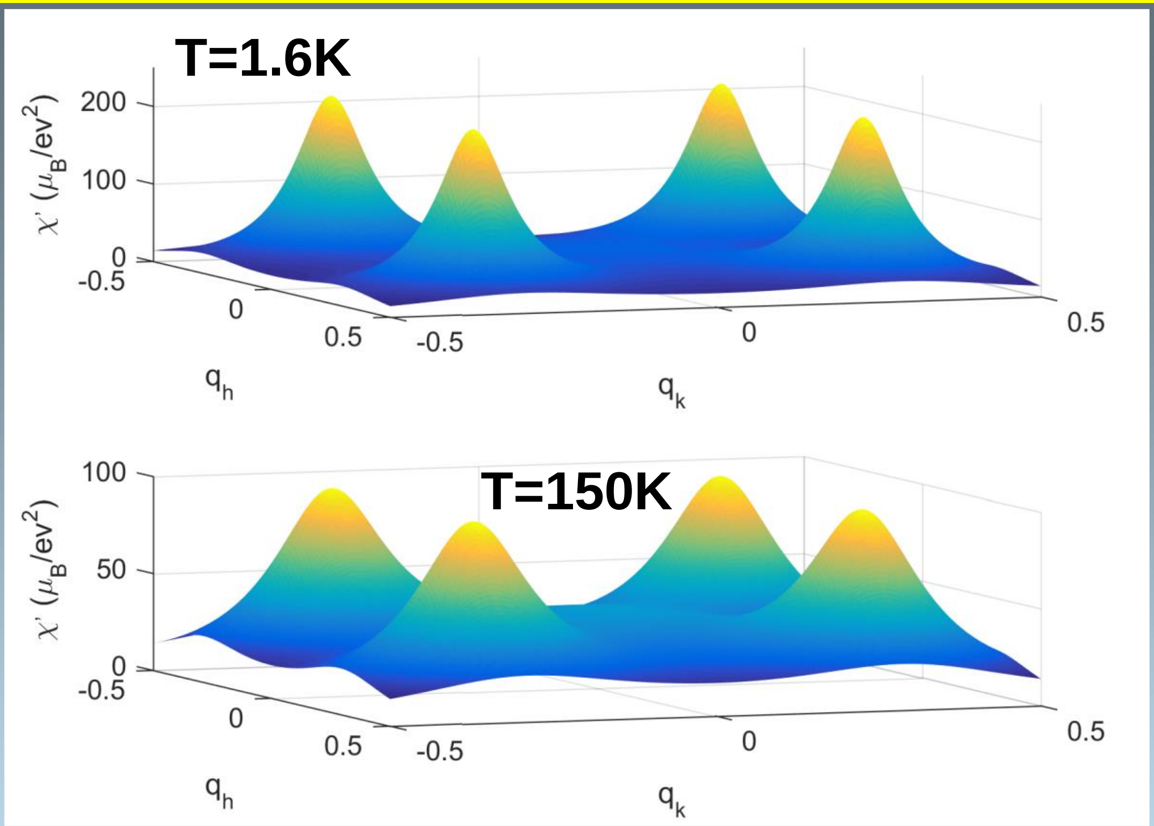
$$\chi_{inc}' = 213\mu_B{}^2/eV \quad \Gamma_{inc} = 11.1meV \quad \xi = 9.7A$$

$$\chi_{fm}' = 22\mu_B{}^2/eV \quad \Gamma_{fm} = 15.5meV \quad W = 0.53\frac{2\pi}{a}$$

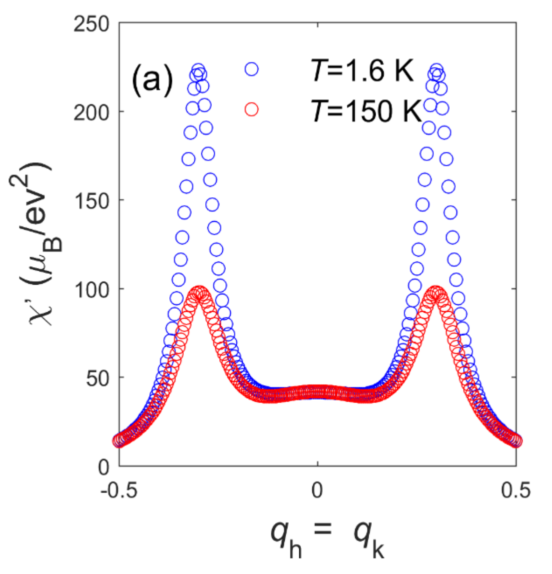
$$\mu_B{}^2/eV \approx 3\cdot10^{-5}emu/mol$$

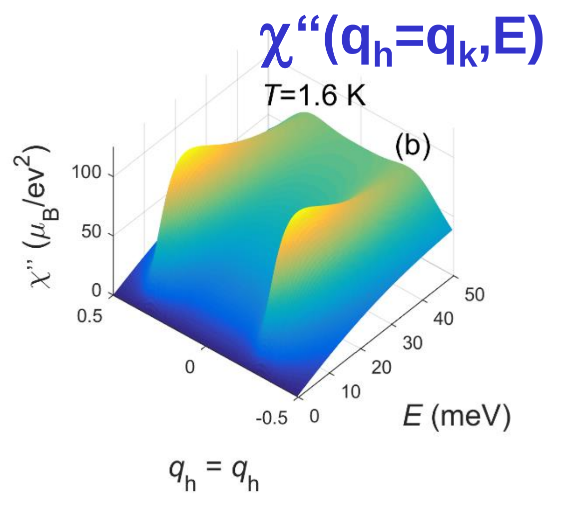
P. Steffens, Y. Sidis, J. Kulda, Z. Q. Mao, Y. Maeno, I. I. Mazin, and M. Braden, Phys. Rev. Lett. **122**, 047004 (2019).

two-component model


T=1.6K

T=150K




$\chi''(q_h=q_k,E)$

agrees with :

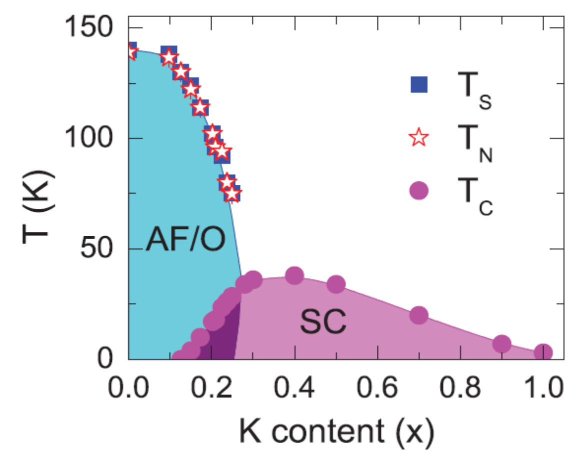
- **susceptibility** ☺
- **NMR-data** ☺
- **specific heat-coefficient** ☺

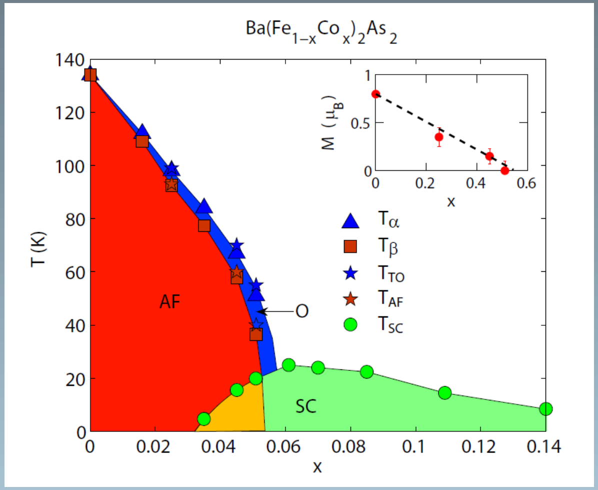
- **FM contribution is sharper than expected**
- **Triplet pairing cannot be explained**

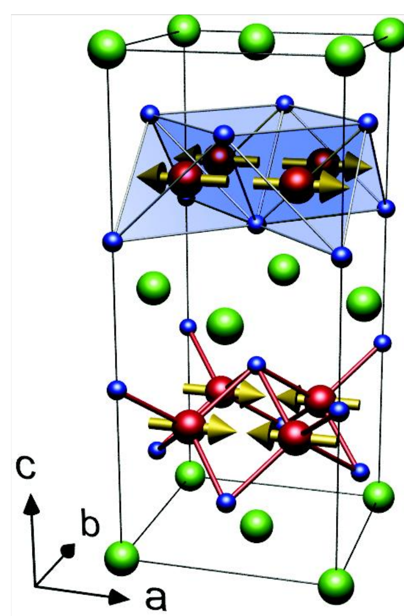
P. Steffens, Y. Sidis, J. Kulda, Z. Q. Mao, Y. Maeno, I. I. Mazin, and M. Braden, Phys. Rev. Lett. **122**, 047004 (2019).

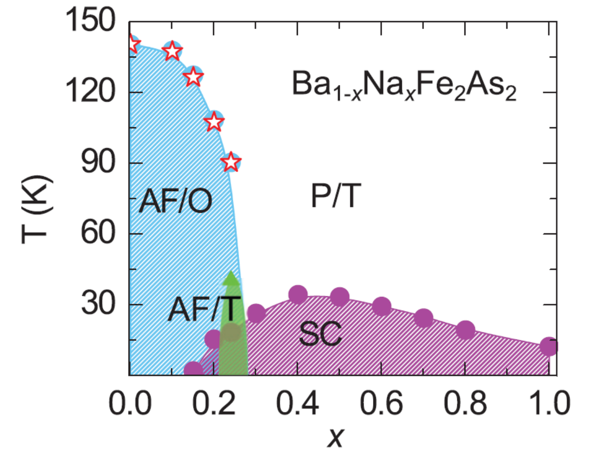
phase diagrams of FeAs superconductors

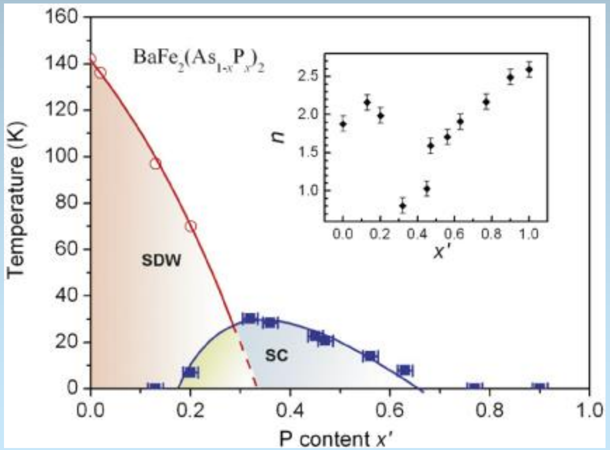
superconductivity appears close to a SDW phase either by doping or by pressure

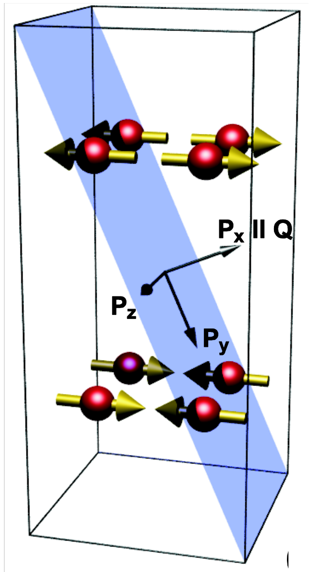








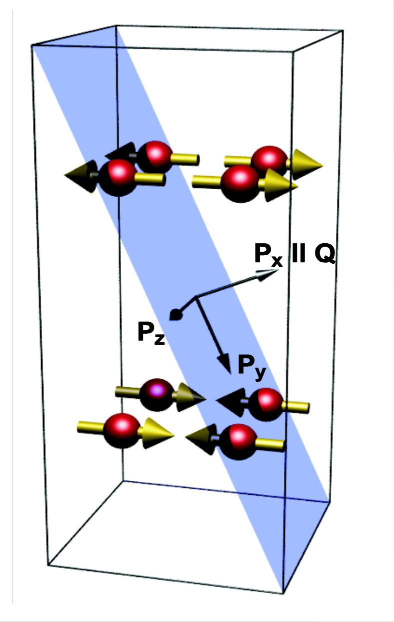


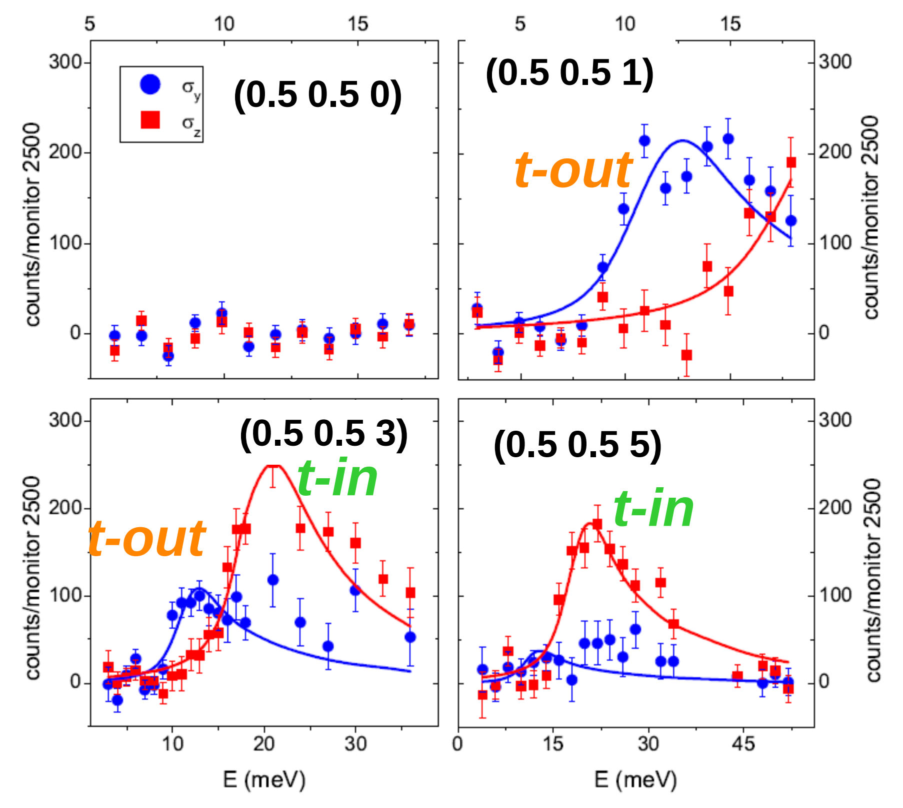


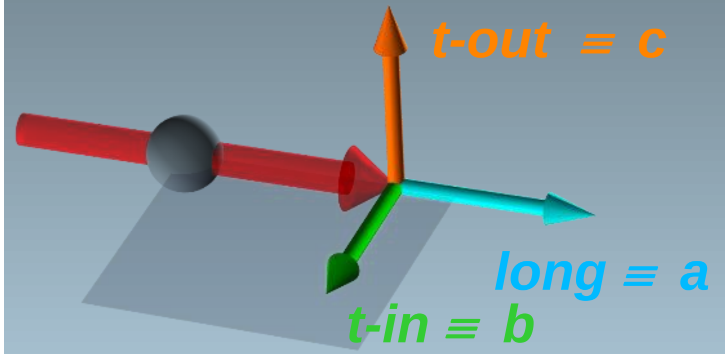
Avci et al., PRB 85, 184507 (2012)
Avci et al., PRB 88, 094510 (2013)

C. Lester et al., RRB 79, 144523 (2009).
S.Jiang et al. JPhConMat 21, 382203 (2009).

Magnetic anisotropy in $BaFe_2As_2$





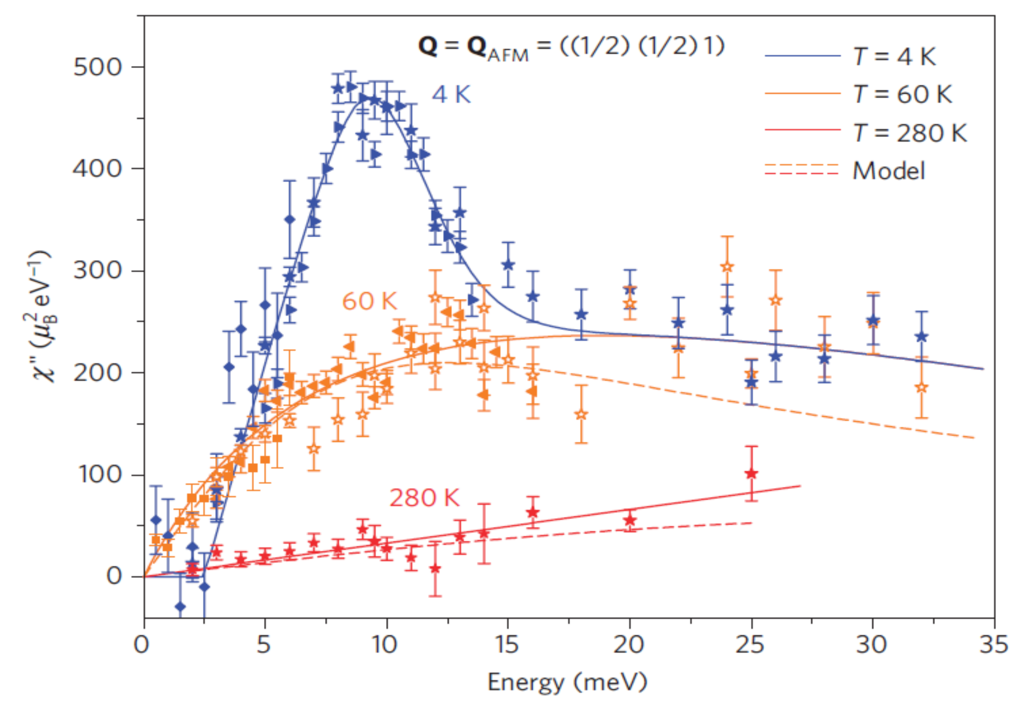


Static moment parallel a ➔ SFz senses the out-of-plane modes
SFy senses the transversal in-plane modes

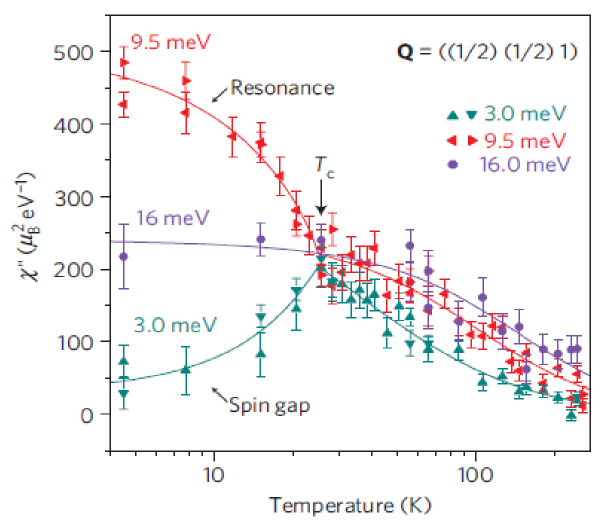
Λ_b=1.16(2)meV Λ_c=0.44(1)meV *N. Qureshi et al.*, ***Phys. Rev. B 86, 060410(R) (2012).***

Resonance mode in SC Ba(Fe/Co)$_2$As$_2$

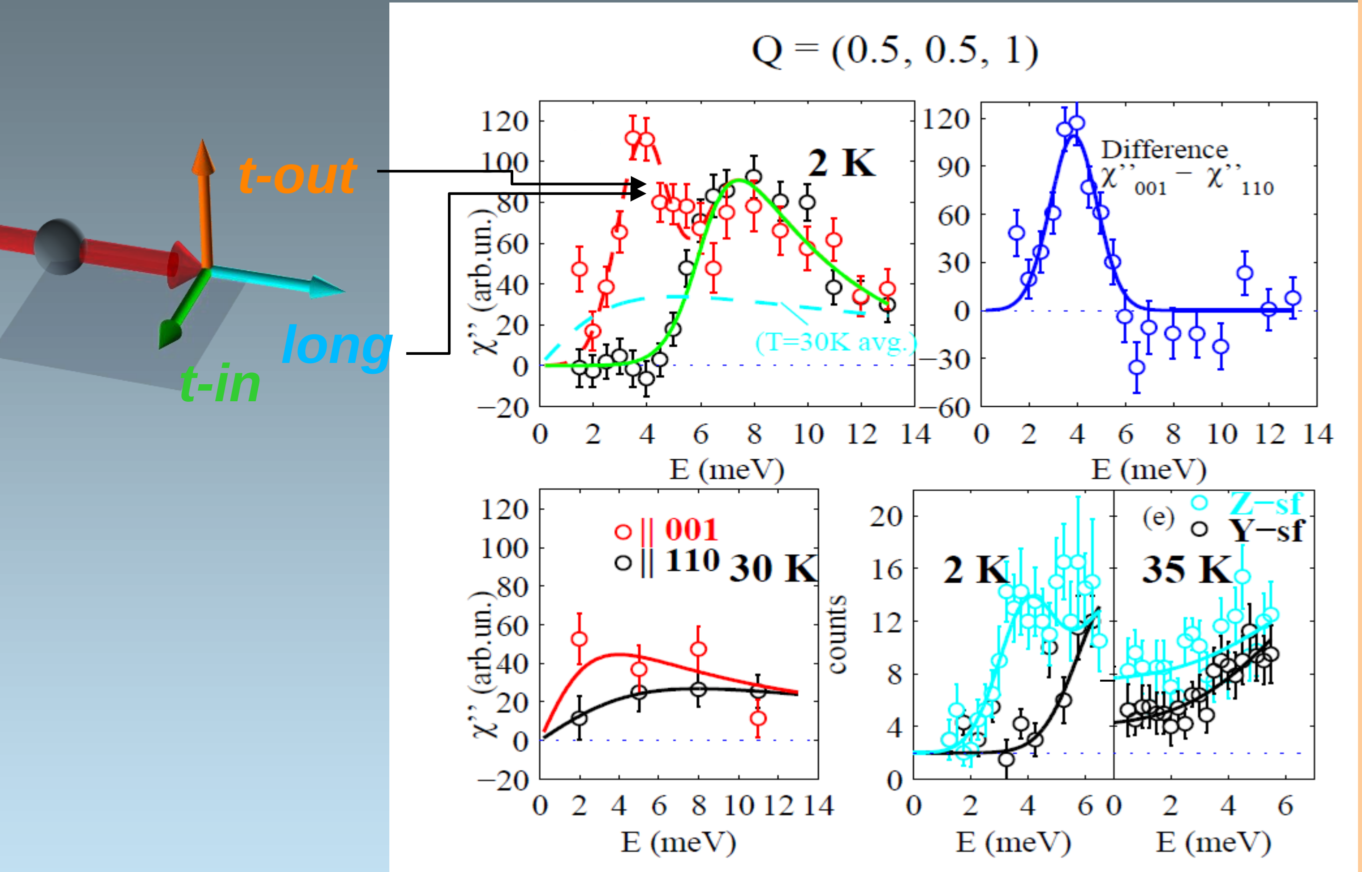
A.D. Christianson et al., Nature 456, 930 (2008).
M. D. Lumsden et al., Phys. Rev. Lett. 102, 107005 (2009).
S. Chi et al., Phys. Rev. Lett. 102, 107006 (2009).
A. D. Christianson et al., Phys. Rev. Lett. 103, 087002 (2009) …



D. Inosov et al., nat. phys. 6, 178 (2010).



Resonance mode in $Ba(Fe_{0.94}Co_{0.06})_2As_2$



Co-doped $BaFe_2As_2$

x=0.06 opt. doped T_c=24K

Steffens et al., Phys. Rev. Lett. **111**, 107006 ('13); Waßer et al., Sci. Rep. **7**, 10307 (2017)

Ni-doped $BaFe_2As_2$

x=0.048 opt. doped T_c=19.8K

H. Luo et al., Phys. Rev. Lett. **111**, 107006 ('13).

K-doped $BaFe_2As_2$ x=0.33 T_c=38K

Chenglin Zhang et al.,
Phys. Rev. B **87**, 081101 (2013).

K-doped $BaFe_2As_2$ x=0.50 T_c=36K

N. Qureshi et al.,
Phys. Rev. B **90**, 100502(R) (2014).

Co-doped NaFeAs

C. Zhang *et al.*, *Phys. Rev. B* **90**, 140502(R) (2014). *Phys. Rev. Lett.* **111**, 207002 (2013).

LiFeAs

N. Qureshi et al.,
Phys. Rev. B **90**, 144503 (2014).

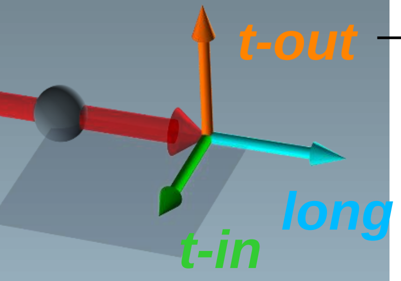
Na-doped $BaFe_2As_2$ x=0.39 T_c=29K

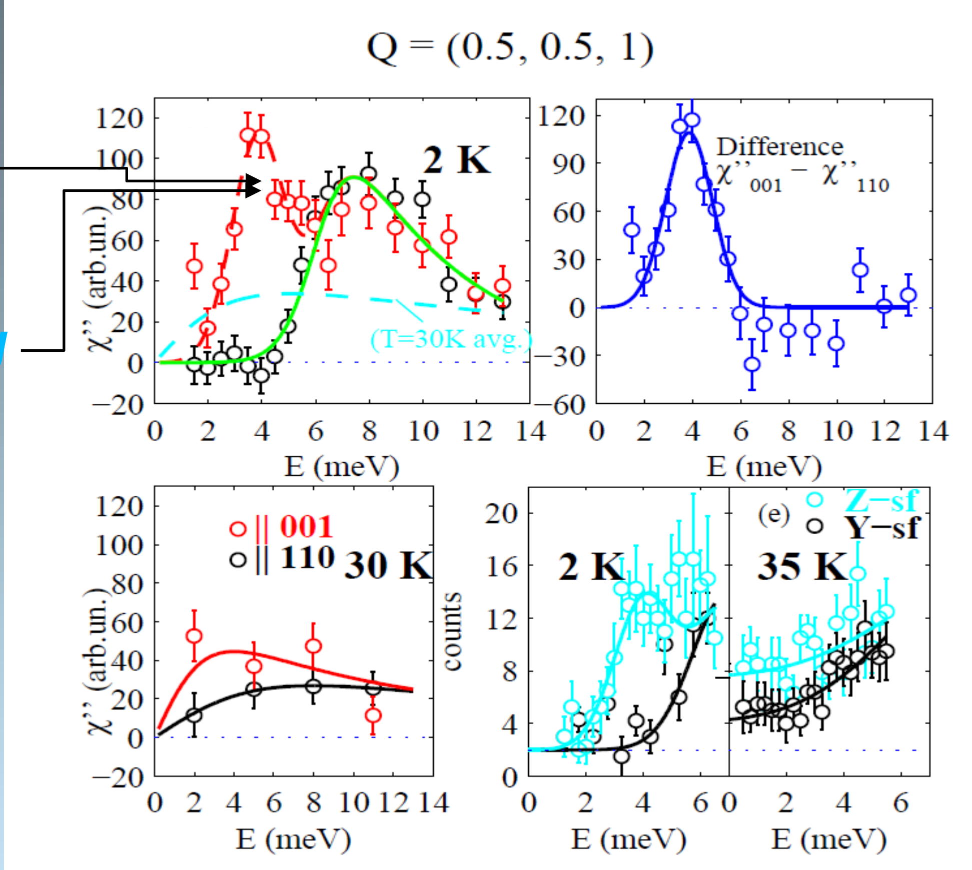
F. Waßer et al., npj QM **4**, 59 (2019)

P. Steffens et al., Phys. Rev. Lett. 110, 137001 (2013)

- **resonance mode is split : extra low-E anisotropic mode in long & t-out**
- **similarity with parent compound: transversal in-plane is hard direction!**

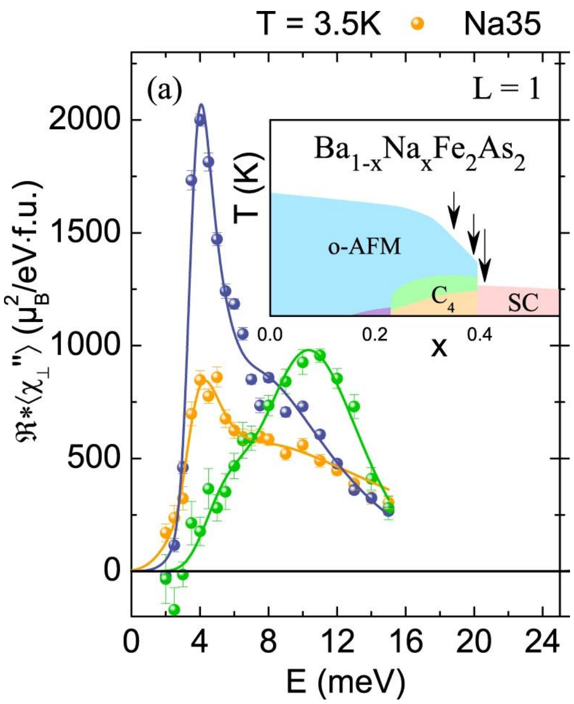
Resonance mode in $Ba(Fe_{0.94}Co_{0.06})_2As_2$





$Ba_{0.61}Na_{0.39}Fe_2As_2$

T_c=29K



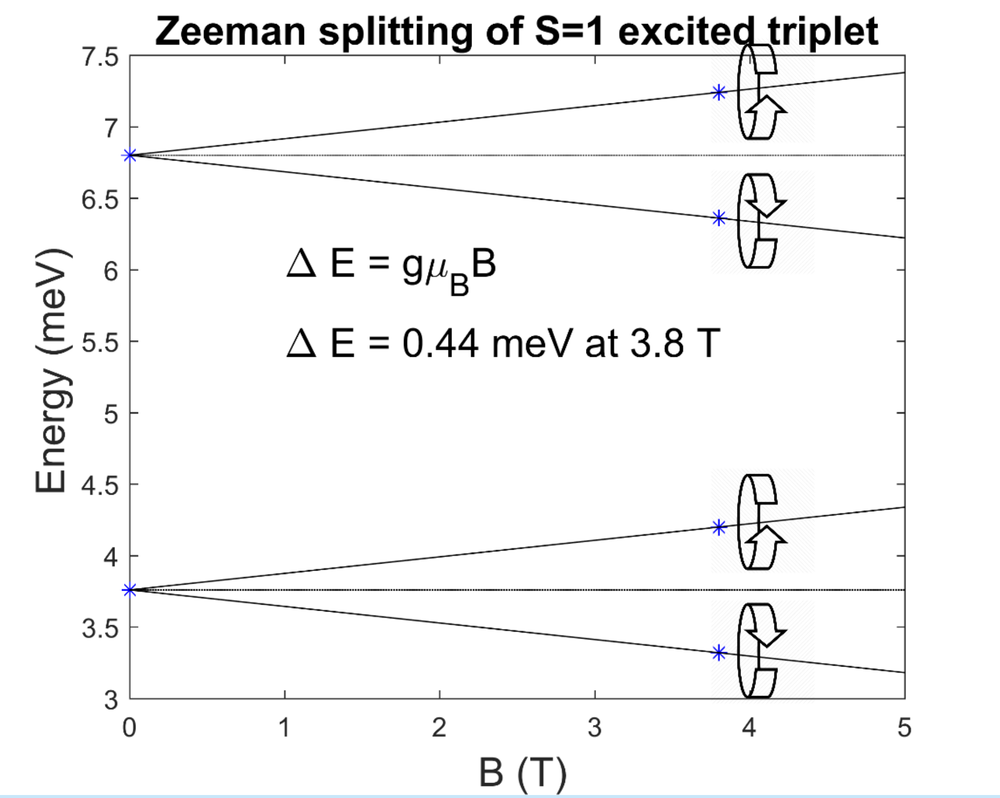
F. Waßer et al., npj QM **4**, 59 (2019)

P. Steffens et al., Phys. Rev. Lett. 110, 137001 (2013)

- **resonance mode is split : extra low-E anisotropic mode in long & t-out**
- **similarity with parent compound: transversal in-plane is hard direction!**

Chirality in $Ba(Fe_{0.94}Co_{0.06})_2As_2$

What is the character of the two SRM's? Singlet – triplet exciton ?



horizontal cryomagnet @ ILL
compatible with neutron polarization analysis

Conclusions

polarized inelastic neutron scattering can

- quantitatively detect broad quasiferromagnetic fluctuations in Sr_2RuO_4
- reveal magnetic anisotropy in AFM $BaFe_2As_2$
- show split and anisotropic spin-resonance modes in FeAs-based superconductors

There is an urgent need for more powerfull instrumentation!

Thanks for the attention!