



MAX-PLANCK-GESELLSCHAFT



Three axis spin echo - examples from TRISP

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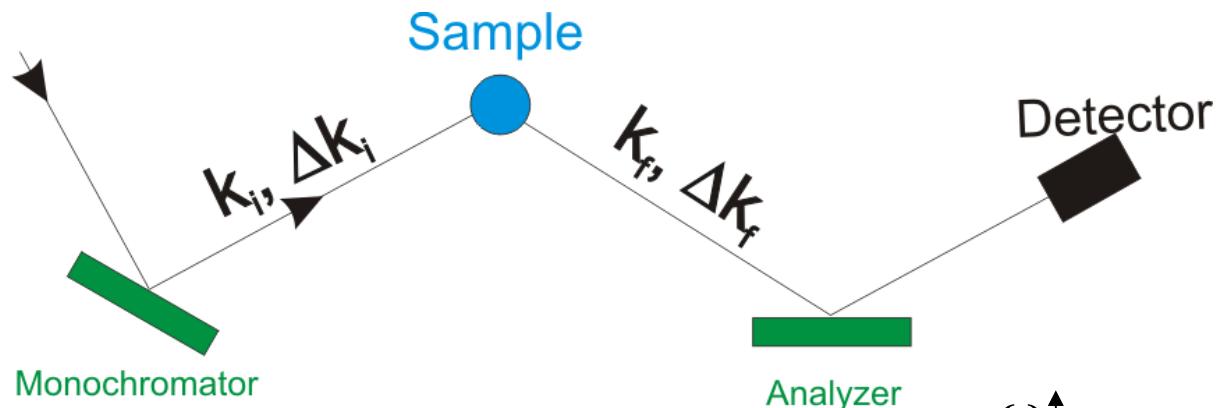
outline



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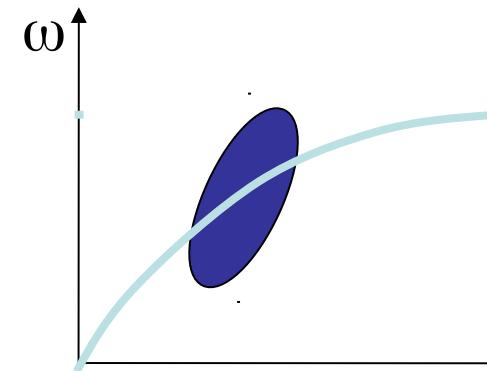
- basic principles of spin-echo TAS
- phonon lifetimes in elemental superconductors
- magnon lifetimes, critical scattering
- high resolution diffraction (Larmor diffraction)

conventional triple axis spectrometer



$$\hbar\omega = \frac{\hbar^2}{2m} (\mathbf{k}_i^2 - \mathbf{k}_f^2)$$

$$\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$$



excitation energy: <100meV

energy resolution: typ. 10%

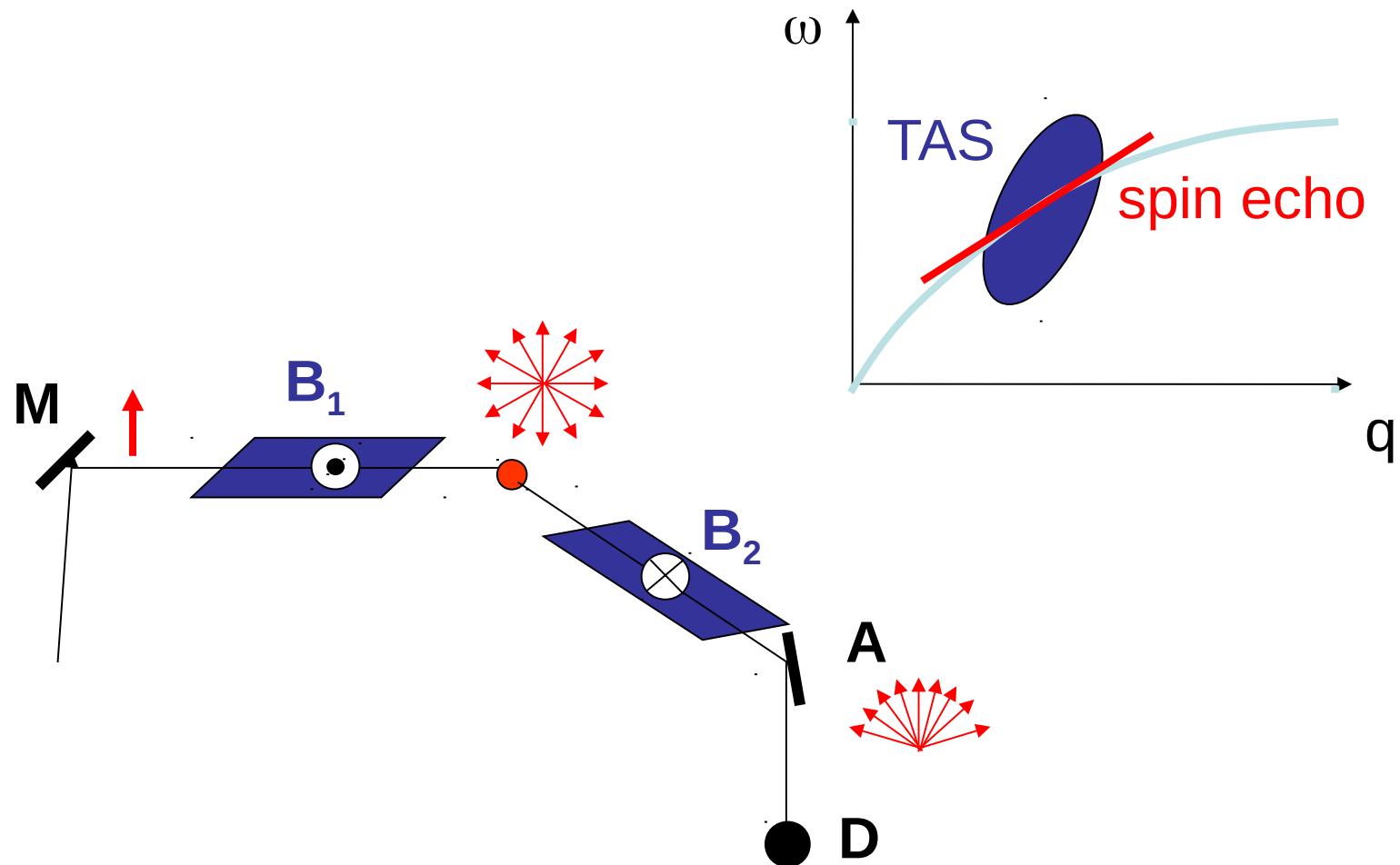
resolution $\sim 1/\text{intensity}$

-> not sufficient to resolve linewidths

solution Mezei 1977: spin echo + TAS tilted coil technique



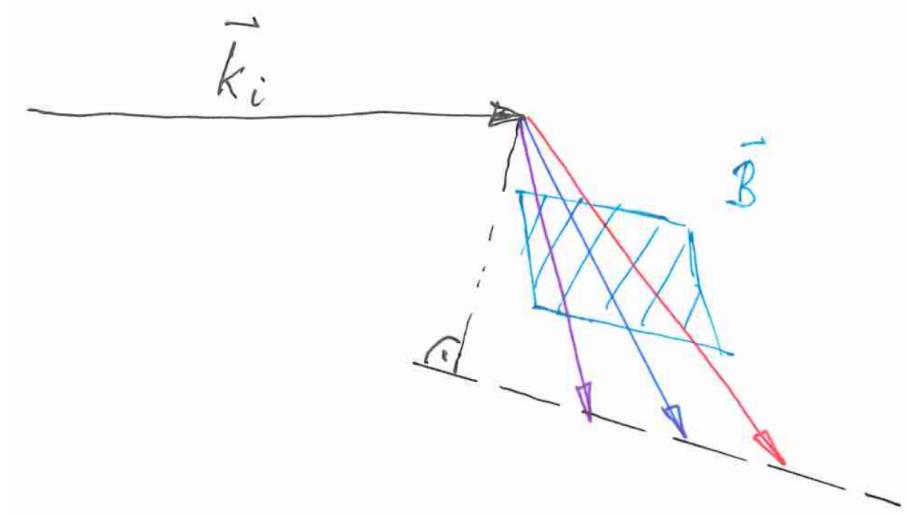
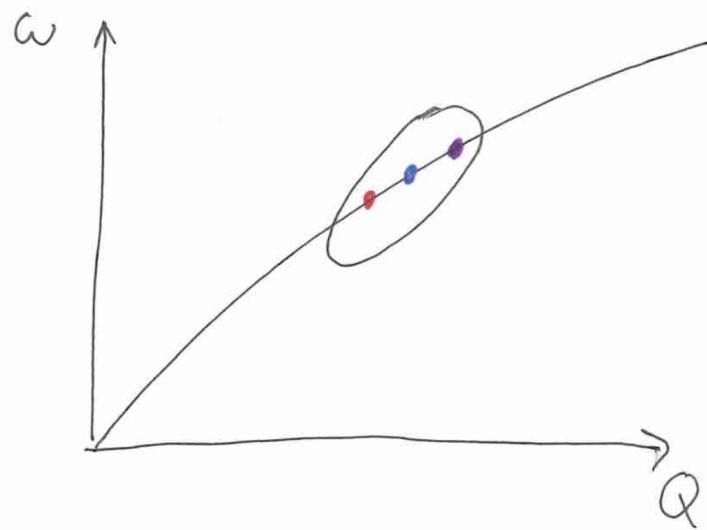
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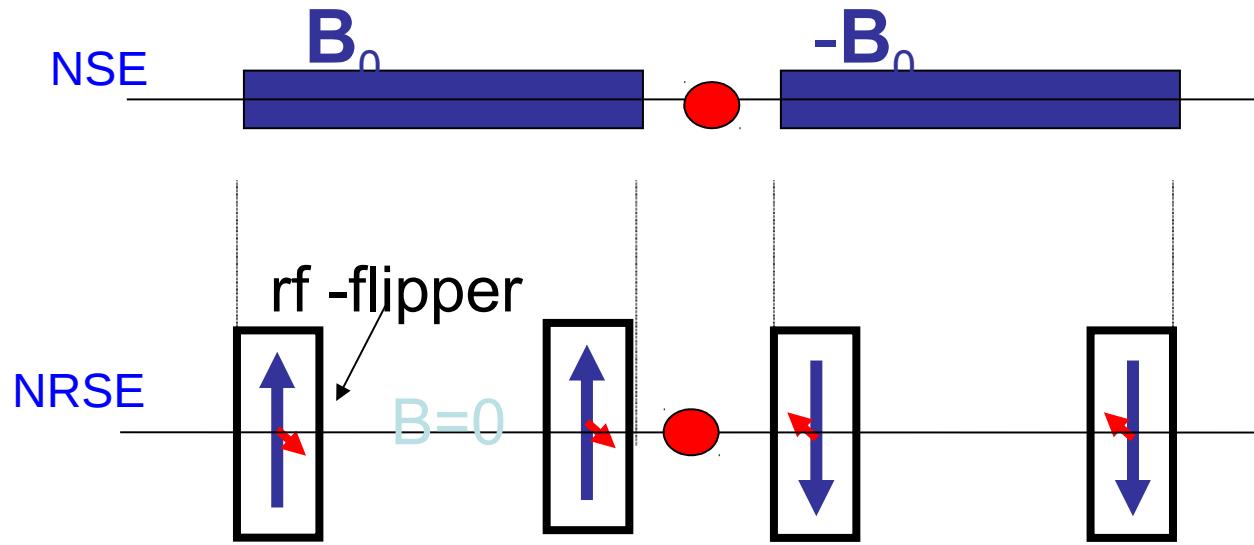
focusing I - Pynn picture



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NRSE (neutron resonance SE)



+ NRSE:

- precise field boundaries (windings of rf -flipper)
- high stability (RF oszill. vs. large DC coil)
- no stray fields (*bootstrap* coils)
- mu-metal shield possible
- dispersive excitations (phonons, magnons)
-

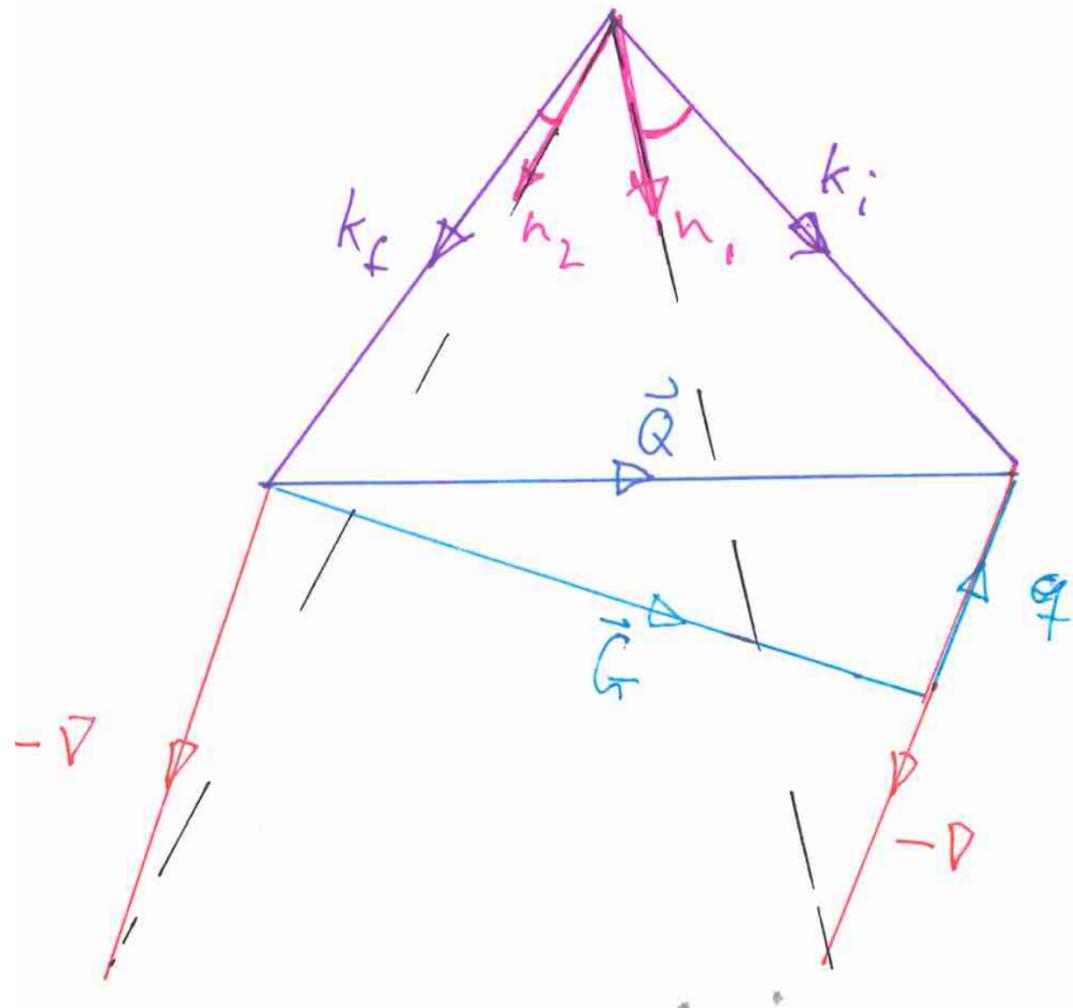
+ NSE:

- better resolution for quasielastic small Q
- multidetector setups



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focusing II - scattering triangle



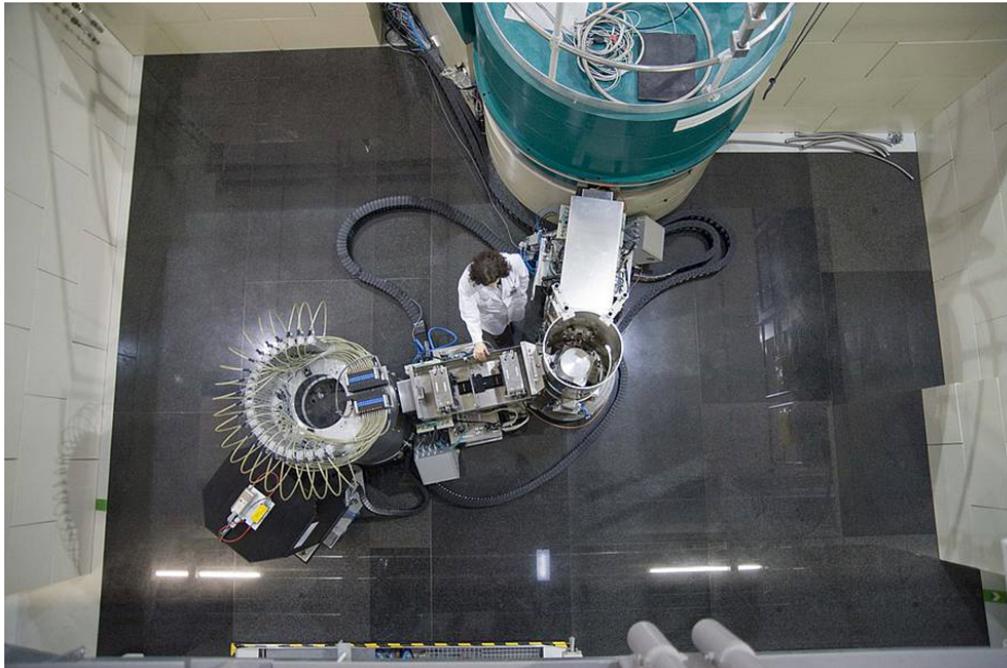
$$\vec{n}_i \parallel \vec{k}_i - \frac{d\omega}{dq}$$

$$\vec{n}_f \parallel \vec{k}_f - \frac{d\omega}{dq}$$

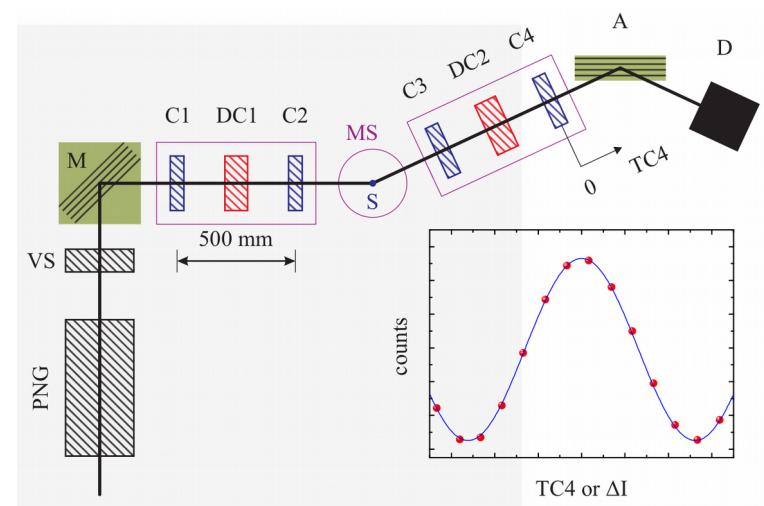
TAS spin-echo and Larmor diffraction



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thermal $E = 0.4 - 60 \text{ meV}$
resolution $1-10 \mu\text{eV}$
LD mode: $\Delta d/d \sim 10^{-6}$



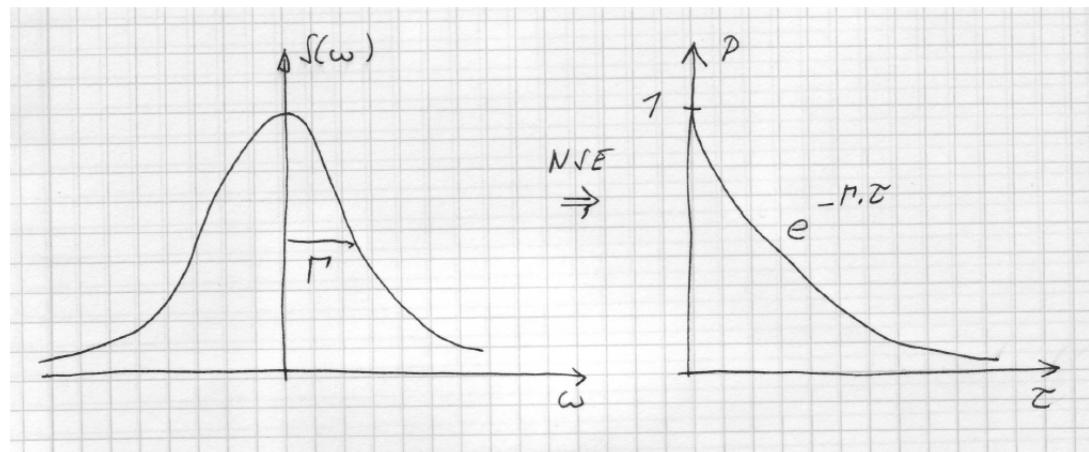
spin echo polarization



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$$P(\tau) = P_{\text{res}} \times \cos(\omega_0 \tau) \times \int S(\omega) \cos(\omega \tau) d\omega$$

Lorentzian: $S(\omega) = \frac{1}{\pi} \cdot \frac{\Gamma}{\Gamma^2 + \omega^2}$ $P(\tau_{\text{NSE}}) = \exp(-\Gamma \cdot \tau_{\text{NSE}})$



$$P = \frac{1}{N} \int \exp\left(-\frac{1}{2} \tilde{\mathbf{J}}^T \tilde{\mathbf{L}}_I \tilde{\mathbf{J}}\right) d\tilde{J}_n \\ \times \int S(\omega) \exp(-i\tau\Delta\omega) d\Delta\omega + \text{c.c.}$$

resolution matrix includes:

- TAS resolution (Popovici)
- sample mosaic, d-spacing spread
- curvature of dispersion sheet

missing:

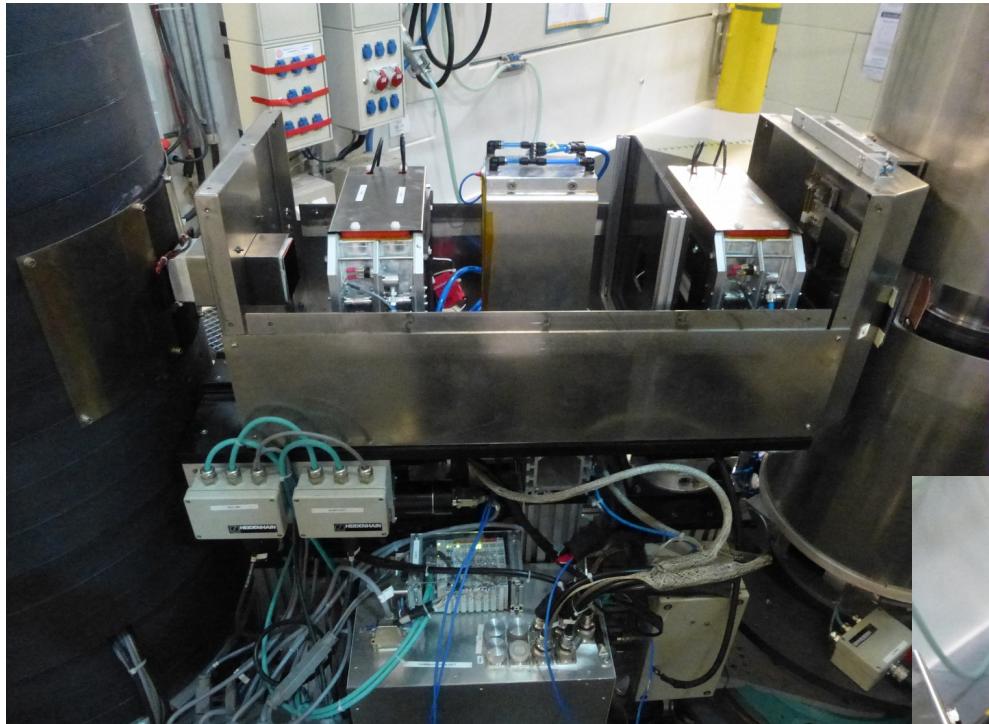
detuning, mode splitting, several branches

Habicht, J. Appl. Cryst. 36, 1307 (2003)

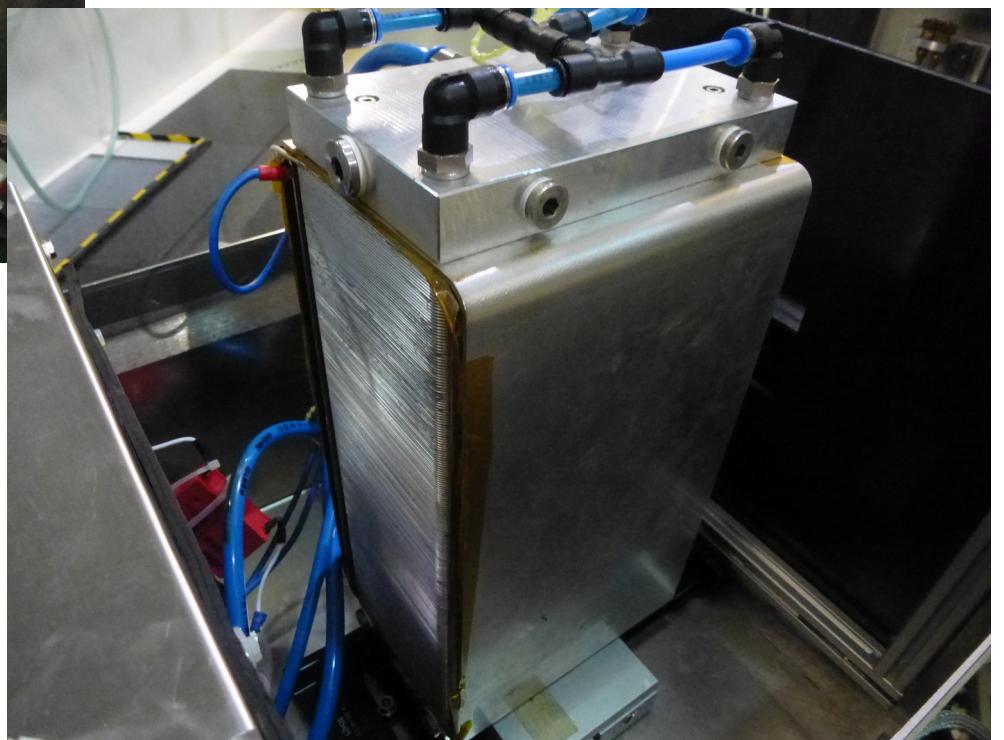


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coils

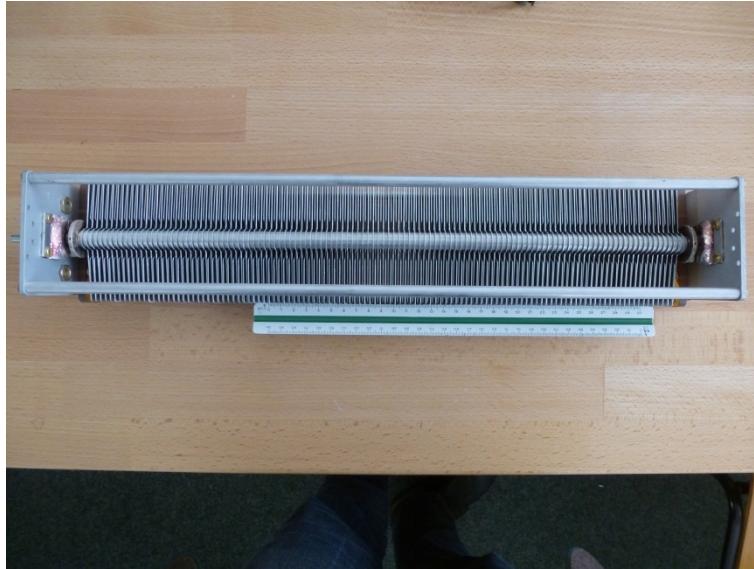
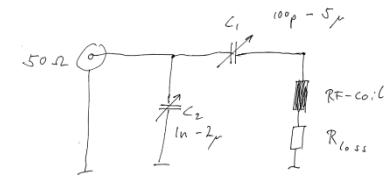
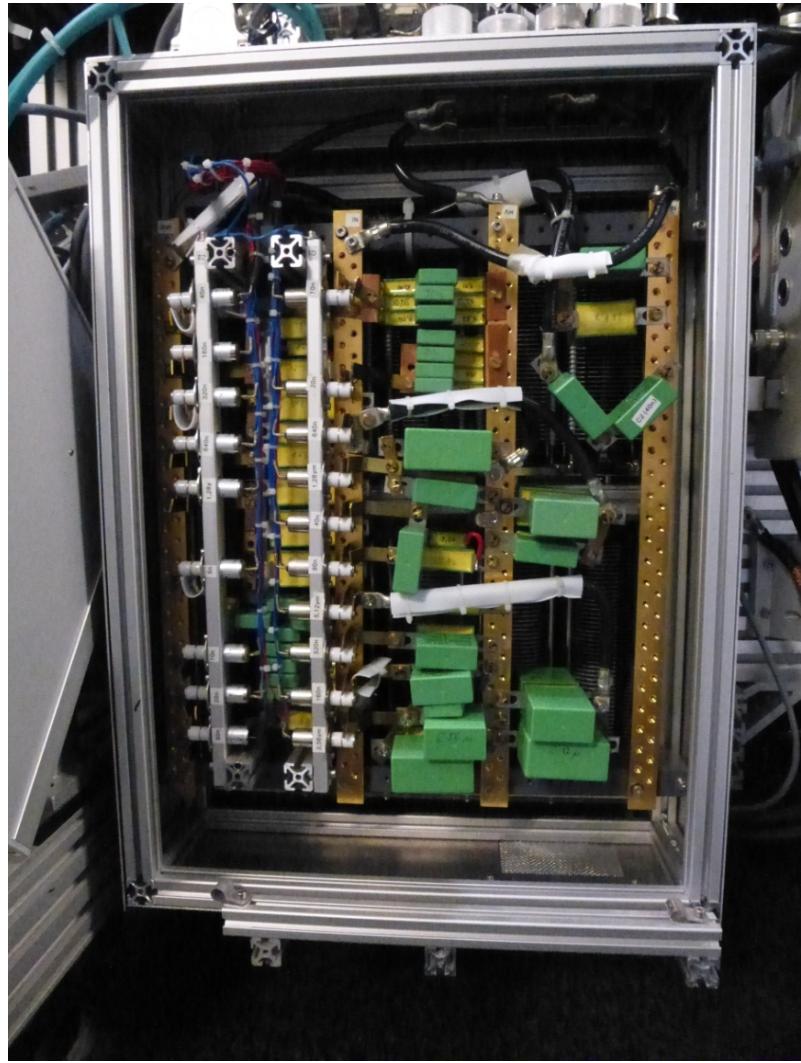


small τ DC coil



RF flippers

impedance matching



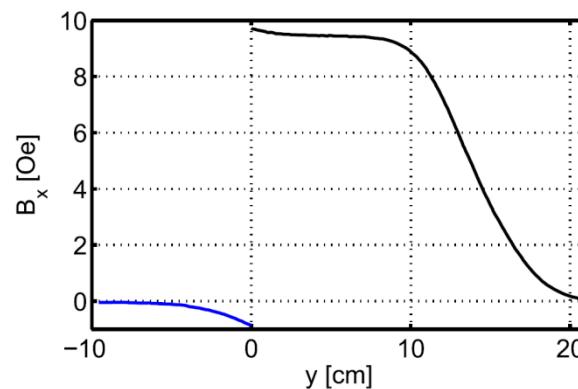
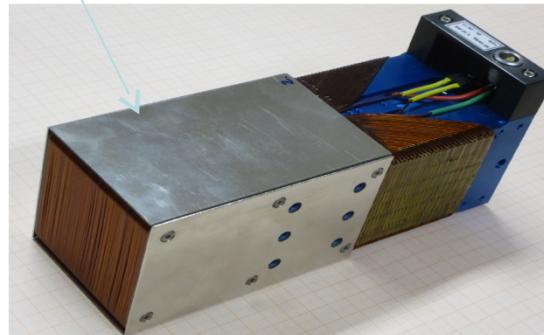
coupling coil



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mu-metal yoke (design Felix Groitl)



1mm wire, 0.7A

sample space



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mu-metal connection (movable) from box
to sample cylinder

sample space



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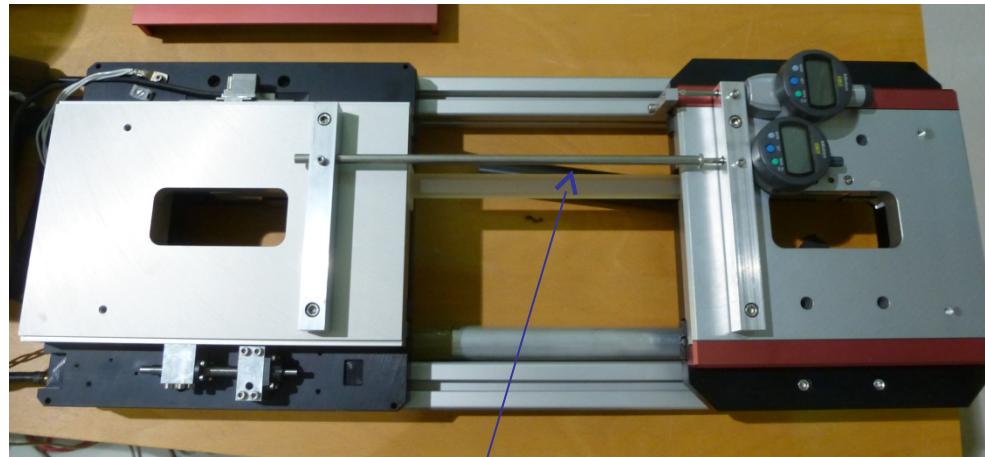
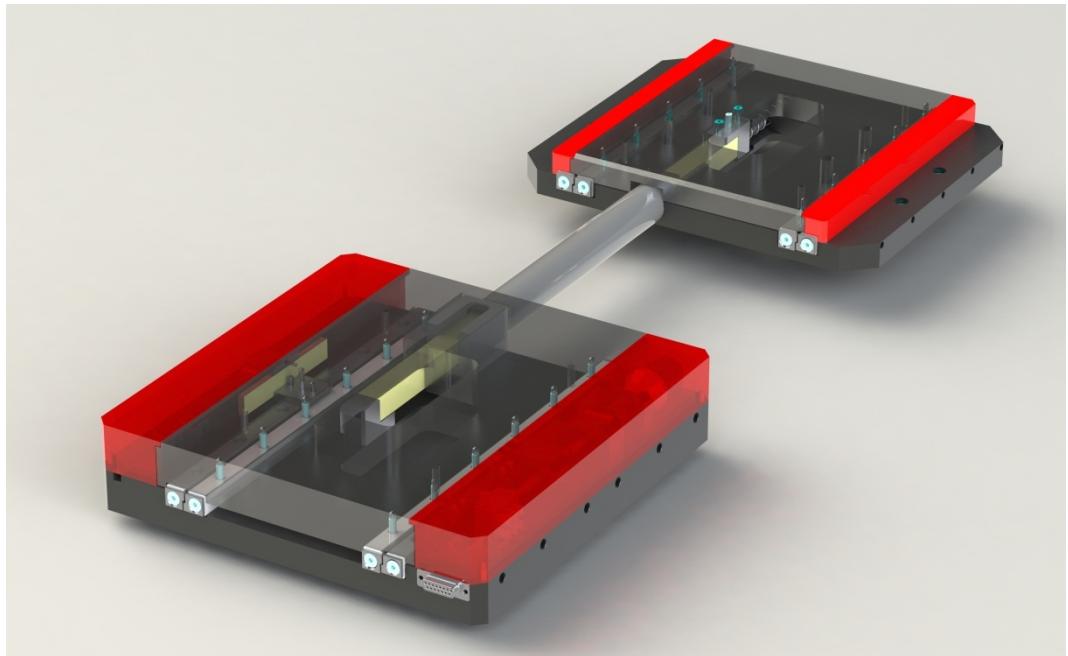
compensation coil for
longitudinal field on
mu-mutual chimney



3-D fluxgate (*Stefan Mayer*)
on telescope cylinder



rotation + simple goniometer



thermal drift compensation

Zerodur



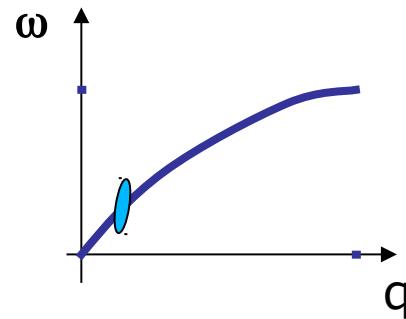
motivation

- e-p interaction -> cooper pairs in BCS theory
- pioneering TAS experiments by Shapiro et al. (Nb, Nb₃Sn)
- *ab-initio* calculations

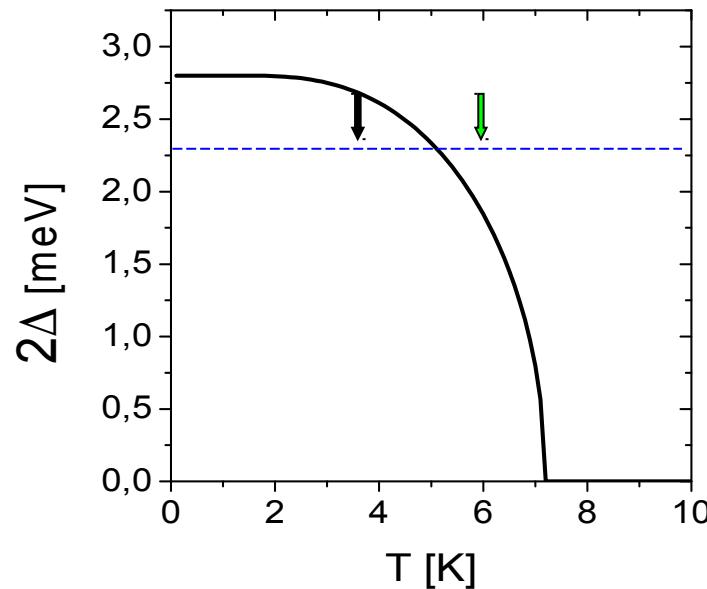
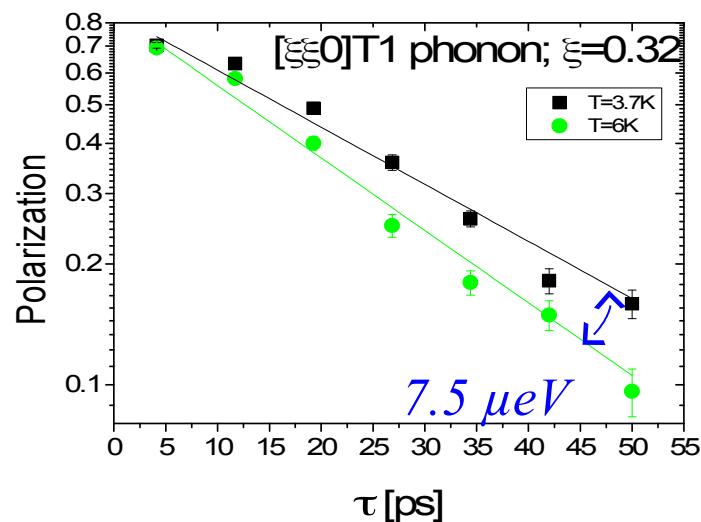
method (Shapiro): how to separate e-p interaction

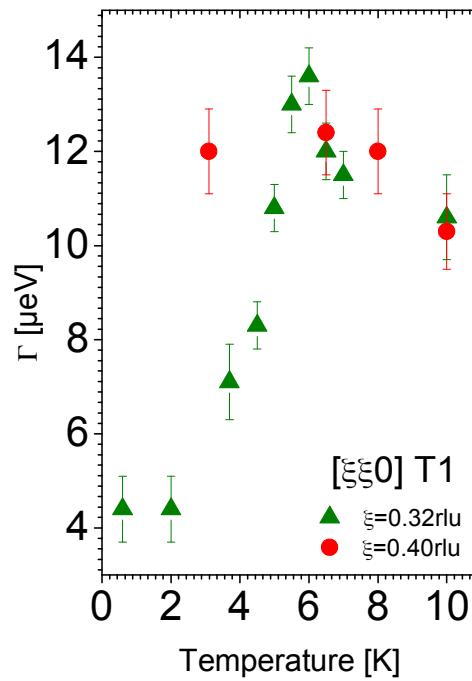
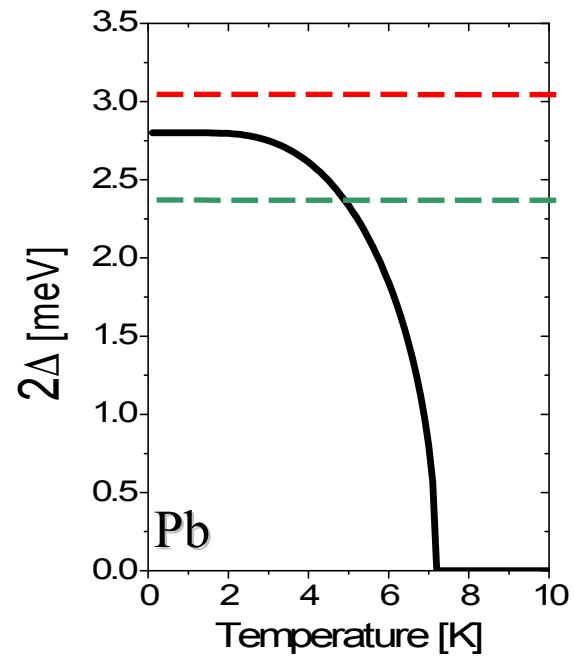


Pb



spin-echo



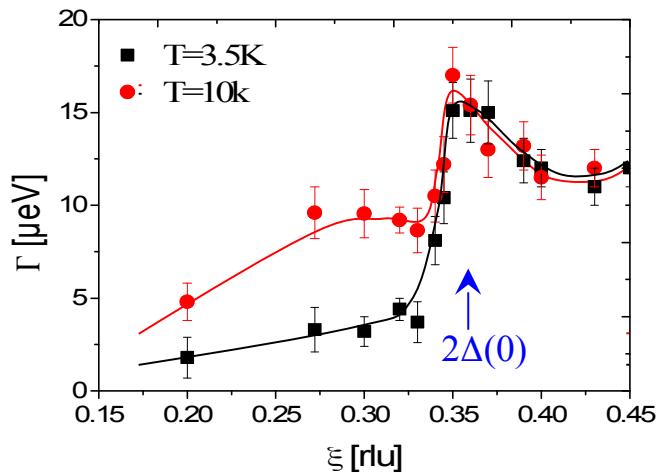


anomaly at 2Δ above Tc

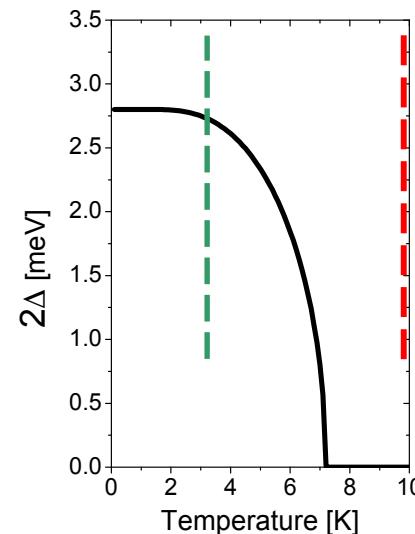
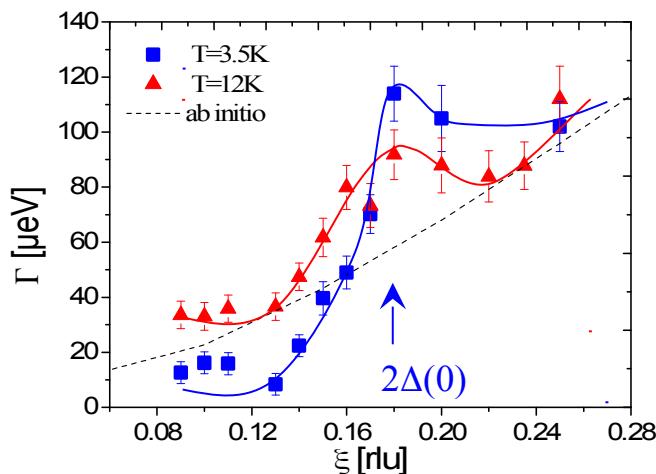


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Pb [110]T1



Nb [100]T

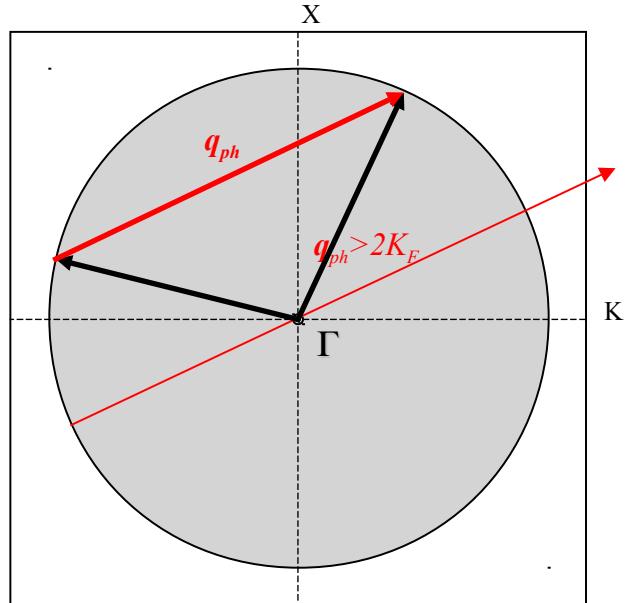


Pb

Aynajian et al., Science 319, 1509 (2008)



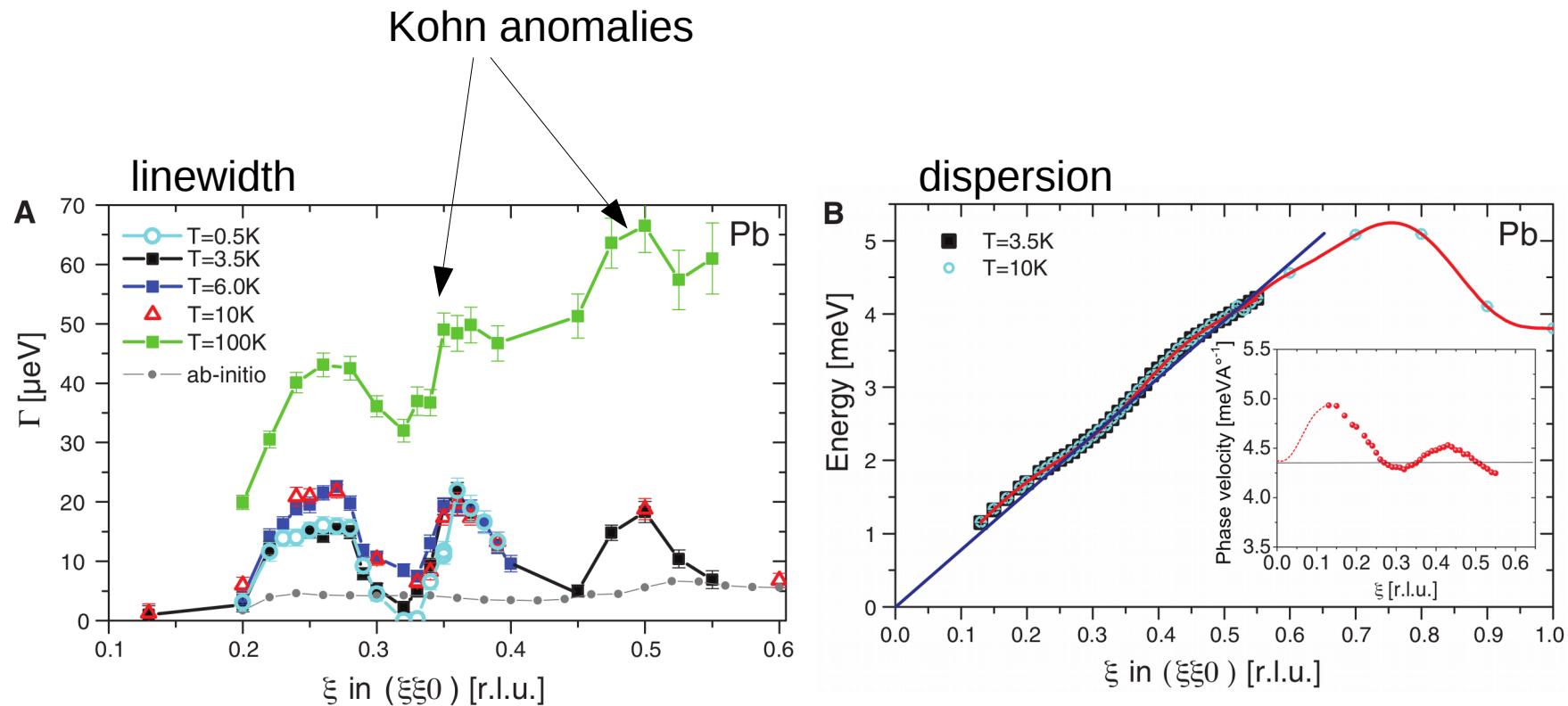
Kohn anomaly



Kohn anomaly

$$|q_{ph} + K| = 2k_F$$

Kohn anomaly limits 2Δ ?

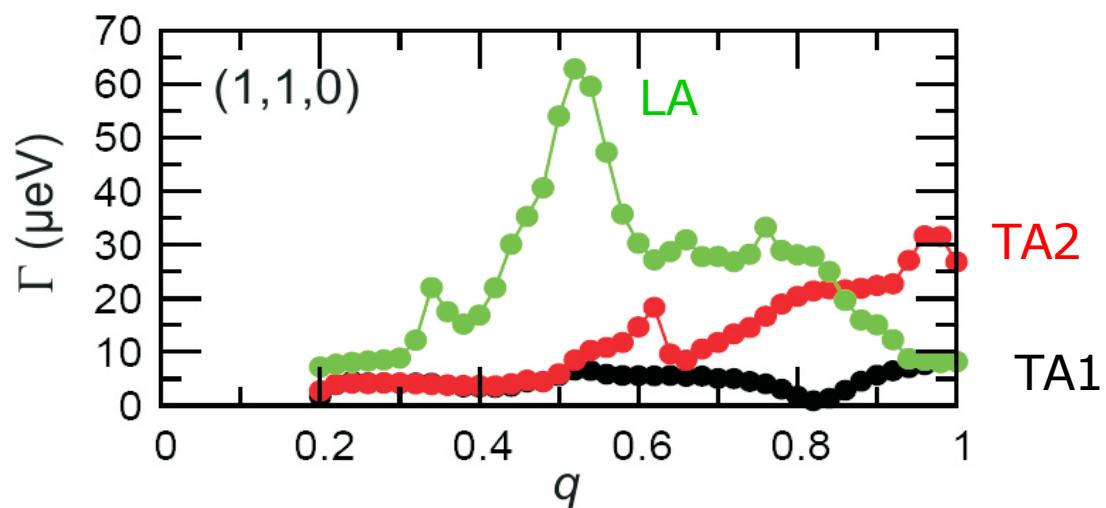


Aynajian et al., Science 319, 1509 (2008)

Pb linewidths ab initio (LDA)



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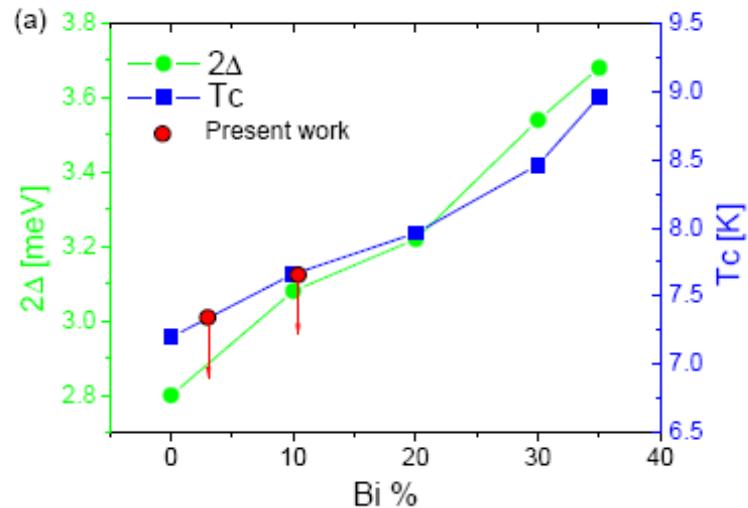


- LDA calculations predict Kohn anomalies for LA, but not TA modes

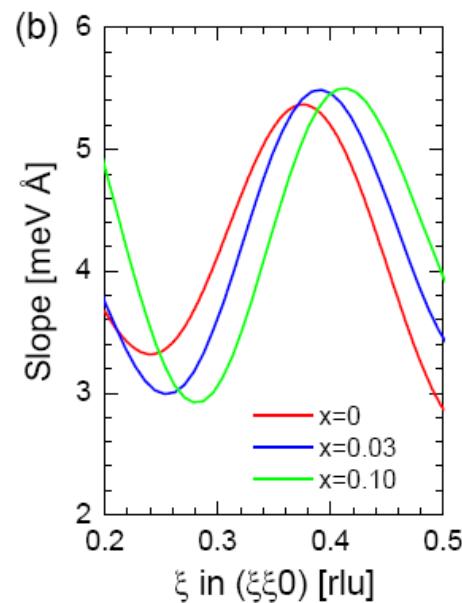
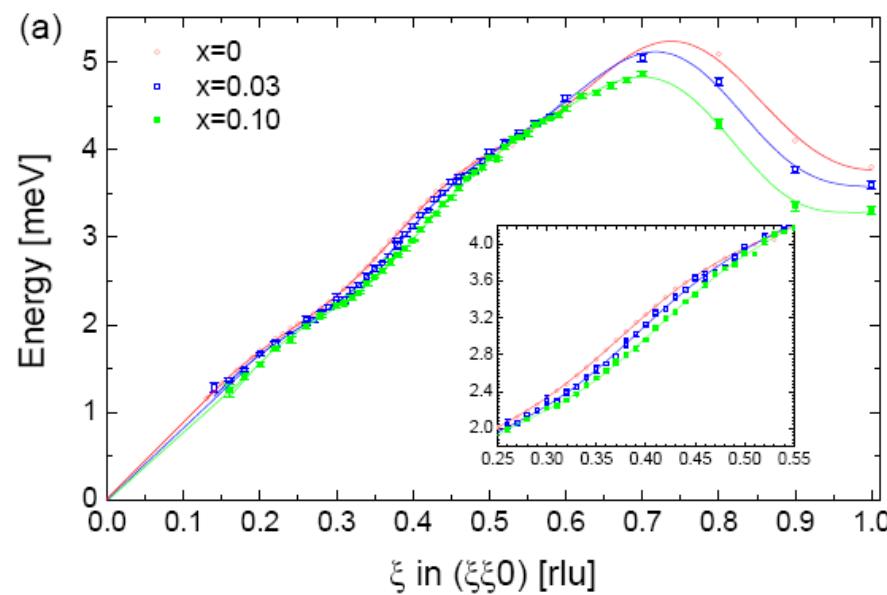
PbBi alloy



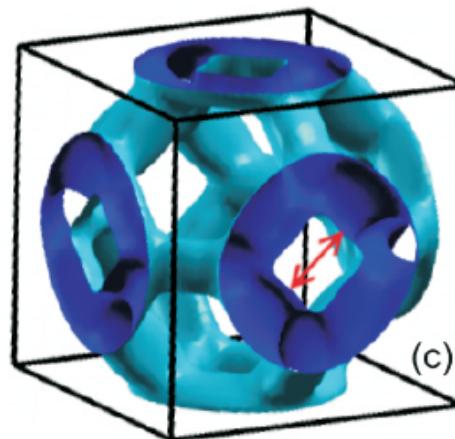
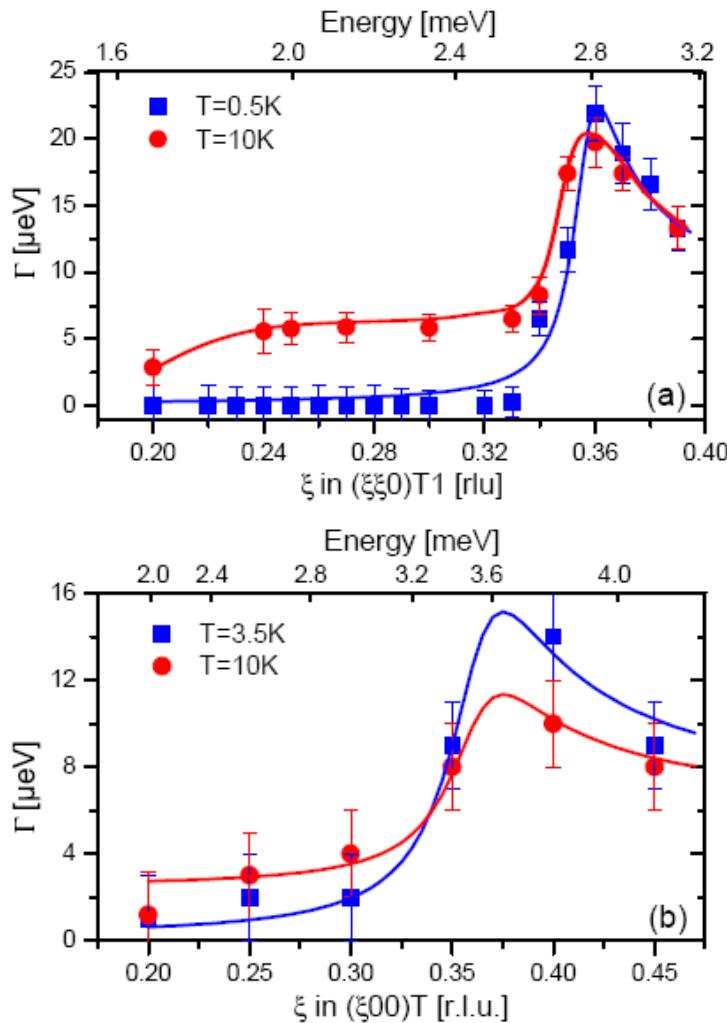
MAX-PLANCK-GESELLSCHAFT



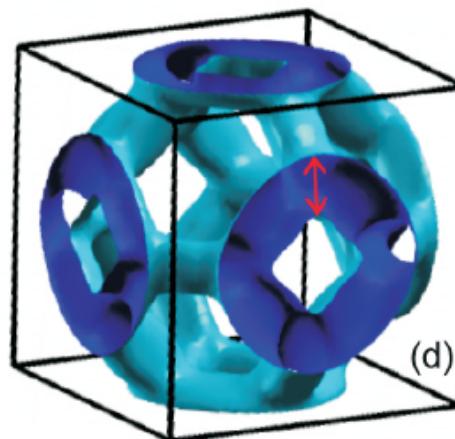
anomaly locked to 2Δ



Gap anisotropy (Pb)



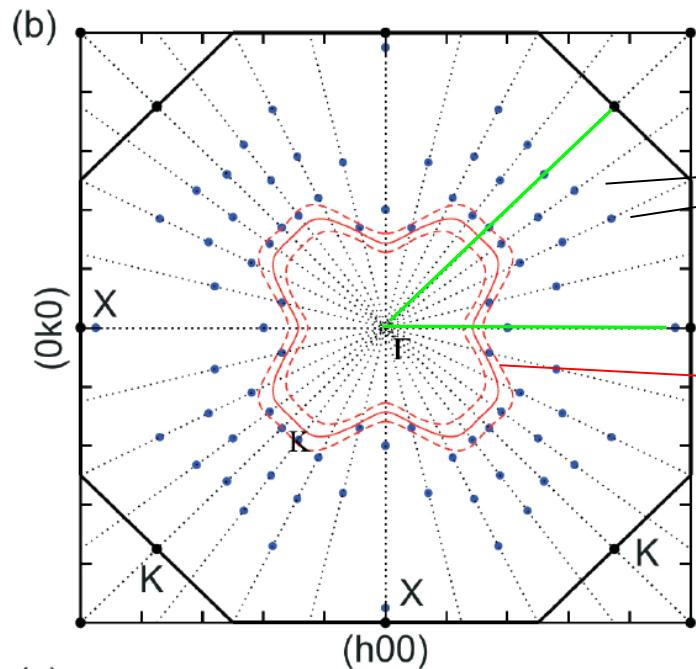
along (110)
 $2\Delta = 2.8 \text{ meV}$



along (100)
 $2\Delta = 3.6 \text{ meV}$

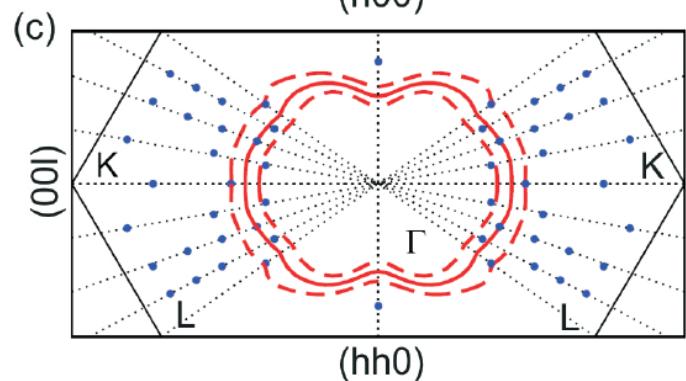
lock-in to Kohn anomaly generates 20% gap anisotropy

Kohn anomaly surface (LDA)



computed Kohn anomalies

tunneling gap (2.8 meV) \pm 10 %



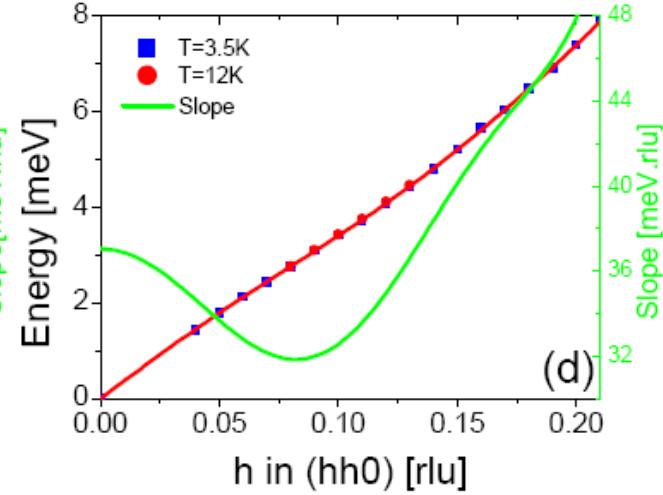
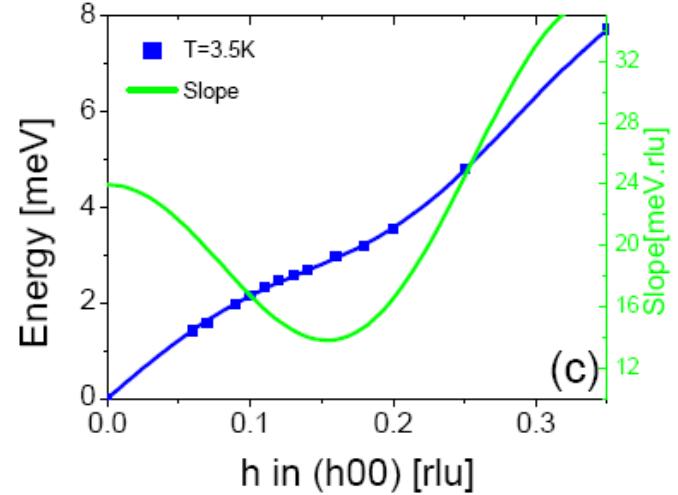
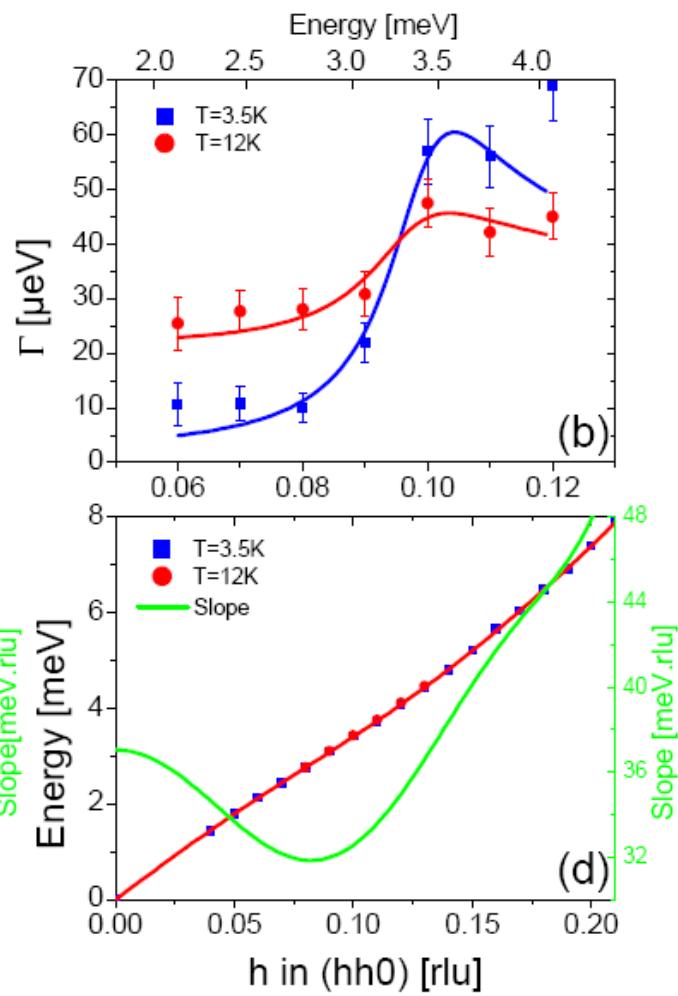
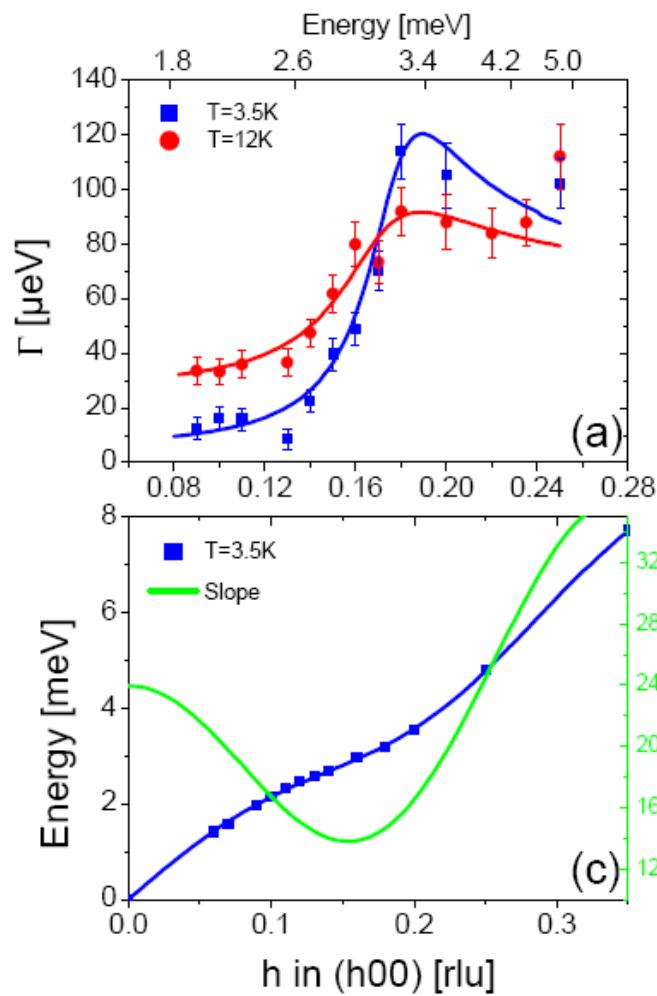
locking $2\Delta(\mathbf{q}) < - >$
lowest-energy Kohn anomaly

-> $\Delta(\mathbf{q})$ can be obtained by
geometrical construction

Niobium

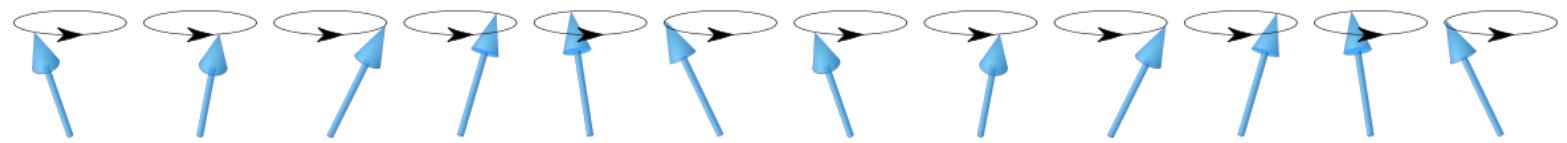


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smaller gap anisotropy, same coincidence

spin excitations

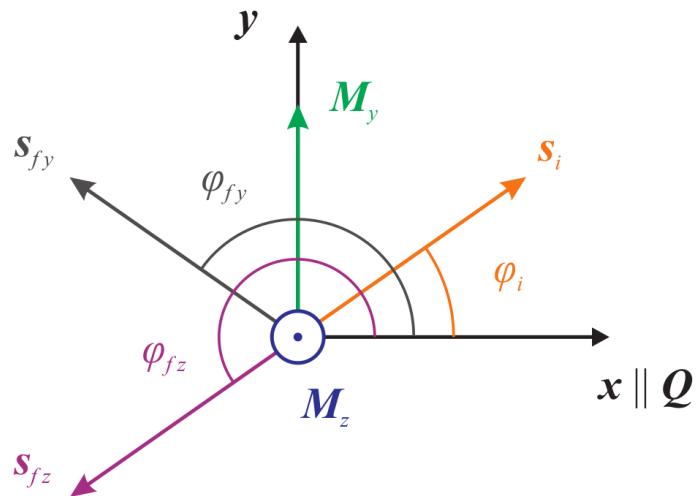


selection rule:

- scattering only by spin fluctuations $\perp \mathbf{Q}$
- pi-flip around fluctuation

spin-echo on spin excitations

-> spin flips at the sample



$$\phi_2 = \pi - \phi_1$$

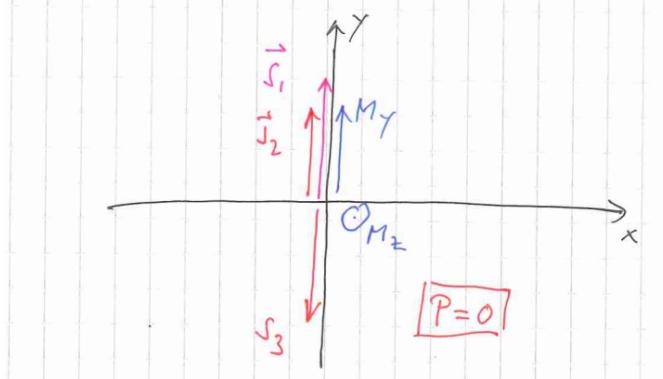
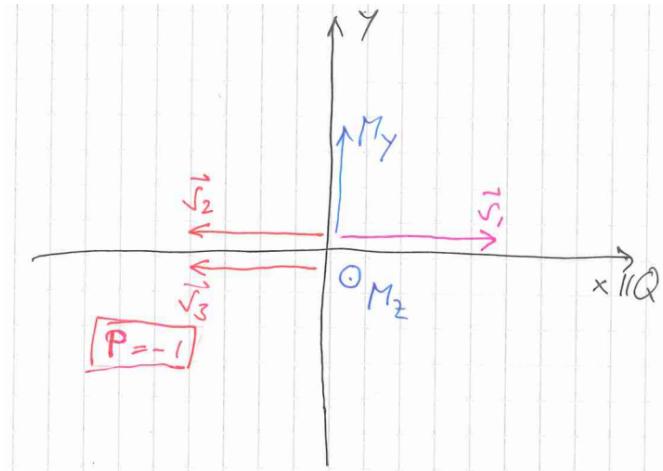
minus sign acts like pi-flipper -> parallel fields

$$\phi_3 = \pi + \phi_1$$

-> conventional case, antiparallel fields
additional pi phase shifts echo group



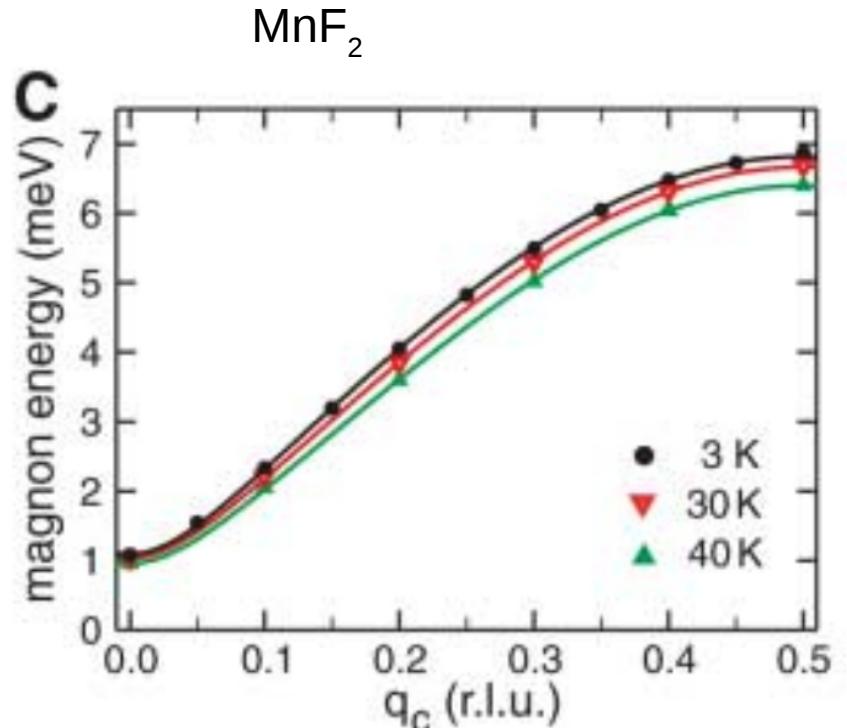
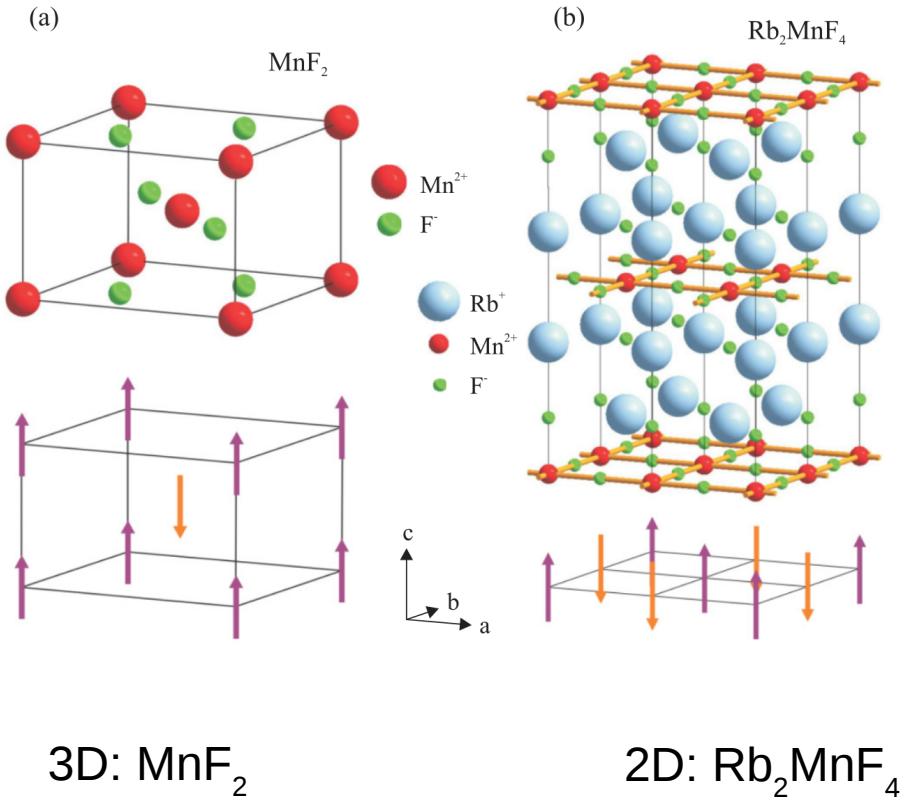
mixing M_y and M_z



magnon linewidths and critical dynamics in s=5/2 AFs



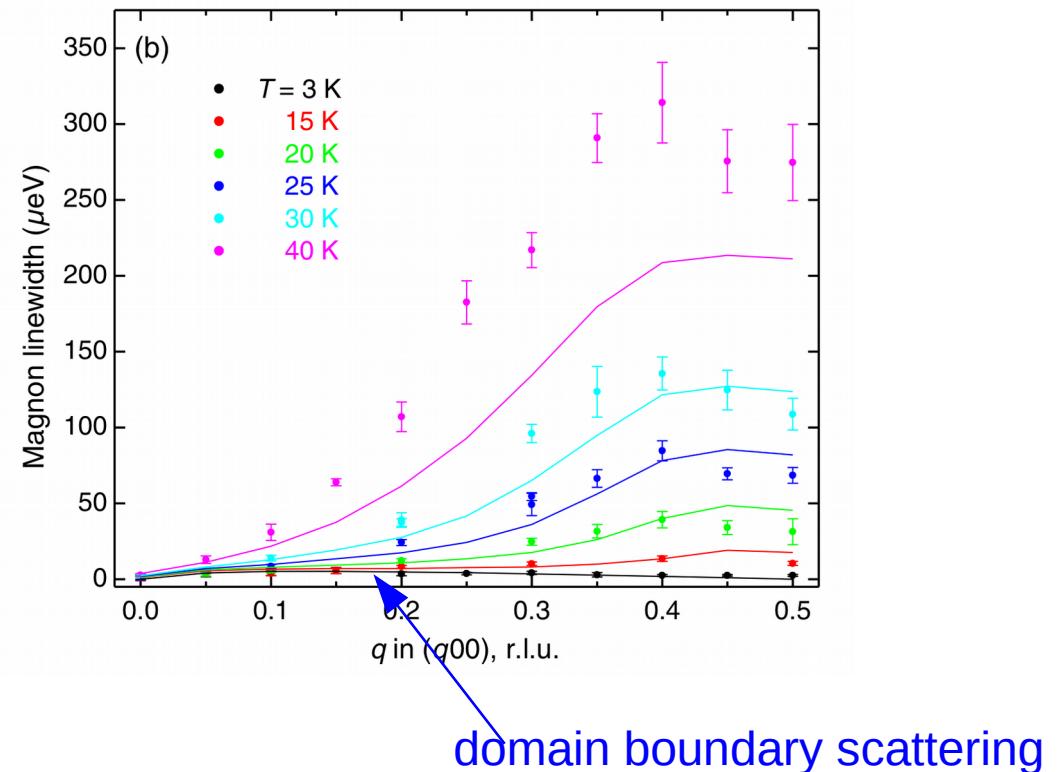
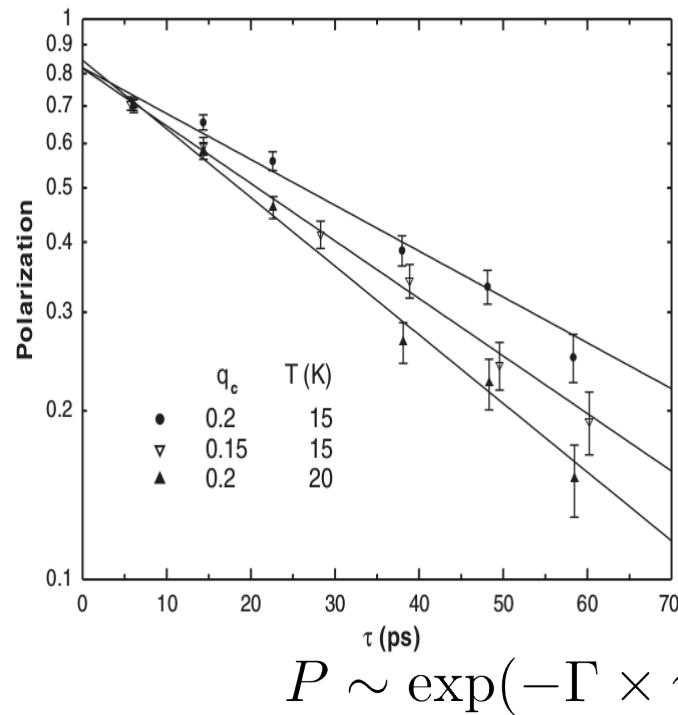
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Heisenberg AFs + small uniaxial anisotropy (dipolar)

Tseng, PRB 94, 014424 (2016)

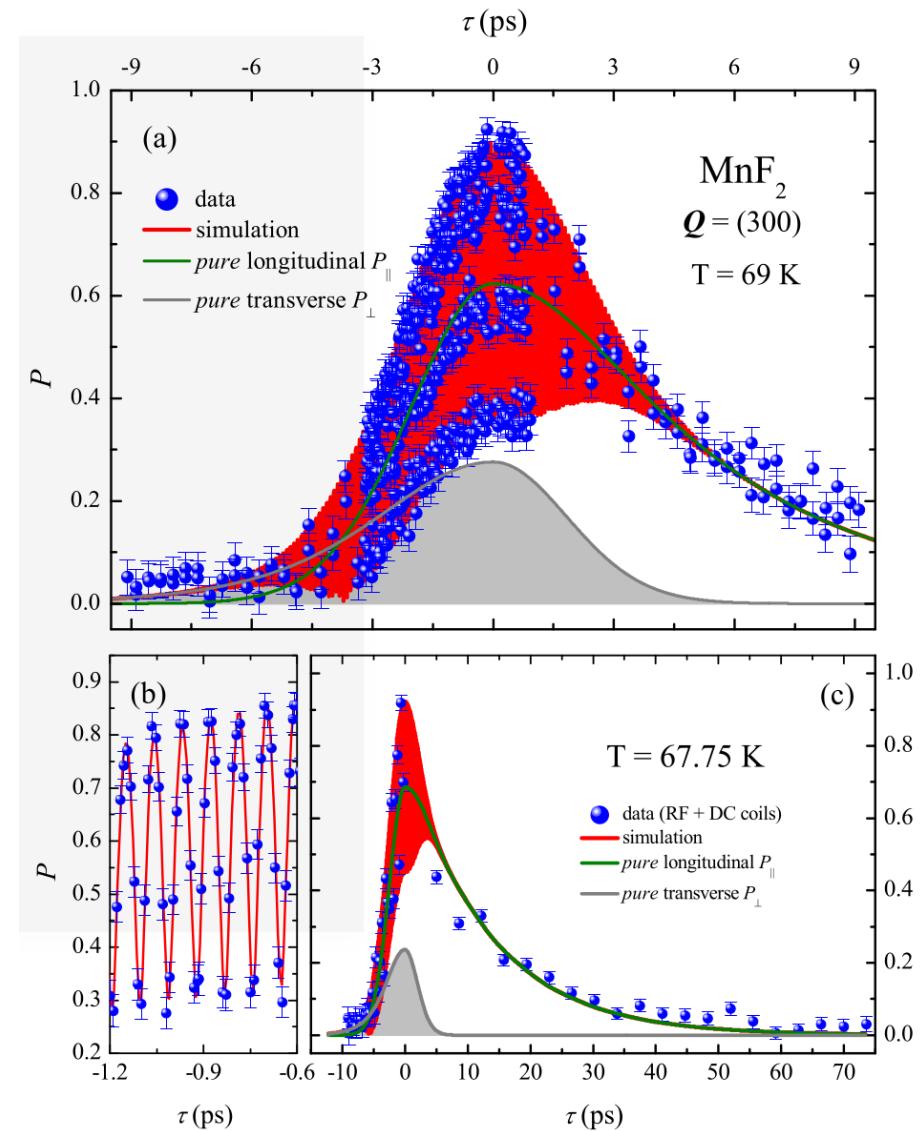
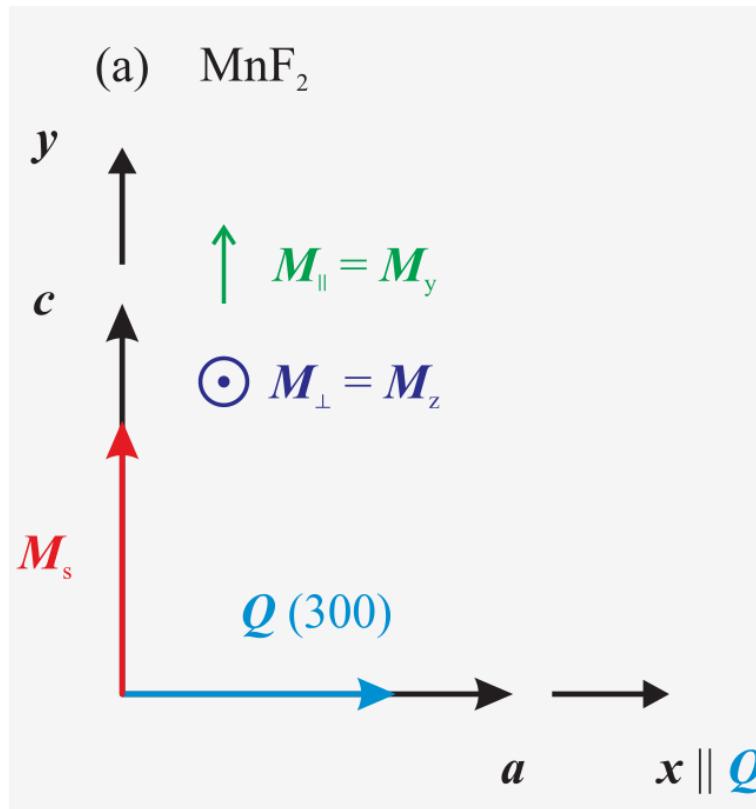
only M_y visible -> conventional signals



critical scattering



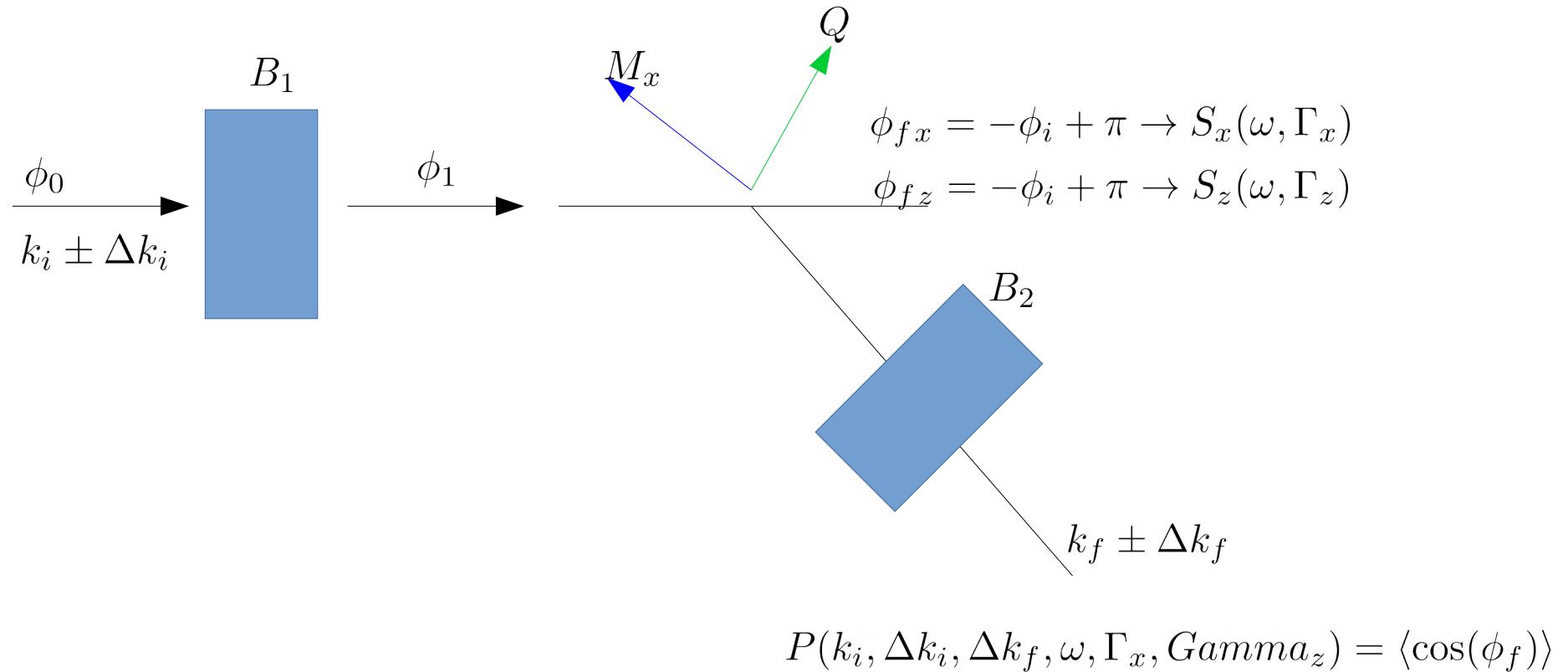
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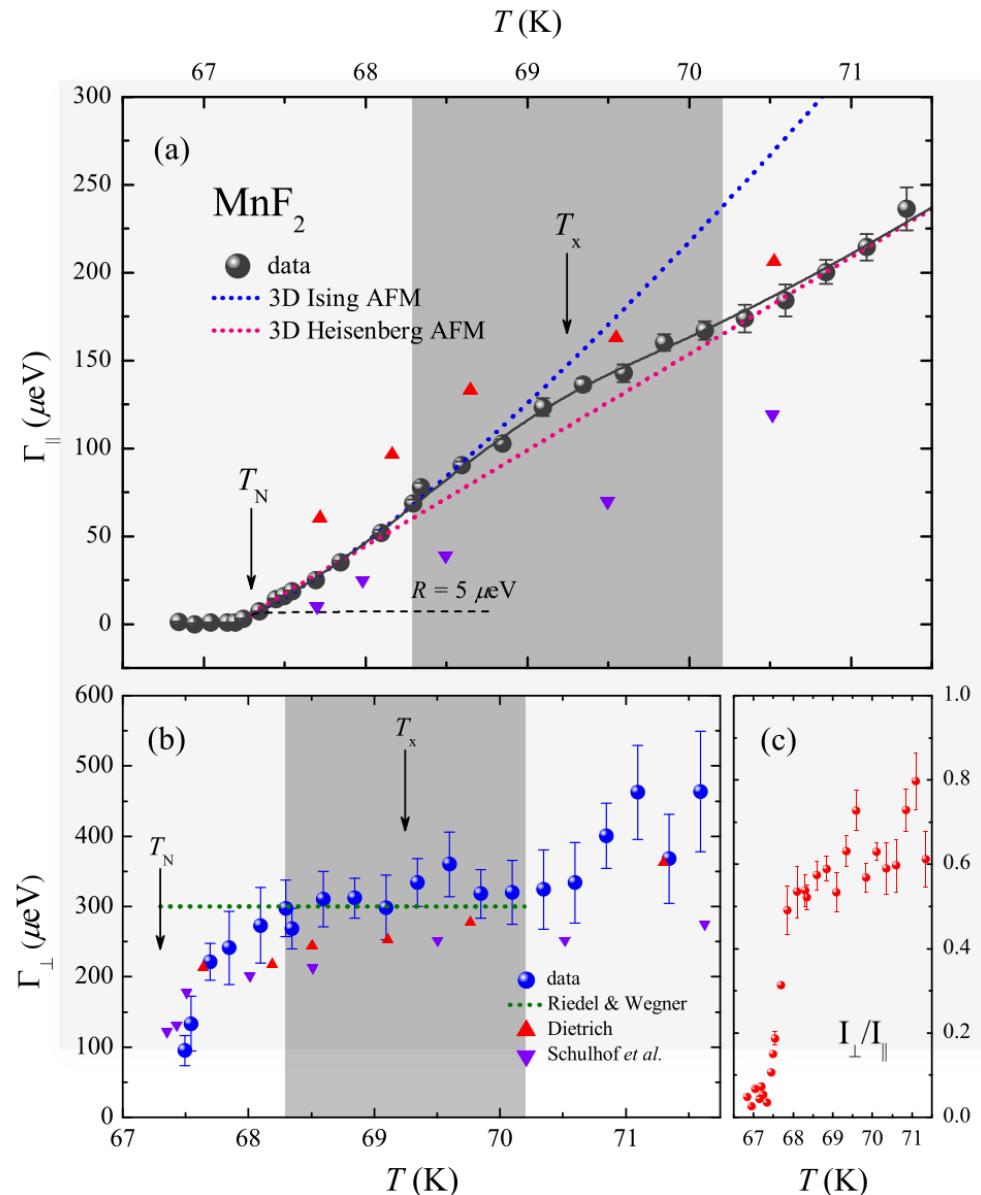
global fit, simulation of the spectrometer

Tseng, PRB 94, 014424 (2016)

simplified ray tracing



MnF₂ critical scattering



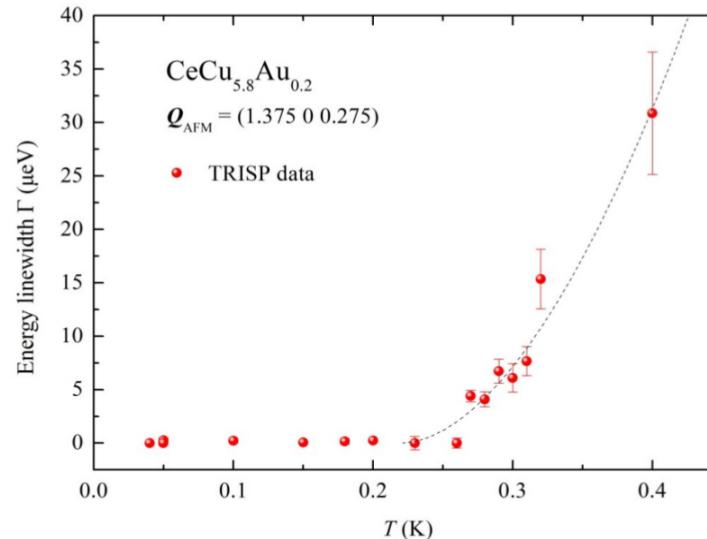
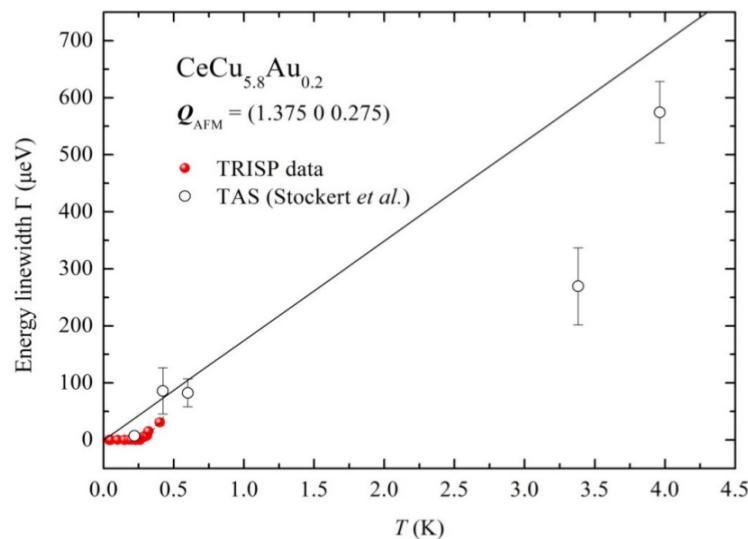
$$\Gamma \sim \xi^{-z}$$

CeCu_{6-x}Au_x critical fluctuations

$x = 0.2$

$T_N = 220\text{mK}$

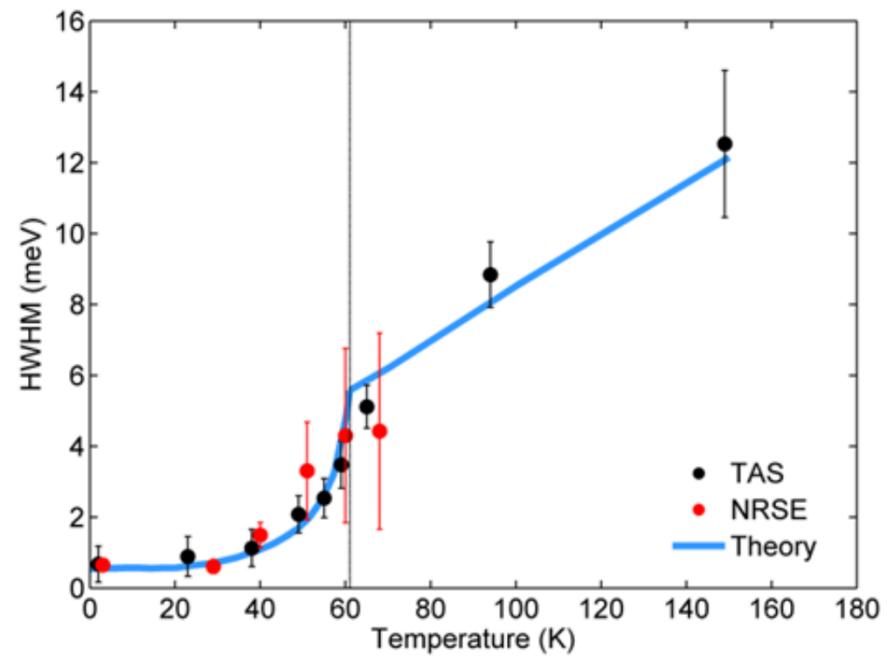
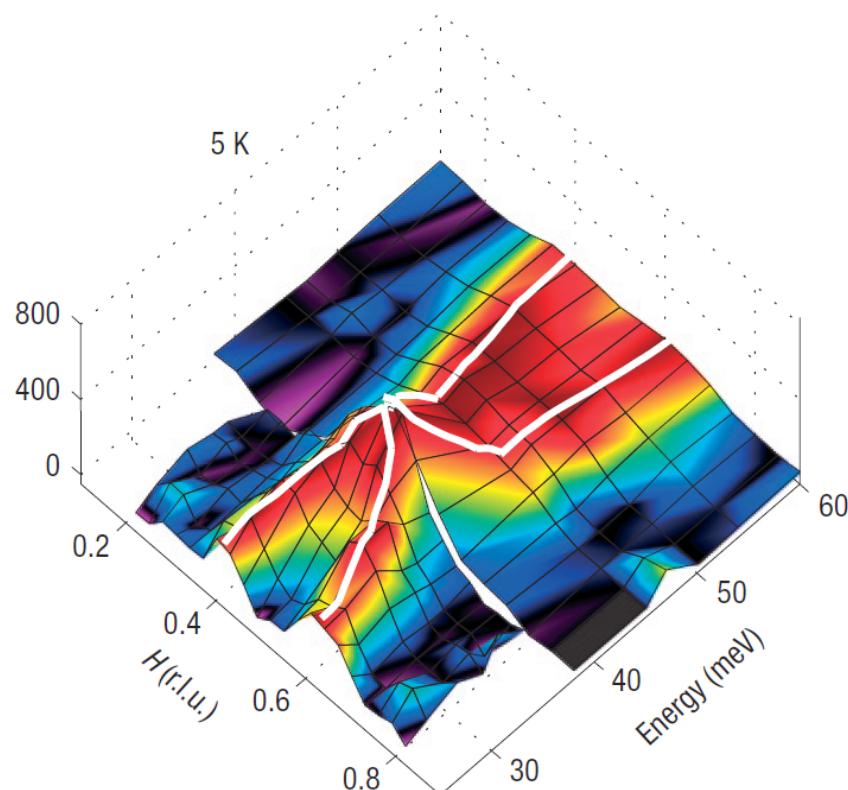
QC for $x=0.1$ or $p \sim 3\text{kbar}$



TAS: $\Gamma \sim T$

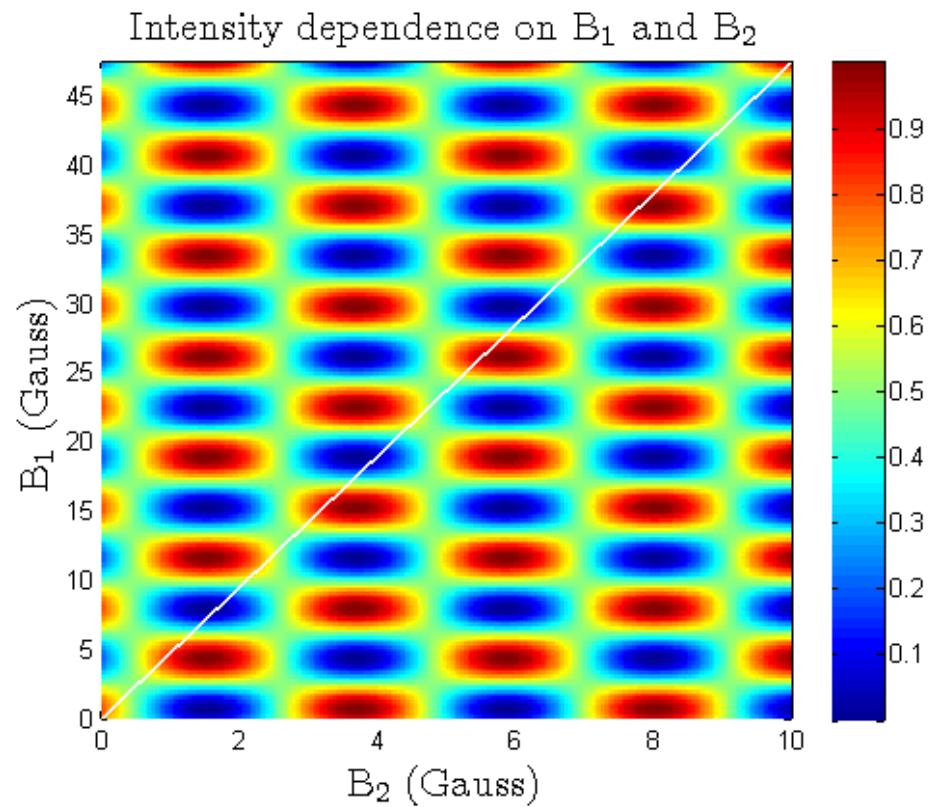
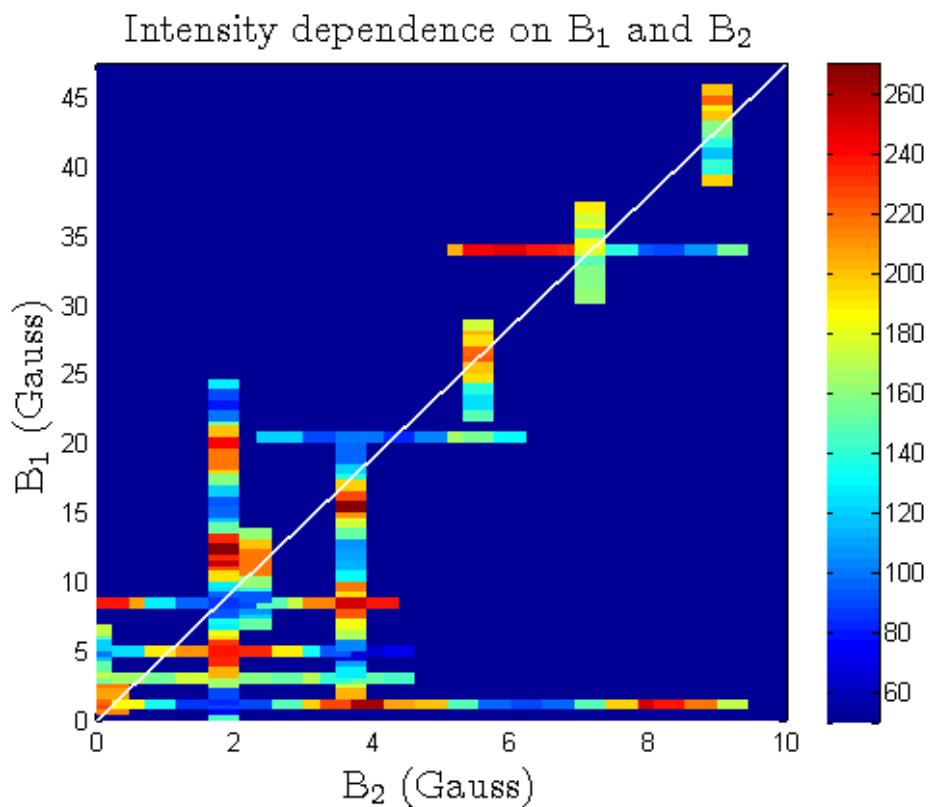
SE: crit. exponent $z=1.75$ (2DIA)

'resonance mode' $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$



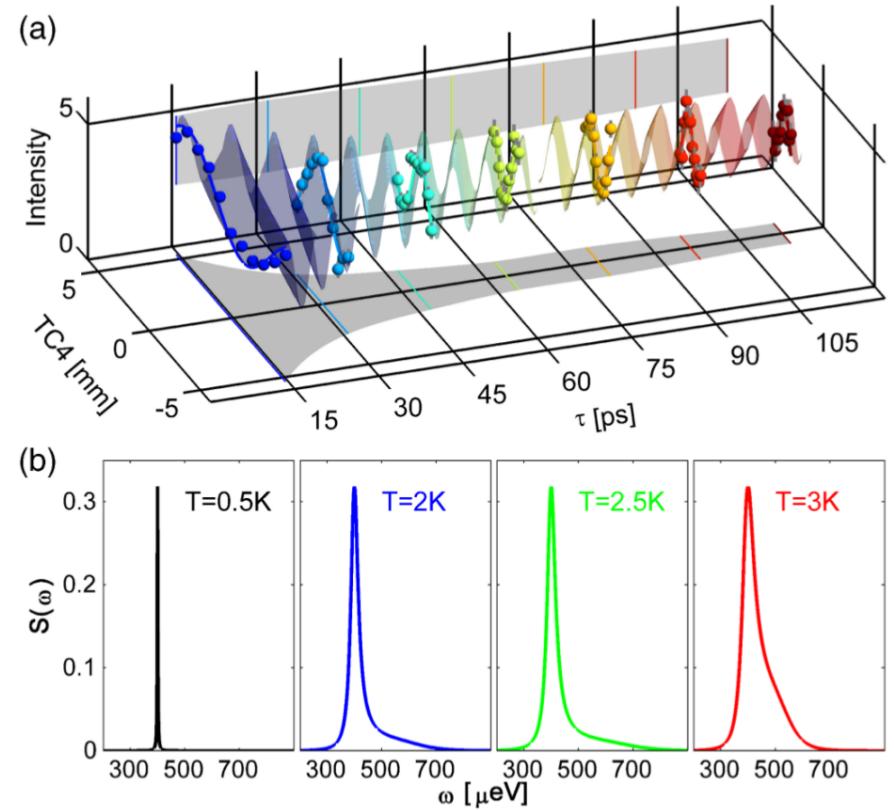
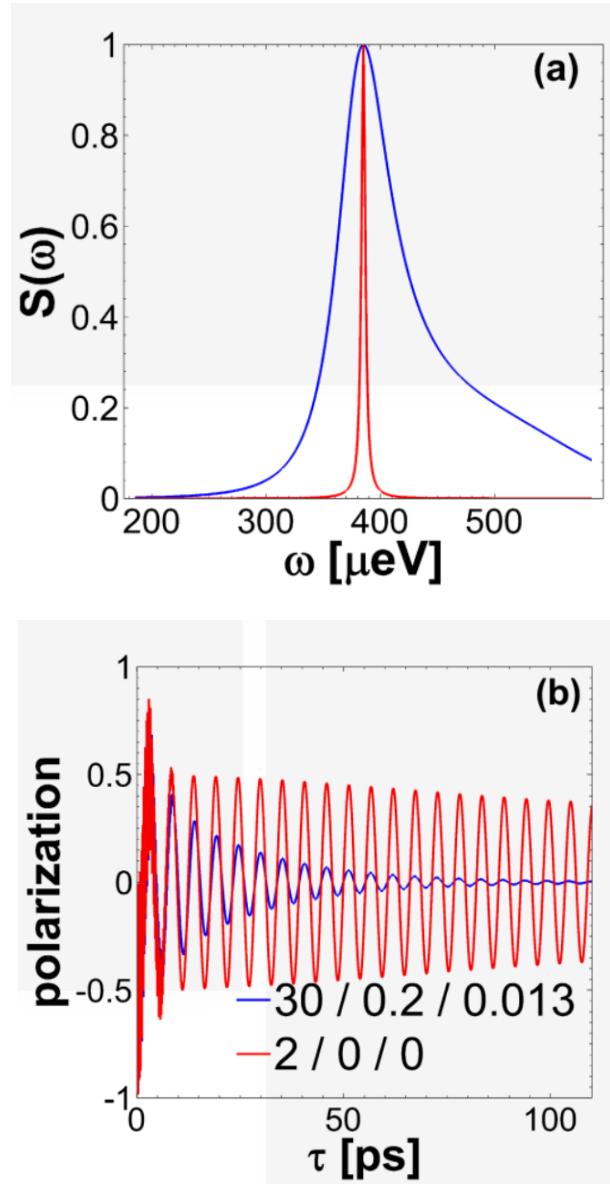
signature of d-wave symmetry
persists up to $T^* = 230\text{K}$
low T:

YBCO6.5 polarization signal

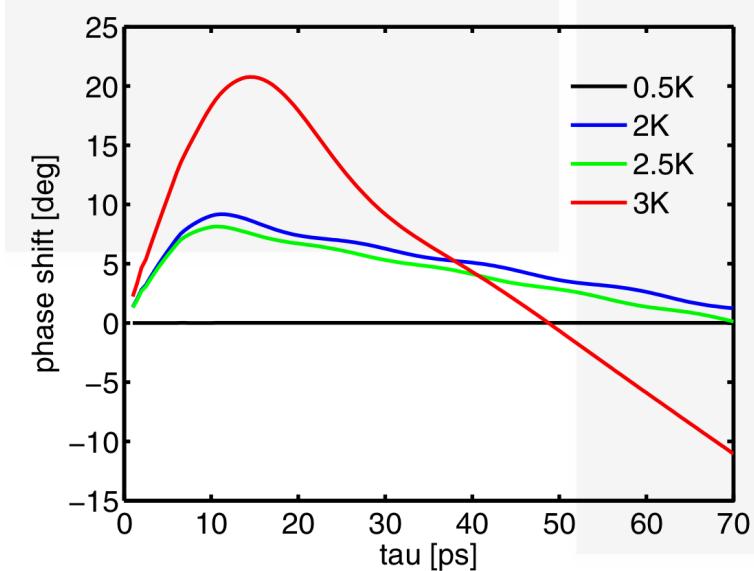


non-Lorentzian $S(\omega)$

$\text{Cu}(\text{NO}_3)_2 \cdot 2.5\text{D}_2\text{O}$, 1D bond alternating Heisenberg chain

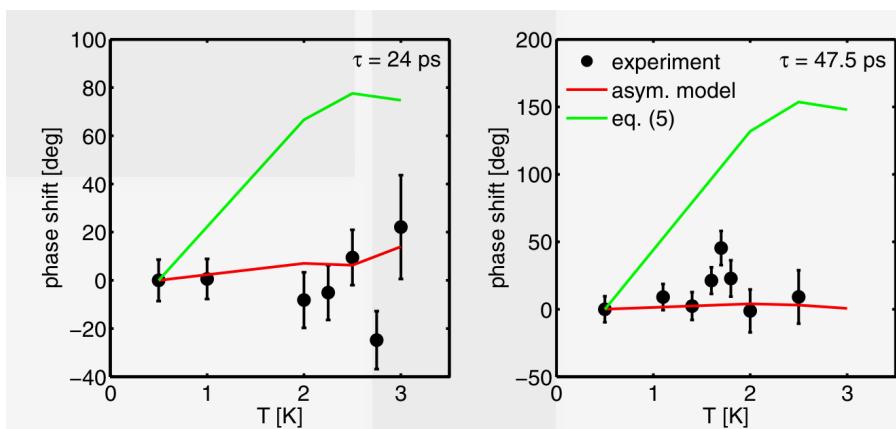


phase, non-Lorentzian



$$\Delta\phi = \Delta\omega \times \tau$$

only for symmetric $S(\omega)$





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Larmor diffraction

LD technique: Rekveldt , 1999
first experiments at FLEX
resolution $\Delta d/d = 10^{-6}$

current interest:

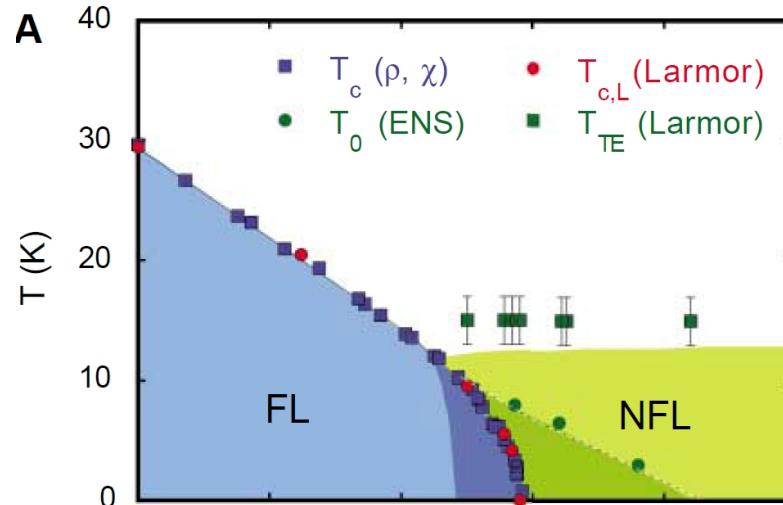
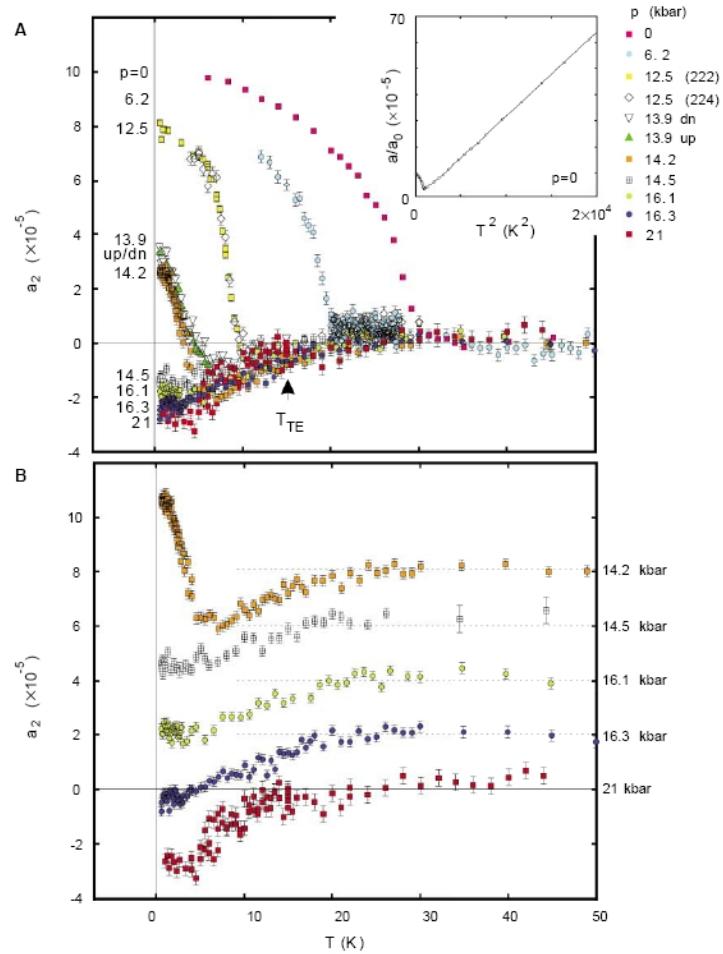
- thermal expansion p, low T
- distribution of d-values, peak splitting
- absolute d-values (calibration)

dilatometry <-> pressure

high resolution x-ray diffraction (10^{-5}) <-> temperature

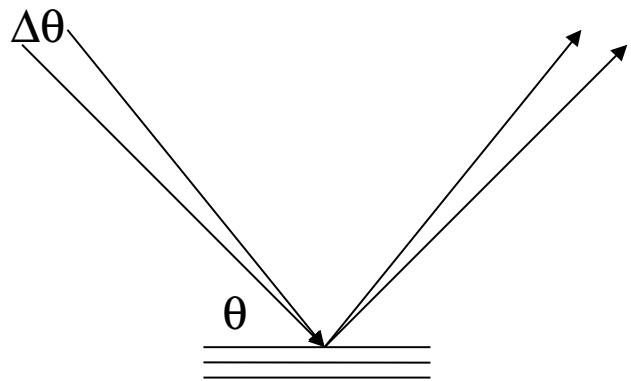
neutron diffraction <-> resolution (10^{-4})

motivation: thermal expansion, pressure



MnSi

Pfleiderer et al., Science 316, 1871, (2007)



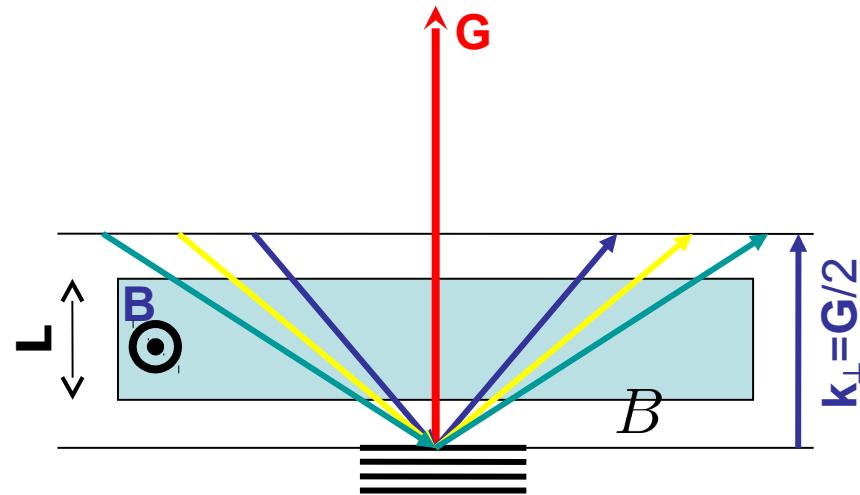
resolution=1/intensity

neutron: $\Delta d/d = 10^{-4}$

x-ray: 10^{-5}

$$\frac{\Delta d}{d} = \frac{\Delta k}{k} + \Delta\theta \cdot \cot\theta$$

aim: try to measure d by a spin echo technique

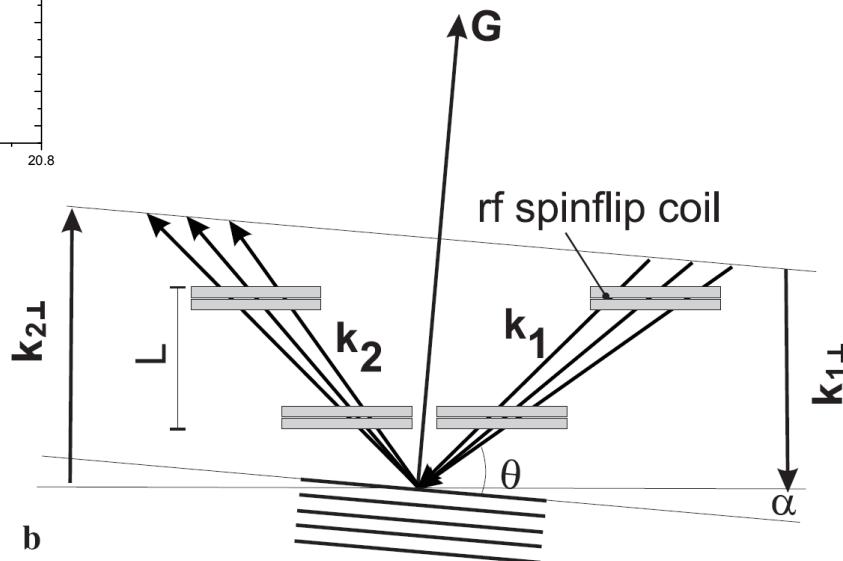
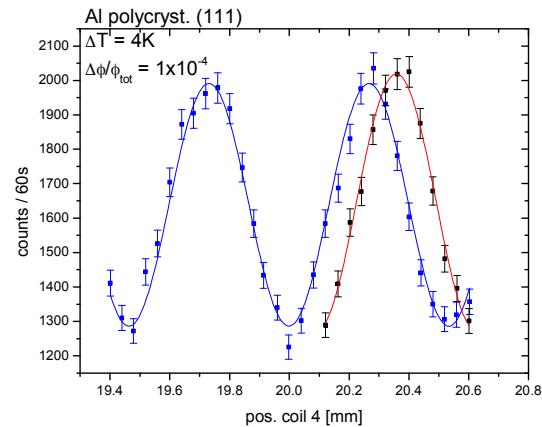


$$\phi_{Larmor} = \omega_L \cdot T = \omega_L \cdot \frac{2L}{v_\perp} = \frac{2\pi\hbar}{m} \cdot \omega_L \cdot L \cdot d$$



MAX-PLANCK-GESELLSCHAFT

LD using NRSE

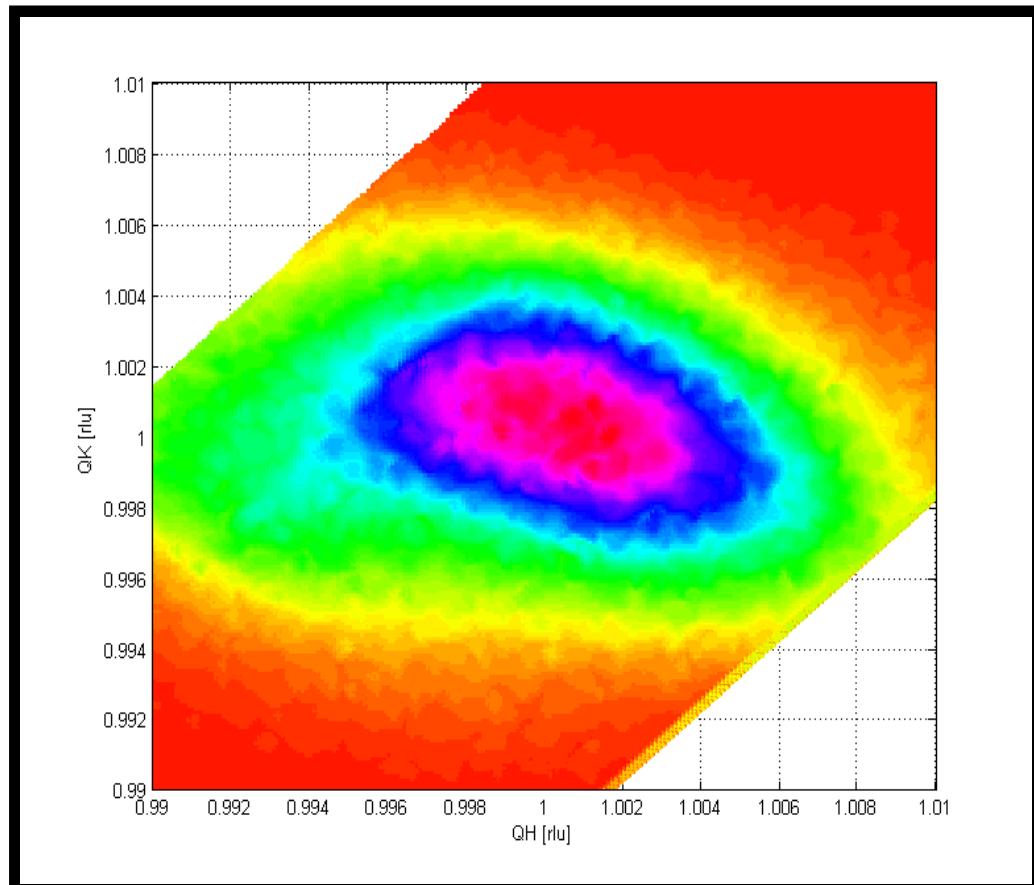
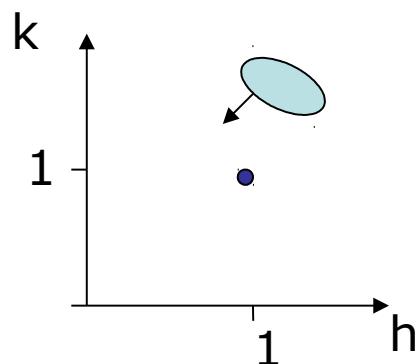


$\Delta d/d$ resolution at TRISP: 1.6×10^{-6}

resolution ellipsoid

(110) Bragg reflection
Larmor diffraction (MnF_2)

TAS only
NRSE off

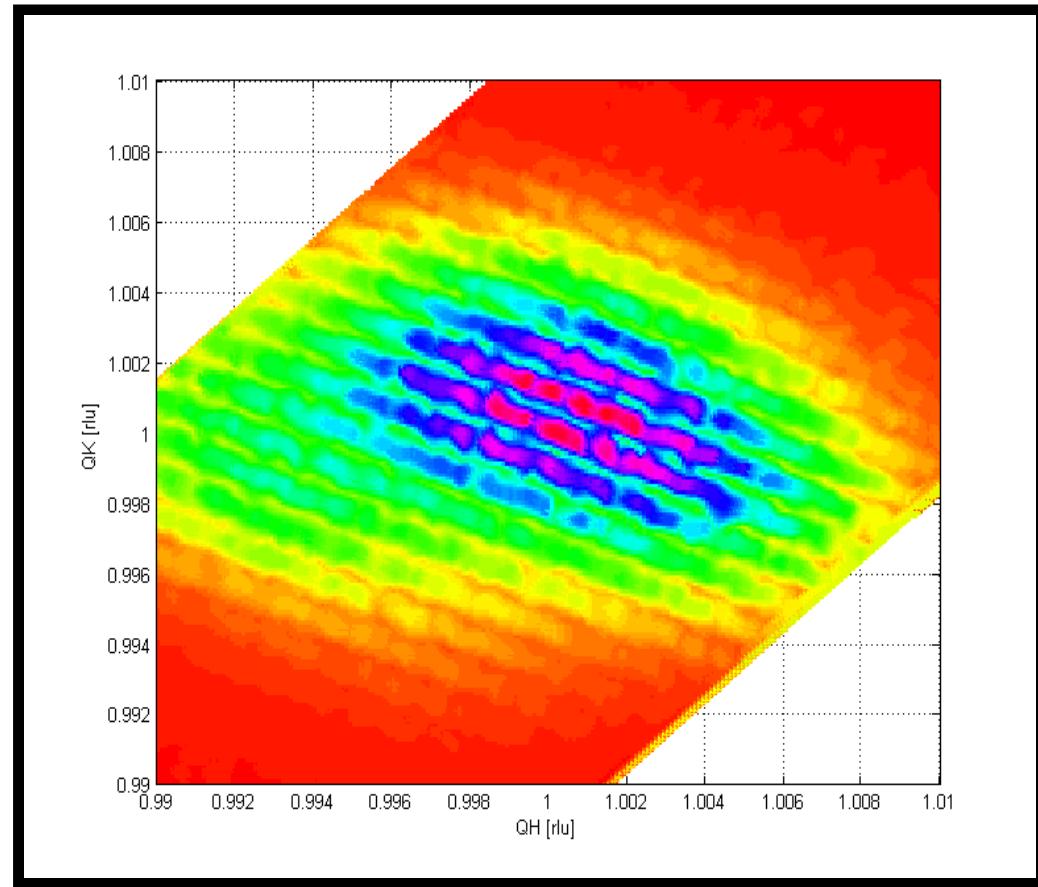




MAX-PLANCK-GESELLSCHAFT

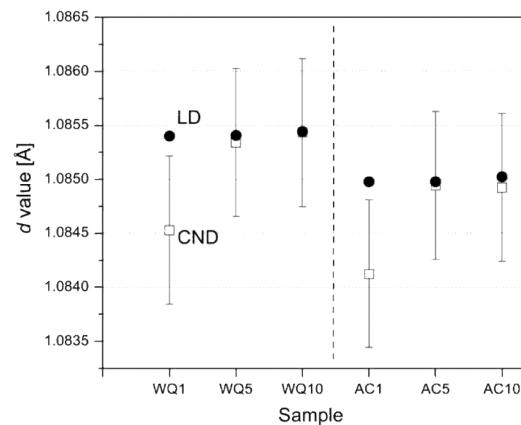
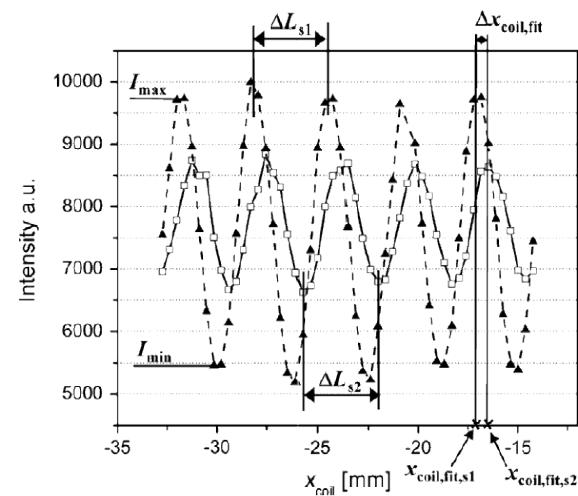
lines of constant Larmor phase

TAS +
NRSE on



K. Habicht, FLEX

materials science: Inconel 718 strain



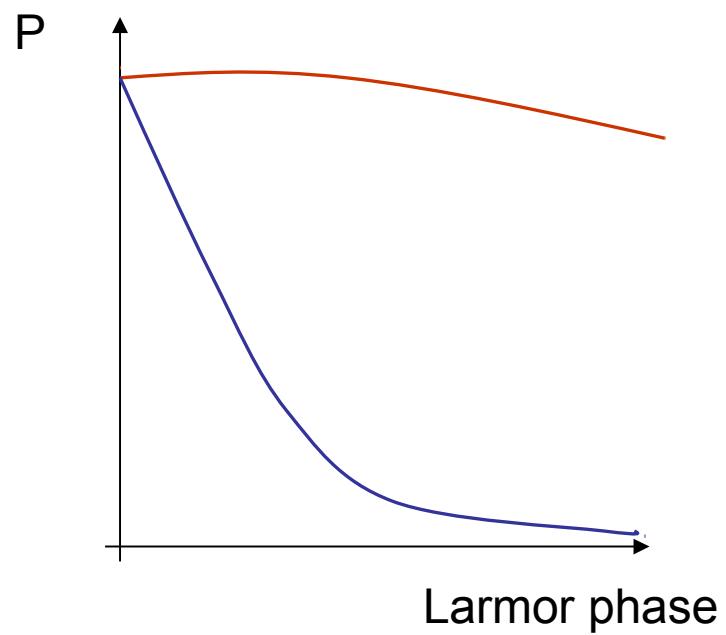
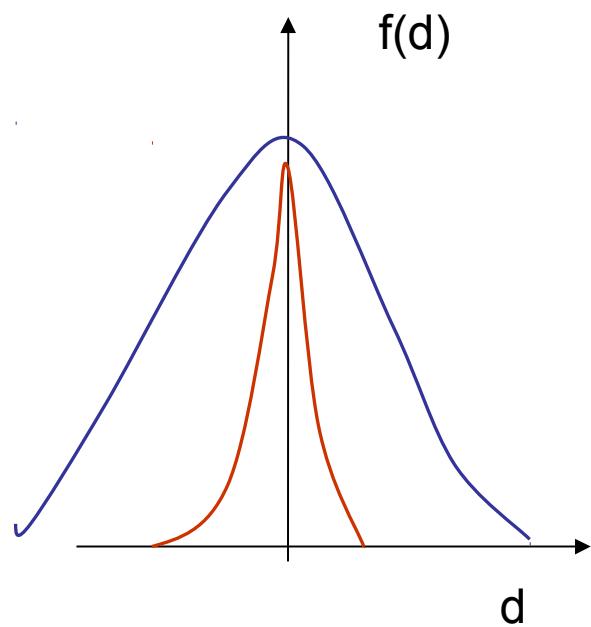
absolute d
distributions of d

J. Repper, Acta Materialia 58, 3459 (2010)

spread of d



MAX-PLANCK-GESELLSCHAFT

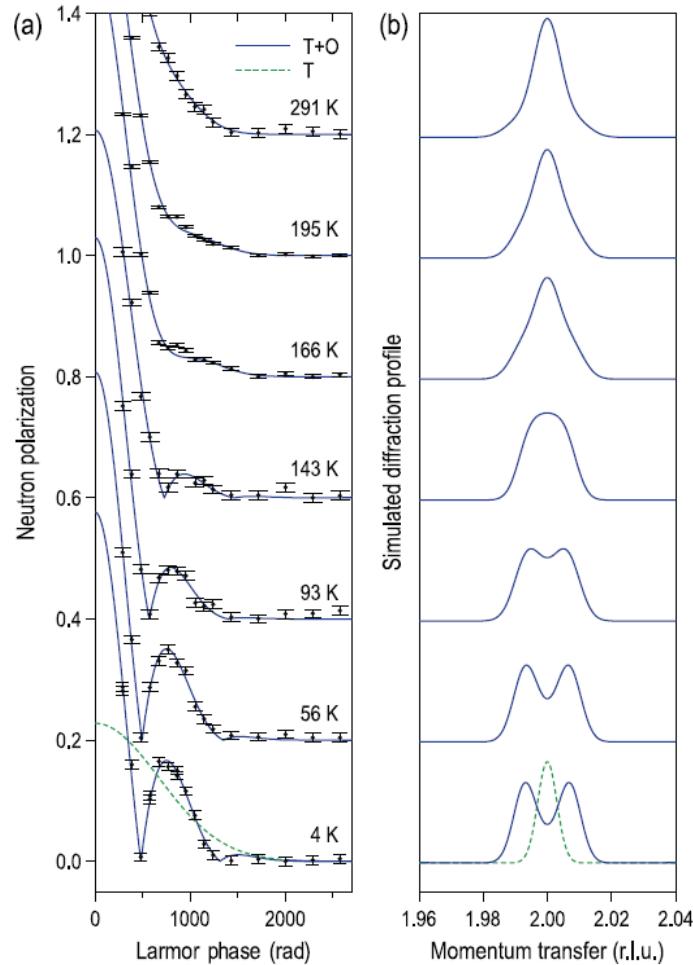


$$P(\Phi) = \int f(d) \cos(d \cdot \Phi) dd$$

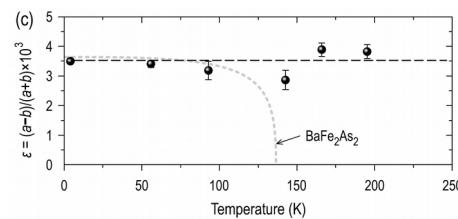
peak splitting



MAX-PLANCK-GESELLSCHAFT



$\text{Ba}(\text{Fe}_{1-x}\text{Mn}_x)\text{As}_2$ (12%)
tetragonal \rightarrow orthorombic
(coexistence)

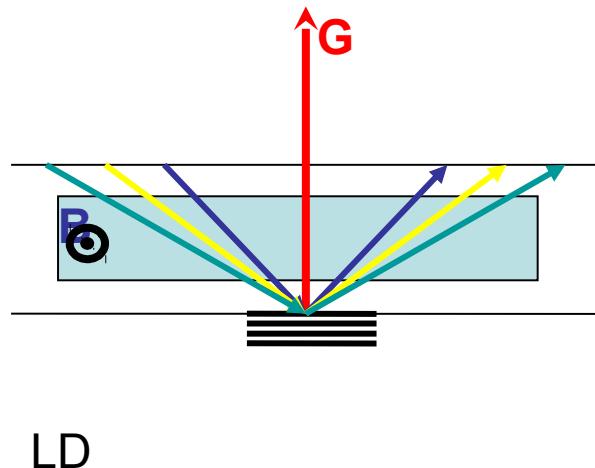


Inosov, Walters, Park et al., PRB 87, 224425 (2013)

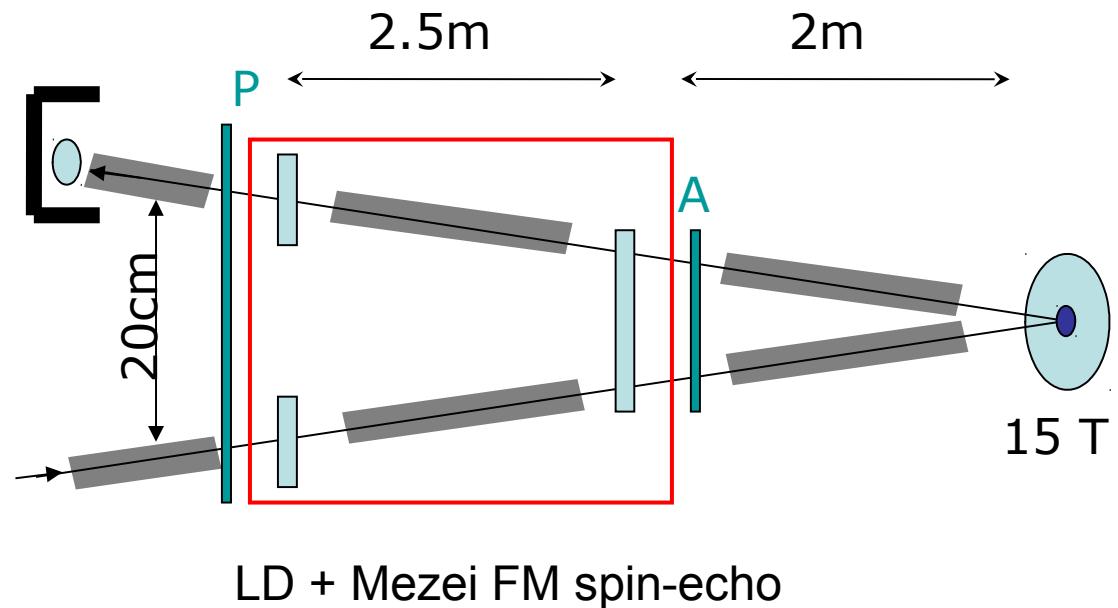


MAX-PLANCK-GESELLSCHAFT

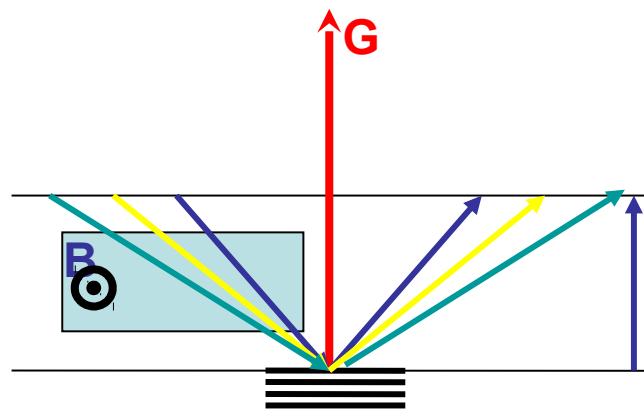
appendix 1: Larmor alternatives



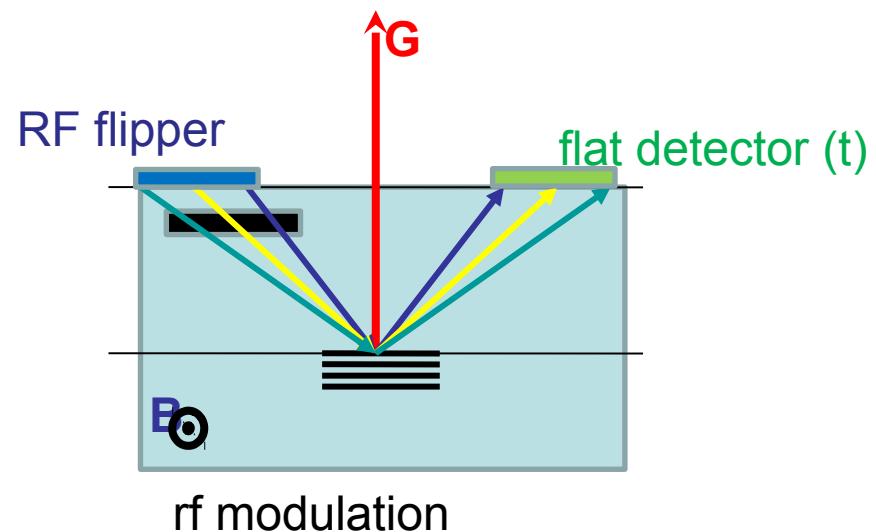
LD



LD + Mezei FM spin-echo



Rekveldt 1-arm



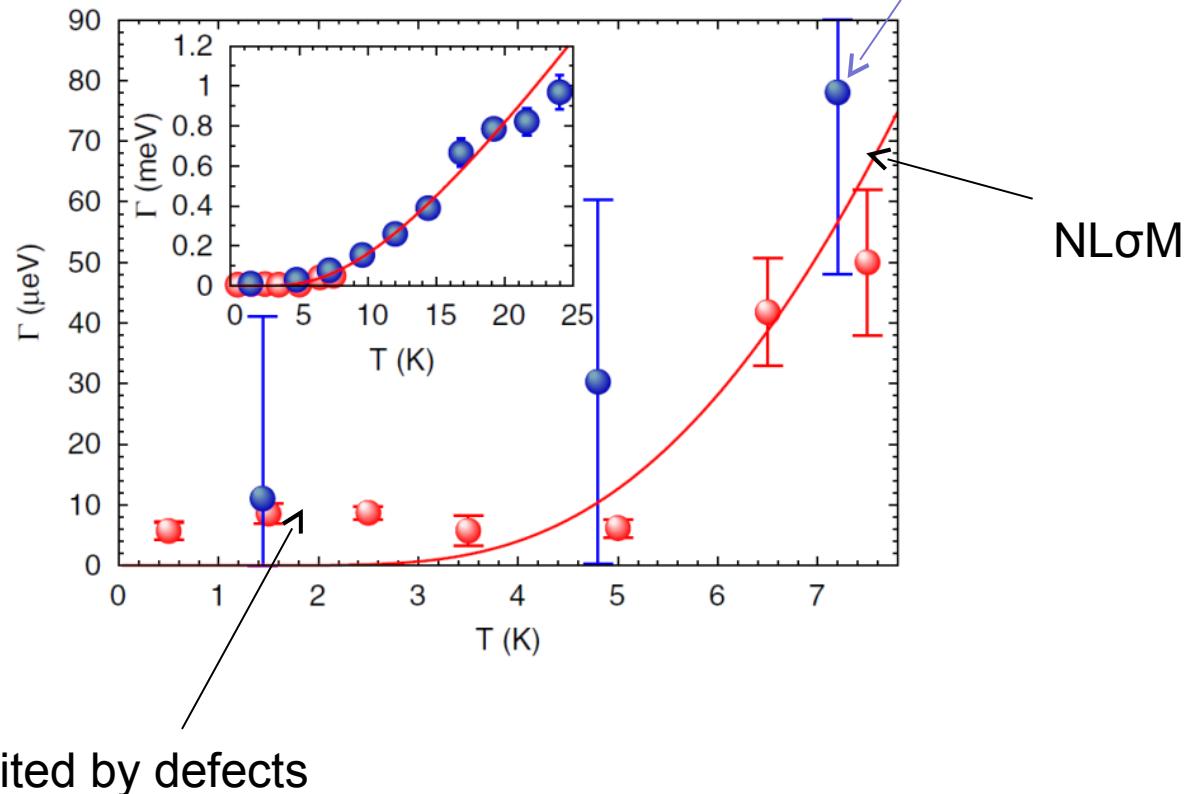
rf modulation

appendix



MAX-PLANCK-GESELLSCHAFT

spin ladder IPA-CuCl₃(1D)



Γ limited by defects

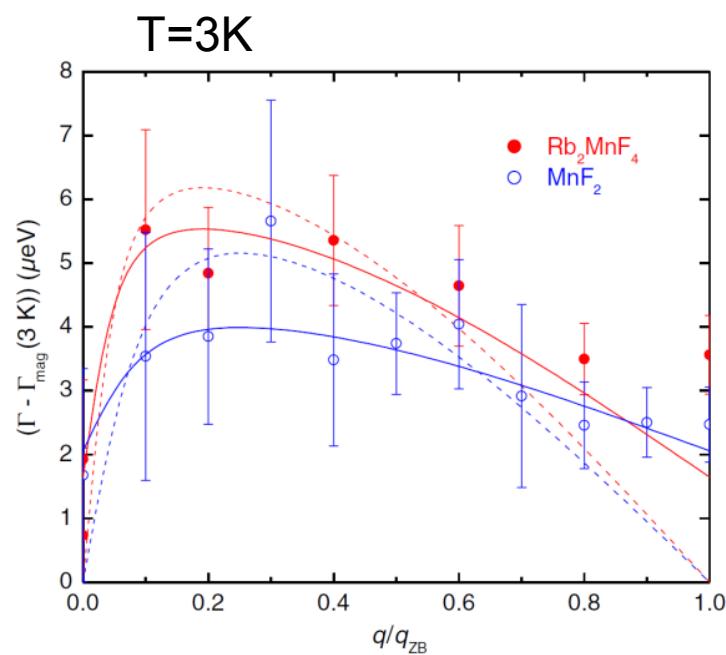
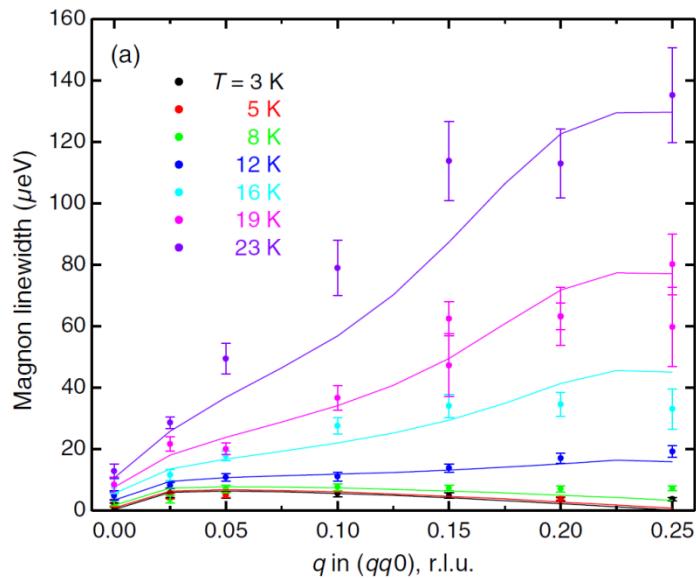
Nafradi, PRL 106, 177202 (2011)

magnons in Rb_2MnF_4 (2D) MnF_2 (3D)



MAX-PLANCK-GESELLSCHAFT

Rb_2MnF_4



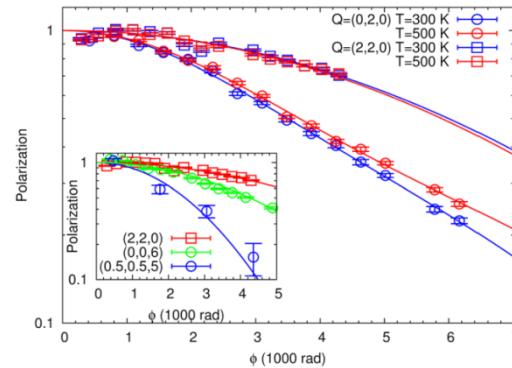
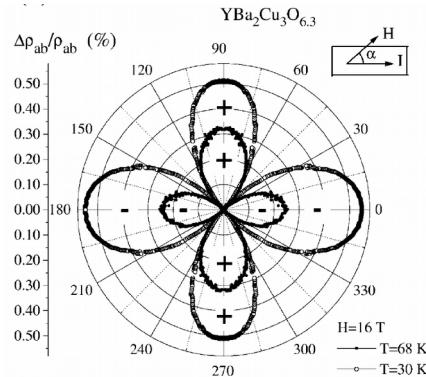
-> Γ limited by antiferromagnetic domains
thermal transport
LD: domains $\sim 500 \text{ nm}$

Bayrakci, Tennant, PRL 111, 017204 (2013)

heterogeneity -> transport

magneto-resistance $\text{YBa}_2\text{Cu}_3\text{O}_6$
-> reorientation of antiferromagnetic domains

domain size 300nm



Ando, PRL **83**, 2813 (1999)

Náfrádi, PRL **116**, 047001 (2016)

empty



MAX-PLANCK-GESELLSCHAFT