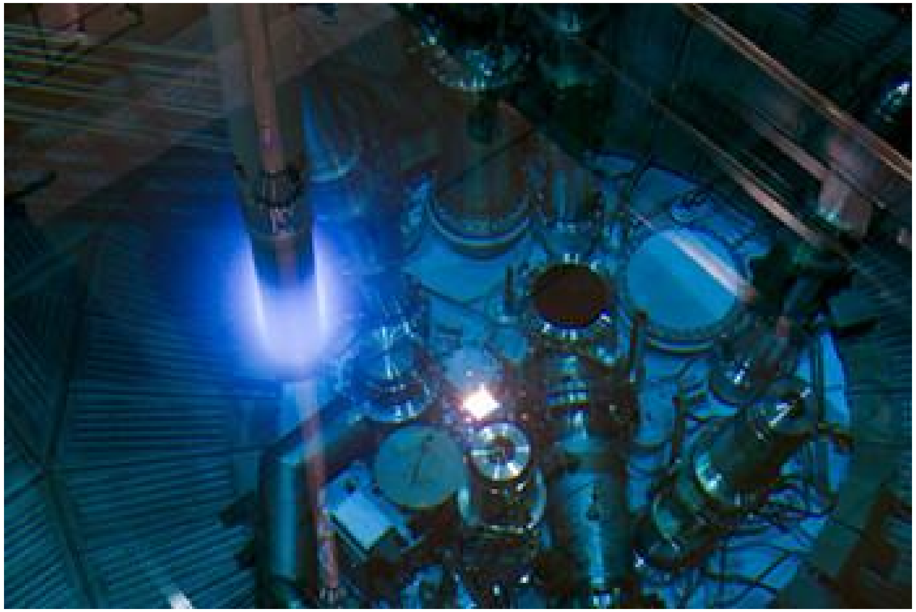
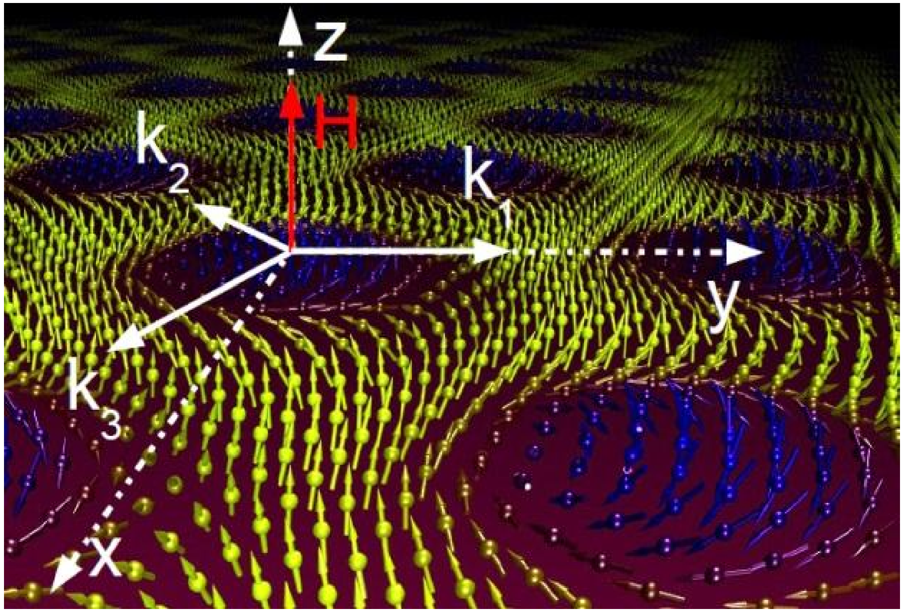
FRM II
Forschungs-Neutronenquelle
Heinz Maier-Leibnitz

MLZ
Heinz Maier-Leibnitz Zentrum

Physics with Neutrons I, WS 2015/2016





Lecture 12, 18.1.2016

MLZ is a cooperation between:

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technische Universität München

Reminder: Coherent and Incoherent Scattering, Fermis Golden Rule

Coherent	Incoherent
	
Spatial and temporal correlations between different atoms	Spatial and temporal correlations between the same atom

- Interference effects:
- Given by average of b
  Bragg scattering

- Constant in Q
- Given by variations in b due to spin, disorder, random atomic motion....

Master formula for coherent inelastic scattering

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}\omega} = \frac{4\pi^3}{v_0 M} \cdot \frac{k'}{k} \langle b \rangle^2 e^{-2W(\boldsymbol{Q})} \sum_{s,\boldsymbol{q}} \frac{(\boldsymbol{Q} \cdot \boldsymbol{e}_s(\boldsymbol{q}))^2}{\omega_s(\boldsymbol{q})}$$

$$\times \Bigg[\underbrace{(n_s(\boldsymbol{q}) + 1)\delta\left(\omega - \omega_s(\boldsymbol{q})\right) \sum_{\boldsymbol{\tau}} \delta(\boldsymbol{Q} - \boldsymbol{q} - \boldsymbol{\tau})}_{\text{Phonon emission}}$$

$$\underbrace{+ n_s(\boldsymbol{q})\delta\left(\omega + \omega_s(\boldsymbol{q})\right) \sum_{\boldsymbol{\tau}} \delta(\boldsymbol{Q} + \boldsymbol{q} - \boldsymbol{\tau})}_{\text{Phonon absorption}} \Bigg] .$$

Reminder: Inelastic Incoherent scattering

Inelastic incoherent scattering: Phonon DOS

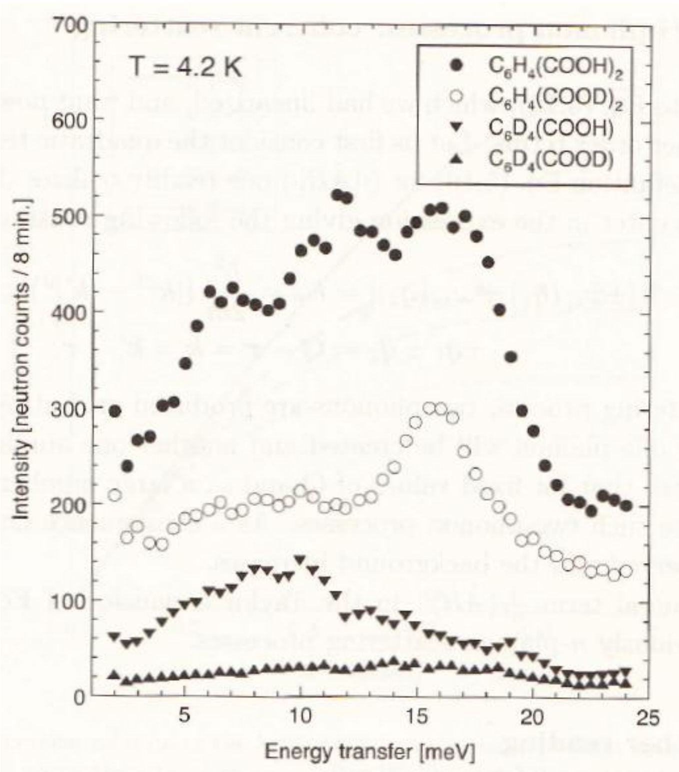
$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{1}{2M}\frac{k'}{k}\left(\langle b^2\rangle - \langle b\rangle^2\right) e^{-2W(\boldsymbol{Q})} \sum_{s,\boldsymbol{q}} \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s(\boldsymbol{q}))^2}{\omega_s(\boldsymbol{q})}$$
$$\times \left[\underbrace{(n_s(\boldsymbol{q})+1)\delta(\omega-\omega_s(\boldsymbol{q}))}_{\text{Phonon emission}} + \underbrace{n_s(\boldsymbol{q})\delta(\omega+\omega_s(\boldsymbol{q}))}_{\text{Phonon absorption}}\right]$$

Phonon emission

Phonon absorption

For a (cubic) Bravais lattice only

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{1}{12M}\frac{k'}{k}\left(\langle b^2\rangle - \langle b\rangle^2\right) e^{-W(\boldsymbol{Q})} Q^2$$
$$\times \frac{g(\omega)}{\omega} \cdot \left[\coth\frac{\hbar\omega}{2k_BT} \pm 1\right].$$



➡ Inelastic incoherent scattering directly measures phonon DOS g(ω)

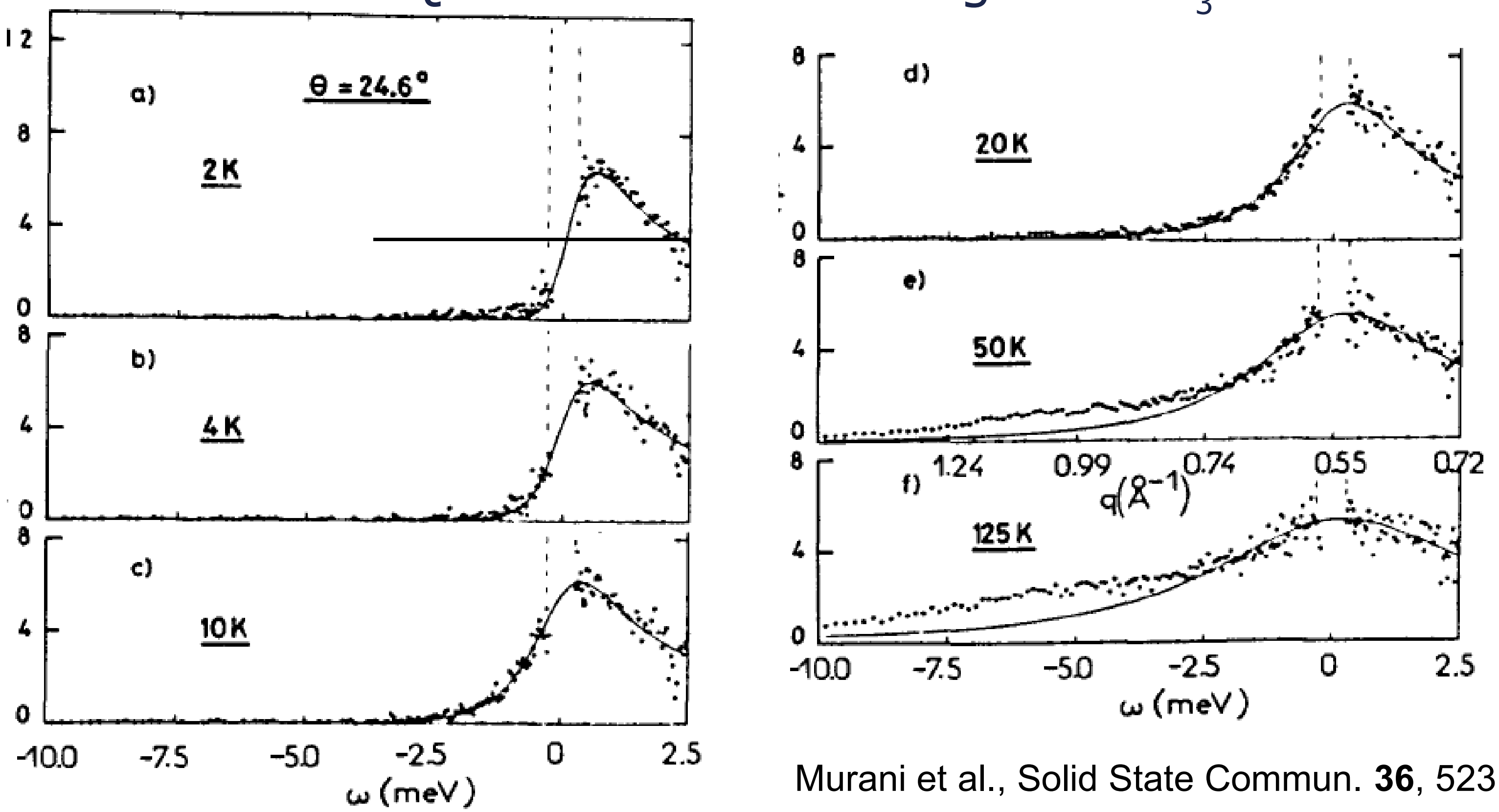
Phonon spectroscopy: Principle of detailed balance

Phonons (and magnons) obey Bose-Einstein statistics

$$n_s(\boldsymbol{q}) = \left(\exp\left(\frac{\hbar\omega_s(\boldsymbol{q})}{k_B T}\right) - 1\right)^{-1}$$

$$S(-q, E) = \exp(-E/k_B T)\, S(q,E)$$

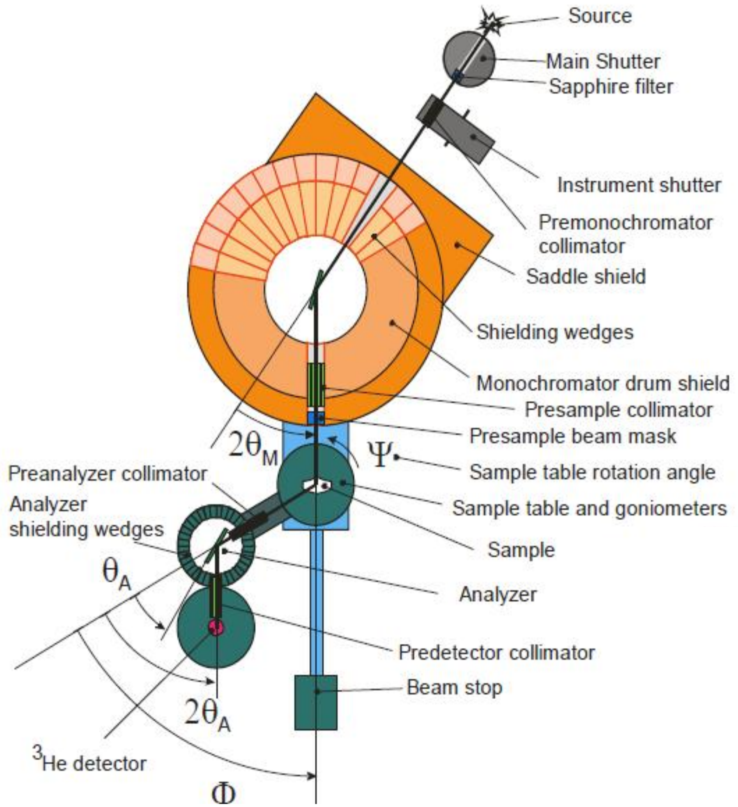
Quasielastic scattering in $CeAl_3$

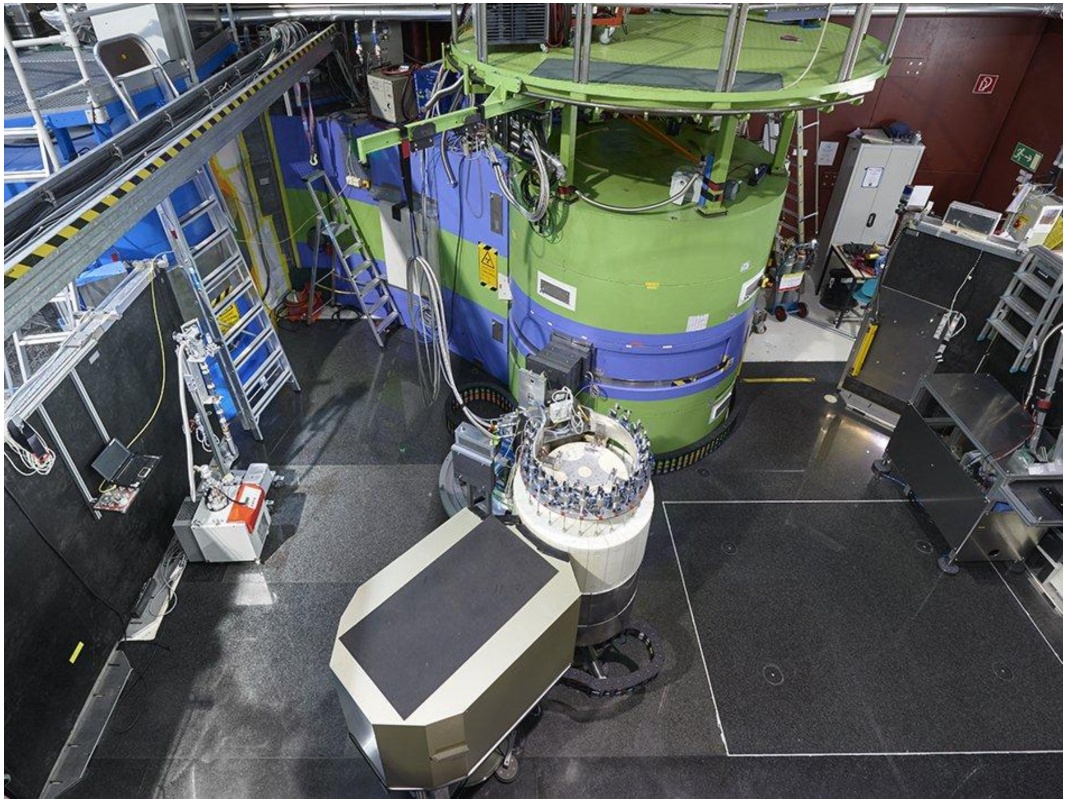


Murani et al., Solid State Commun. **36**, 523 (1980).

Inelastic scattering: TAS

Triple axis spectrometer: Workinghorse for phonons and magnons





„Working horse" for phonons/magnons in magnetism/superconductivity
Clean data at a fixed point in momentum/energy space
Slow, wasting a lot of neutrons

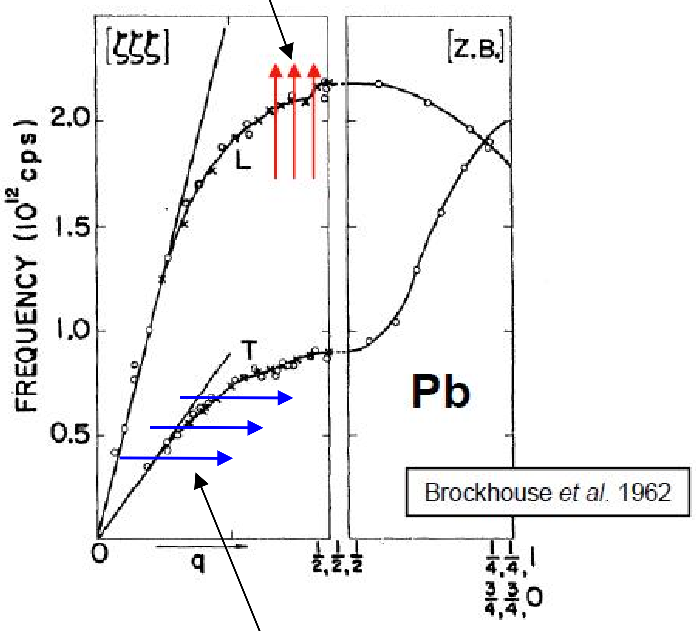
Cold TAS (PANDA)
Best energy resolution: 20µeV
Energy transfer <20meV
Momentum transfer <6Å^{-1}

Thermal TAS (PUMA)
Best energy resolution: 600µeV
Energy transfer <100meV
Momentum transfer <12Å^{-1}

Triple axis spectrometer: Scattering „triangle" S(q,w)

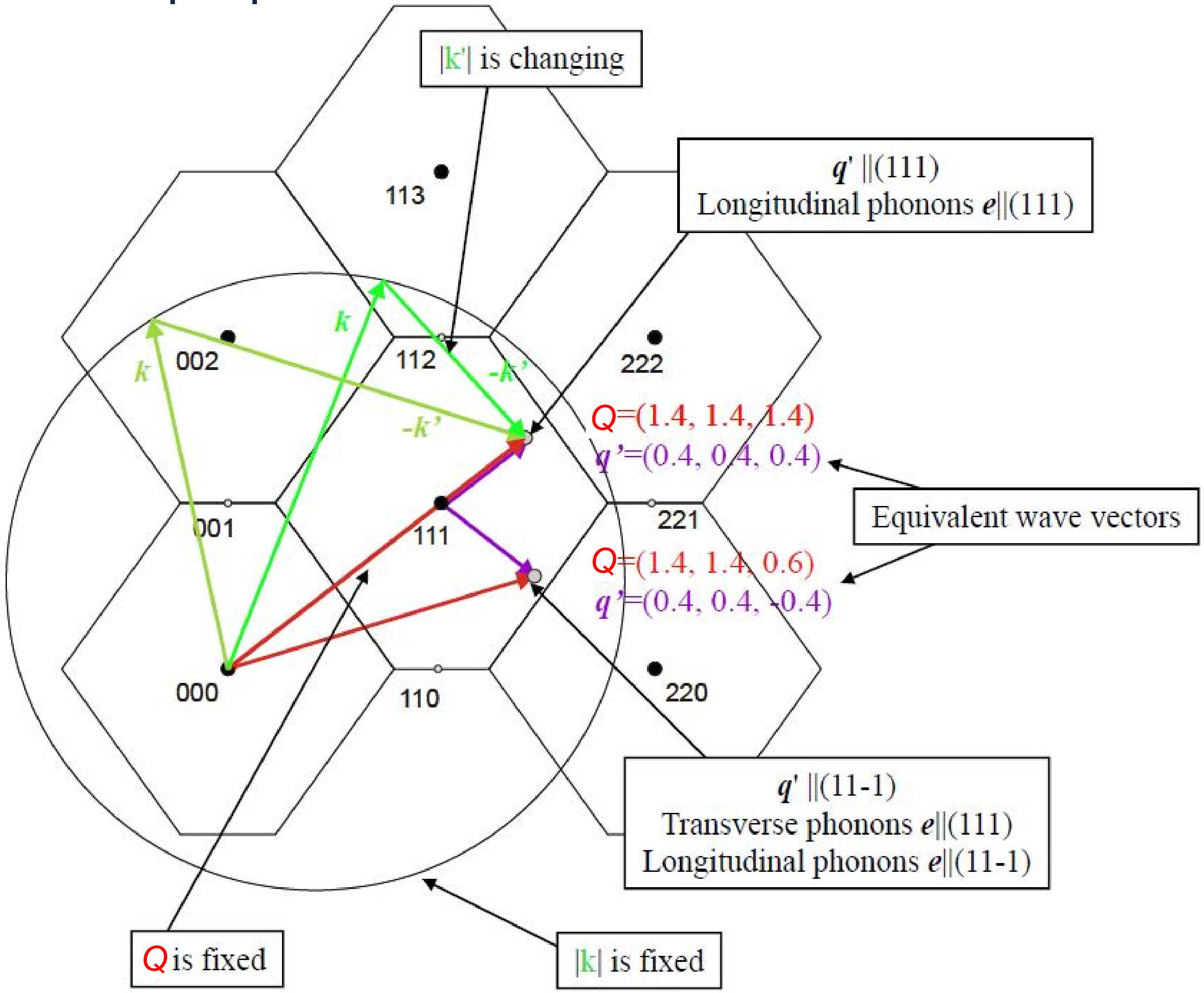
Scanning S(Q,w):

constant *q* scan

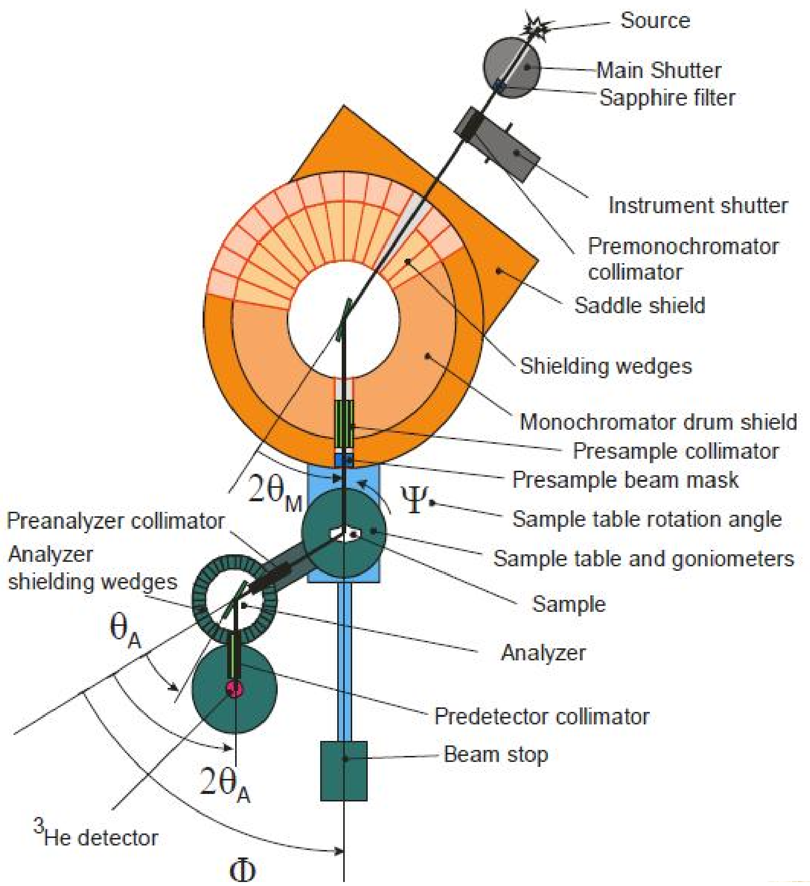


constant *E* scan

Fixed k_i constant *q* scan: Measure the properties of normal vibrational modes

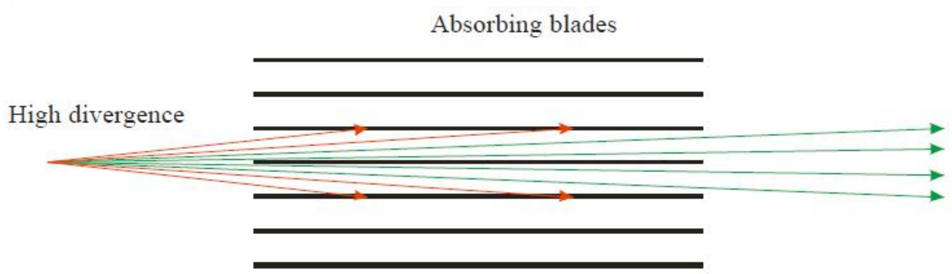


Triple axis spectrometer: Resolution function of a TAS

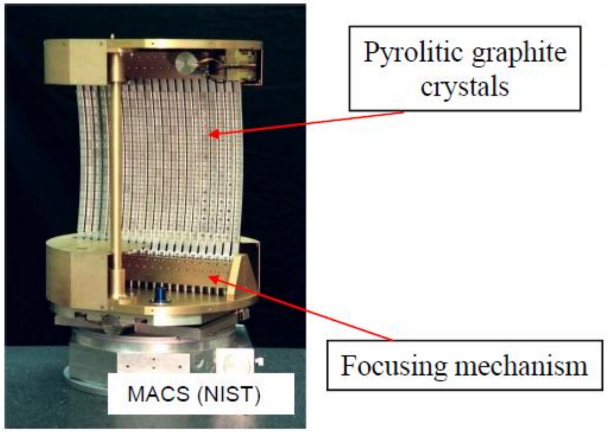


Coupling of resolution and intensity:

Definition of divergency: Collimator



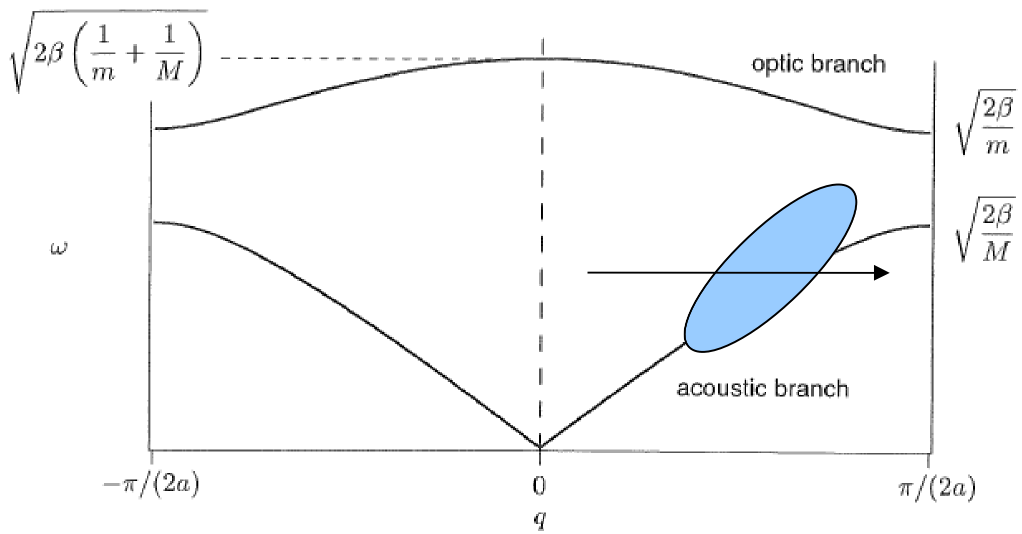
Definition of energy resolution: Single crystal monochromator



Triple axis spectrometer: Resolution function of a TAS

Coupling of *q* and *E* resolution

⇨ Resolution ellipsoid



Treatment as Gaussian functions for *q* and *E*-resolution

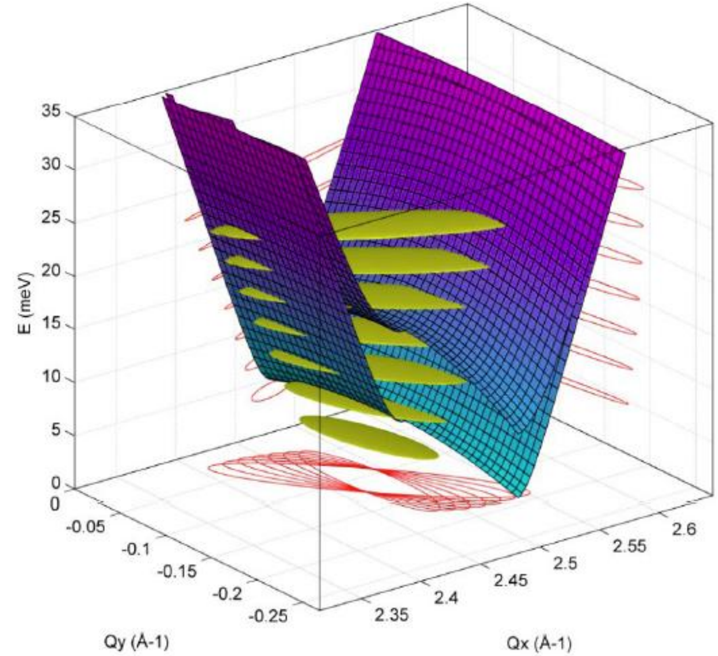
$$I\Big|_{\substack{\vec{k}-\vec{k}'=\vec{q}_0\\ E-E'=\hbar\omega_0}} \approx R_0(\vec{Q}_0)\iiiint\left[\frac{d\sigma}{d\Omega\, dE'}\Big|_{\substack{\vec{k}-\vec{k}'=\vec{q}\\ E-E'=\hbar\omega}}\right]\exp\left[-\frac{1}{2}(Q^i-Q_0^i)(Q^j-Q_0^j)M_{ij}(\vec{Q}_0)\right]d^4\vec{Q}$$

$$\vec{Q}=(q_x, q_y, q_z, \hbar\omega)$$

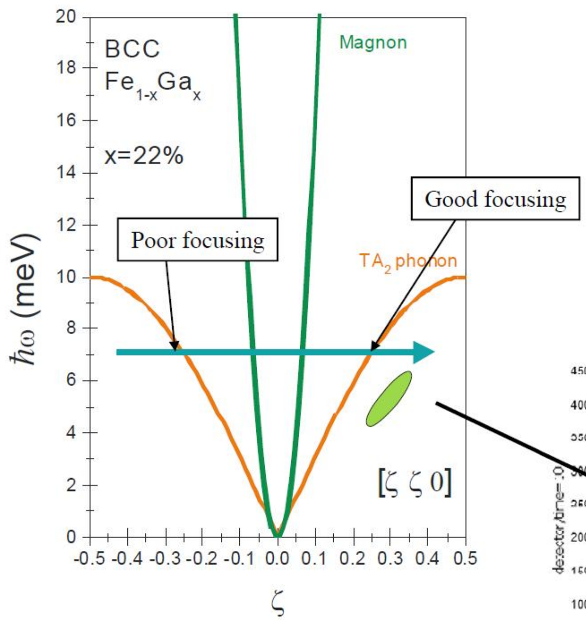
Why? Convolution of Gaussian functions still is a Gaussian!

Triple axis spectrometer: Resolution function of a TAS

Deconvolution of data? - Not possible (not bijective)



→ Instead: Convolute a model with resolution function and fit to the data!



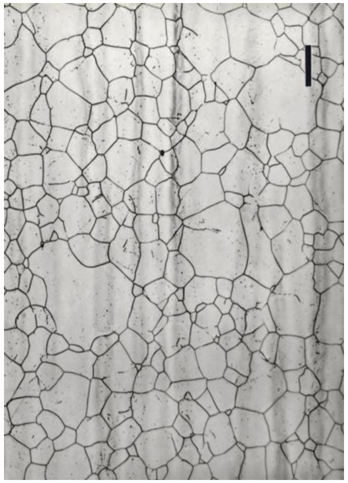
Coupling of q and E resolution: Focusing/defocusing

→ Matching the slope of the resolution ellipsoid to the dispersion of the excitation

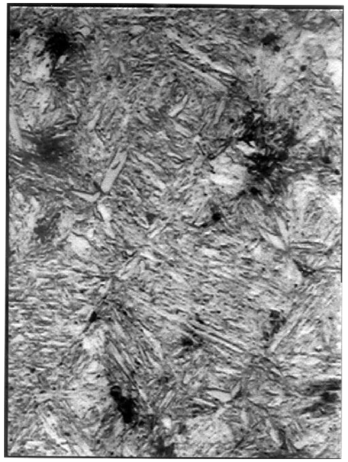
Inelastic scattering: Example I

Phonon softening at the austenitic/martensitic transition in Ni-Fe-Ga alloys

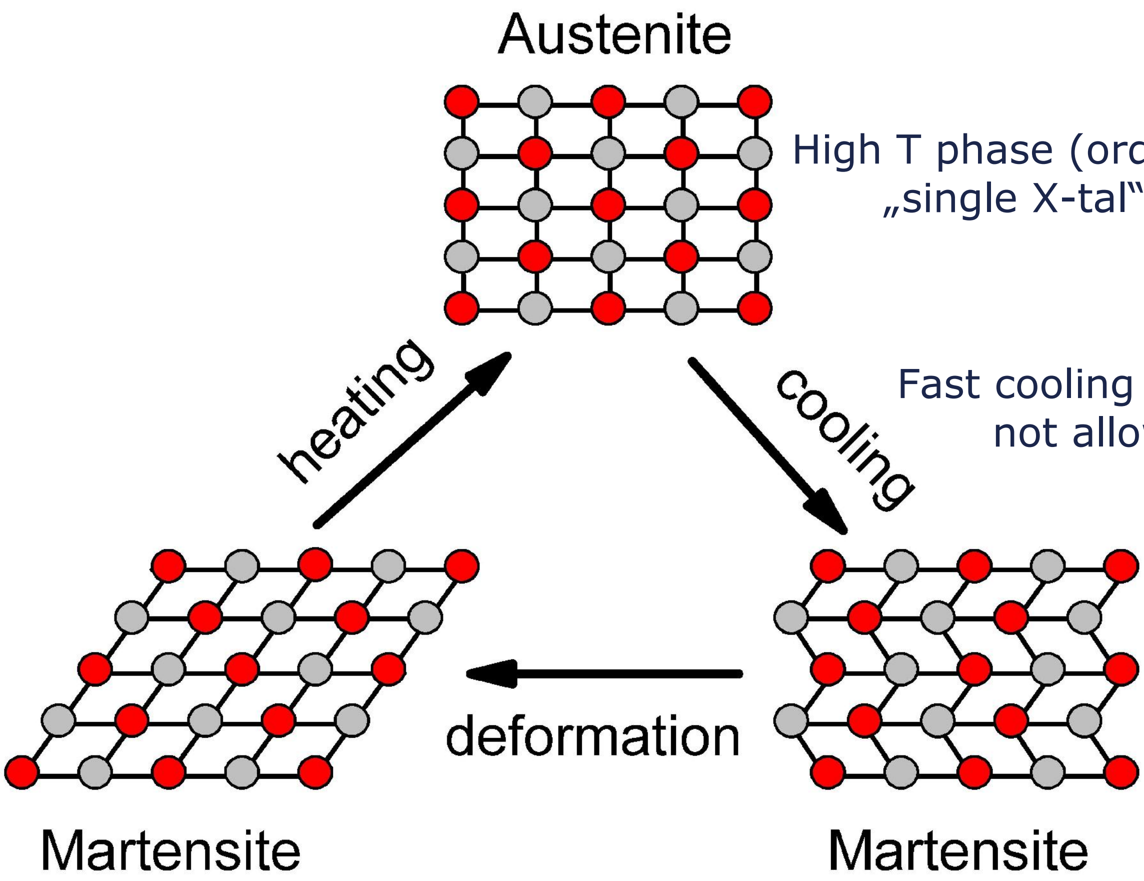
Austenitic – Martensitic phase transition & SMA



Austenitic steel



Martensitic steel
(0.35%C)



High T phase (ordered, „single X-tal")

Fast cooling (quench), does not allow diffusion

Diffusionless, cooperative shear movement
Crystallites form
Very hard and brittle
Small displacements

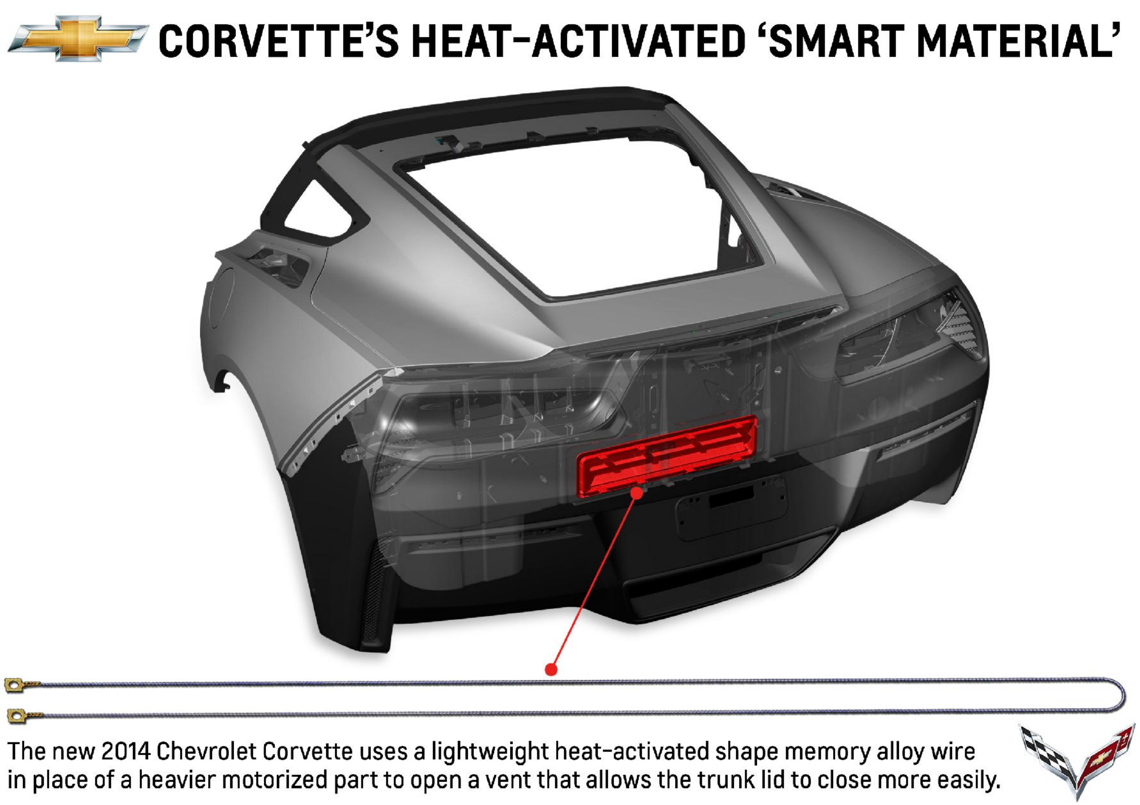
Shape Memory Effect (shear, strain)

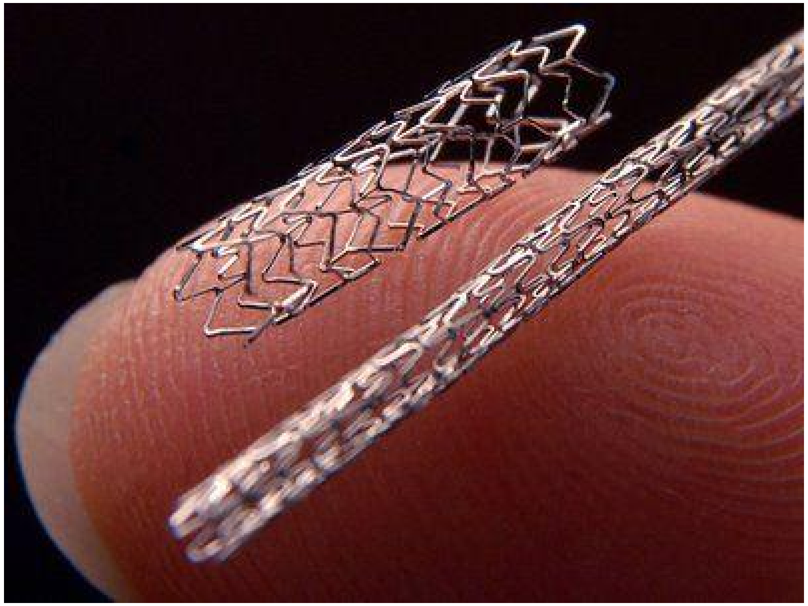
Magnetic Shape Memory Effect (magentic field)

Phonon softening at the austenitic/martensitic transition in Ni-Fe-Ga alloys

Shape Memory Alloys
Applications:

- Powerful and lightweight actuators
- Medicine (stents)





Phonon softening at the austenitic/martensitic transition in Ni-Fe-Ga alloys

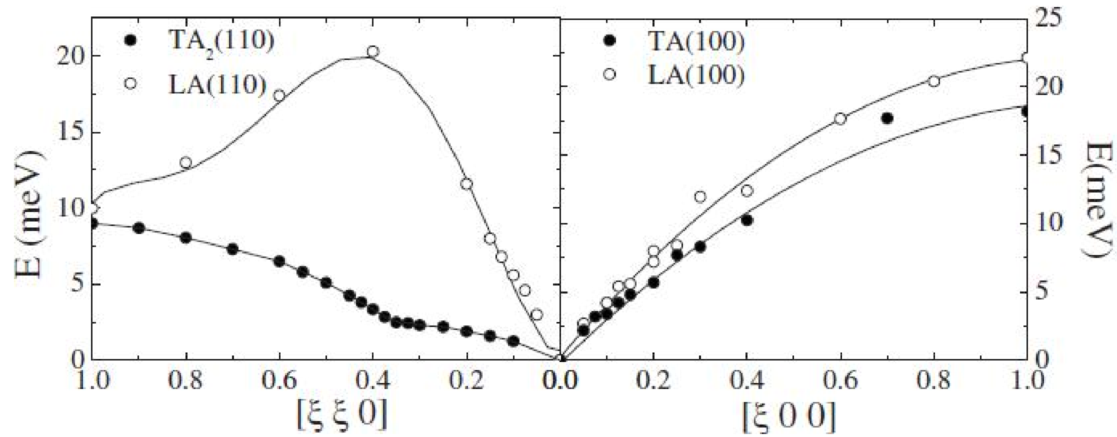
Ferromagnetic shape memory effect in Ni_2FeGa

Thermoelastic martensitic transition at 110K

TABLE I. Refined structural and magnetic parameters (300 K) corresponding to the $L2_1$ cubic phase obtained by single-crystal neutron diffraction.

$T=300$ K	Site	Atom	Occupancy
Lattice parameters (Å) $a=b=c=5.7495$	$4a$ (0 0 0)	Fe	0.86(1)
		Ni	0.06(1)
		Ga	0.08(1)
	$4b$ (0.5 0.5 0.5)	Ga	1.00(1)
	$8c$ (0.25 0.25 0.25)	Ni	1.00(1)
	Magnetic moment (μ_B)	Fe	0.82(2)
		Ni	−0.07(2)
	χ^2		16.58

Neutron diffraction: Structure of austenitc phase



Neutron spectroscopy: Phonon dispersion relation

Influence of phonons?
Influence of magnetic field?

Phys. Rev. B 80, 144301 (2009)

Phonon softening at the austenitic/martensitic transition in Ni-Fe-Ga alloys

Ferromagnetic shape memory effect in Ni_2FeGa

Thermoelastic martensitic transition at 110K

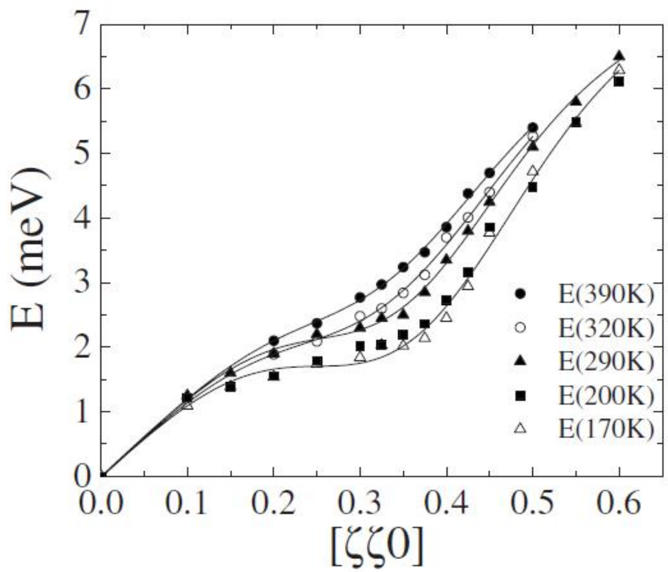
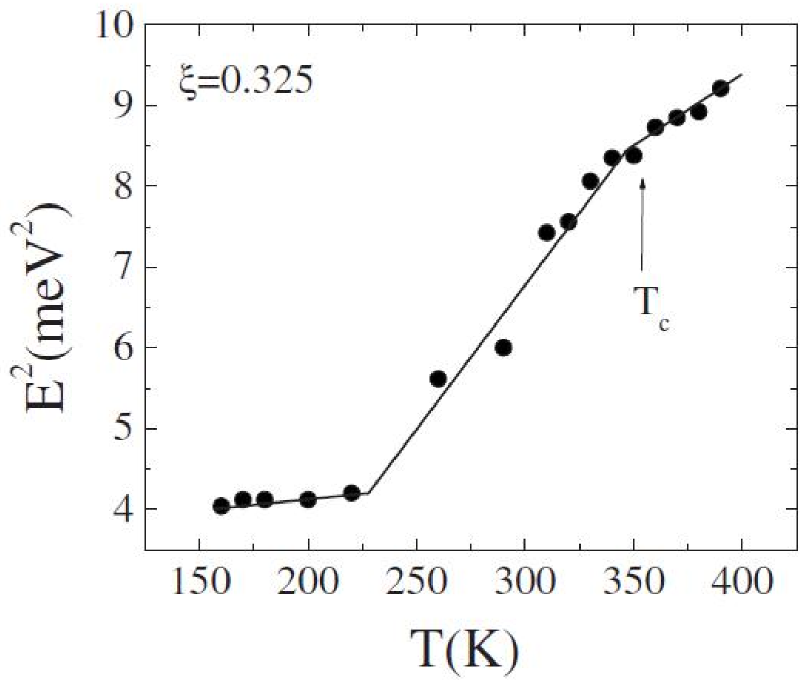


FIG. 3. Temperature dependence of the TA_2 phonon branch along the [110] direction of the $L2_1$ phase.



Prescursor effect: Softening of the TA_2 phonon at (0.35,0.35,0) far above T_m

Phys. Rev. B 80, 144301 (2009)

Phonon softening at the austenitic/martensitic transition in Ni-Fe-Ga alloys

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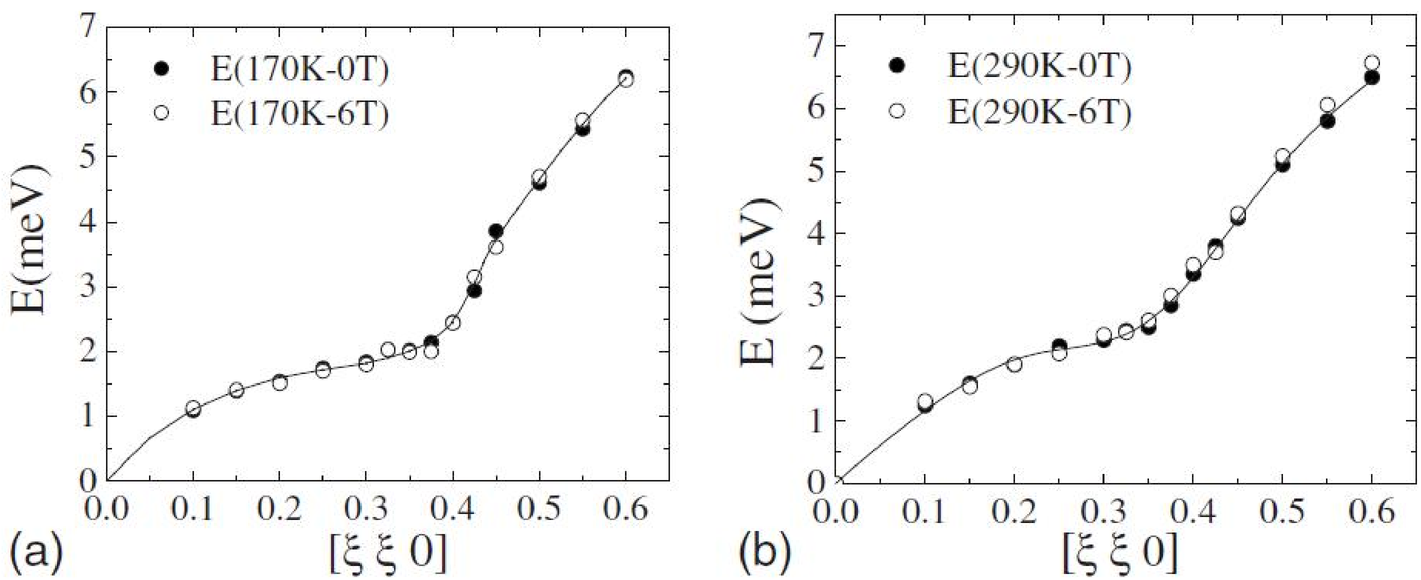


FIG. 6. TA_2 phonon branch along the [110] direction measured at (a) 170 K and (b) 290 K in a external field $H=0$ T (●) and $H=6$ T (○).

Negligible influence of magnetic field

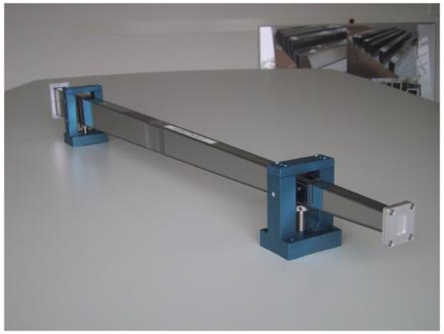
Premartensitic effects, induced by the crystal lattice

Phys. Rev. B 80, 144301 (2009)

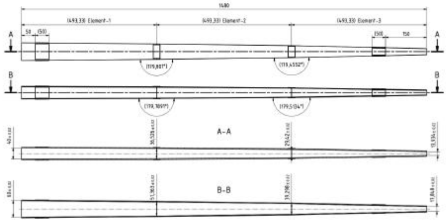
Work Student Physics Project:
Installation and commissioning of advanced neutron optics for the PANDA triple-axis instrument

Inelastic neutron scattering is a unique technique to study magnetic excitations in quantum systems, low-dimensional magnets and heavy fermion systems. PANDA here at TUM/FRM2 is one of the world-leading triple-axis spectrometers serving an international community. Today's focus shifts gradually to **new systems with exotic behaviour**, in order to study quantum phenomena, criticality, frustration etc. For this purpose, we optimized and purchased a dedicated **neutron-focusing device**, which now needs to be **installed on PANDA**. Once this is done, the **commissioning with a neutron beam** will take place. The final device will ensure a top-class spectrometer for the years to come, to study more exotic properties of matter in combination with more stringent sample environment conditions (extreme pressures, magnetic fields and temperatures).

PANDA spectrometer



Focusing Supermirror



PANDA guide drawing

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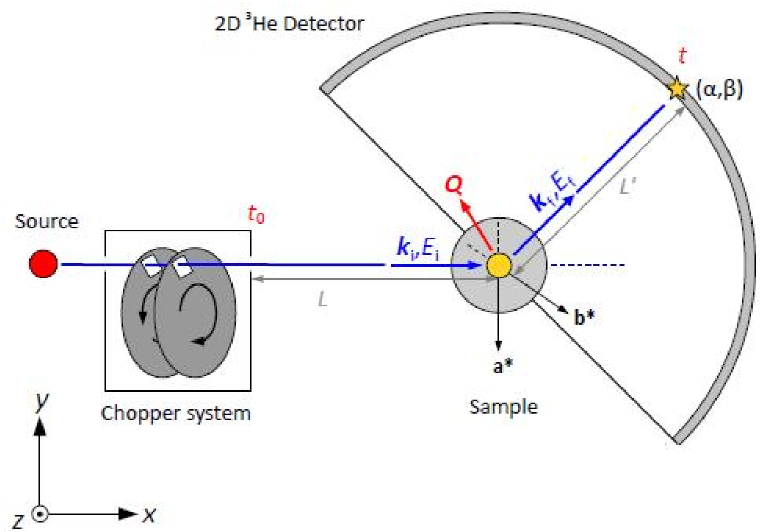
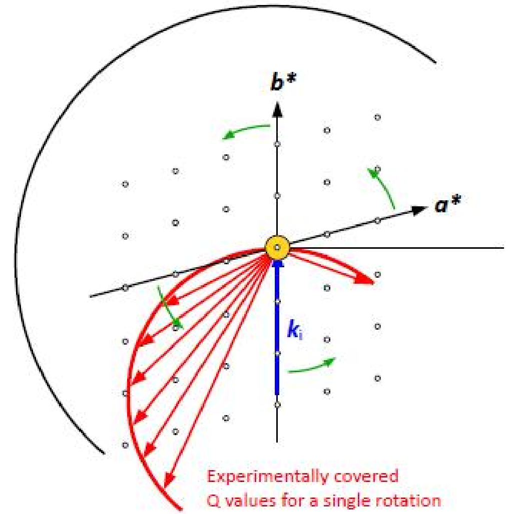
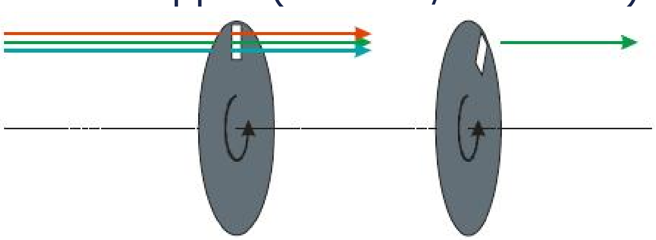
Inelastic scattering: TOF

Time of Flight (TOF) Spectroscopy

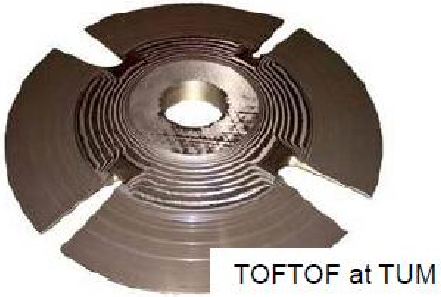




Disc chopper (AIRBUS/ASTRIUM)



Perfect for diffuse excitations (low D magnetism, melts...)
Covers a large region of momentum/energy space simultaneously
Flexible resolution
Data treatment tricky
Fast measurements
Perfectly suited for pulsed neutron sources



Introduction: Low D magnetism in a nutshell

- T=0

	Ising	XY	Heisenberg
d=1	Order	Quasi-LRO or Disorder	Quasi-LRO or Disorder
d=2	Order	Order	Order
d=3	Order	Order	Order

- T>0

	Ising	XY	Heisenberg
d=1	Disorder	Disorder	Disorder (Mermin-Wagner Th.)
d=2	Order (Onsager)	Quasi-LRO (Kosterlitz-Thouless)	Disorder (Mermin-Wagner Th.)
d=3	Order	Order	Order

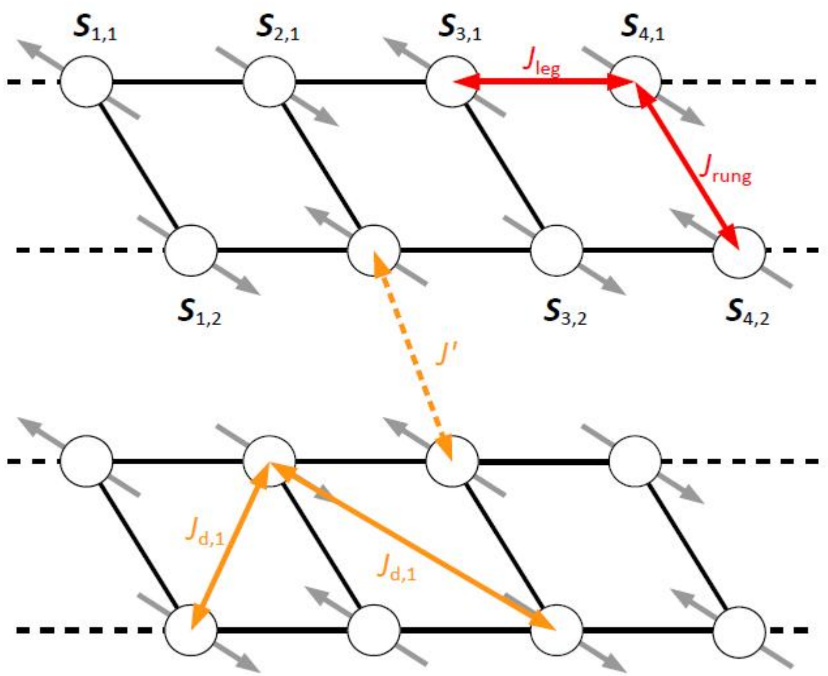
- No long-range order = static spin correlations = ***no magnetic diffraction***!

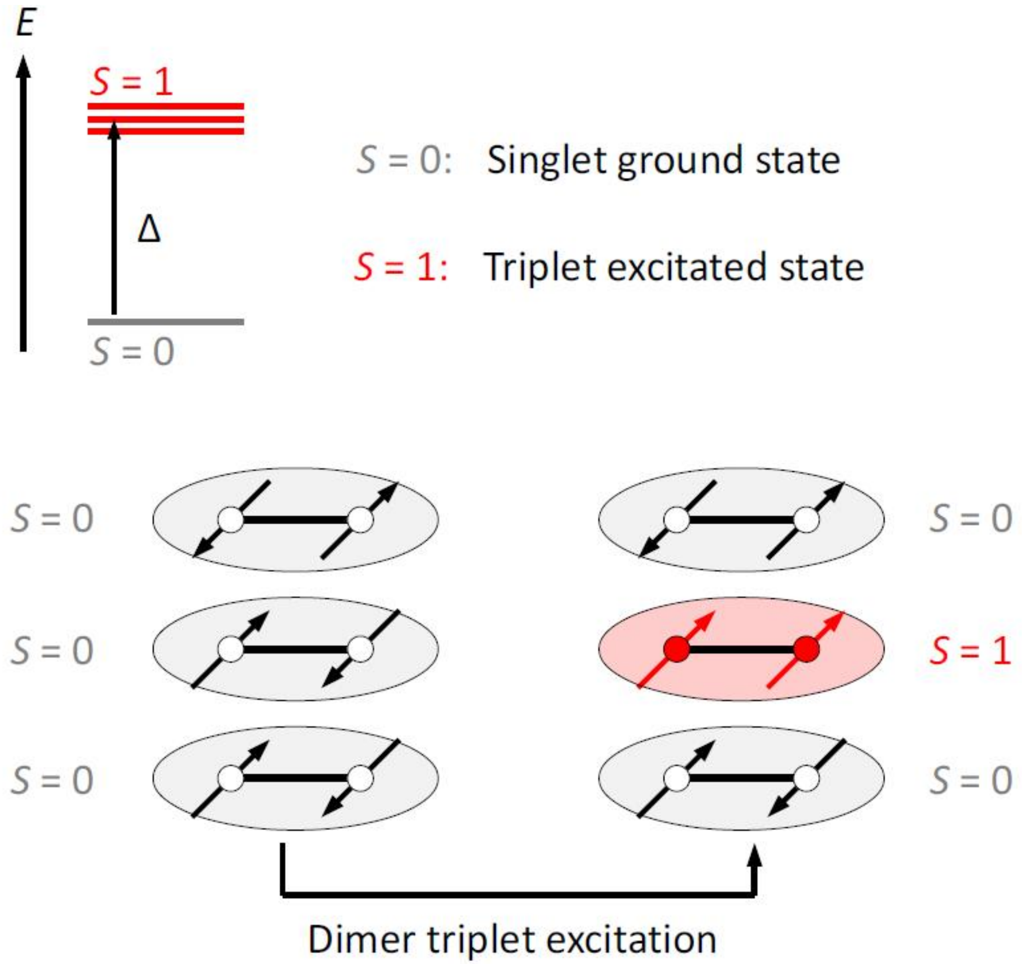
- No long-range order = no waves in the order parameter = ***no spin waves***!

Low D magnetism: Completely new physics + nice model system

Why low-D magnetism? Generic system spin-ladder

1D-spin ladder made of coupled S=1/2 spins



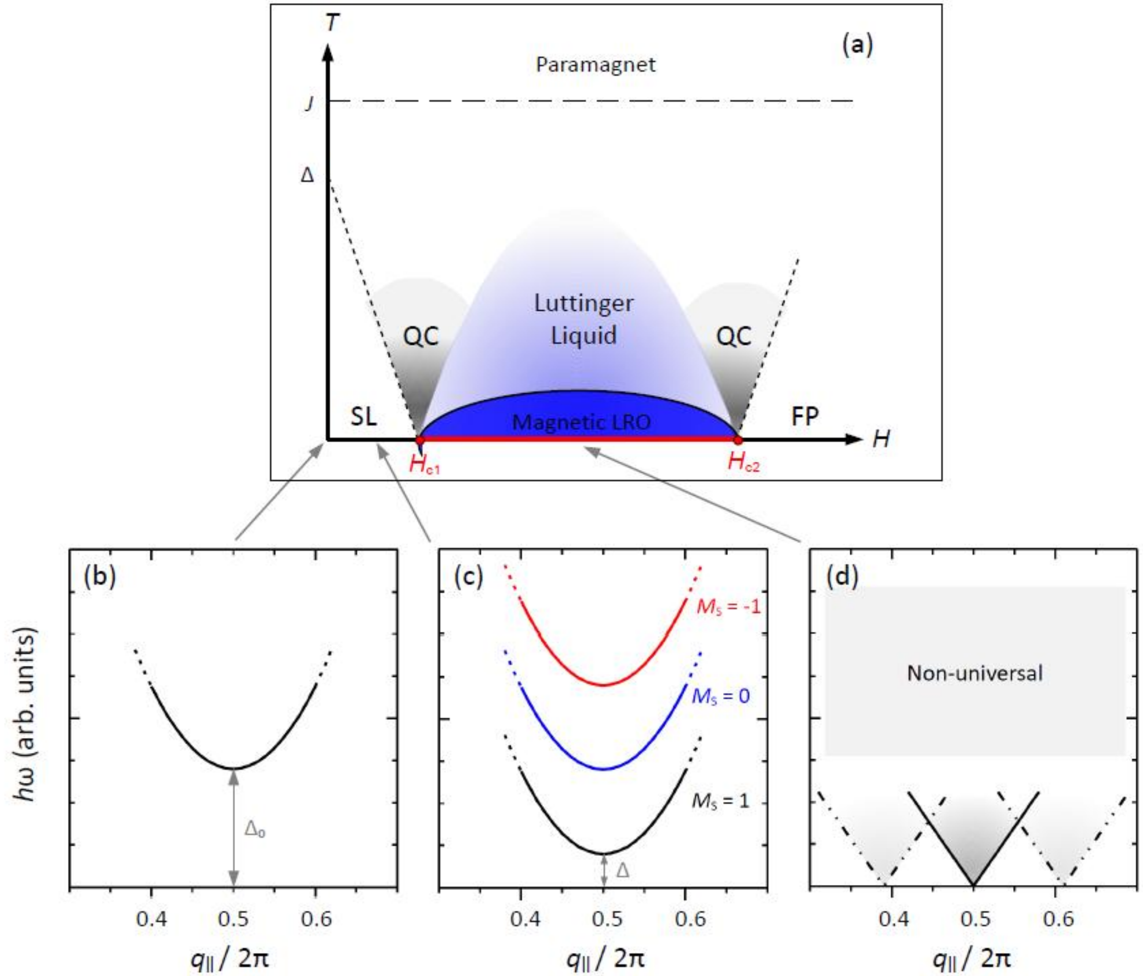


Clean model system for Bose Einstein Condensation!

Inelastic scattering: Example II

Why low-D magnetism? Generic system spin-ladder

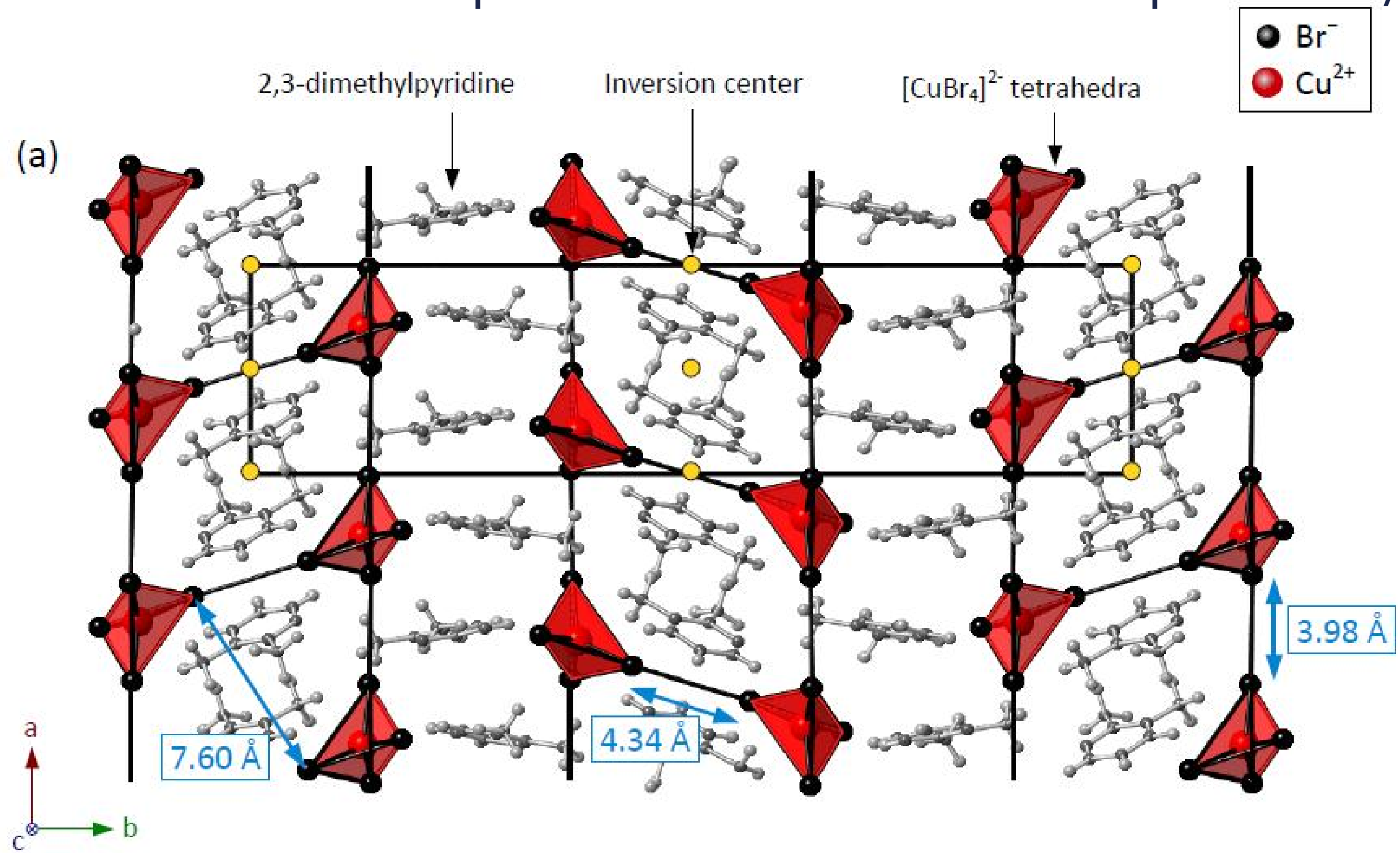
1D-spin ladder made of coupled S=1/2 spins



Clean model system for Bose Einstein Condensation!

Why low-D magnetism? Generic system spin-ladder DIMPY

DIMPY: Realization of a 1D-spin AF ladder made of coupled S=1/2 spins



Copper S=1/2 spins
Convenient energy scales for cold neutrons (few K,T)
$(CuBr_4)^{-2}$ tetrahedra + organic spacer
Wet chemistry gives nice X-tals

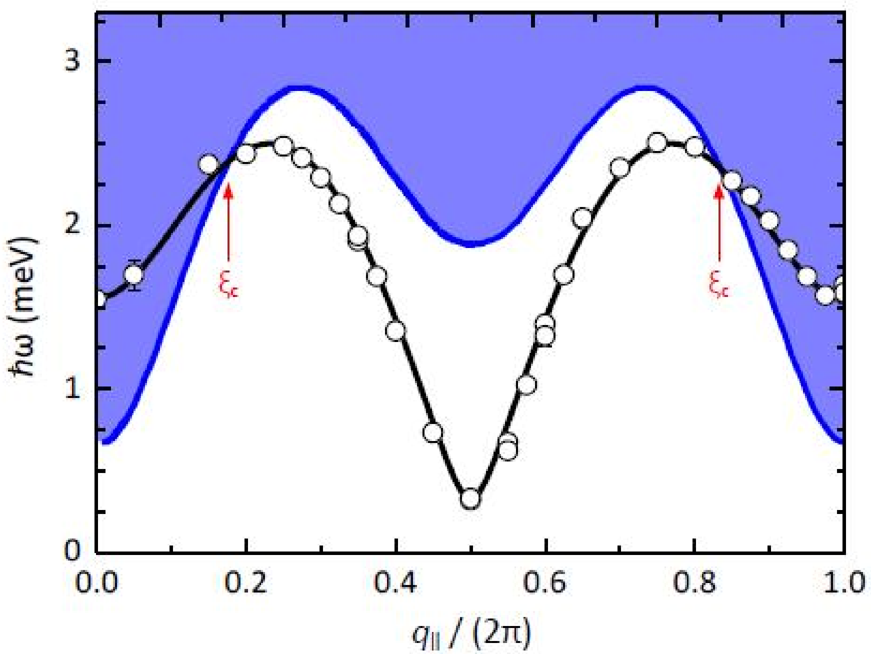
Inelastic scattering: Example II

Why low-D magnetism? Generic system spin-ladder DIMPY

DIMPY: Realization of a 1D-spin AF ladder made of coupled S=1/2 spins

- Due to 1D nature: Dispersion flat perp. to ladder direction
  Integration in (*q*,*E*) possible

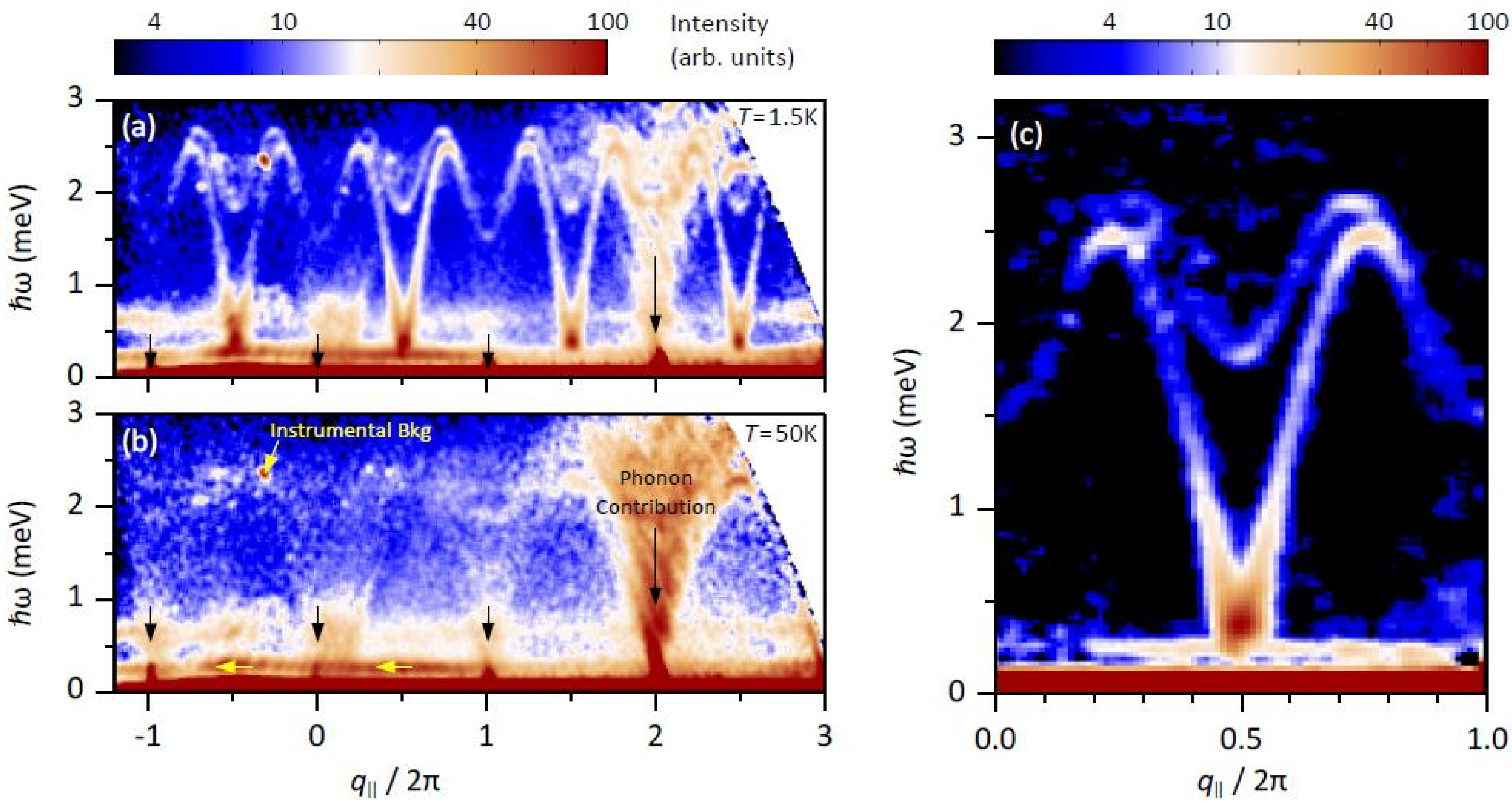
  Ideal for TOF -instrument
- Non-universal excitations in Luttinger liquid
  Weak continua (2magnon) + sharp excitations (1 magnon)



Why low-D magnetism? Generic system spin-ladder DIMPY

DIMPY: Realization of a 1D-spin AF ladder made of coupled S=1/2 spins

Data taken at CNCS (SNS, Oak Ridge, USA)



Why low-D magnetism? Generic system spin-ladder DIMPY

DIMPY: Realization of a 1D-spin AF ladder made of coupled S=1/2 spins

Note the appendix: Removal of background

A. Appendix A: Background subtraction

In the following Appendix, we briefly describe the background subtraction procedure. It is a standard approach and was performed in a similar way in e.g. Refs. 3, 40. For the present experiment, two sources of background were assumed: (1) Temperature-independent background both from the cryostat and other equipment as well as coherent and incoherent scattering from the sample[26] and (2) inelastic phonon scattering from the sample, proportional to the bose-factor $n(\omega)+1$. The total signal $\mathcal{I}(\mathbf{Q},\omega,T)$ at $T_1 = 50$ K and $T_2 = 110$ K was modelled as

$$\mathcal{I}(\mathbf{Q},\omega,T) = \mathcal{A}(\mathbf{Q},\omega) + \mathcal{B}(\mathbf{Q},\omega)(n(\omega,T)+1) \quad (8)$$

with $n(\omega) = (e^{\hbar\omega/k_B T} - 1)^{-1}$ and $\mathcal{A}$, $\mathcal{B}$ describing the T-independent and T-dependent background, respectively. The background contributions can be calculated by

$$\mathcal{B}(\mathbf{Q},\omega) = \frac{\mathcal{I}_1(\mathbf{Q},\omega) - \mathcal{I}_2(\mathbf{Q},\omega)}{n(\omega,T_1) - n(\omega,T_2)} \quad (9)$$

$$\mathcal{A}(\mathbf{Q},\omega) = \mathcal{I}_1(\mathbf{Q},\omega) - \mathcal{B}(\mathbf{Q},\omega)(n(\omega,T_1)+1). \quad (10)$$

The background subtracted signal at base temperature $T_0 = 1.5$ K is therefore

$$\mathcal{I}^{\mathrm{sub}}(\mathbf{Q},\omega) = \mathcal{I}_0(\mathbf{Q},\omega) - \mathcal{A}(\mathbf{Q},\omega) - \mathcal{B}(\mathbf{Q},\omega)(n(\omega,T_0)+1). \quad (11)$$