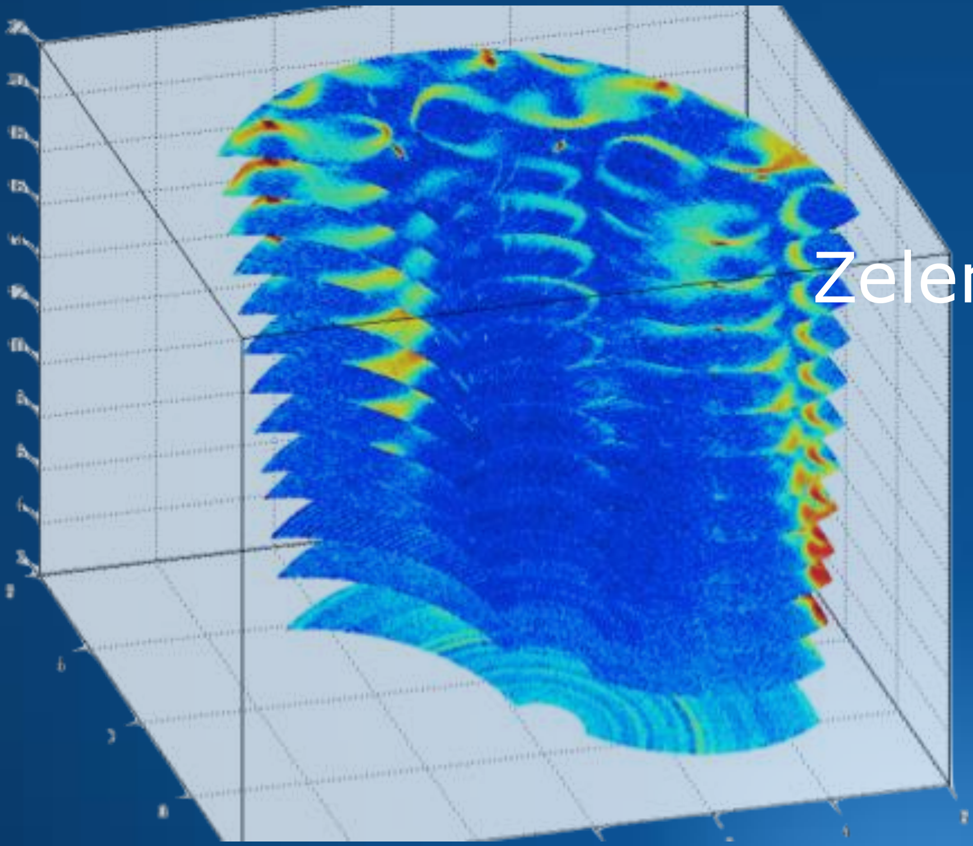
Spectroscopy on TAS instruments



Martin Boehm, ILL, Grenoble

Zelenogorsk, 15th March 2016

Outline

Science with neutron spectroscopy

Short TAS description

Examples

TAS development

Challenges

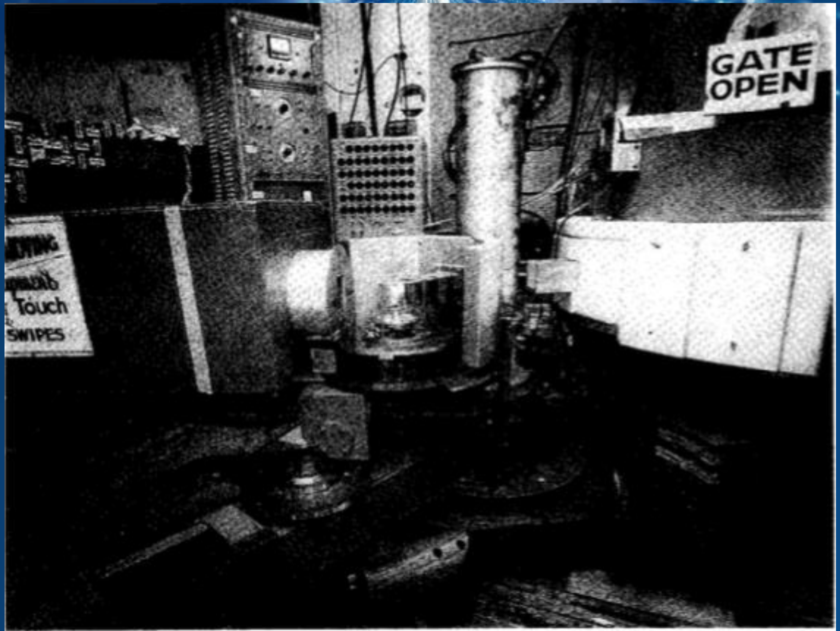


Fig. 9: Photograph (1959) of the original triple-axis spectrometer at the NRU reactor at Chalk River. The

B.N. Brockhouse, C.G. Shull, Chalk River, 1959
From the Nobel prize lecture 1994

Well established method in condensed matter physics.

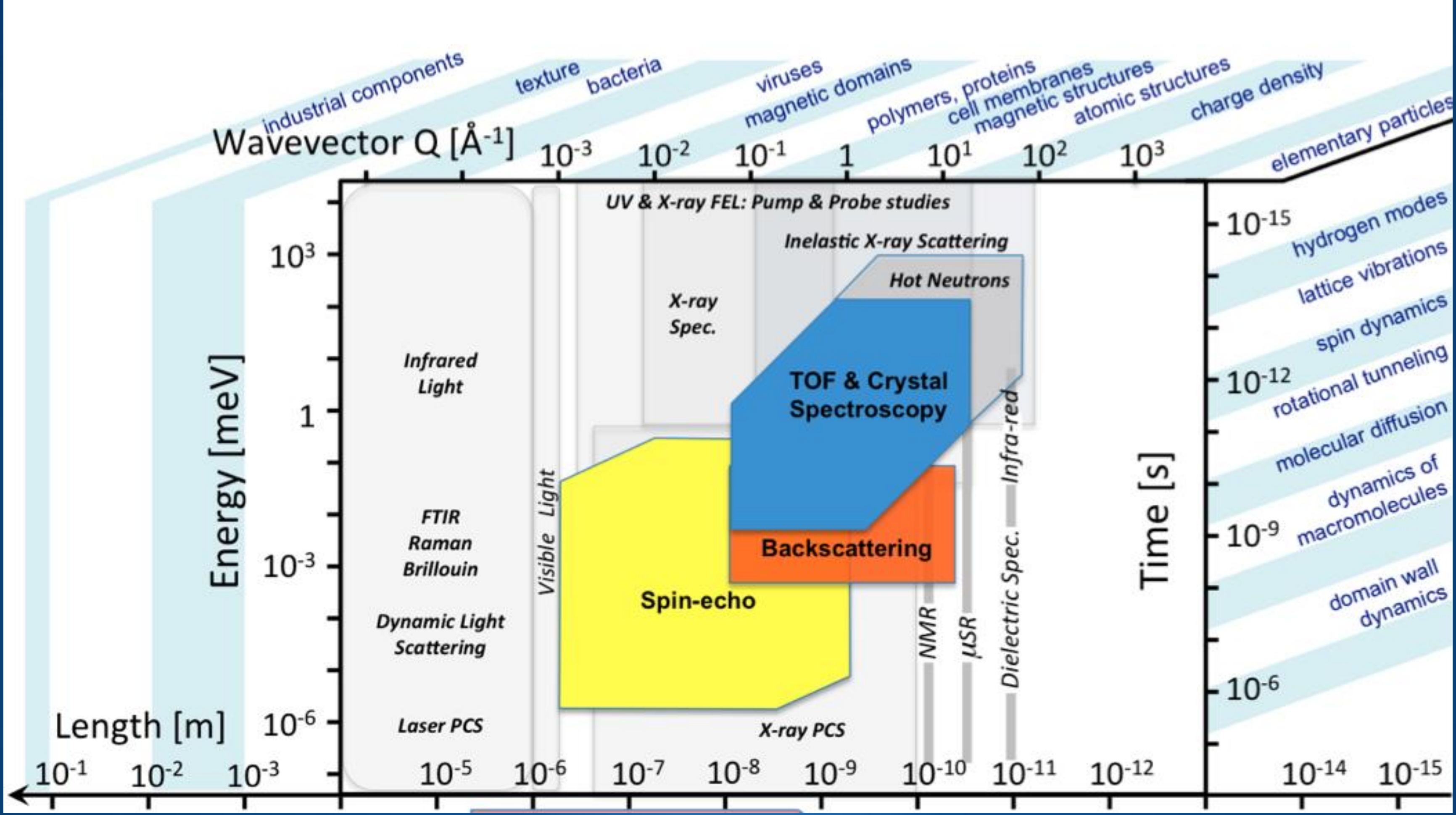
Reactor based experimental technique.

Probes collective lattice and magnetic excitations.

ILL reactor

Versatile experimental technique.

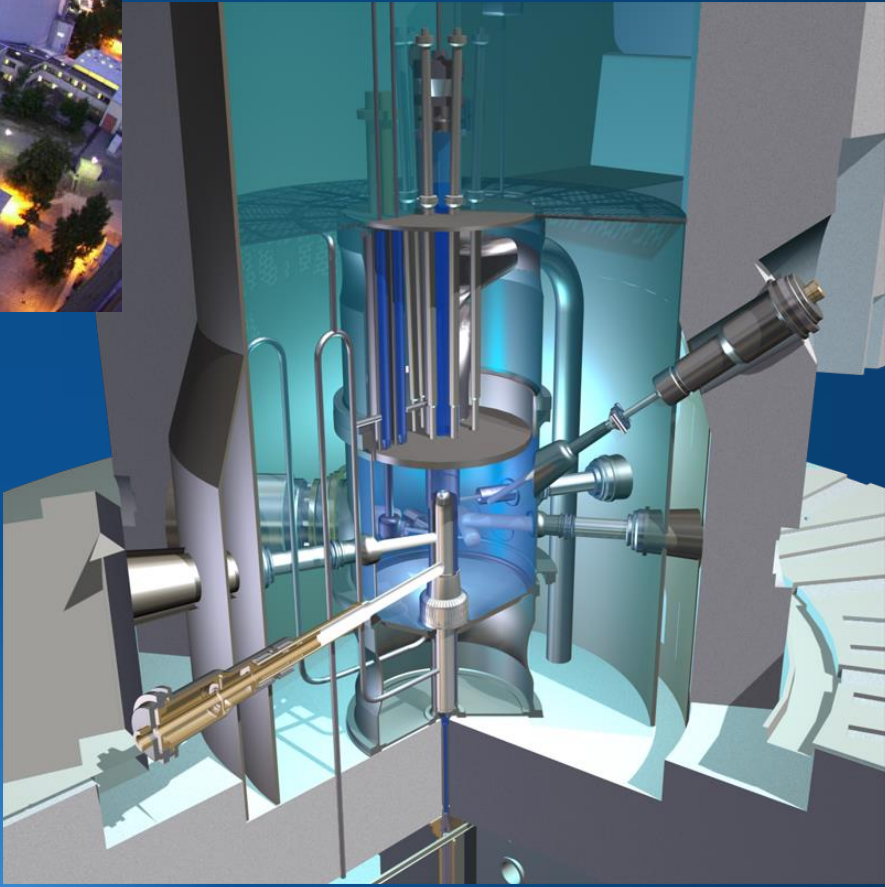
‘Large’ volume samples.



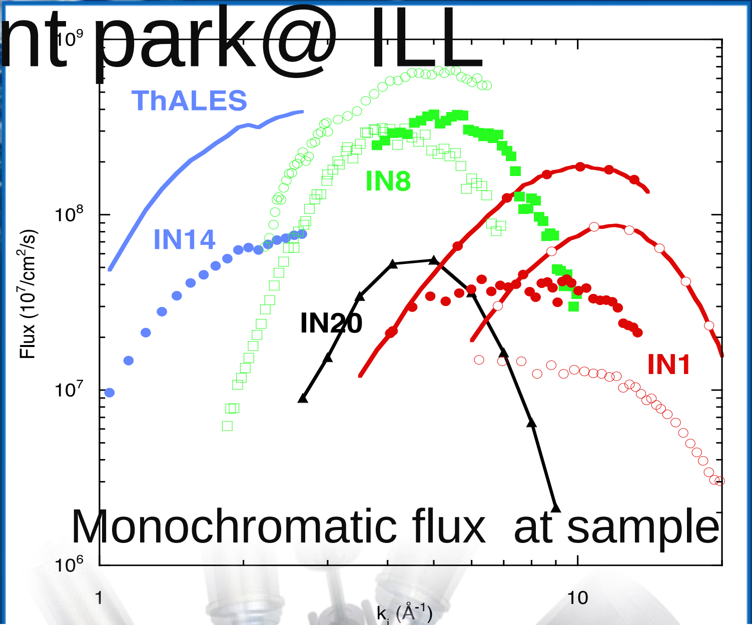
Taken from ESS Technological Documentation, 2013

The ILL Reactor

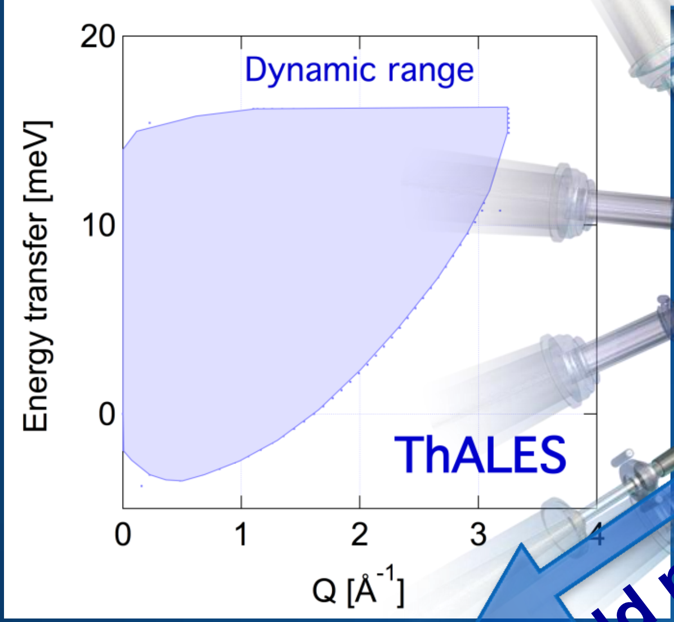
Operating 200 days/year
58 MW reactor - 4 cycles/year

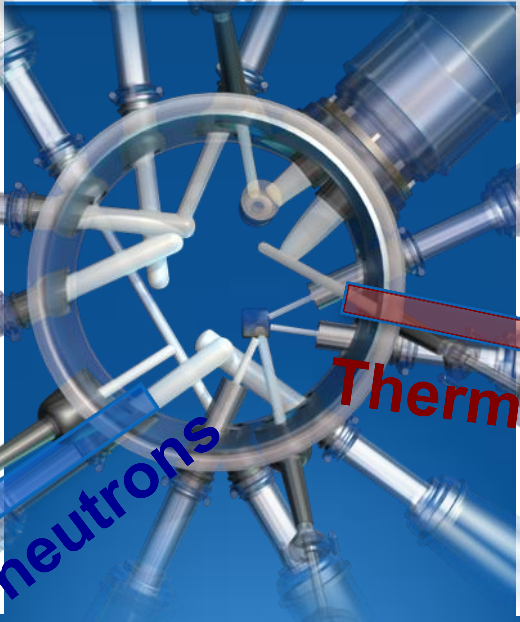


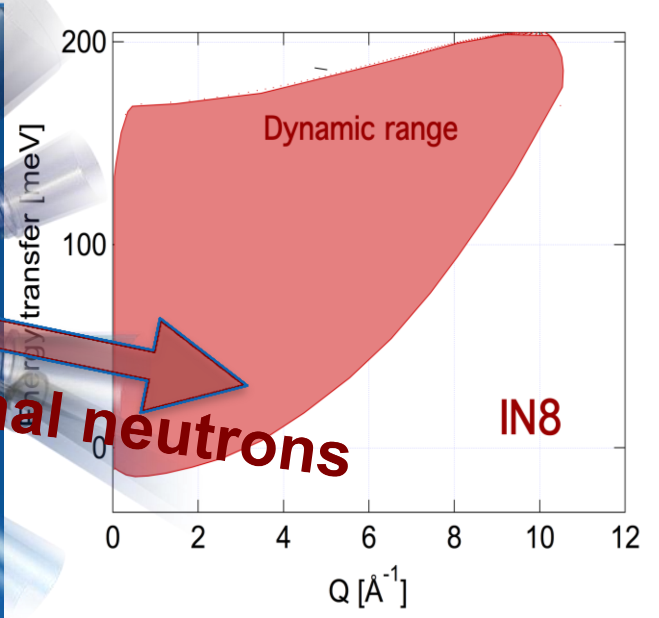
TAS Instrument park@ ILL



Monochromatic flux at sample







Cold neutrons

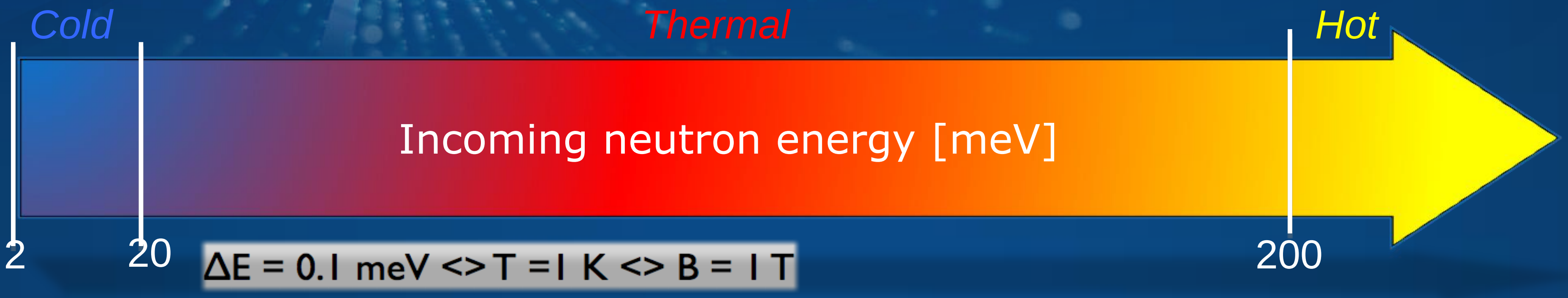
Thermal neutrons

Spectrometers:

ThALES
IN12 (CRG)

IN8 high flux
IN20 polarized
IN22 (CRG)

Lagrange



$\Delta E = 0.1$ meV <> T = 1 K <> B = 1 T

Scientific fields:

Heavy fermions physics
Oxide physics
Quantum criticality
Exotic ordering
Unconventional superconductors
Multiferroics
Skyrmions
Frustration, quantum magnetism

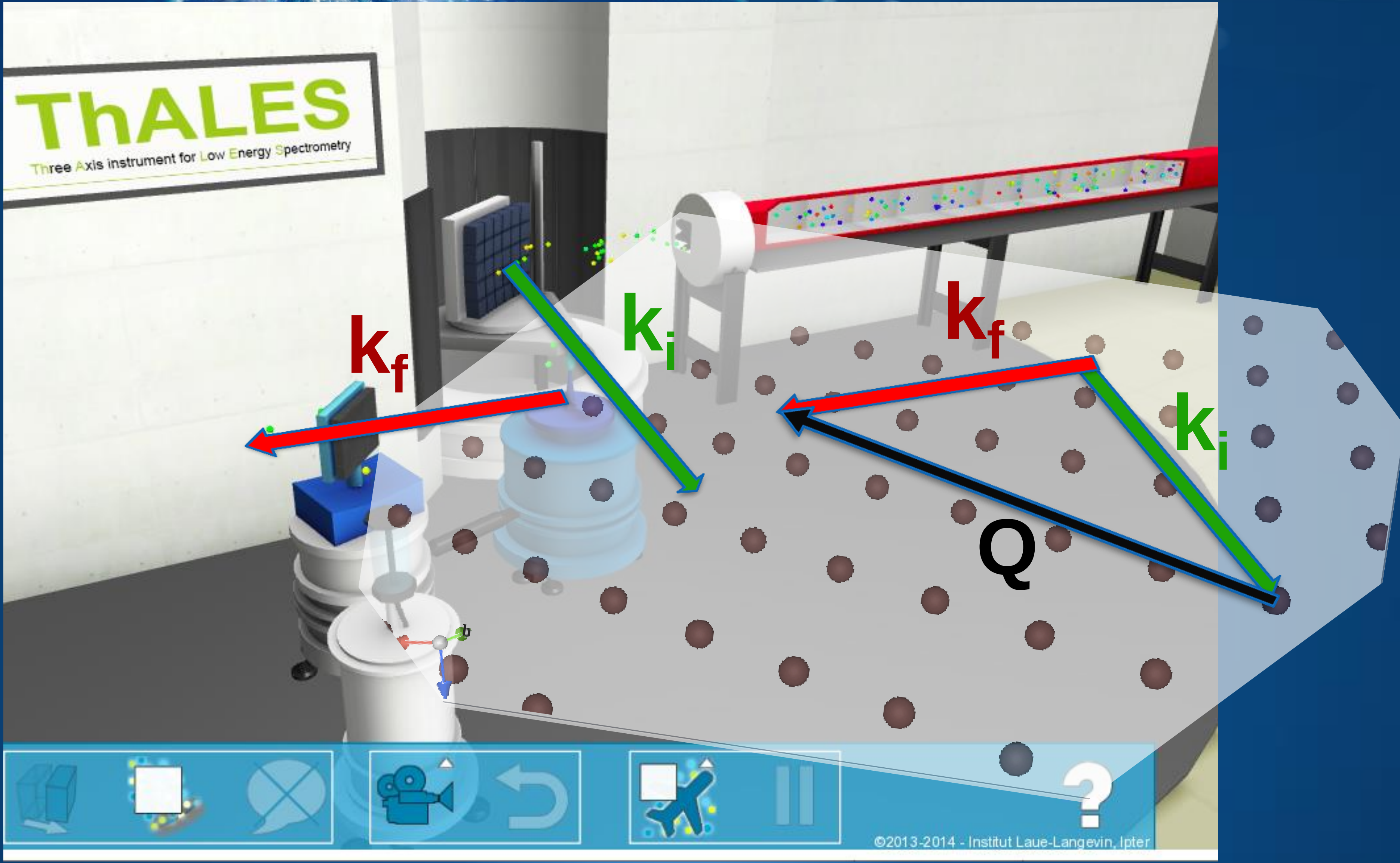
Phonons, magnons and electromagnons
Superconductors
Carbon-based materials
Multiferroics
Relaxors
Amorphous, liquid matter
Materials at extreme pressure

Life science: H-bonding
Energy storage: hydrides of metals
Zeolites and metallic catalysts
Nano-crystalline materials : fullerenes, nanotubes polymers,
amorphous materials and composites, surfaces and porous media
Geochemistry matters for earth science

Three axis spectroscopy – *a cartoon*

https://www.ill.eu/en/html/about/movies/animations/instrument-animations/

Three axis spectroscopy – *a cartoon*



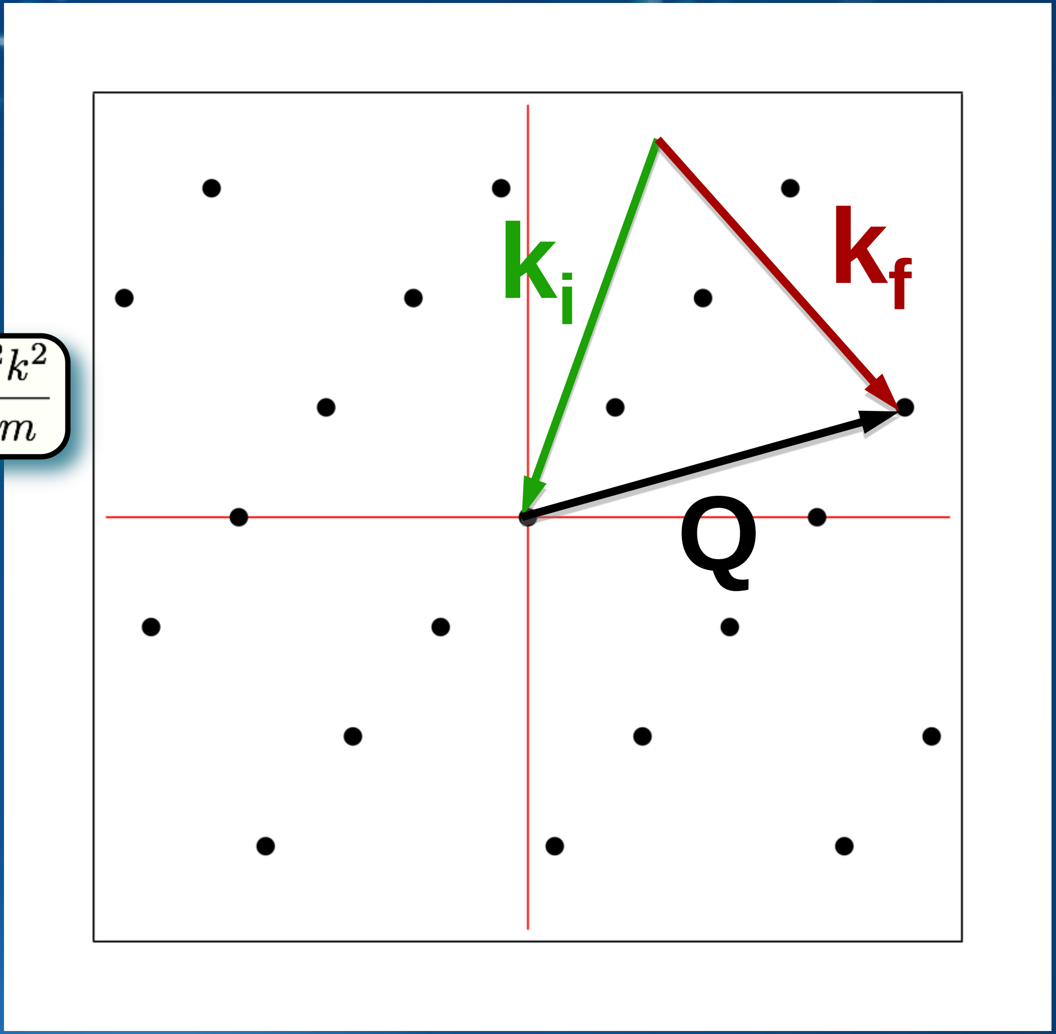
Three axis spectroscopy

$$\hbar\vec{Q} = \vec{p}_i - \vec{p}_f \qquad \vec{p} = \hbar\vec{k}$$

Conservation of momentum

$$\Delta E = E_i - E_f \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Conservation of energy



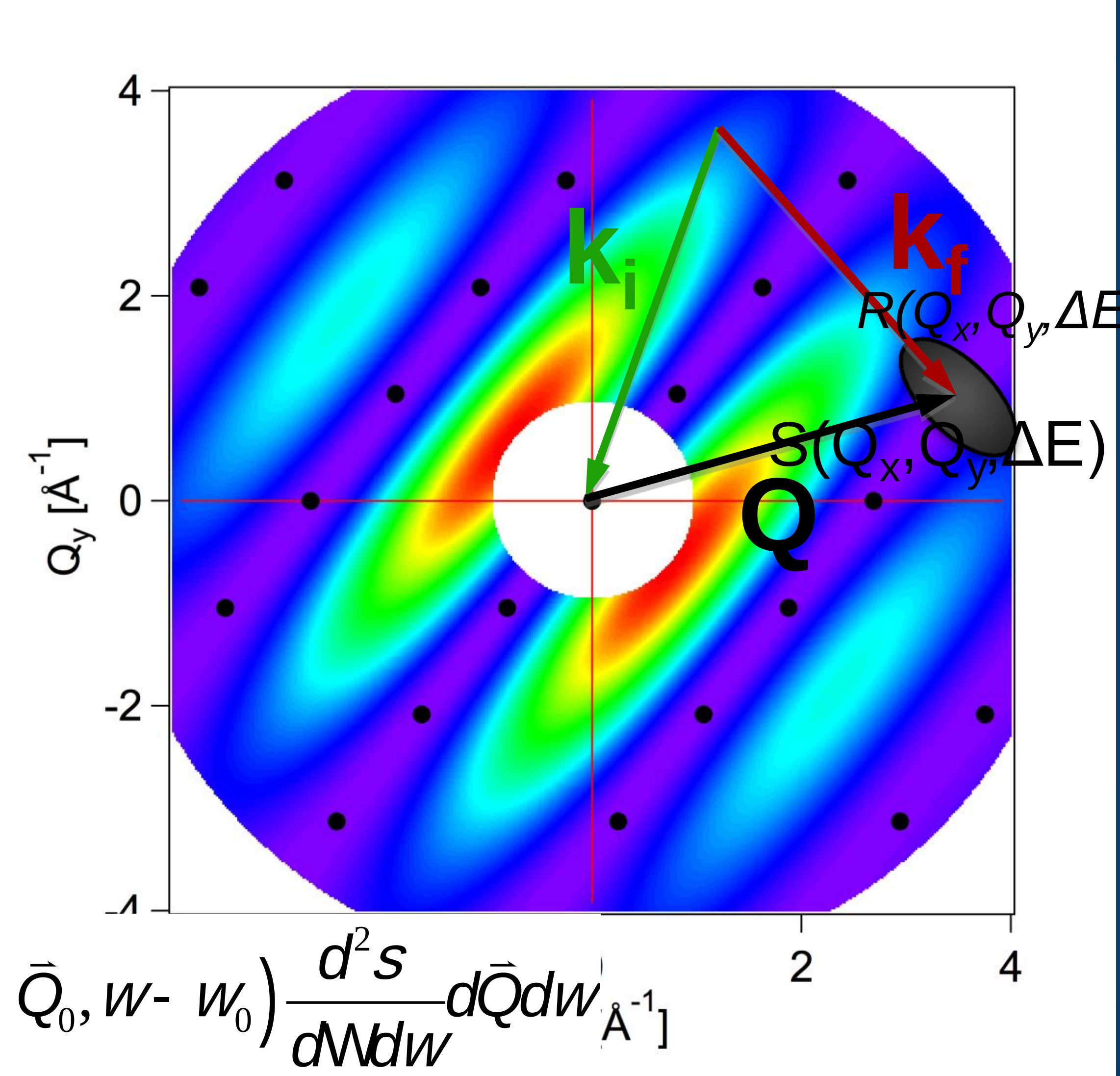
Three axis spectroscopy

Exploring S(**Q**,ω) in a 4D space spanned by **Q**=(Q_x,Q_y,Q_z) and ΔE=ħω.

$$\frac{d^2\sigma_{\vec{k}_i \rightarrow \vec{k}_f}}{d\Omega dE_f} = \frac{k_f}{k_i} S\left(\vec{Q},\omega\right)$$

S: Scattering function

R: Resolution function



$$I\left(\vec{Q}_0, w_0\right) = NA\left(\vec{k}_i\right) \square R\left(\vec{Q} - \vec{Q}_0, w - w_0\right) \frac{d^2 s}{dWdw} d\vec{Q} dw$$

Coherent one-phonon neutron cross-section (energy loss):

$$S(\vec{Q},\omega) \propto \exp\left(-2W\right) \sum_{s} \sum_{\tau} \frac{\left(\vec{Q}\cdot\vec{e}_s\right)^2}{\omega_s} \left\langle n_s + 1 \right\rangle \delta\left(\omega - \omega_s\right) \delta\left(\vec{Q} - \vec{q} - \vec{\tau}\right)$$

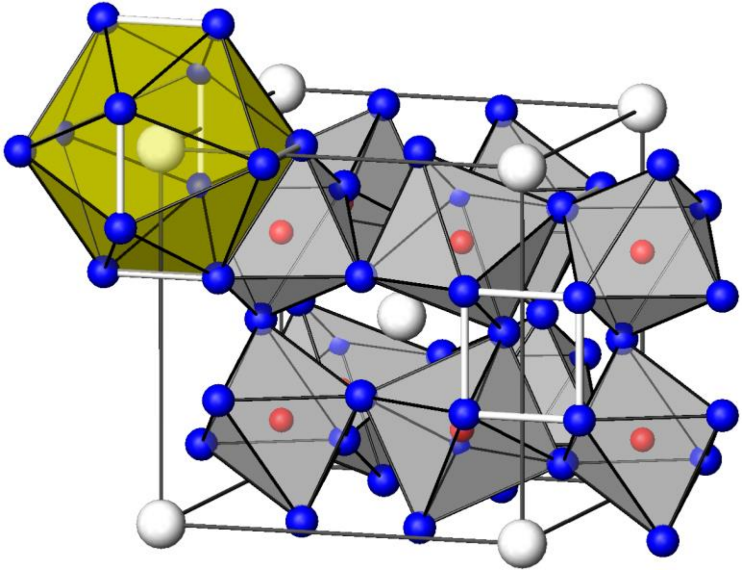
Classical phonon study in the skutterudite $LaFe_4Sb_{12}$:

M. Koza et al.

Reduced thermal conductivity in $M_{1-x}Fe_yCo_{4-y}Sb3$ (M= e.g. La, Ce)

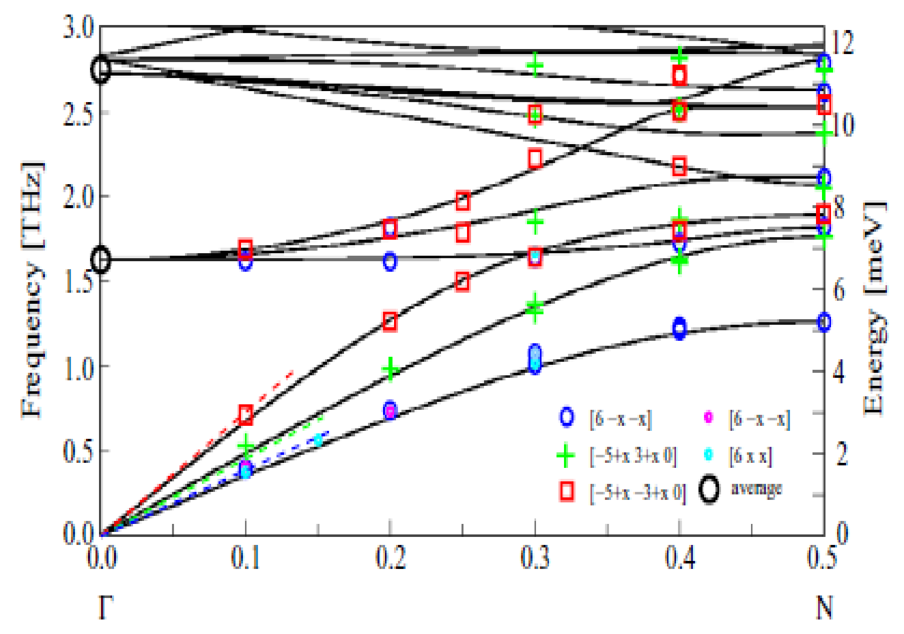
Vibrational modes 5 to 10 meV

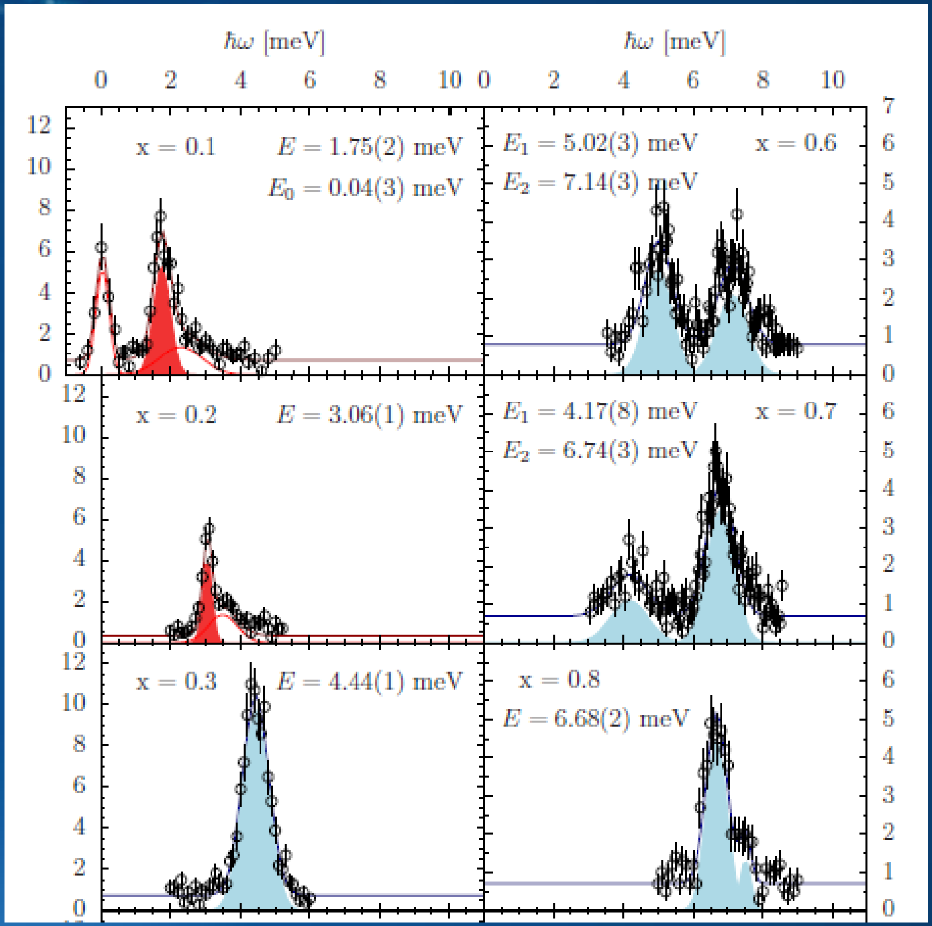
Small sample mass, good energy resolution



Koza, M. M.; Boehm, M.; Sischka, E.; Schnelle, W.; Mutka, H.; Leithe-Jasper, A.; *Physical Review B* **2015**, *91*, 014305.

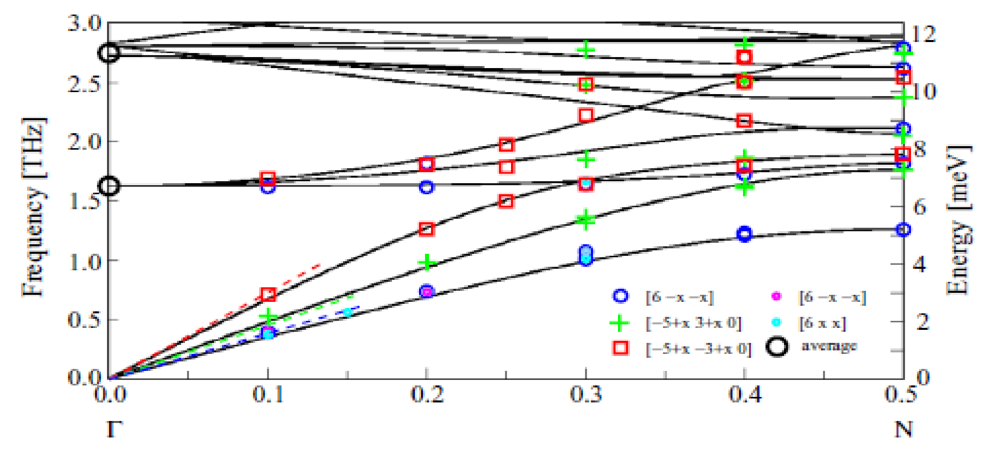
Classical phonon study in the skutterudite LaFe$_4$Sb$_{12}$:

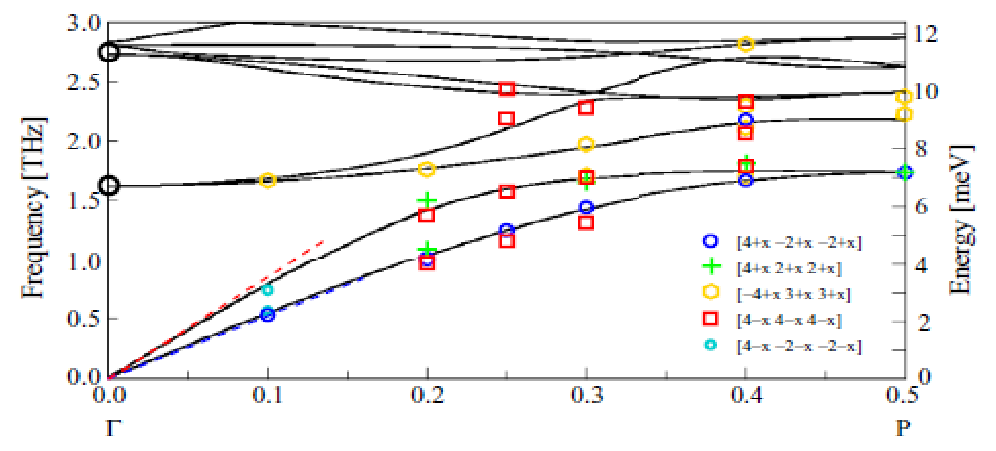




Koza, M. M.; Boehm, M.; Sischka, E.; Schnelle, W.; Mutka, H.; Leithe-Jasper, A.; *Physical Review B* **2015**, *91*, 014305.

Classical phonon study in the skutterudite $LaFe_4Sb_{12}$:





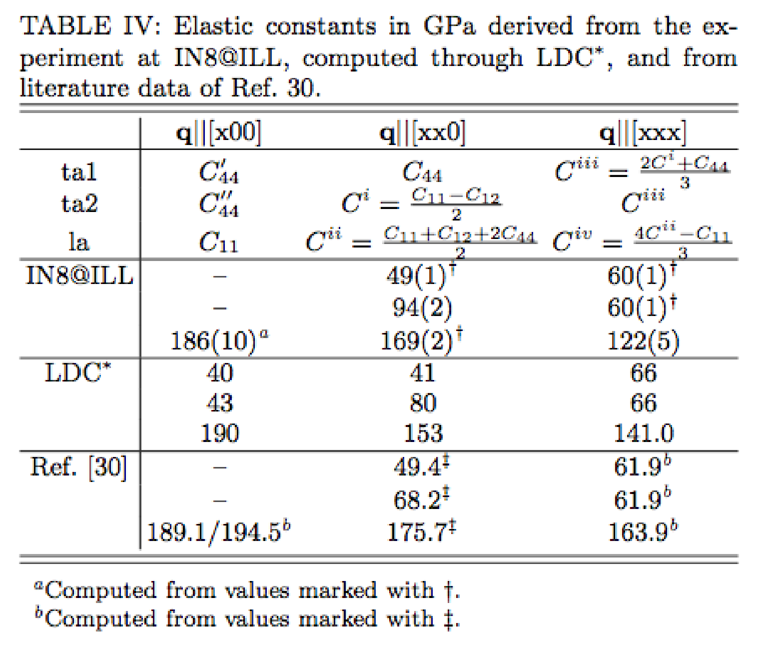


TABLE IV: Elastic constants in GPa derived from the experiment at IN8@ILL, computed through LDC*, and from literature data of Ref. 30.

	q||[x00]	**q**||[xx0]	**q**||[xxx]
ta1	C'_{44}	C_{44}	$C^{iii} = \frac{2C^{i}+C_{44}}{3}$
ta2	C''_{44}	$C^{i} = \frac{C_{11}-C_{12}}{2}$	C^{iii}
la	C_{11}	$C^{ii} = \frac{C_{11}+C_{12}+2C_{44}}{2}$	$C^{iv} = \frac{4C^{ii}-C_{11}}{3}$
IN8@ILL	–	49(1)†	60(1)†
	–	94(2)	60(1)†
	186(10)^a	169(2)†	122(5)
LDC*	40	41	66
	43	80	66
	190	153	141.0
Ref. [30]	–	49.4‡	61.9^b
	–	68.2‡	61.9^b
	189.1/194.5^b	175.7‡	163.9^b

[a] Computed from values marked with †.
[b] Computed from values marked with ‡.

Calculations indisponsible

Experimental calibration with TAS

No anomalies in life-time

Koza, M. M.; Boehm, M.; Sischka, E.; Schnelle, W.; Mutka, H.; Leithe-Jasper, A.; *Physical Review B* **2015**, *91*, 014305.

Quantum magnetism: close to QCPs

Magnetic (dipole-dipole) interaction:

$$S^{\alpha,\beta}(\vec{\kappa},\omega)=\frac{1}{2\pi\hbar}\sum_{ll'}\exp\left(i\vec{\kappa}\left(\vec{r}_l-\vec{r}_{l'}\right)\right)\int_{-\infty}^{\infty}\exp\left(-i\omega t\right)\left\langle S_l^{\alpha}(0)\,S_{l'}^{\beta}(t)\right\rangle dt$$

$$\frac{d^2\sigma}{d\Omega d\omega}=\left(\frac{\gamma r_0}{2}\right)^2\frac{k'}{k}\left(gf\left(\vec{Q}\right)\right)^2\exp\left(-2W\left(\vec{Q}\right)\right)\sum_{\alpha\beta}\left(\delta_{\alpha,\beta}-\hat{Q}_\alpha\hat{Q}_\beta\right)S^{\alpha,\beta}\left(\vec{Q},\omega\right)$$

Spin-spin correlation function

Polarization factor: → Dipole-dipole interaction

Magnetic form factor: → scattering at spatial distributed e^-'s.

Quantum magnetism: close to QCPs

Magnetic (dipole-dipole) interaction:

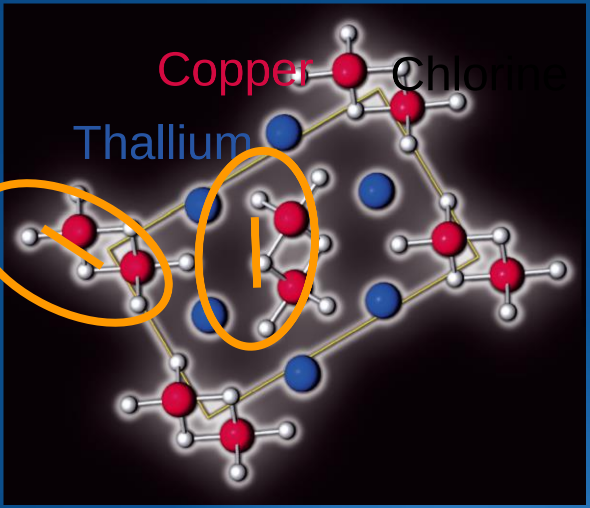
$$S^{\alpha,\beta}(\vec{\kappa},\omega)=\frac{1}{2\pi\hbar}\sum_{ll'}\exp\left(i\vec{\kappa}\left(\vec{r}_l-\vec{r}_{l'}\right)\right)\int_{-\infty}^{\infty}\exp(-i\omega t)\left\langle S_l^{\alpha}(0)\,S_{l'}^{\beta}(t)\right\rangle dt$$

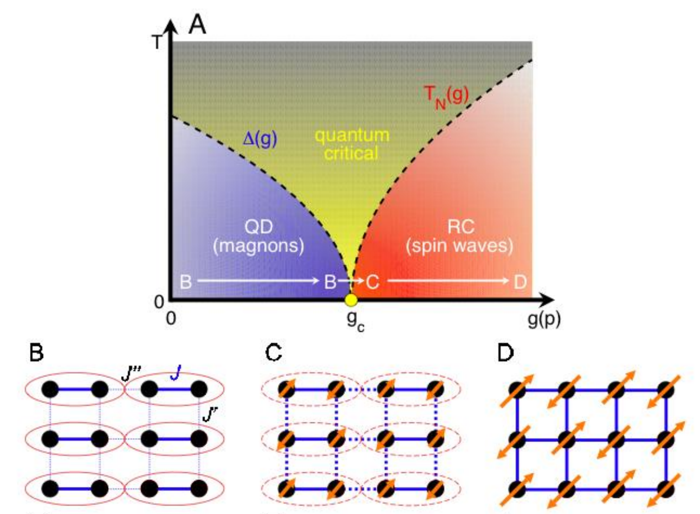
$$\frac{d^2\sigma}{d\Omega\, d\omega}=\left(\frac{\gamma r_0}{2}\right)^2\frac{k'}{k}\left(gf(\vec{Q})\right)^2\exp\left(-2W(\vec{Q})\right)\sum_{\alpha\beta}\left(\delta_{\alpha,\beta}-\hat{Q}_\alpha\hat{Q}_\beta\right)S^{\alpha,\beta}(\vec{Q},\omega)$$

Quantum magnetism:

Low S

Low D

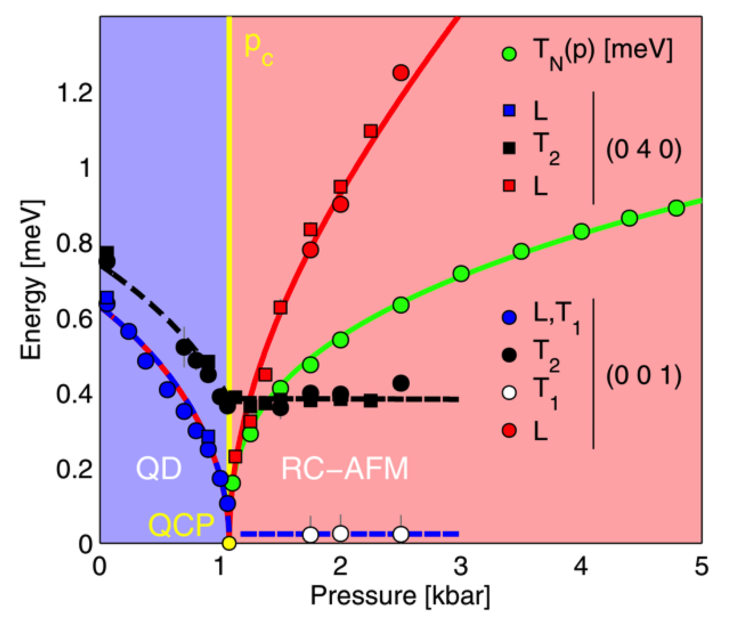


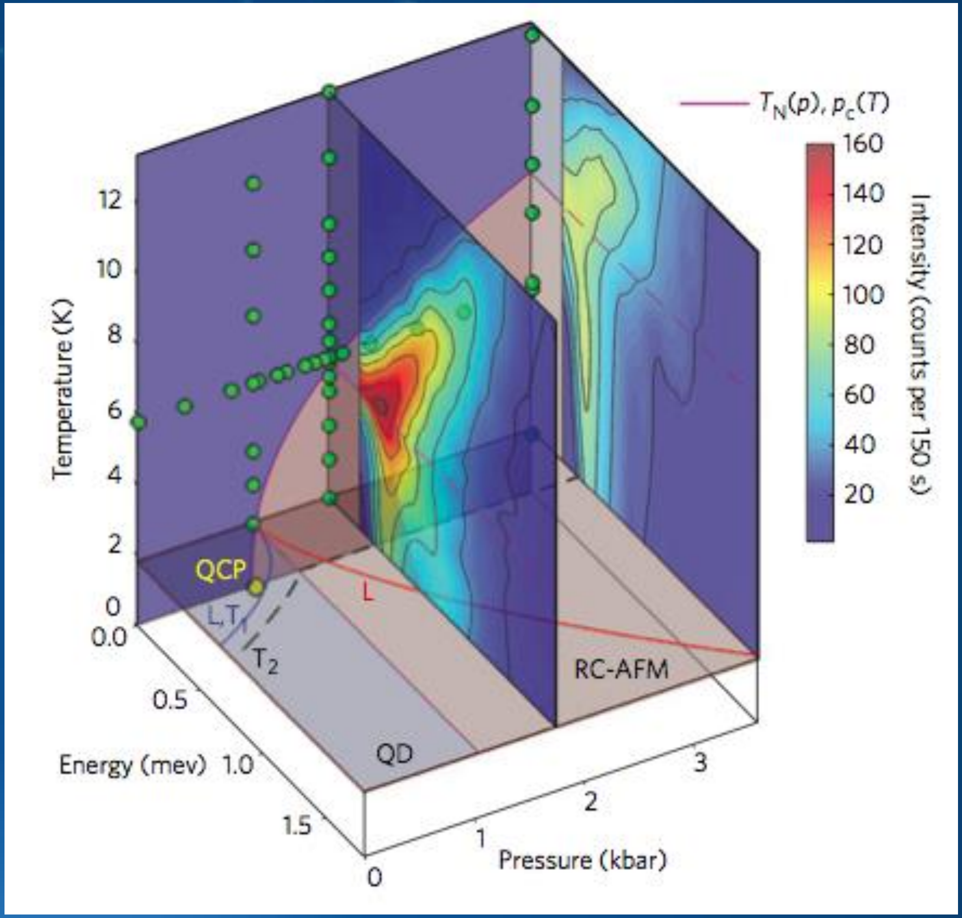


Merchant and al., Nature Physics ***10*** *(2014), p.373-379, and references.*

Quantum magnetism: close to QCPs

Probing the parameter space in restricted momentum space: Q= (0,4,0)





Merchant and al., Nature Physics ***10*** *(2014), p.373-379.*

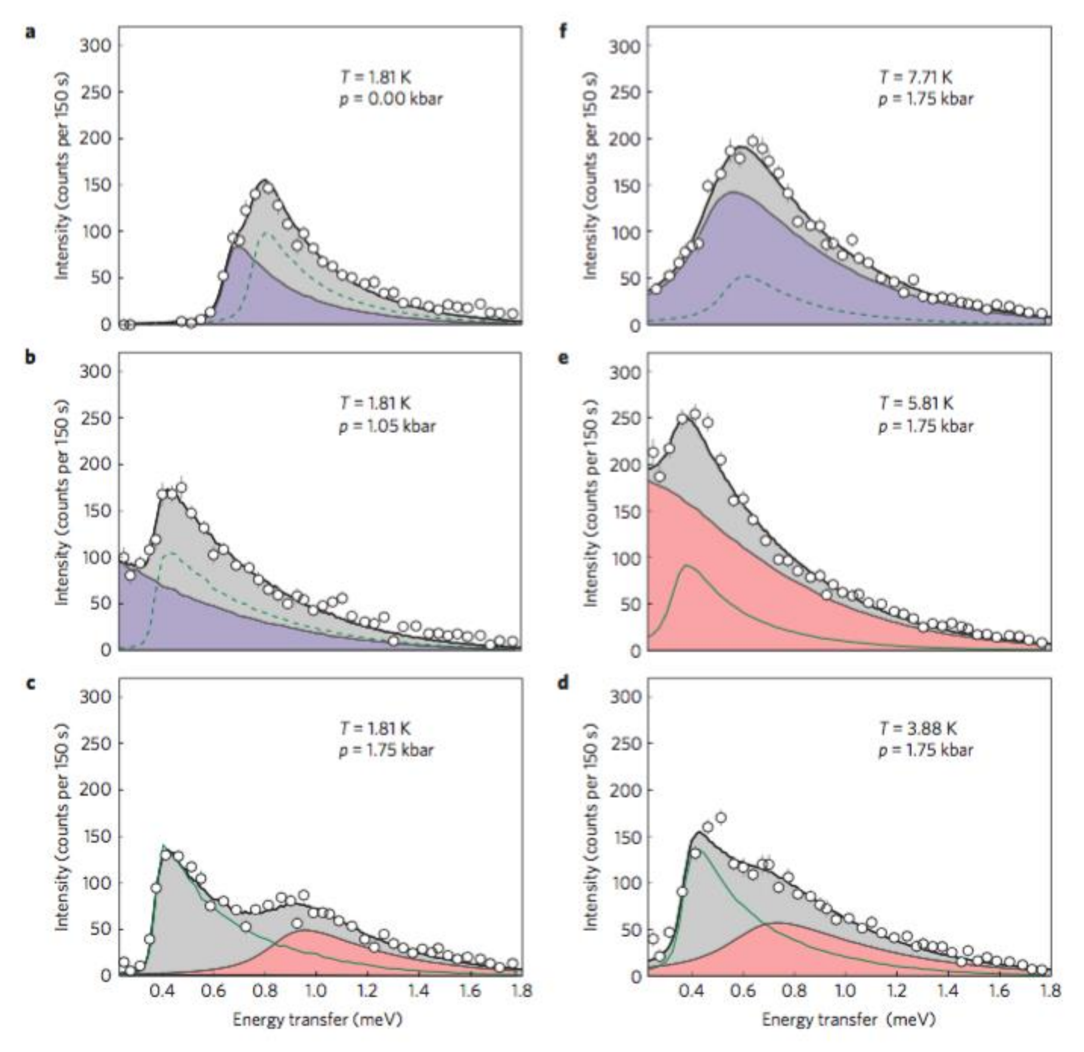
Quantum magnetism: close to QCPs

Probing parameter space in restricted momentum space.

Information from polarization dependence (L,T).

Strong theoretical support.

Detailed knowledge of resolution ellipsoid (MC).

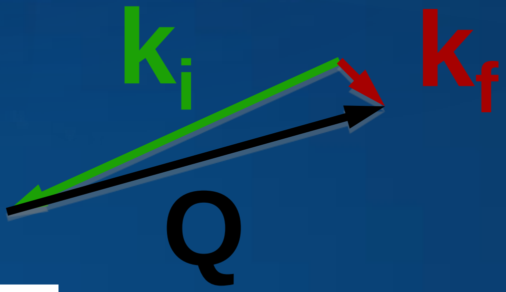


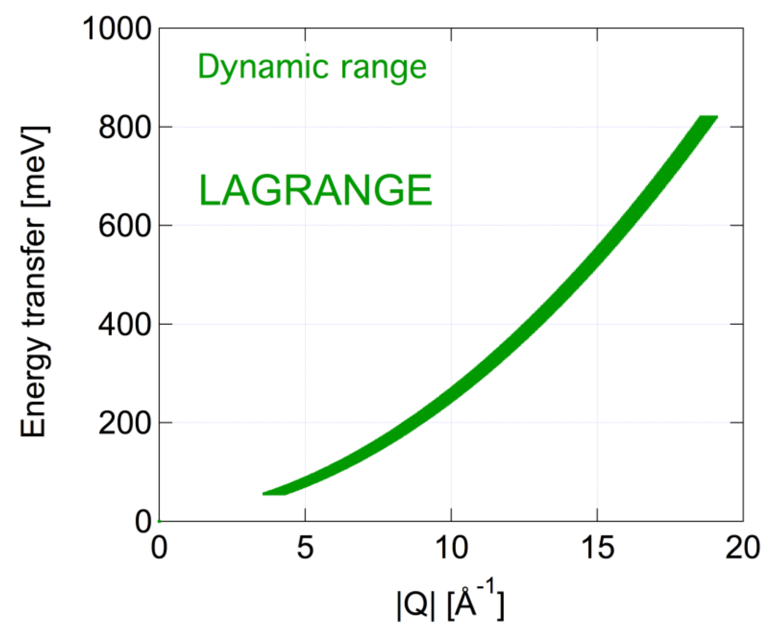
Merchant and al., Nature Physics ***10*** *(2014), p.373-379.*

Hot neutrons ki >> kf: LAGRANGE

$$\left|\vec{Q}\right| \approx k_i$$

$$\Delta E \approx \frac{\hbar^2}{2m} k_i^2$$



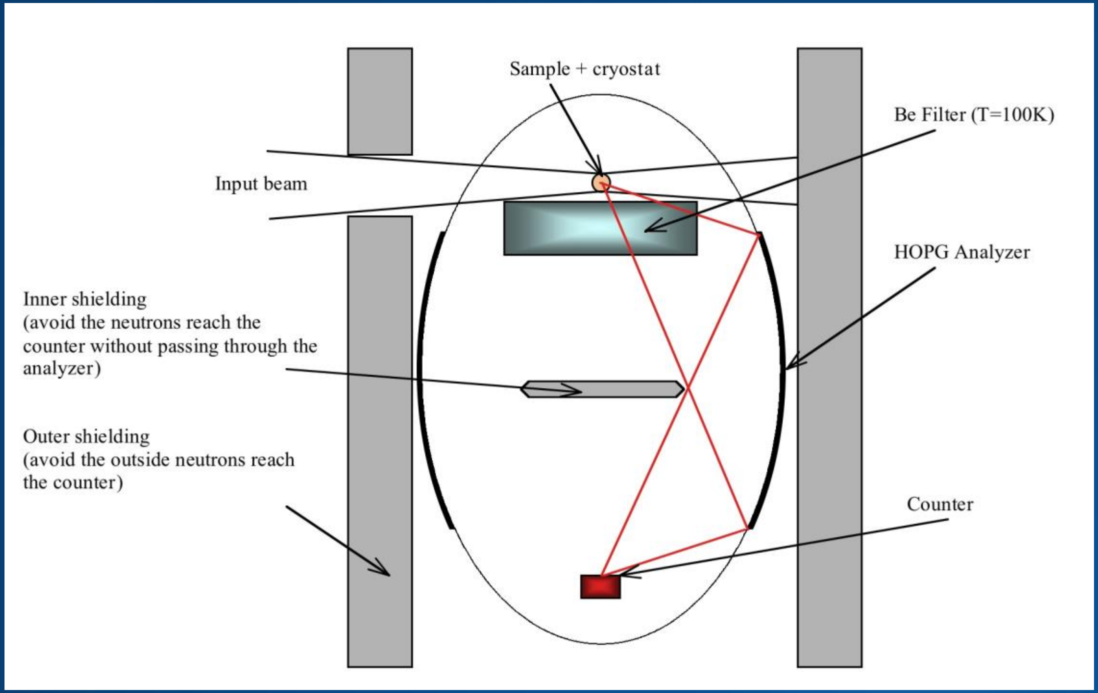


pDOS on powder samples and liquids

Hot neutrons ki >> kf: LAGRANGE

LArge GRaphite ANalyser for Genuine Excitations

Collecting scattered neutrons in a very large solid angle using space focussing
Millenium project (ILL) + spanish contribution



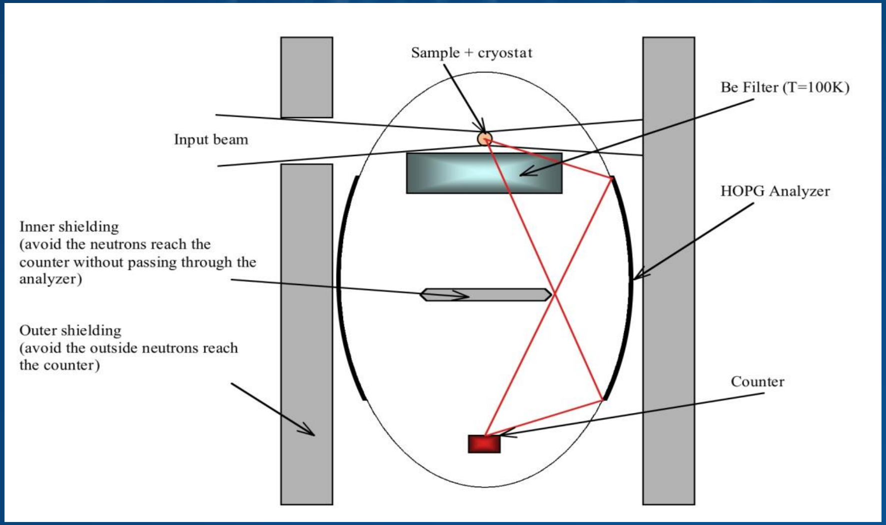
Vertical axis

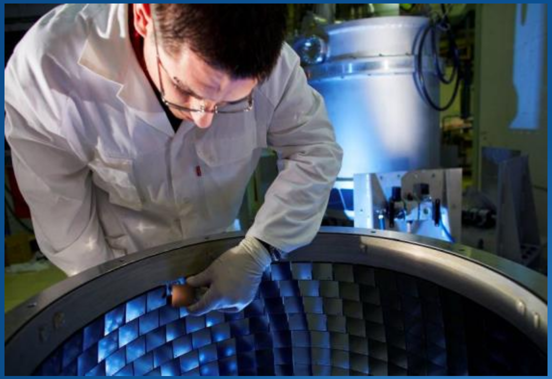
using space focussing:
a small single counter -
increase in solid angle
(2.5 Sterad or 20% of 4π)
without multiplying
counting volume

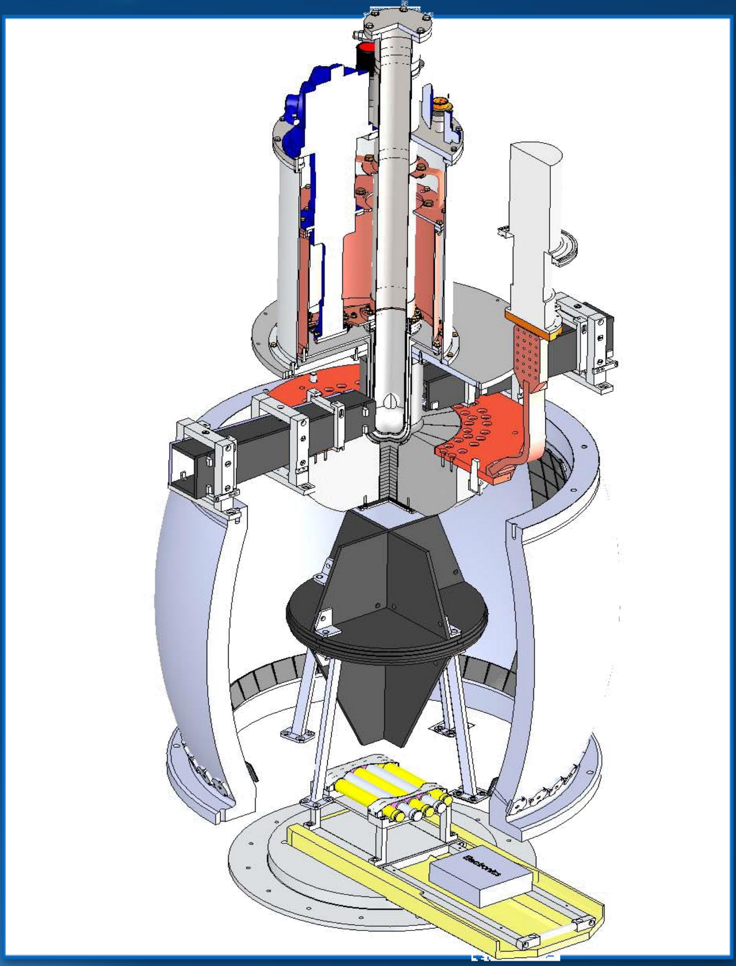
characteristic instrument volume ~1 m^3

Hot neutrons ki >> kf: LAGRANGE

LArge GRaphite ANalyser for Genuine Excitations



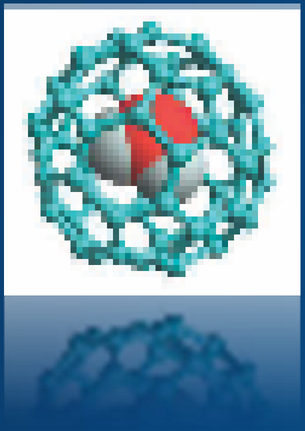


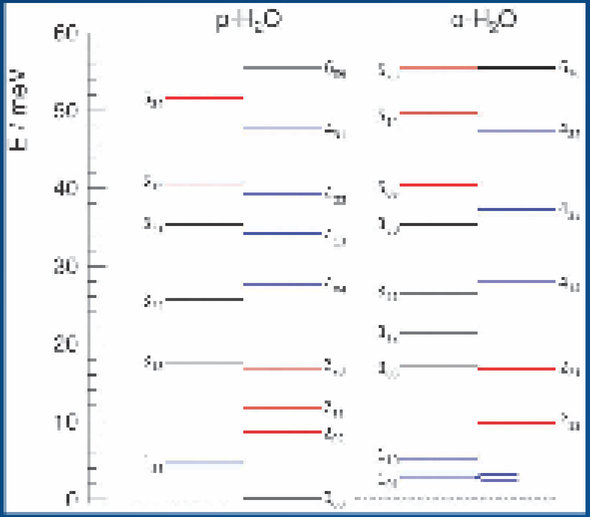


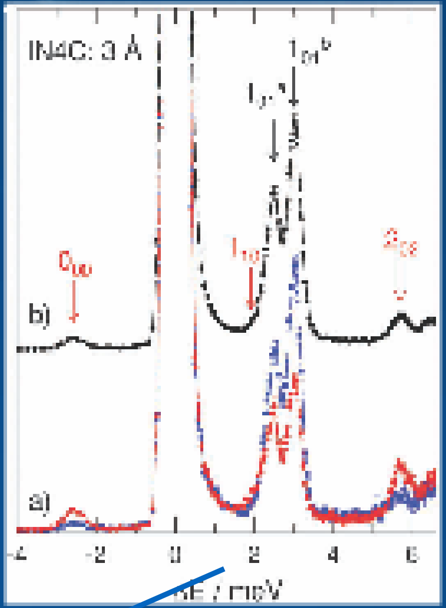
Quantum molecular dynamics: H2O@C60:

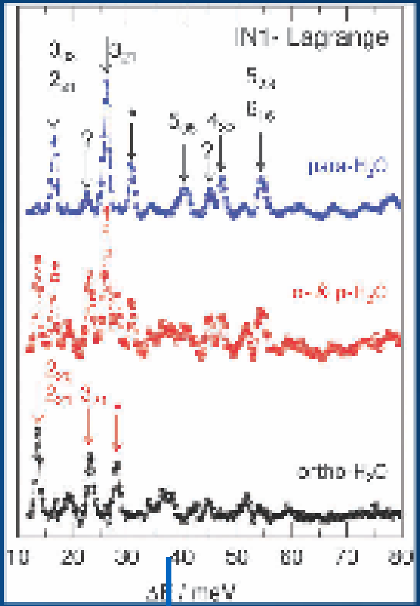
A.J. Horsewill *et al.* (Univ. Nottingham)

Unique opportunity to study isolated water molecules in a highly symmetric environment.









The ground *o*- state is split —> Symmetry-breaking interaction of the water environment

Free from strong interactions, the water molecule has a high degree of rotational freedom enabling its nuclear spin isomers, *o*-H2O and *p*-H2O to be separately studied.

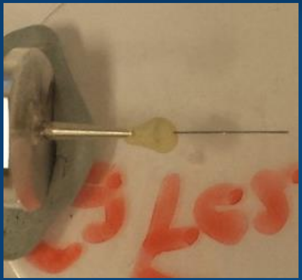
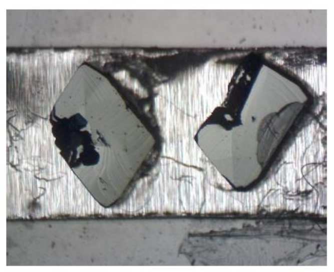
K. Goh, M. Jiménez-Ruiz, M.R. Johnson *et al.* Physical Chemistry Chemistry Physics **16**, 21330 (2014)
M. Xu, M. Jiménez-Ruiz, M.R. Johnson, *et al.* Physical Review Letters **113**, 123001 (2104)

Challenges – remain competitive for users

Neutrons in the detector:

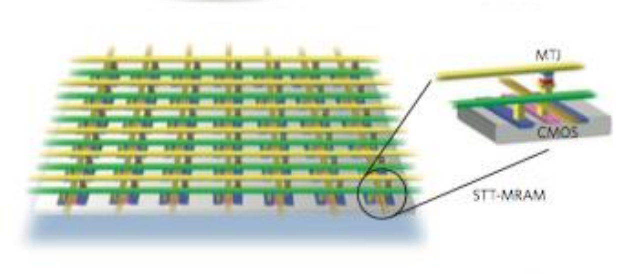
$$\Delta I \propto \Delta\phi(k_i) \times \boxed{N} \times \int_{-\infty}^{+\infty} ..\boxed{\langle S_0^{\alpha}(0)S_l^{\beta}(t)\rangle} exp(-i\omega t)dt \times \Delta\Omega_f \times \Delta E_f$$

Chemistry:

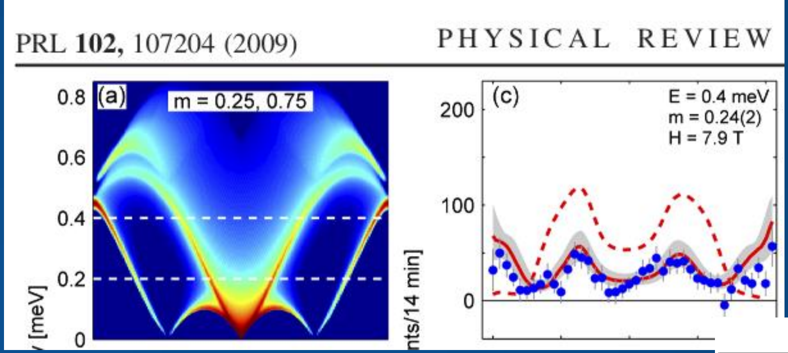
"*Millenium step*": 2000 to now
From > 100 mg to < 10 mg …

… but, no 'tailored' systems:



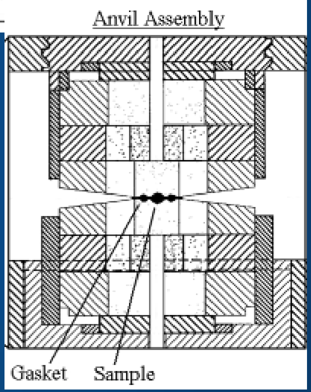
Physics (In extreme conditions):

More than phonons and magnons:


PRL **102,** 107204 (2009) PHYSICAL REVIEW

Polarisation

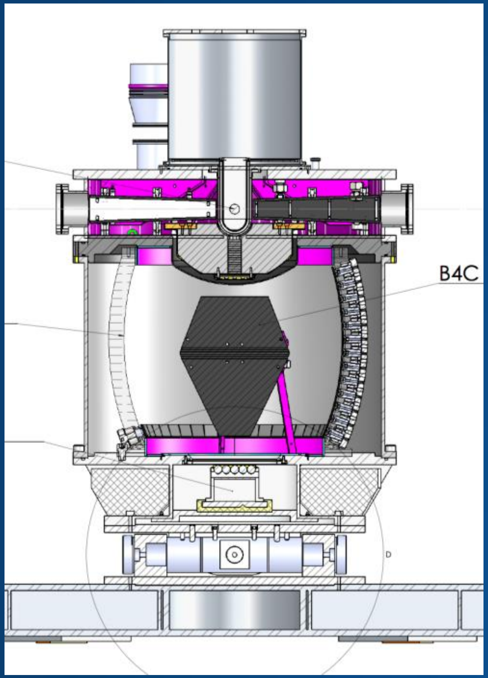
Magnetic fields
Pressure

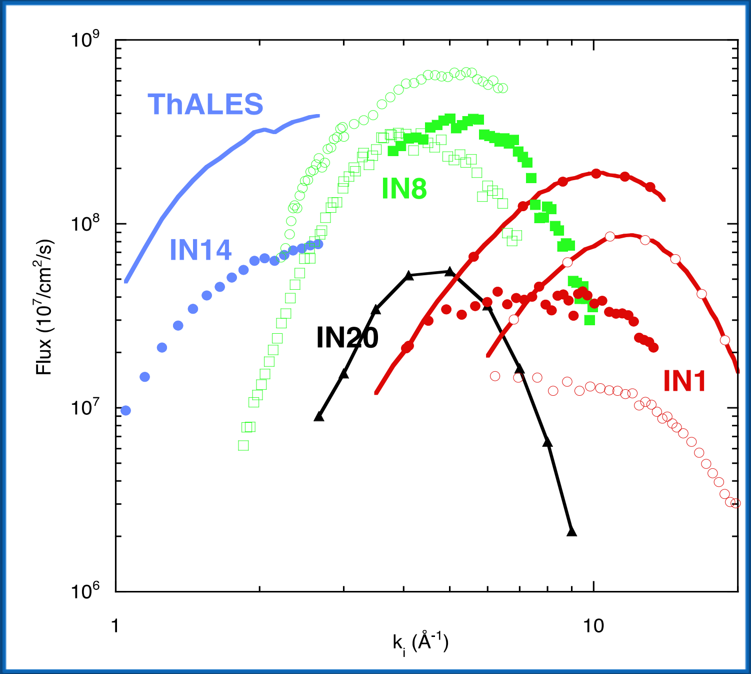


Instrument upgrades - 100%:

$$\Delta I \propto \Delta\phi(k_i) \times N \times \int_{-\infty}^{+\infty} ...\langle S_0^{\alpha}(0) S_l^{\beta}(t)\rangle exp(-i\omega t)dt \times \Delta\Omega_f \times \Delta E_f$$

Millenium step – Instrument up-grades:



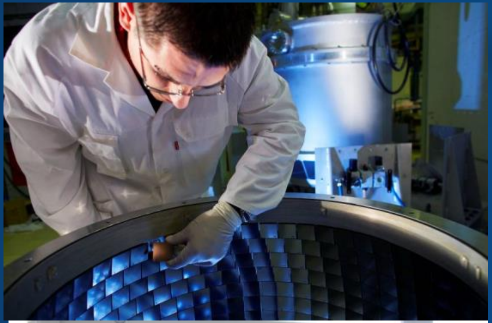


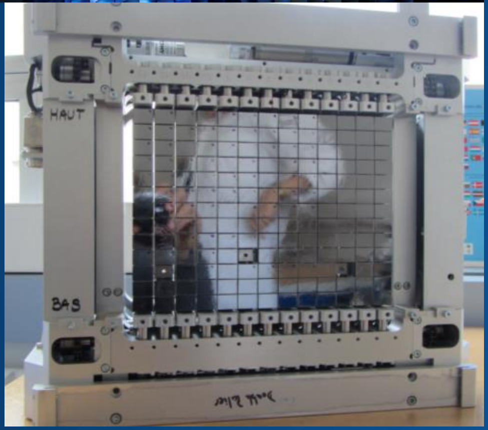
Lagrange

ThALES

New optical components:

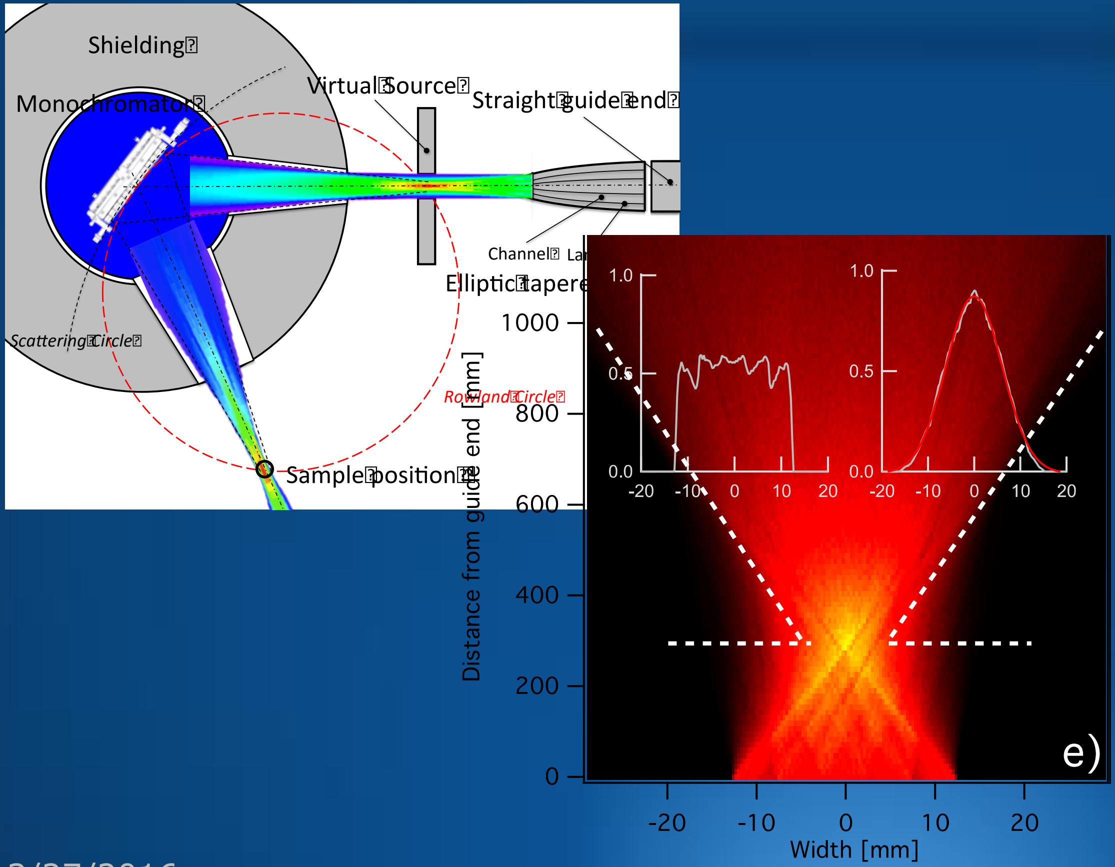
$$\Delta I \propto \boxed{\Delta\phi(k_i)} \times N \times \int_{-\infty}^{+\infty} \ldots \langle S_0^{\alpha}(0) S_l^{\beta}(t) \rangle exp(-i\omega t) dt \times \Delta\Omega_f \times \Delta E_f$$

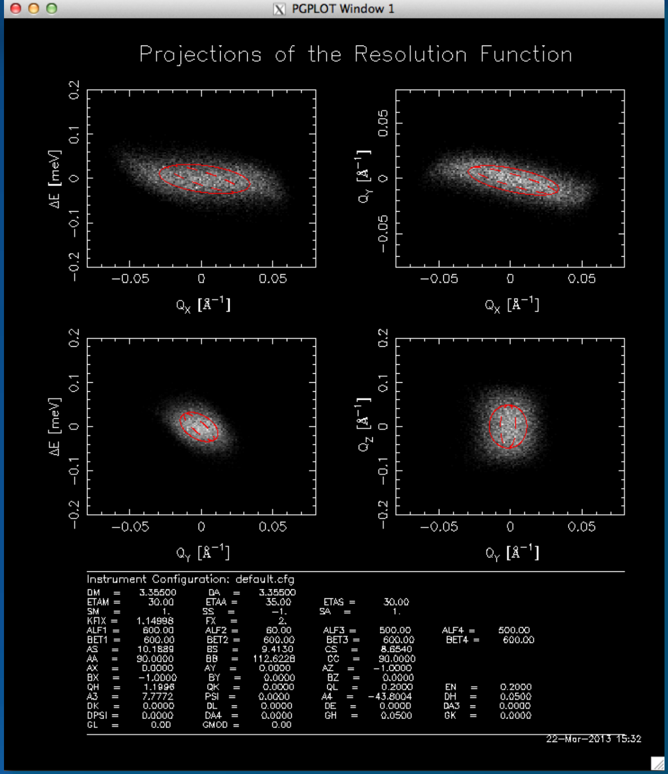




Ray-tracing simulations:

$$\Delta I \propto \Delta\phi(k_i) \times N \times \int_{-\infty}^{+\infty} \ldots\langle S_0^{\alpha}(0)S_l^{\beta}(t)\rangle exp(-i\omega t)dt \times \Delta\Omega_f \times \Delta E_f$$





```
Instrument Configuration: default.cfg
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ETAM =      30.00     ETAA =      35.00     ETAS =      30.00
SM   =         1.     SS   =        -1.     SA   =         1.
KFIX =    1.14998     FX   =         2.
ALF1 =     600.00     ALF2 =      60.00     ALF3 =     500.00     ALF4 =     500.00
BET1 =     600.00     BET2 =     600.00     BET3 =     600.00     BET4 =     600.00
AS   =    10.1889     BS   =     9.4130     CS   =     8.6540
AA   =    90.0000     BB   =   112.6228     CC   =    90.0000
AX   =     0.0000     AY   =     0.0000     AZ   =    -1.0000
BX   =    -1.0000     BY   =     0.0000     BZ   =     0.0000
QH   =     1.1996     QK   =     0.0000     QL   =     0.2000     EN   =     0.2000
A3   =     7.7772     PSI  =     0.0000     A4   =   -43.8004     DH   =     0.0500
DK   =     0.0000     DL   =     0.0000     DE   =     0.0000     DA3  =     0.0000
DPSI =     0.0000     DA4  =     0.0000     GH   =     0.0500     GK   =     0.0000
GL   =       0.00     GMOD =       0.00
                                                          22-Mar-2013 15:32
```
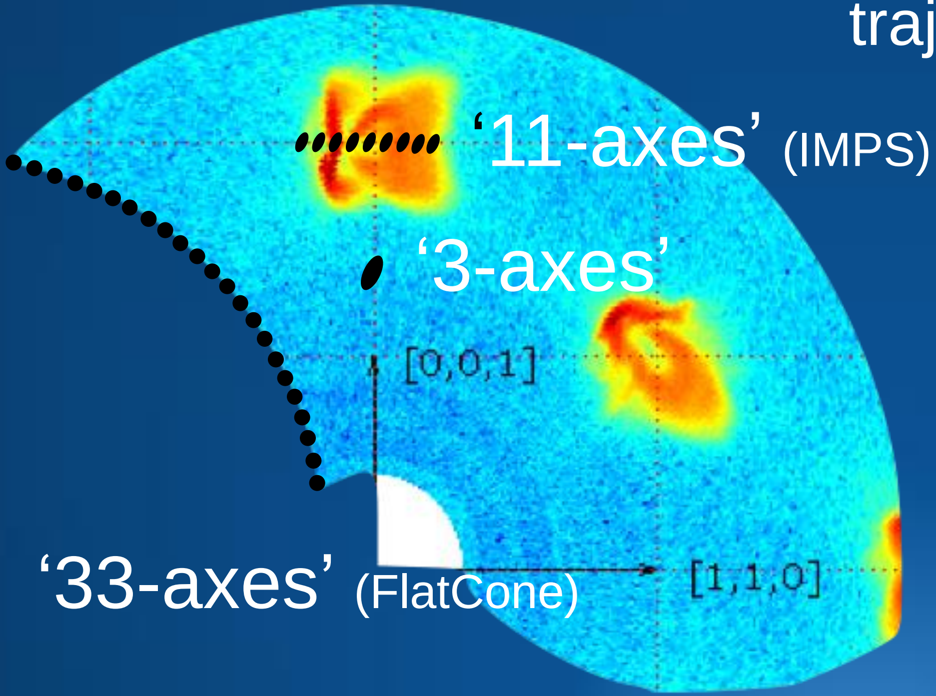

Multiplexing:

$$\Delta I \propto \Delta\phi(k_i) \times N \times \int_{-\infty}^{+\infty} \ldots \langle S_0^{\alpha}(0) S_l^{\beta}(t)\rangle exp(-i\omega t)dt \times \Delta\Omega_f \times \Delta E_f$$

Multiplexing sets constraints in real space leading to predefined trajectories in reciprocal space

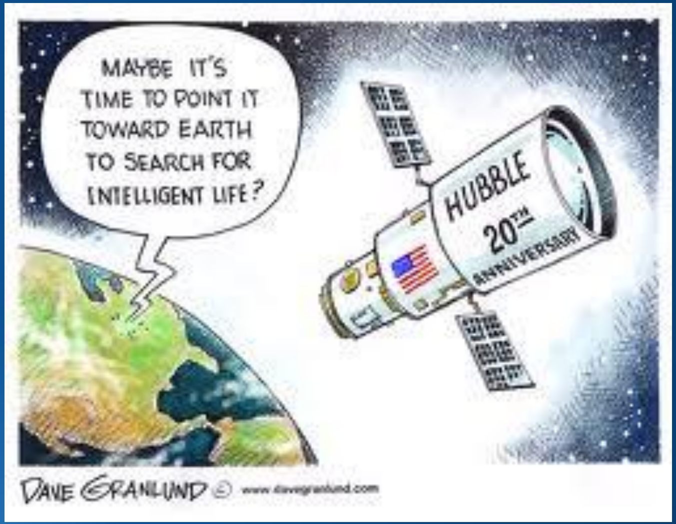


‘11-axes’ (IMPS)

‘3-axes’

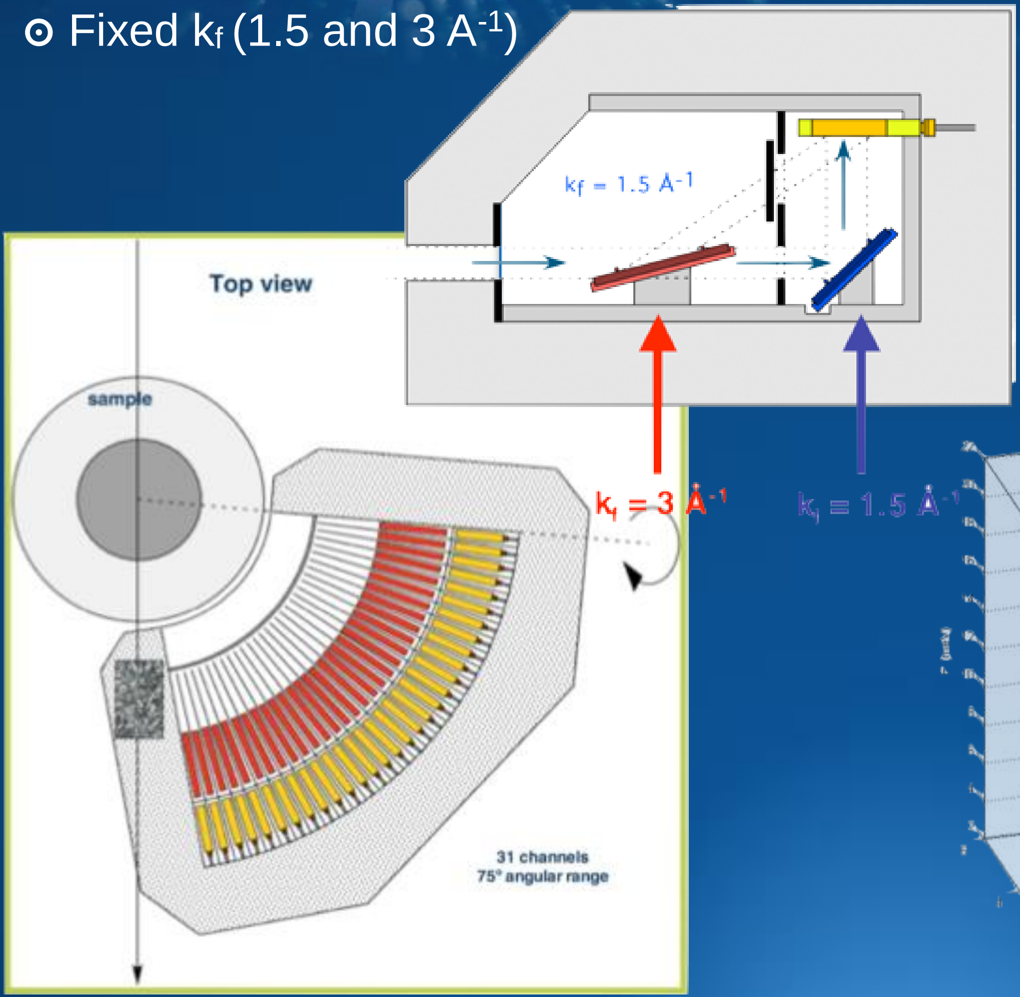
‘33-axes’ (FlatCone)

Measuring strategy?

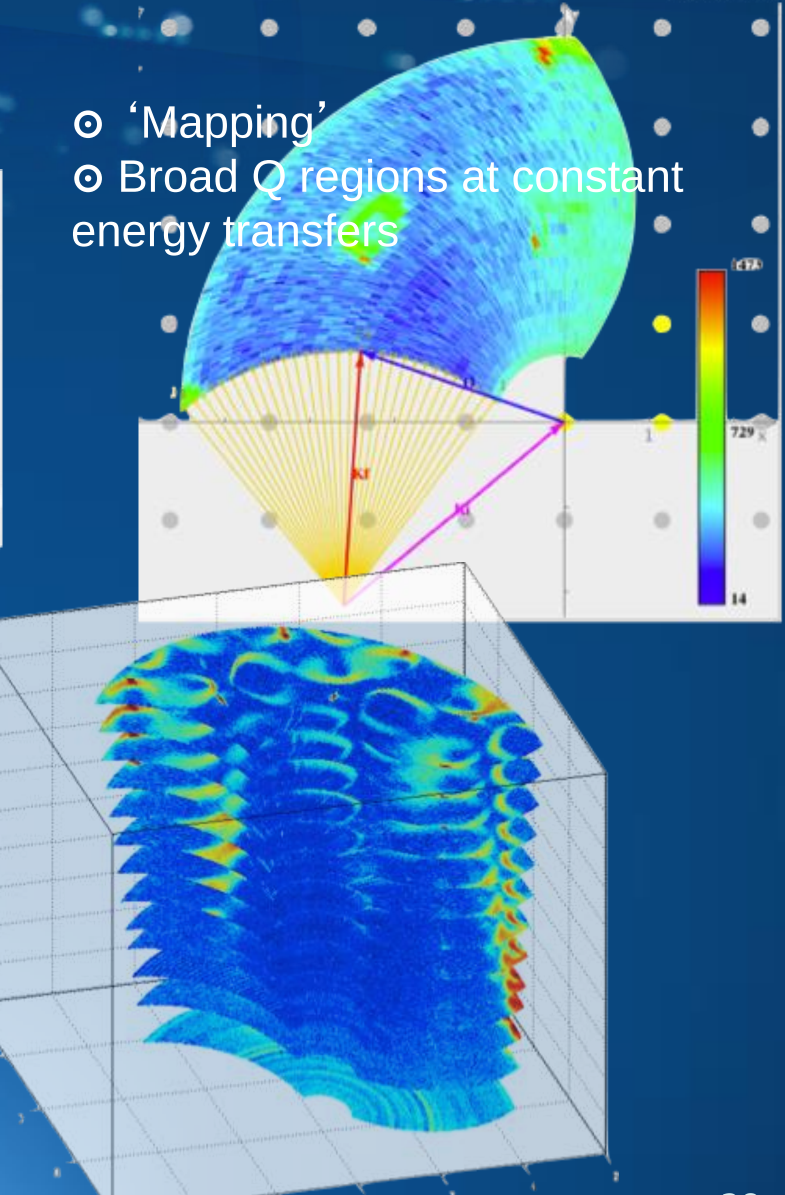


Multiplexing - FlatCone:

- 31 individual analyser-detector channels
- Fixed k_f (1.5 and 3 A^{-1})

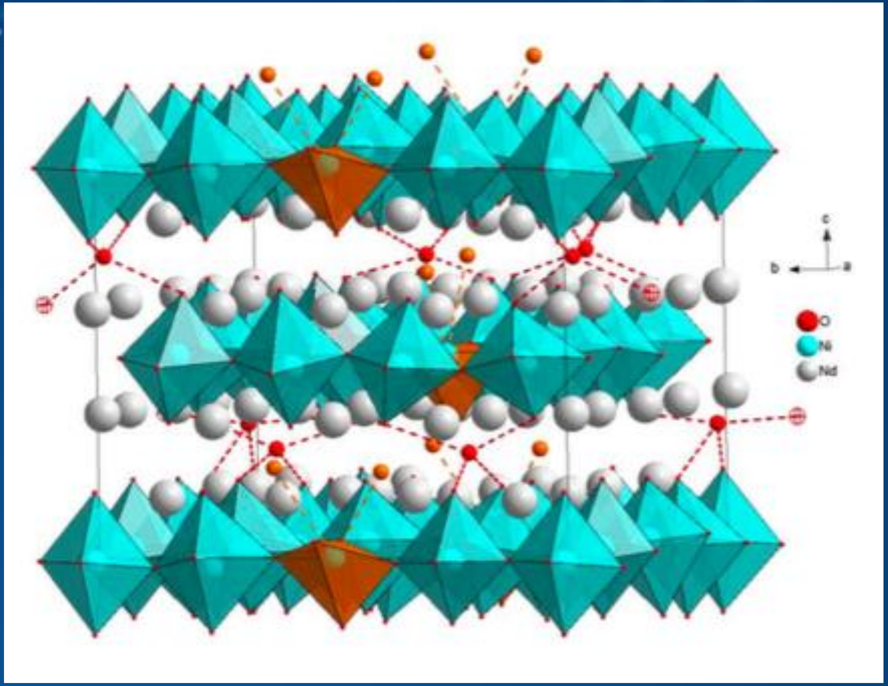


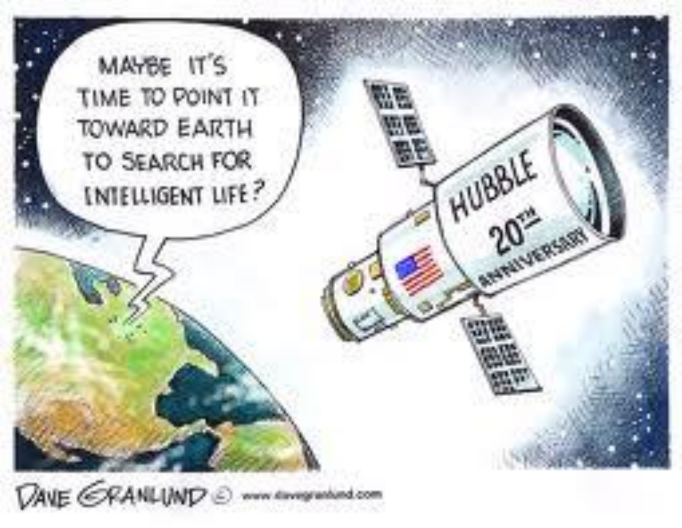
- ‘Mapping’
- Broad Q regions at constant energy transfers



Challenges – small and 'dirty' materials:

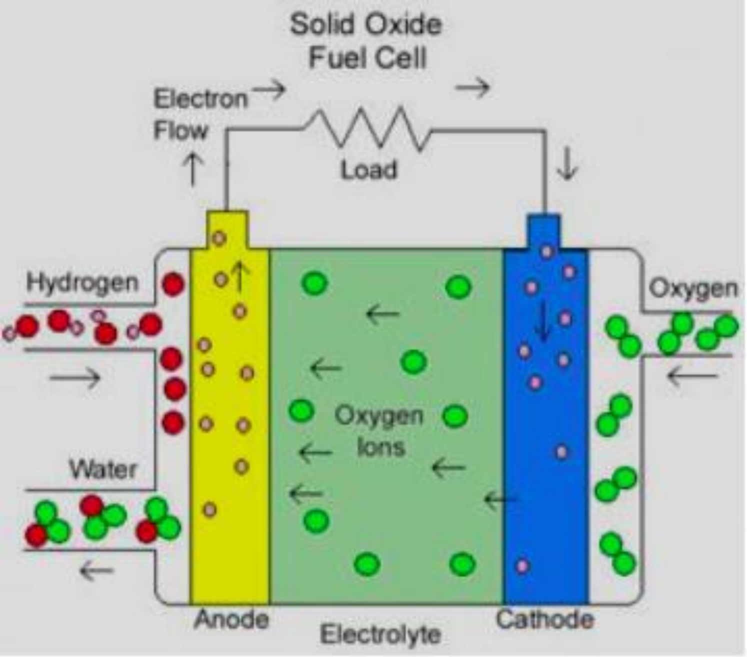
Doped materials





Beyond LDC:
Molecular dynamics

Oxygen ion mobility for solid state ionics:



http://www.iit.edu/

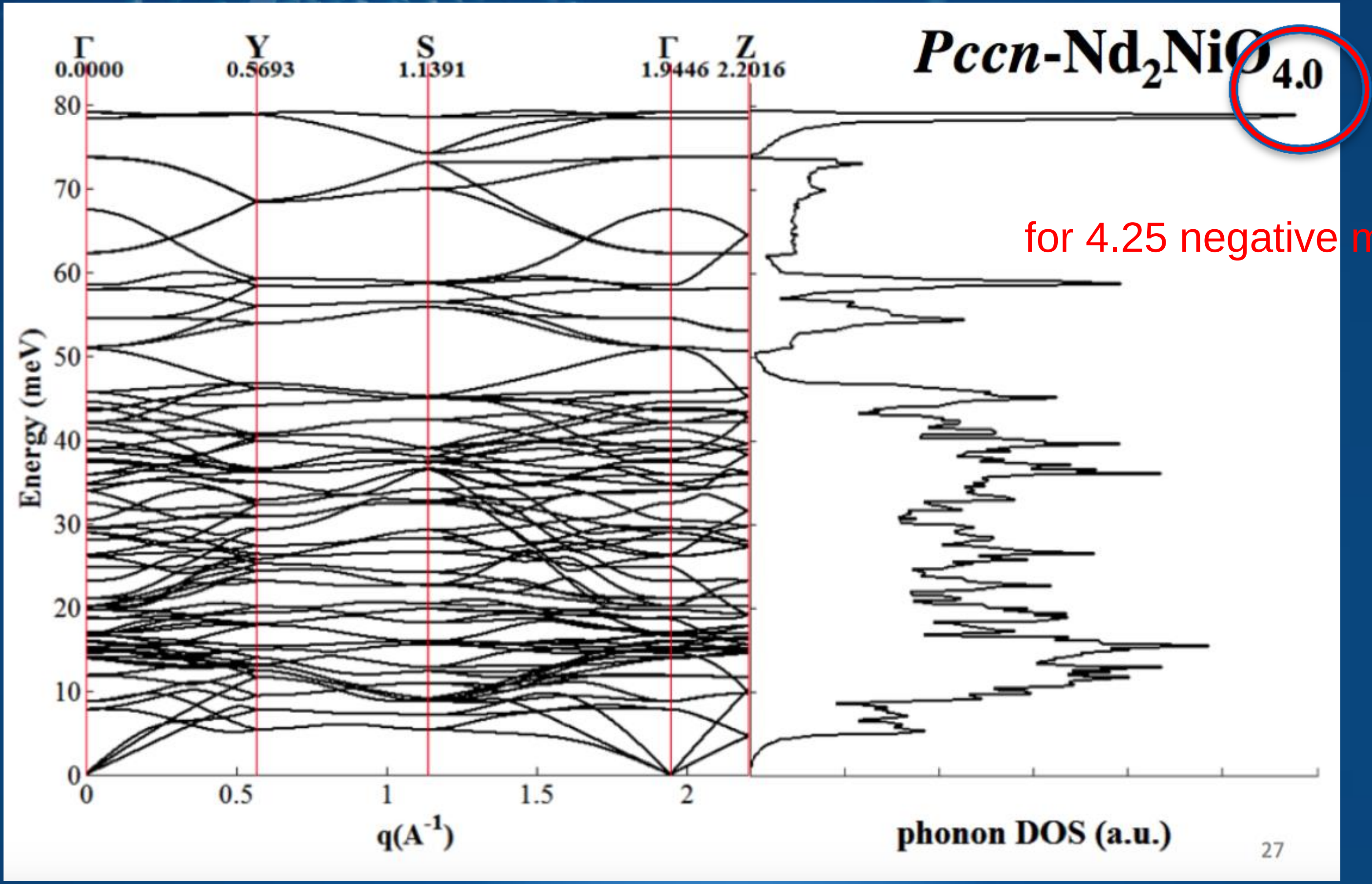
O^{2-} is doubly negative charged, has large VdV radii:

→ High operating temperatures are needed (T>1300K)

→ Issues: cost, stability, cracking

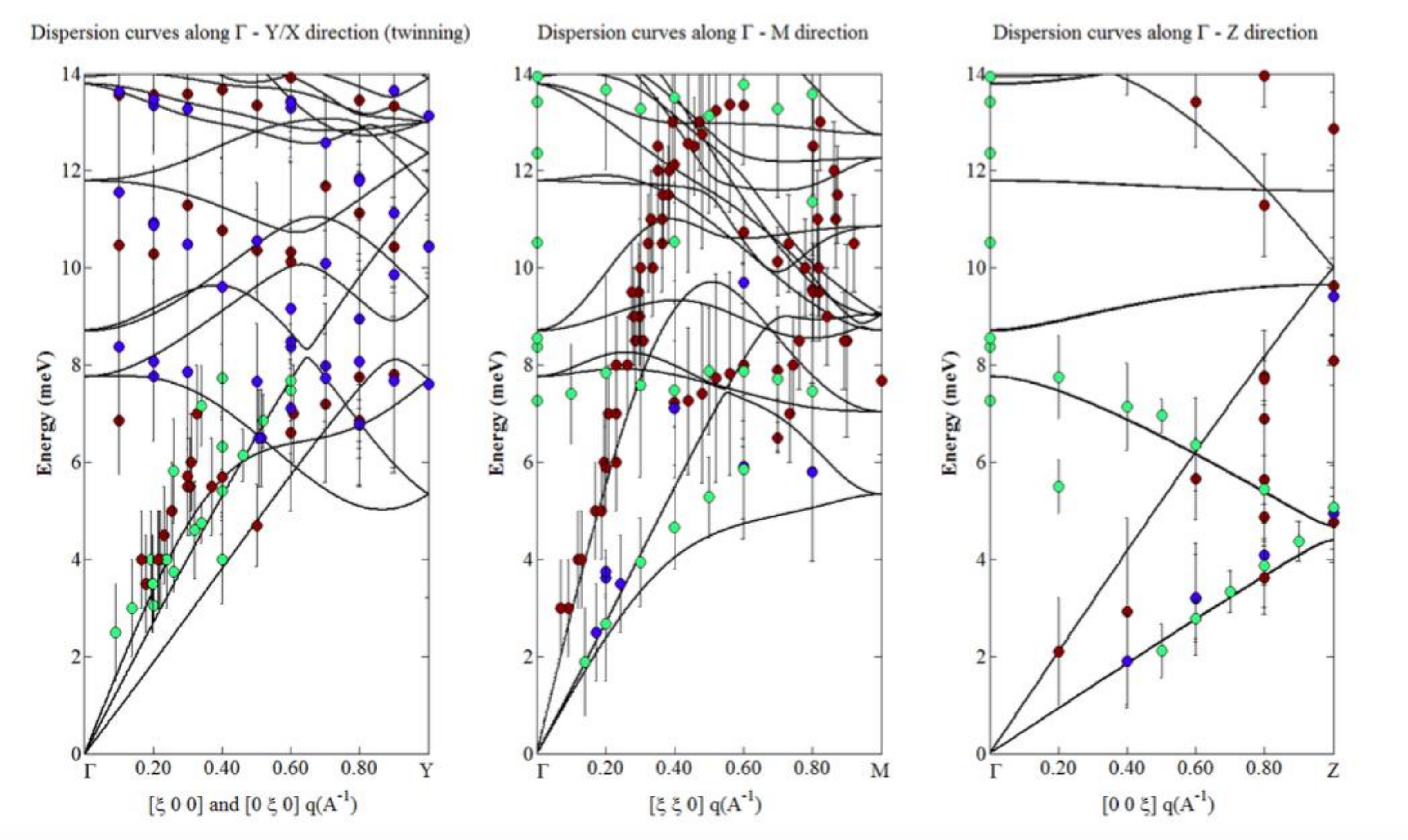
A few exepctions show RT oxygen mobility:
-Brownmillerite oxides (SrFeO2.5, SrCoO2.5
-Non-stoichiometric K_2NiF – type oxides (Re_2MO_{4+d} with *Re*=La,Nd,Pr and *M*=Ni, Co,Cu

DFT calculation with VASP (GGA, PAW-PBE) to get the forces, post-treatment with Parlinski's PHONON code.

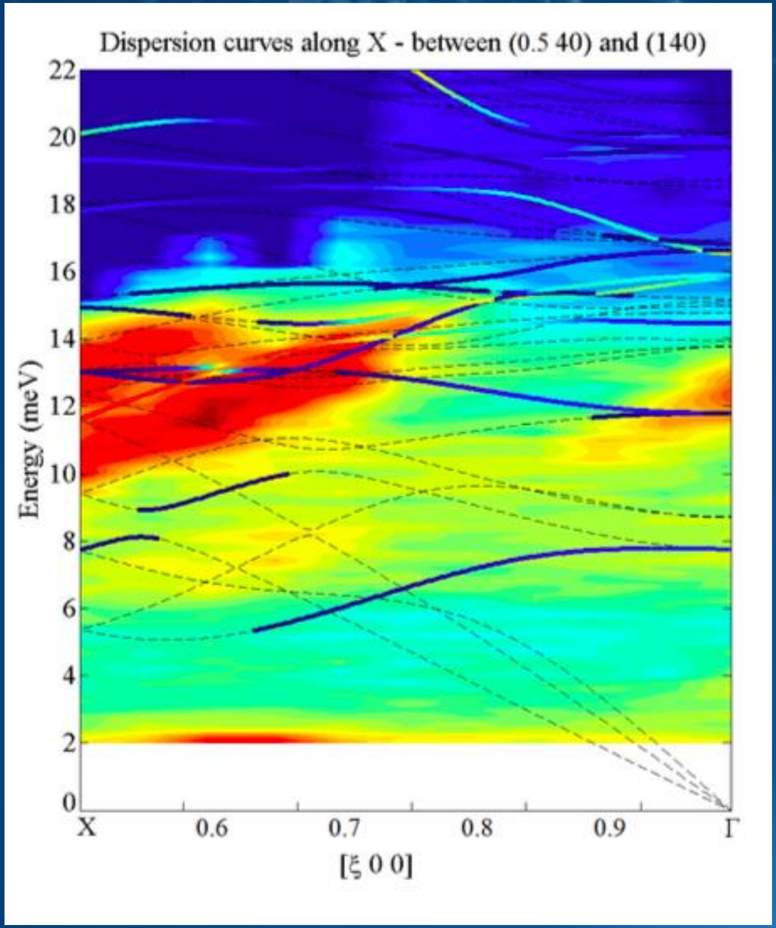


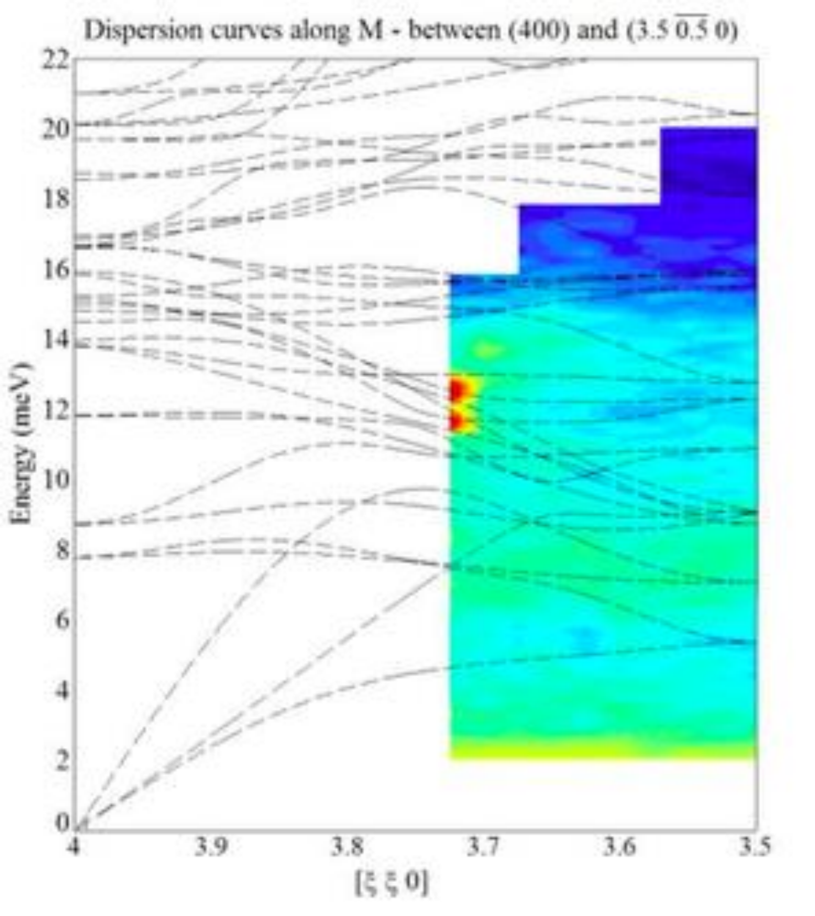
for 4.25 negative modes!

Phonon dispersion – measurements on IN8:



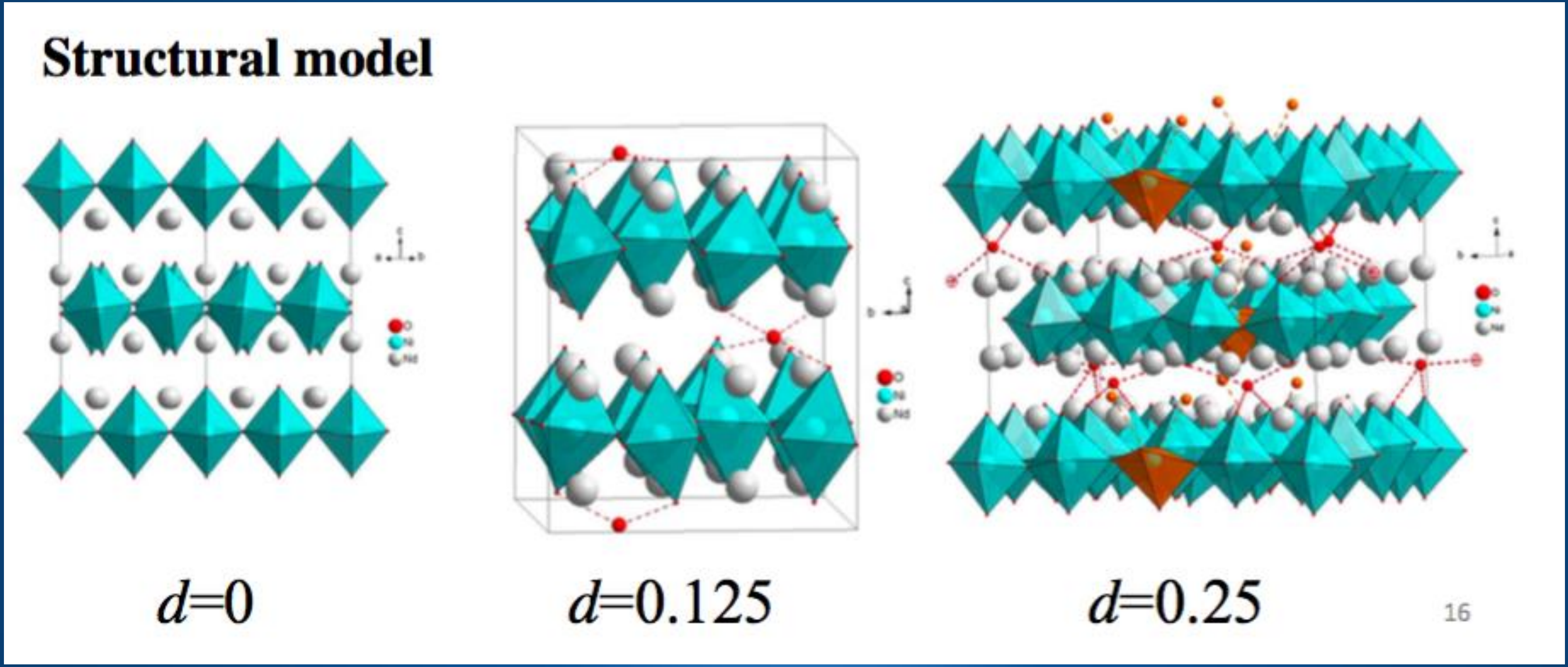
Phonon dispersion – measurements on IN8:





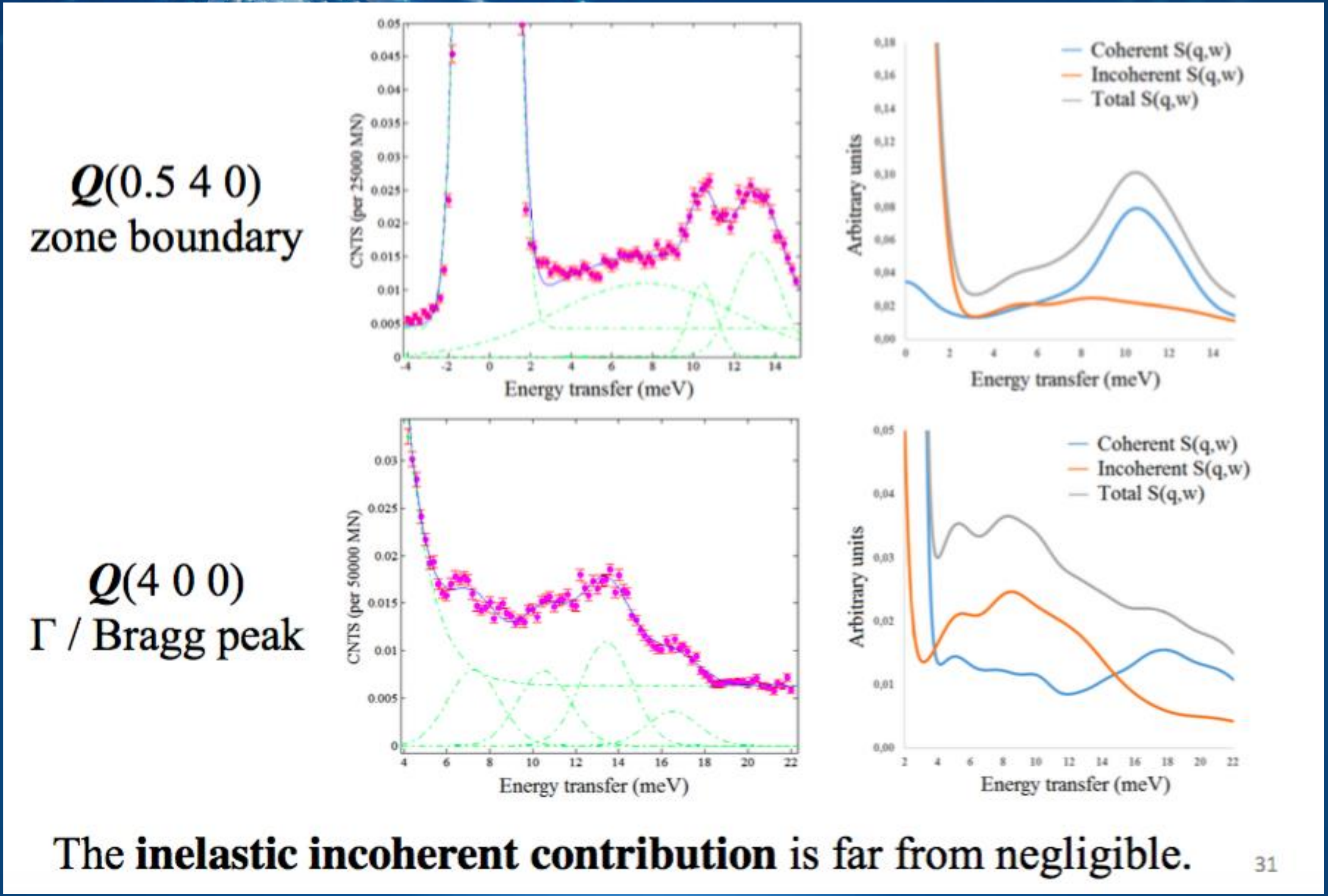
Molecular dynamics:

Molecular dynamics with VASP post-treatment with nMoldyn and Matlab. Calculation of vibrational DOS from velocity auto- correlation function (vDOS weighted by m, σcoh and convoluted with exp. resolution.



Perrichon A. *et al*., Journal of Physical Chemistry C **119,** 1557-1564 (2015).

Phonon dispersion of Nd2NiO4.25 (IN8) – comparison with MD



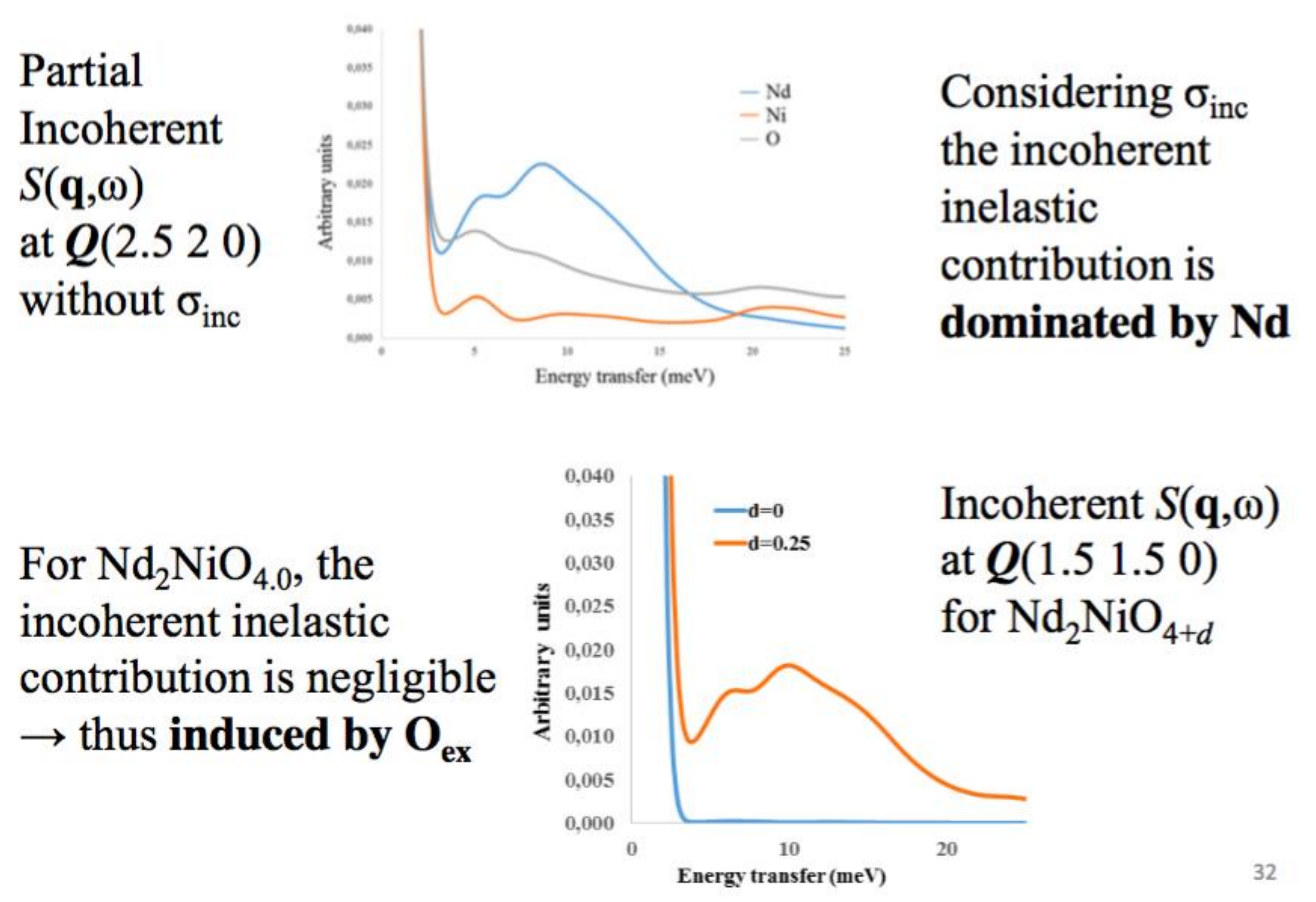
Q(0.5 4 0)
zone boundary

Q(4 0 0)
Γ / Bragg peak

The **inelastic incoherent contribution** is far from negligible.

31

Phonon dispersion of Nd2NiO4.25 (IN8) – comparison with MD

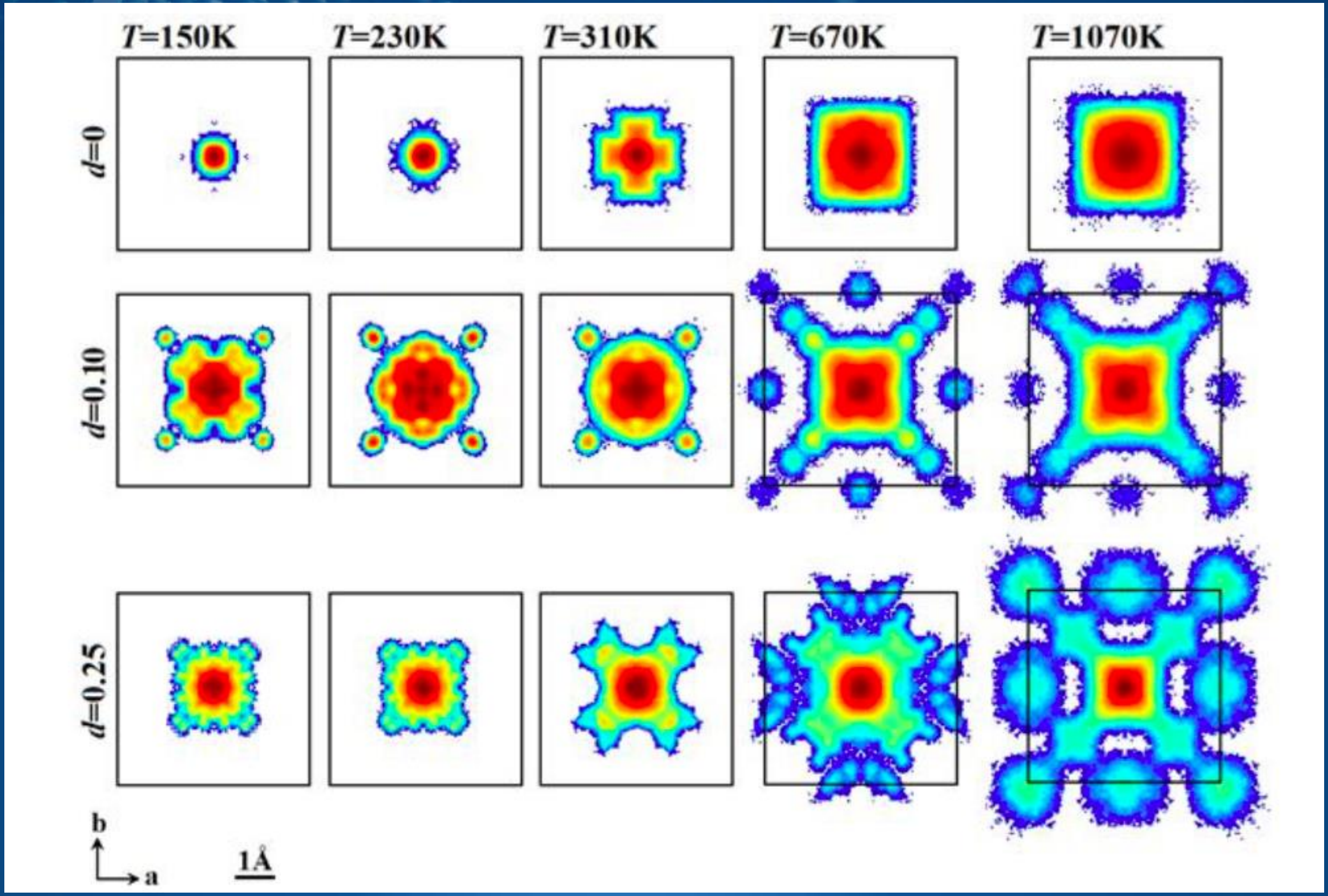


Partial Incoherent $S(\mathbf{q},\omega)$ at $Q(2.5\ 2\ 0)$ without σ_{inc}

Considering σ_{inc} the incoherent inelastic contribution is **dominated by Nd**

For $Nd_2NiO_{4.0}$, the incoherent inelastic contribution is negligible → thus **induced by O_{ex}**

Incoherent $S(\mathbf{q},\omega)$ at $Q(1.5\ 1.5\ 0)$ for Nd_2NiO_{4+d}


T=150K
T=230K
T=310K
T=670K
T=1070K
d=0
d=0.10
d=0.25
b
a
1Å

Conclusions:

TAS is a dinosaur in condensed matter physics.

Its DNA is probed on a competitive environment and sane.

Large scale facilities – reactor based experimental technique.

Gives information on S(Q,w).

Strongest on measuring selected regions in S(Q,w) as functions of external parameters.

External parameters: magnetic field <= 15T, temperatures 50 mK < *T* < 1800 K, Pressures < 100 kb, polarization, …

For optimum efficiency, computing assistance indispensible.

TAS @ ILL:

Lagrange: Monica Jimenez – Ruiz
Alain Bertoni

IN8: Alexander Ivanov
Andrea Piovano

CRG – IN22: Frederic Bourdarot
Stephane Raymond

IN20: Mechthild Enderle
Elisa Wheeler
Philippe Chevallier

Jiri Kulda
Louis-Pierre Regnault

ThALES: Martin Boehm
Paul Steffens
Emmanuel Villard

CRG – IN12: Karin Schmalzl
Wolfgang Schmidt

TAS group at ILL:

Andrea Piovano
Paul Steffens
Jiri Kulda
Sasha Ivanov
Monica Jimenez
Mechthild Enderle
Elisa Wheeler

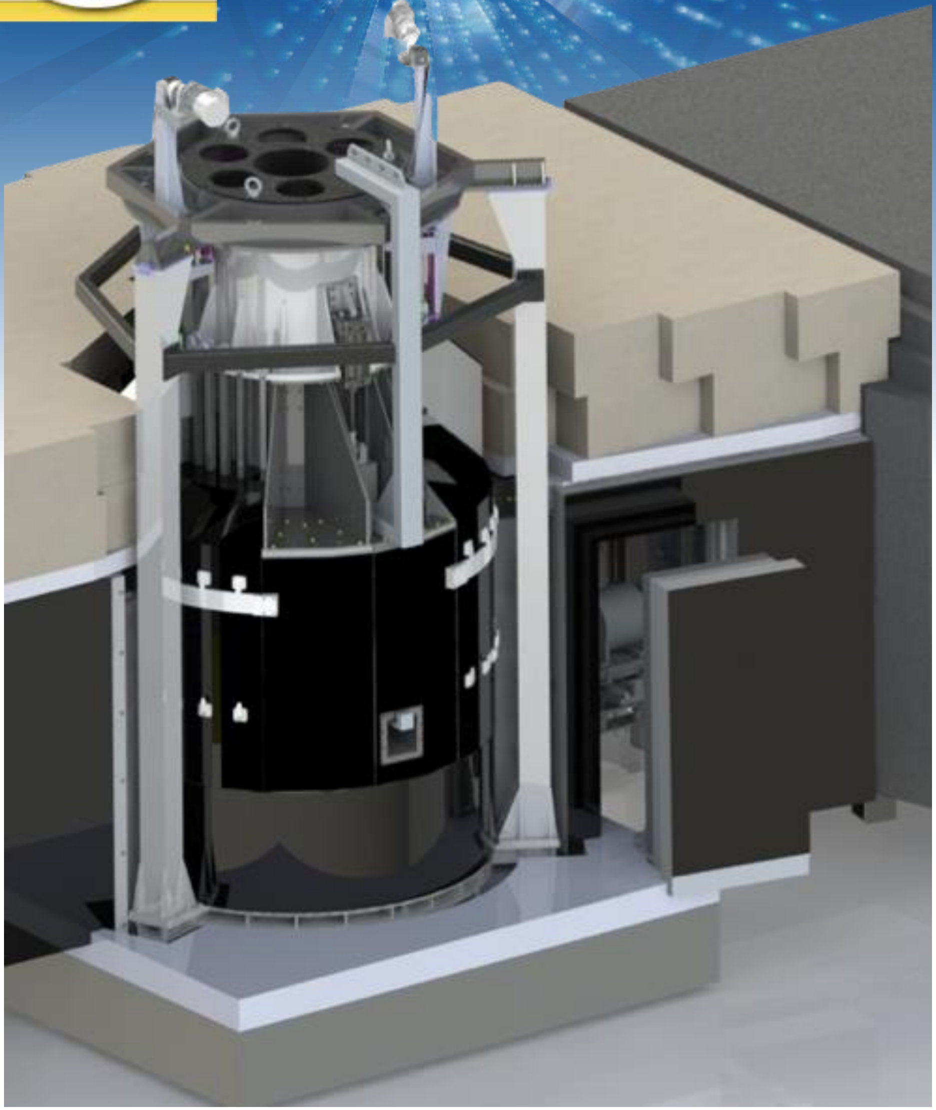
Literature:

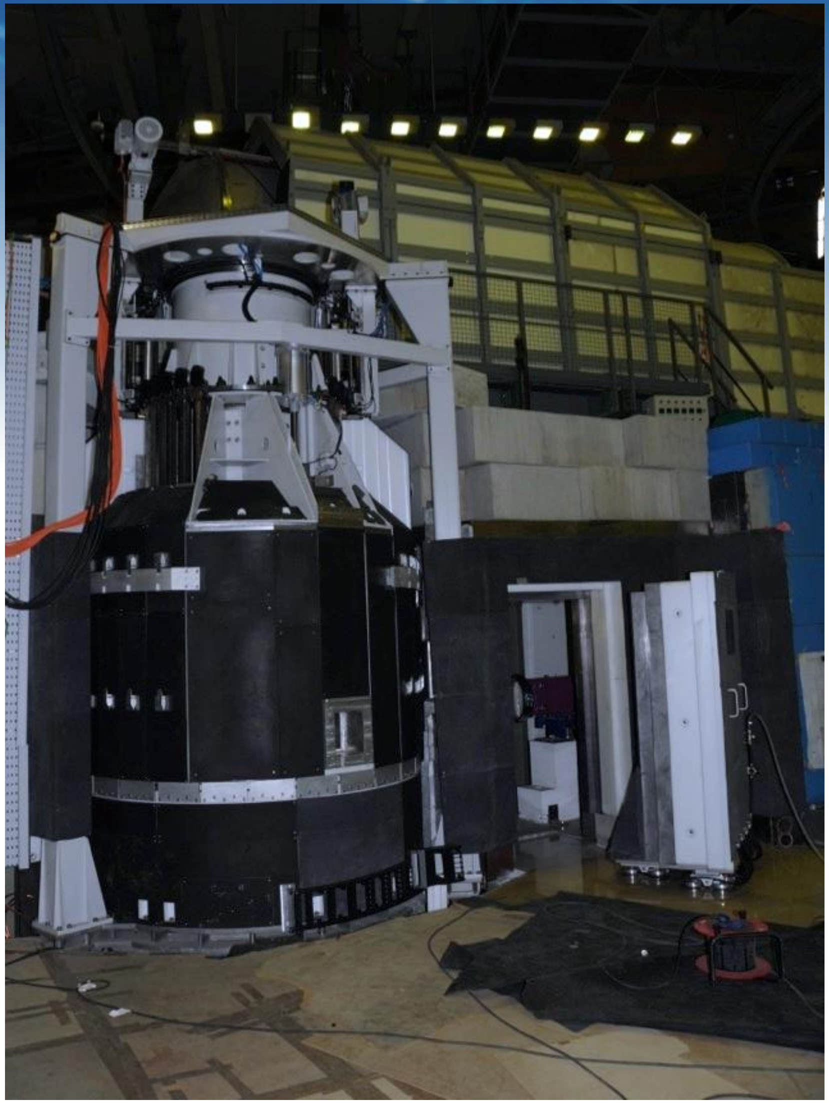
Squires
Marshall and Lowde, Rep. Prog. Phys 31 (1968), 705
Collins
Bertaut

CRG - IN12:

Wolfgang Schmidt
Karin Schmalzl

Thales - Primary spectrometer

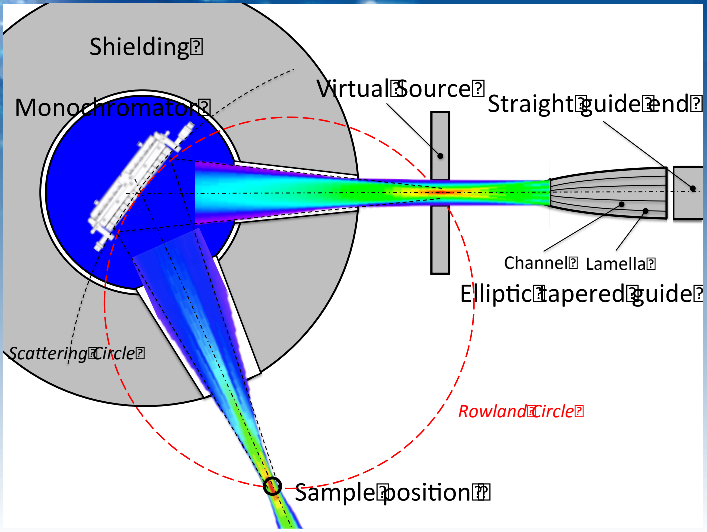




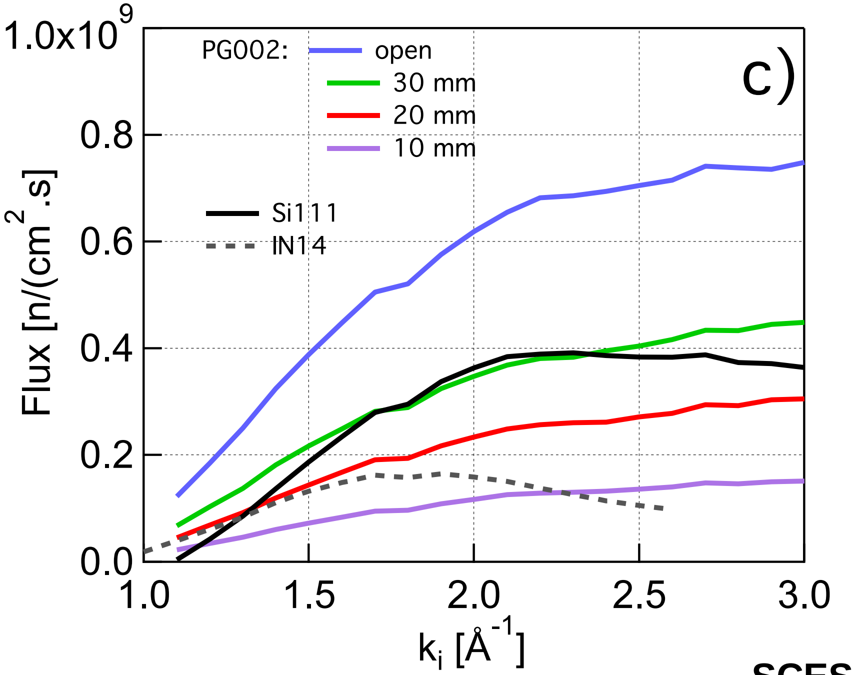
after detailed design study

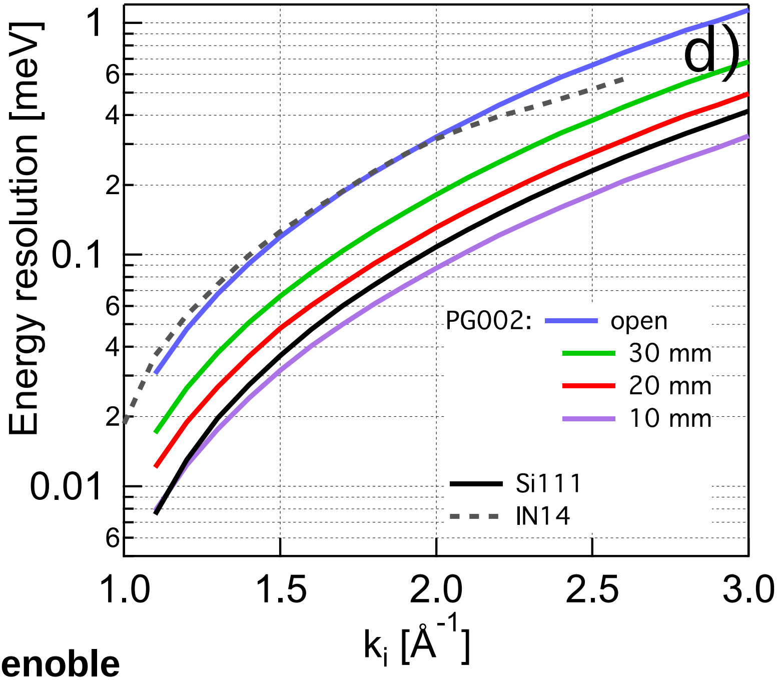
ThALES - Characteristics

Monochromators:
PG002
Si111
Heusler



Guides:
Straight m=3
Elliptically focusing





Efficiency:
Increase in Data Collection Rate

$$\Delta I \propto \Delta\phi(k_i)\frac{d^2\sigma}{d\Omega_f dE_f}\Delta\Omega_f\Delta E_f$$

Multiplexing ....

	IN8	IN4	IN4/IN8
$\Delta\phi$ [n/cm^2/s^2]	2x10^8	5x10^5	0.0025
$\Delta\Omega$ [sr]	0.0044	0.29	66
$\frac{\Delta E}{E_i}$	0.05	1	20-30

IN8-FC
2x10^8
0.042
0.05

PG002, k_i=2.662A-1

$$\frac{\Delta I_{IN4}}{\Delta I_{IN8}} = 5$$

$$\frac{\Delta I_{IN8-FC}}{\Delta I_{IN8}} = 10$$

Efficiency: Increase in publication rate?

Publication Rate

$PR = f(DCR)$

Data Collection Rate

M: Multiplexing

$$PR = f(M*DCR)$$
$$= \cancel{M}*f(DCR)$$

Year	2007	2008	2009	2010	2011	2012
All.Experiment IN4	33	29	28	31		
All.Experiment IN8	18	15	18	19		
Publications IN4				8	11	14
Publications IN8				12	6	8

But, multiplexing for:

Staying competitive

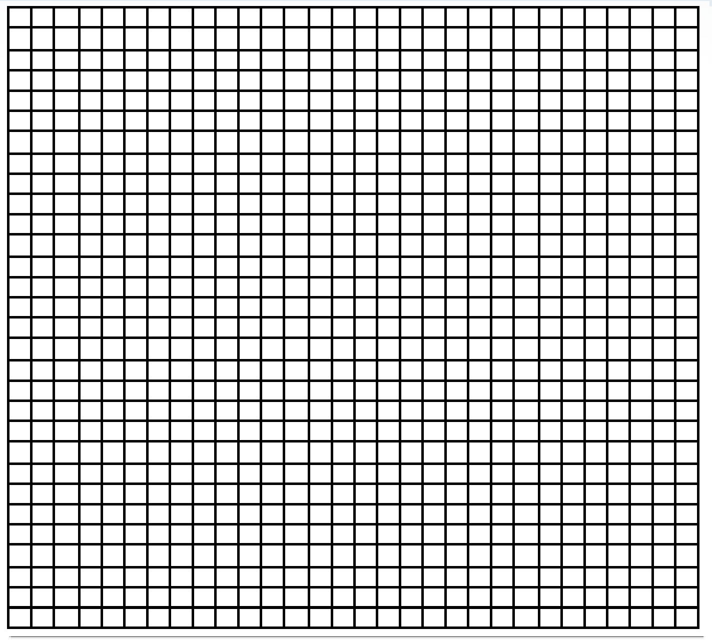
Enhancing data quality

Daring new experiments (e.g. reduction in sample size)

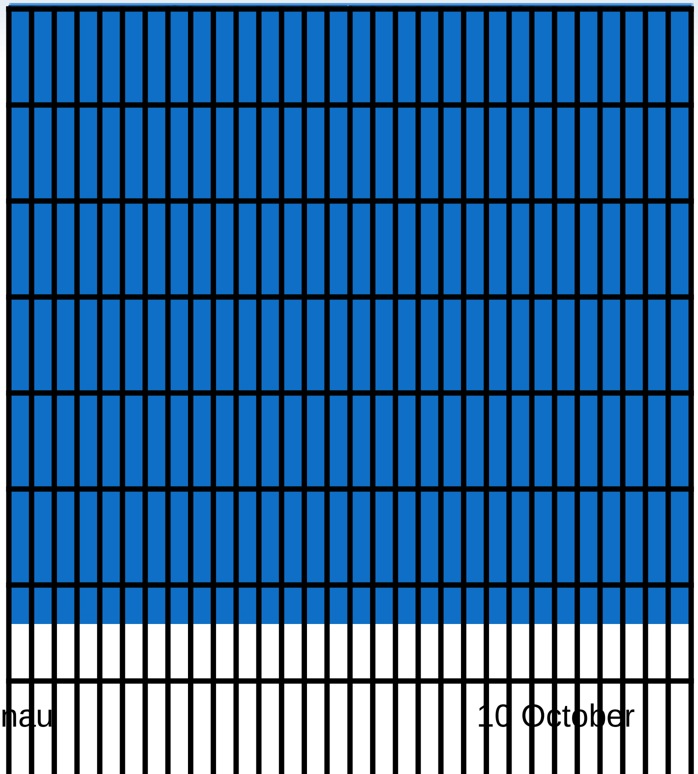
Data Collection Philosophy

The way of the data acquisition influences the mentality of the users
(or the other way round).

Battle-ship gambling mentality (*TAS*)

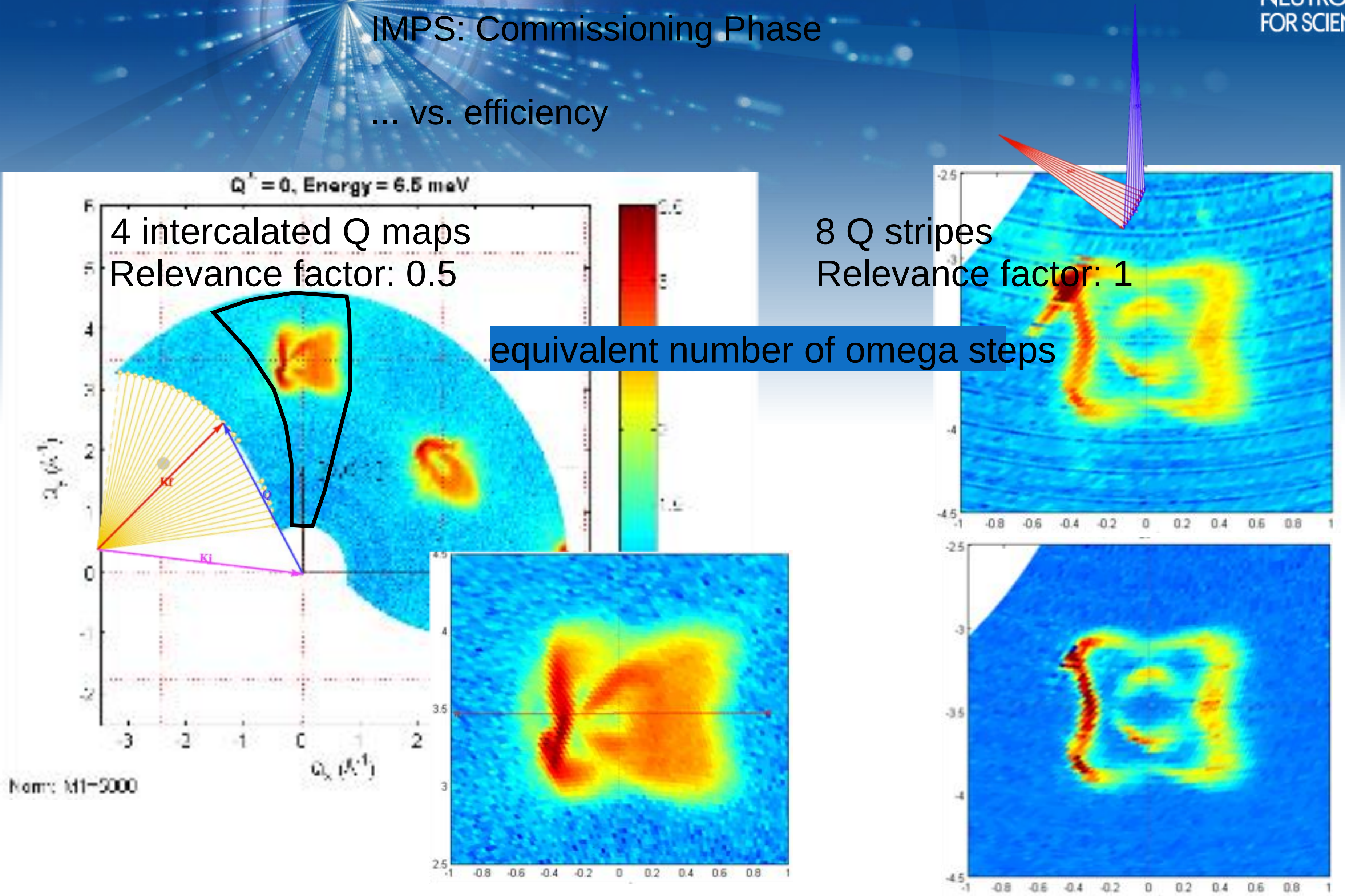


Coffee break mentality (*TOF*)



IMPS: Commissioning Phase

... vs. efficiency

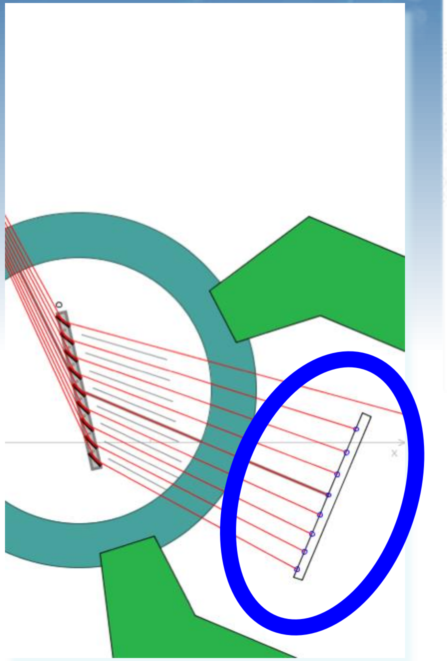


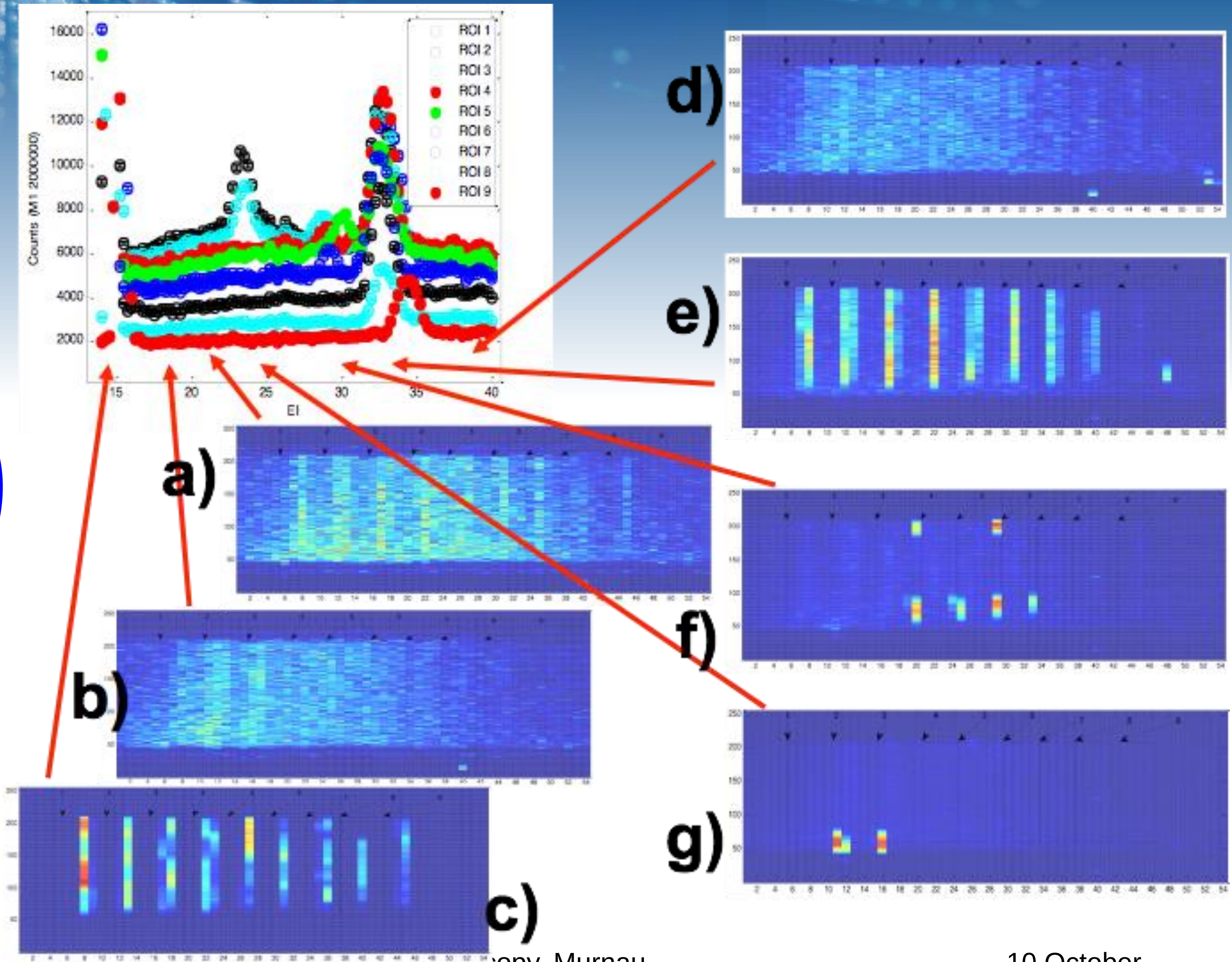
4 intercalated Q maps
Relevance factor: 0.5

8 Q stripes
Relevance factor: 1

equivalent number of omega steps

IMPS: Multidetector





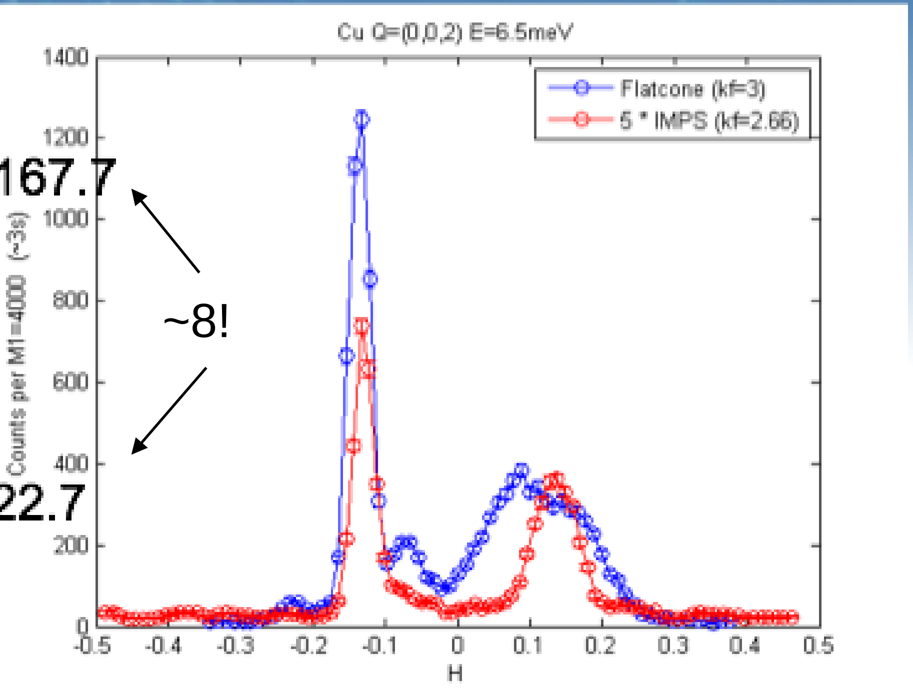
IMPS: Commissioning Phase

IN8-FC:

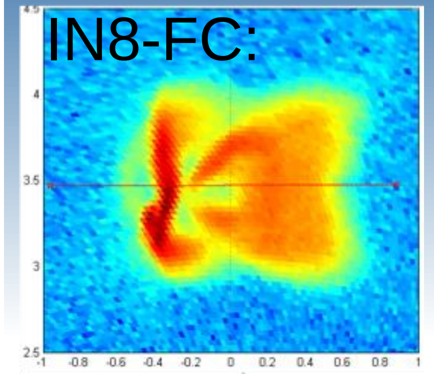
S/N ≈ 402.4/2.4 ≈ 167.7

IN8-IMPS:

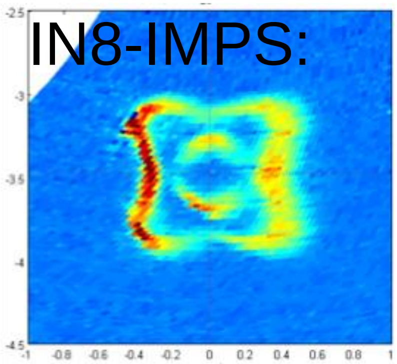
S/N ≈ 43.5/1.92 ≈ 22.7



~8!



IN8-FC:



IN8-IMPS:

Solid angle 0.62
Det. coverage (Cd) 0.7
Crystal shadow (avg) 0.64

→ 28%

Ge crystals

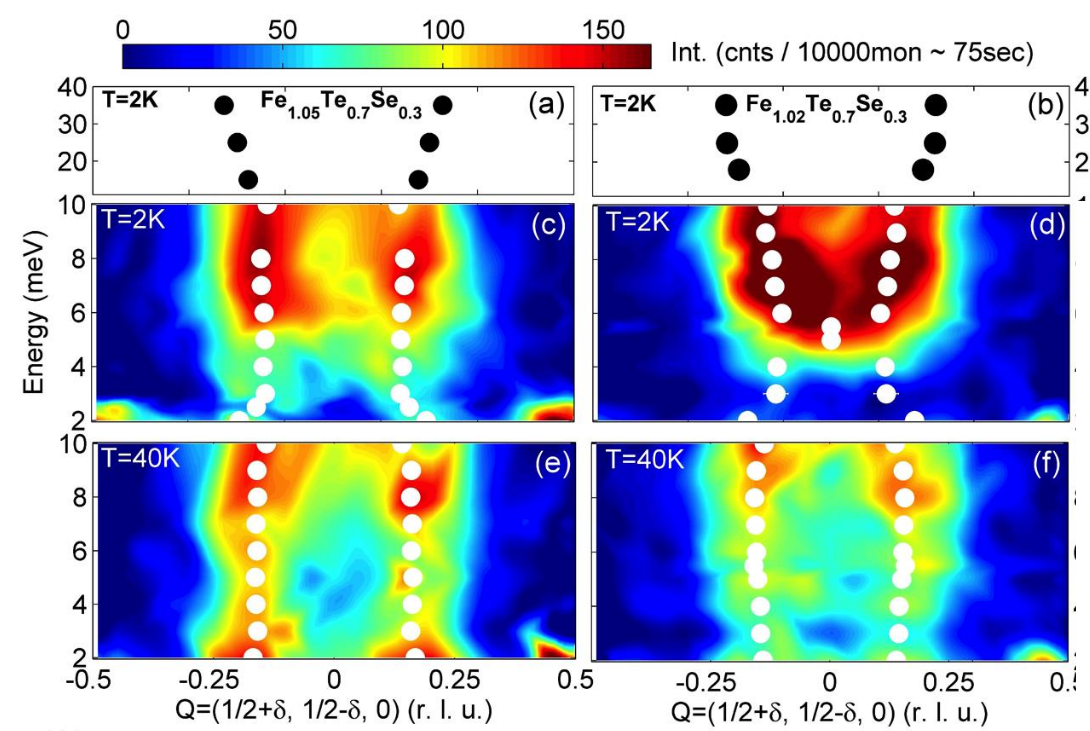
How to distinguish magnetic from other scattering?

$$\frac{d^2\sigma}{d\Omega dE'} = \left(\frac{\gamma r_0}{2}\right)^2 \frac{k'}{k} \left(g f(\vec{\kappa})\right)^2 \exp\left(-2W(\vec{\kappa})\right) \sum_{\alpha\beta} \left(\delta_{\alpha,\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta\right) S^{\alpha,\beta}(\vec{\kappa},\omega)$$

1) Q-dependence
2) PA → Elisa, Mechthild
3) Magnetic properties of the system (dependence in T, H,..)

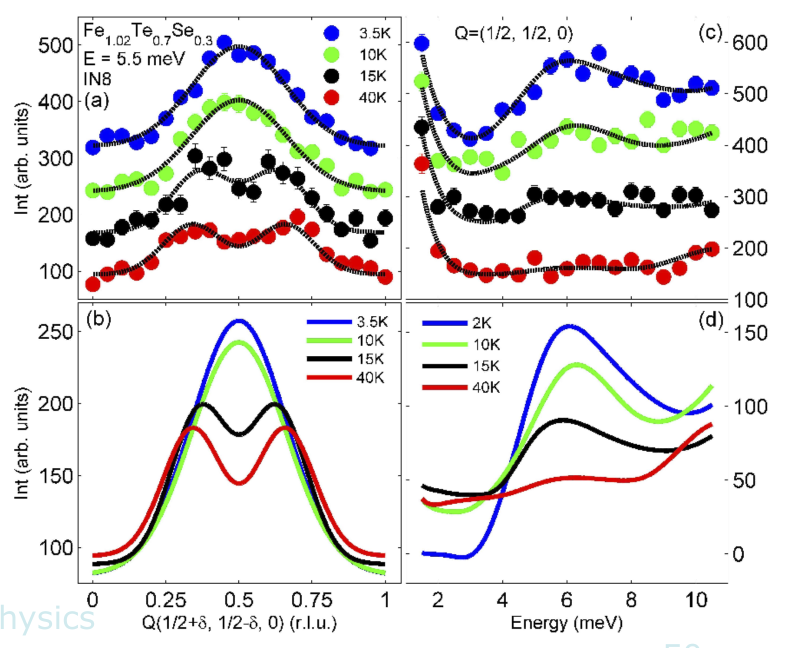
$$S^{\alpha,\beta}(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar} \sum_{ll'} \exp\left(i\vec{\kappa}\left(\vec{r}_l - \vec{r}_{l'}\right)\right) \int_{-\infty}^{\infty} \exp(-i\omega t) \left\langle S_l^\alpha(0) S_{l'}^\beta(t) \right\rangle dt$$

How to distinguish magnetic from other scattering?



FeTeSe

IN8



Tsyrulin et al, submitted

Neutron scattering cross sections

$$\frac{d^2\sigma}{d\Omega d\omega} = \left(\frac{\gamma r_0}{2}\right)^2 \frac{k'}{k}\left(gf\left(\vec{Q}\right)\right)^2 \exp\left(-2W\left(\vec{Q}\right)\right)\sum_{\alpha\beta}\left(\delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right) S^{\alpha,\beta}\left(\vec{Q},\omega\right)$$

Magnetic Form factor

Polarization factor

Scattering function

The Momentum Sum Rule:

$$\frac{1}{N}\sum_{\vec{q}\alpha}\int_{-\infty}^{+\infty} S^{\alpha\alpha}(\vec{q},\omega)\,d(\hbar\omega) = (g\mu_B)^2 S(S+1) = \frac{1}{N}\left\langle S_{tot}^{\alpha\,2}\right\rangle$$

Marshall, p.712
J. Lorenzo et al., PRB **72** (2005), 224511

$$\frac{g^2\mu^2}{Nk_BT}\left(\left\langle S_{tot}^{\alpha\,2}\right\rangle - \left\langle S_{tot}^{\alpha}\right\rangle^2\right) = N\frac{\left\langle \left(M_r^\alpha - \left\langle M_r^\alpha\right\rangle\right)^2\right\rangle}{k_BT} = \chi^{\alpha\alpha}$$

Marshall, p.711

Bragg scattering

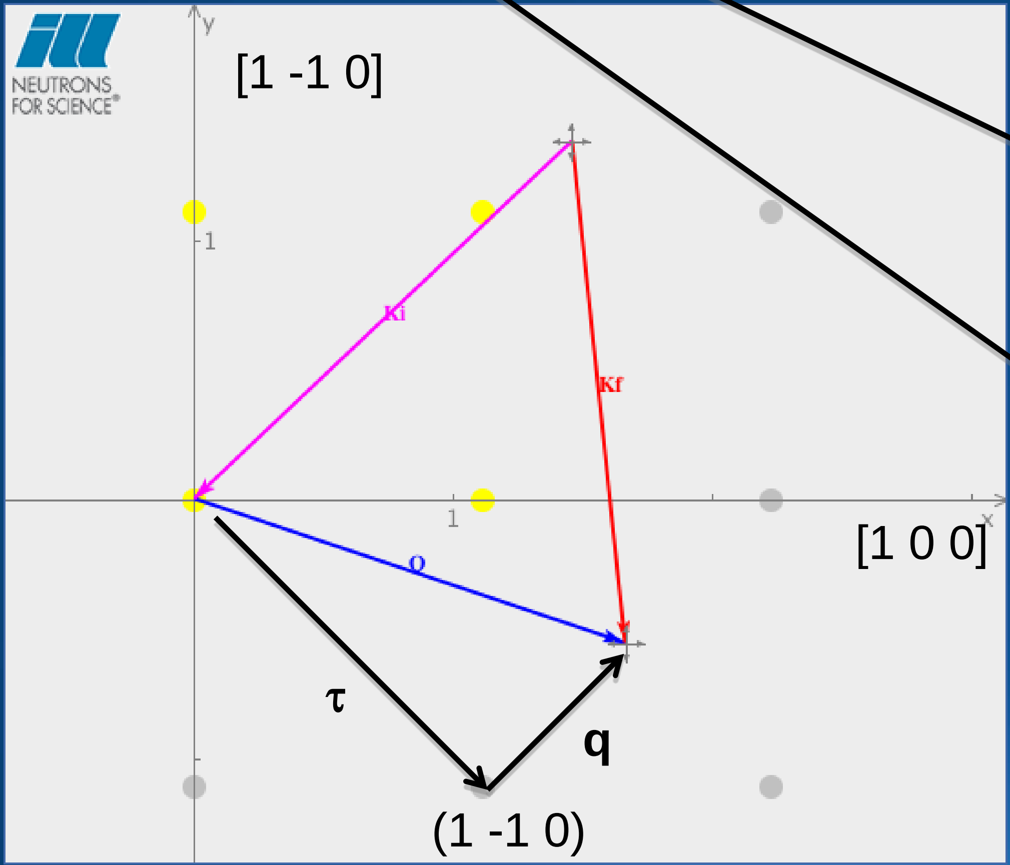
Mean square fluctuation of the magnetization per atom

Spin-Waves:

$$\ldots \propto \sum_{\vec\tau,\vec q} \delta\left(\vec Q - \vec q - \vec\tau\right)\delta\left(\hbar\omega_{\vec q} - \hbar\omega\right)\left\langle n_{\vec q} + 1\right\rangle + \ldots$$

$$= \frac{1}{1 - \exp\left(\frac{\hbar\omega}{k_B T}\right)}$$

Bose factor



Conservation of:

$$\frac{\hbar^2}{2m}\left(k_i^2 - k_f^2\right) = \hbar\omega_{\vec q}$$

energy

$$\vec k_i - \vec k_f = \vec\tau + \vec q$$

momentum

Dispersion relation:

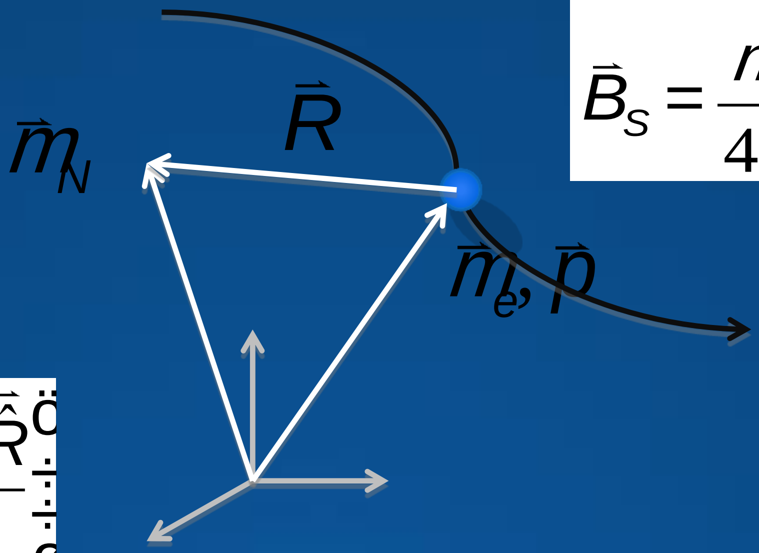
e.g.

$$\hbar\omega_{\vec q} = \hbar\omega\left(\vec q\right) = Dq^2$$

Polarisation factor

Classical ED:

Dipole-dipole interaction between n and e-



$$\vec{B}_S = \frac{\mu_0}{4\pi} \vec{\nabla} \times \left(\frac{\vec{\mu}_e \times \hat{\vec{R}}}{R^2}\right)$$

Dipole

Biot - Savart

$$\vec{B}_L = -\frac{\mu_0}{4\pi}\left(\frac{2\mu_B}{\hbar}\,\frac{\vec{p} \times \hat{\vec{R}}}{R^2}\right)$$

Evaluation of expectation value:

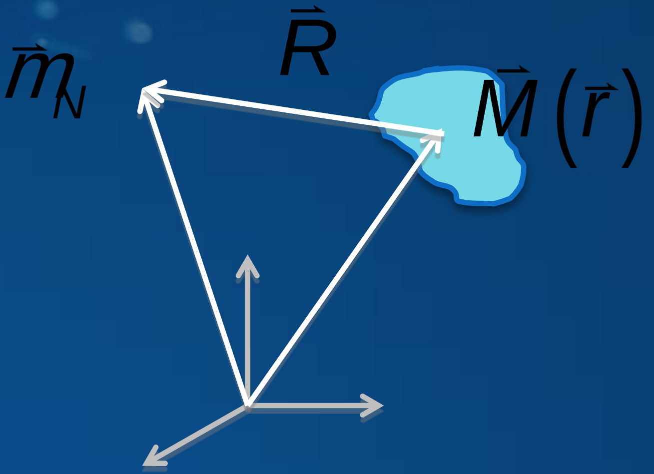
$$\left|\left\langle \vec{k}' s' \lambda' \middle| -\vec{\mu}_N \vec{B} \middle| \vec{k} s \lambda \right\rangle\right|^2$$

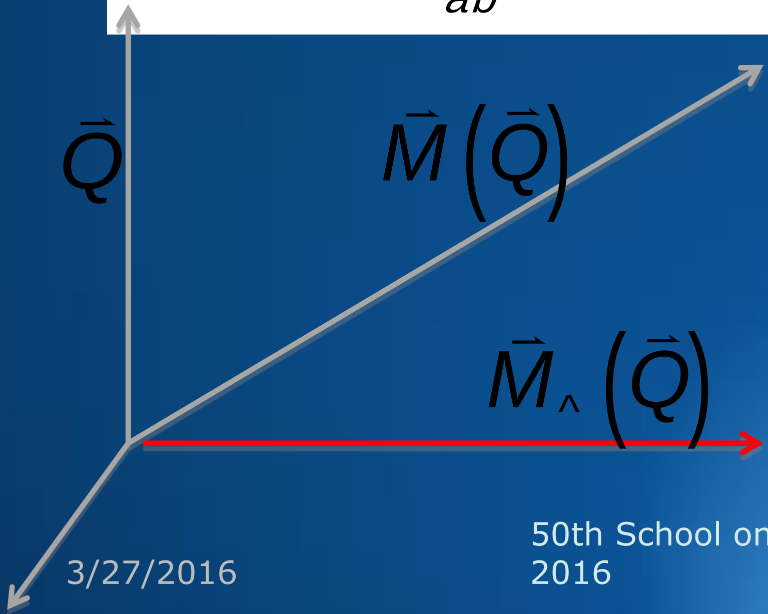
Polarisation factor

Evaluation of expectation value: … Squires pp.131 …

$$\langle \lambda' | \vec{M}_\perp^* \cdot \vec{M}_\perp | \lambda \rangle$$

$$\vec{M}_\perp^* \cdot \vec{M}_\perp = \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right) M_\alpha^* M_\beta$$





$$\vec{M}_\perp(\vec{Q}) = \hat{\vec{Q}} \times \left(\vec{M}(\vec{Q}) \times \hat{\vec{Q}}\right)$$

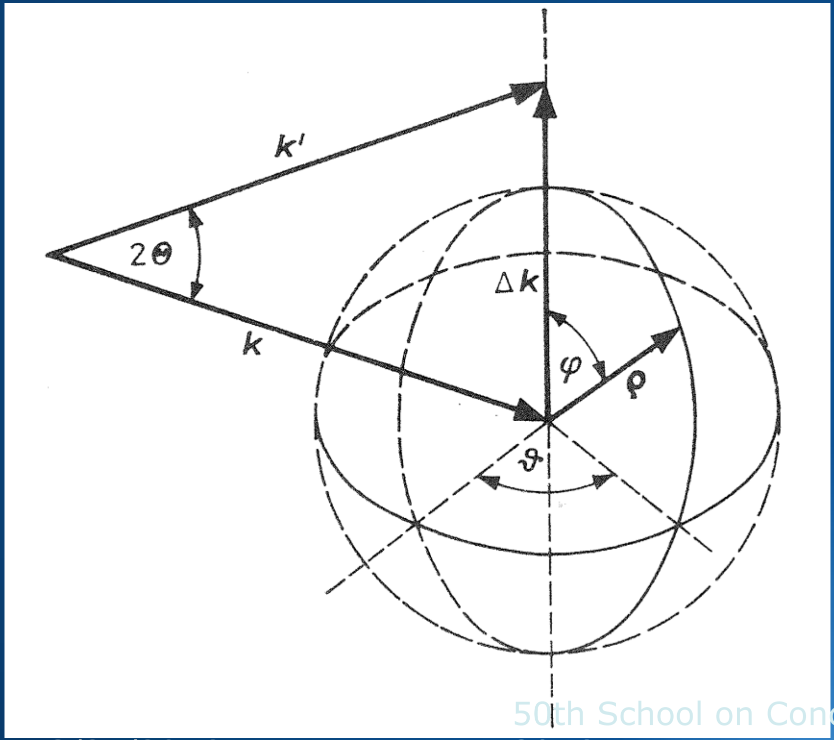
$$\vec{Q} = \vec{k} - \vec{k}'$$

$$\vec{M}(\vec{Q}) = \int \vec{M}(\vec{r}) \exp\left(i\vec{Q}\vec{r}\right) d\vec{r}$$

Magnetic Form factor

Spatial distribution of unpaired electrons

$$\vec{f}\left(\vec{Q}\right) = \int \vec{\rho}_d\left(\vec{r}\right)\exp\left(i\vec{Q}\vec{r}\right)d\vec{r}$$



WH, p.166

JR, Thesis, p.19

Spin-Waves:

Localized electrons

Linear approximation (n<< S)

- ➔ (Approximately) valid for ‘classical’ systems: isolators with large spin quantum number
- ➔ Spin-waves are independent, i.e. non-interacting
- ➔ Only transverse terms, longitudinal term is time independent

$$\frac{d^2\sigma}{d\Omega dE'} = (\gamma r_0)^2 \frac{k'}{k}\frac{(2\pi)^3}{v_0}\frac{1}{2}S\left(1-\hat{Q}_z^2\right)\left\{\frac{1}{2}gf(\vec{Q})\right\}^2 \exp\left(-2W(\vec{Q})\right)$$

Creation of magnons

$$\times\sum_{\vec{\tau},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{\tau})\,\delta(\hbar\omega_{\vec{q}}-\hbar\omega)\langle n_{\vec{q}}+1\rangle +$$

‘Energy loss’

Annihilation of magnons

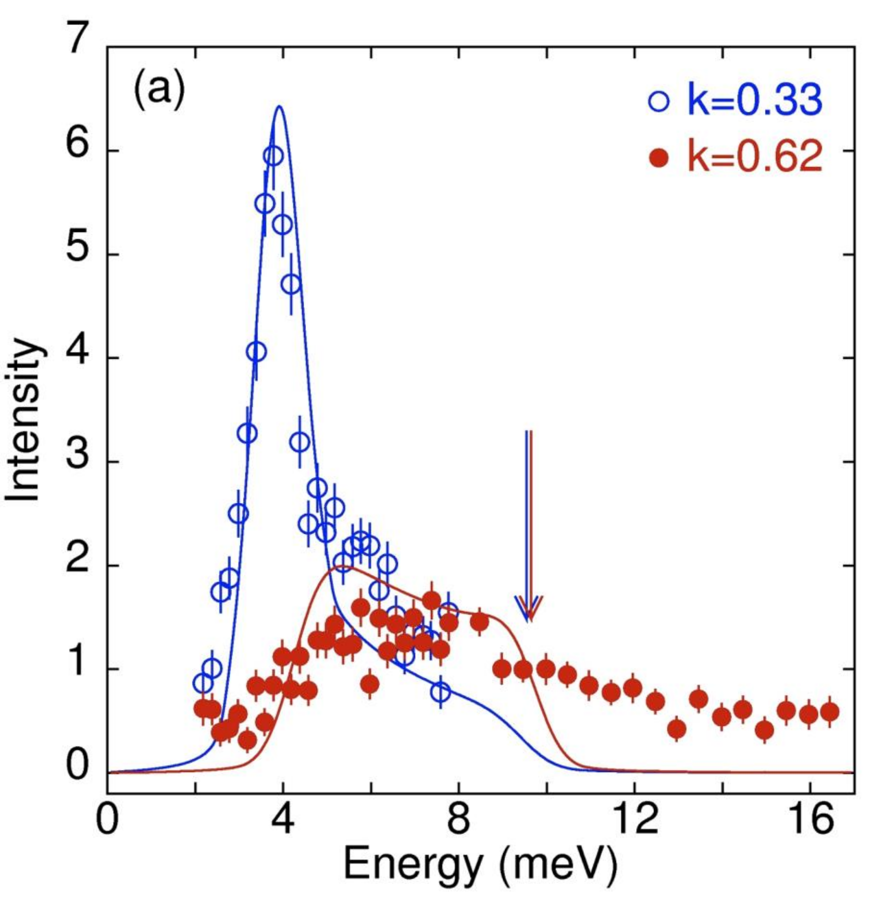
$$+\sum_{\vec{\tau},\vec{q}} \delta(\vec{Q}+\vec{q}-\vec{\tau})\,\delta(\hbar\omega_{\vec{q}}+\hbar\omega)\langle n_{\vec{q}}\rangle$$

‘Energy gain’

Squires, p.163

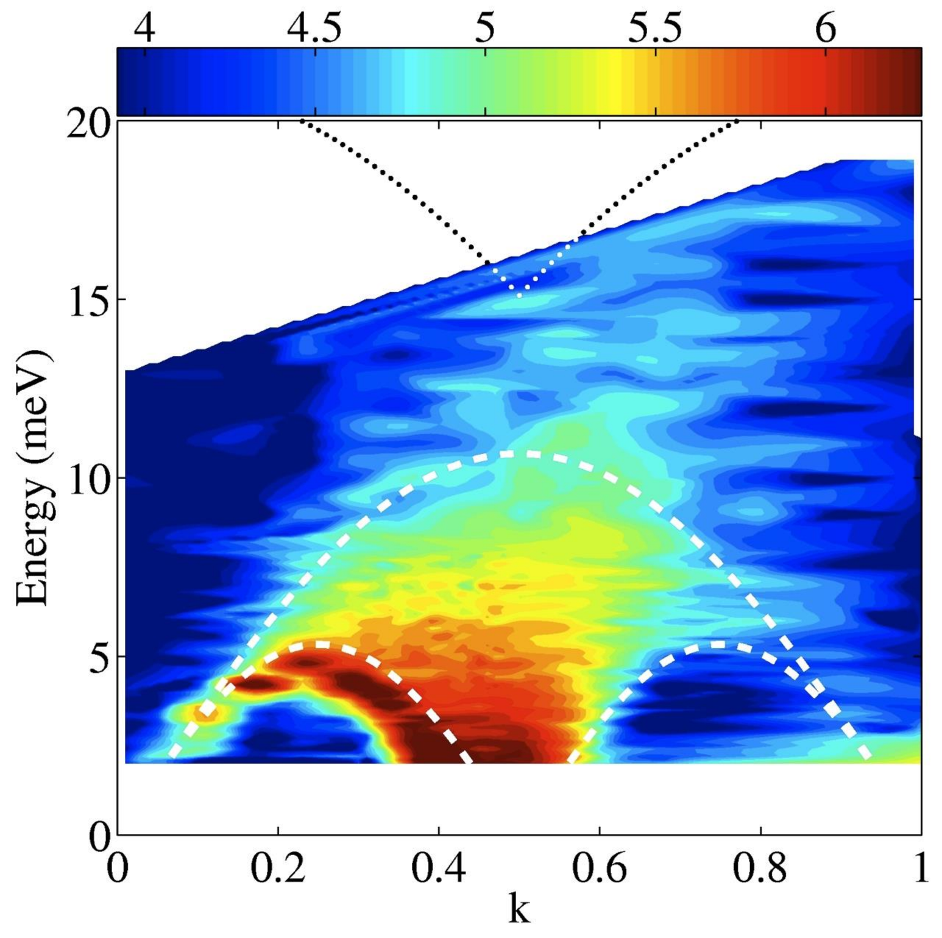
Spin ½ in 1 dimension:

$LiCuVO_4$

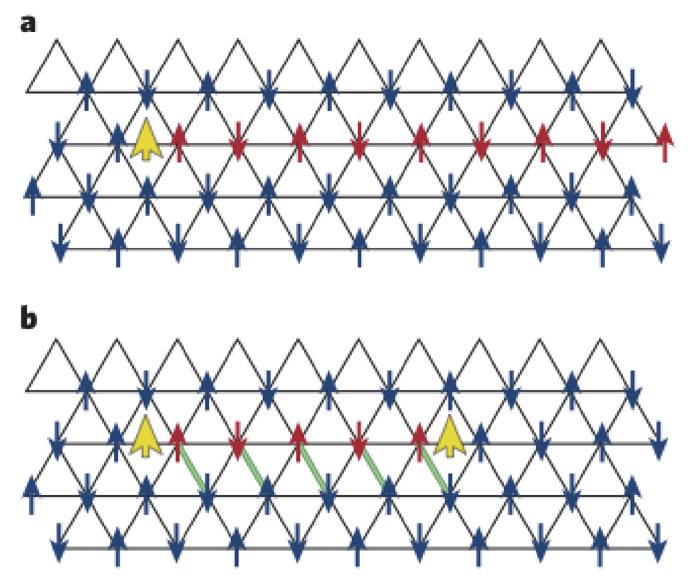


M. Enderle et al., PRL 104 (2010), p.237207

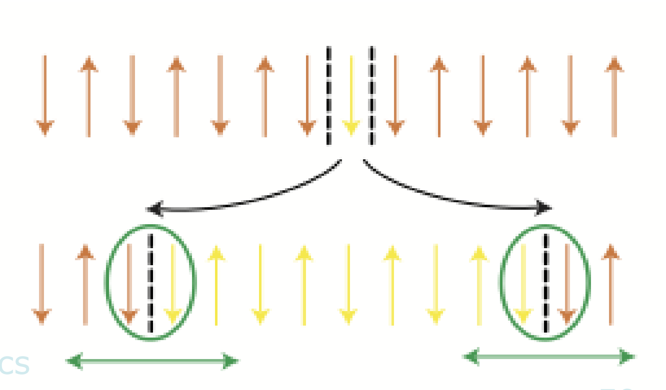
Spin ½ in 1 dimension:



M. Enderle et al., PRL 104 (2010), p.237207



L. Balent, Nature 464 (2010), p.199



DS=±1

H.-B. Braun et al., Nat. Phys.1 (2005), p.159