Choosing the Right Spectrometer

NCNR

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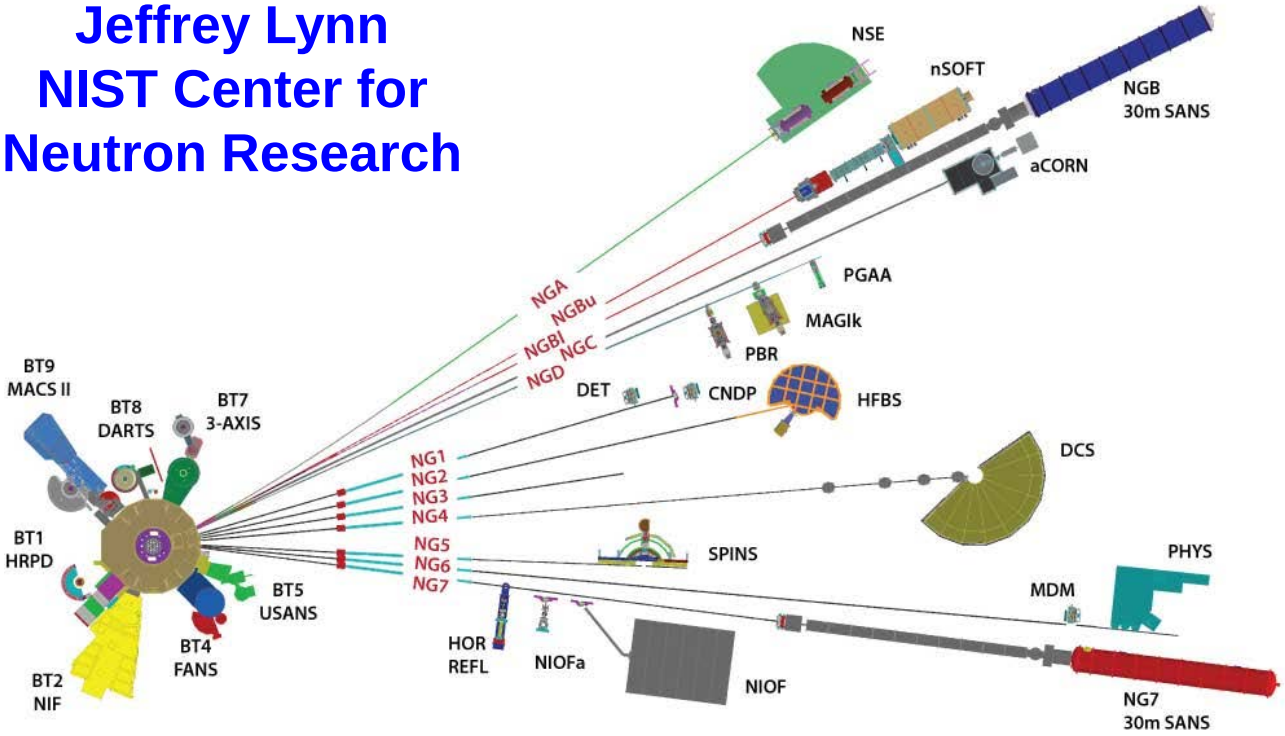
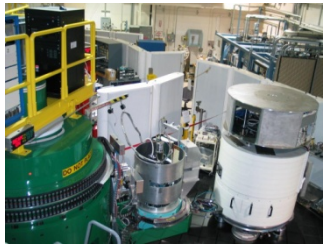
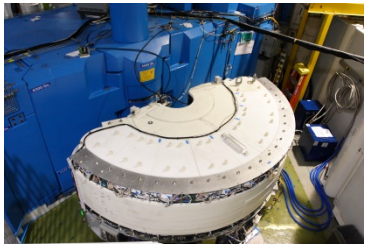
NIST Center for Neutron Research



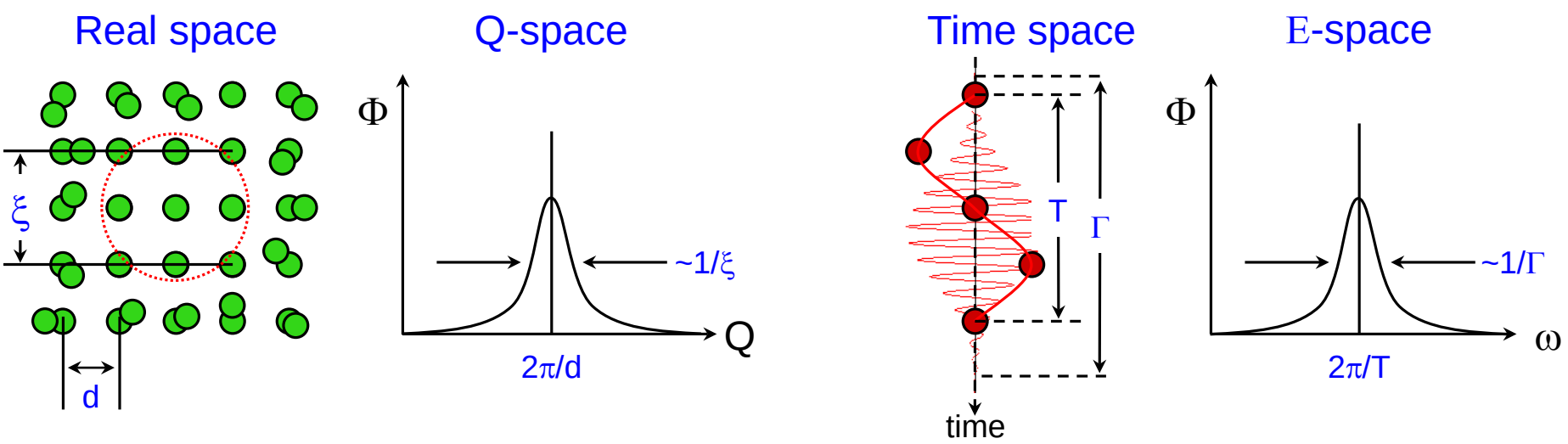




Review: Main Messages of the Week

The scattered neutron flux $\Phi(Q,\hbar\omega)$ is proportional to the space (r) and time (t) Fourier transform of the probability $G(\vec{r},t)$ of finding one or two atoms (*spins*) separated by a particular distance (*angle)* at a particular time.

$$\Phi \propto \frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto \iint e^{i(\vec{Q}\cdot\vec{r}-\omega t)} G(\vec{r},t)\, d^3\vec{r}\, dt$$

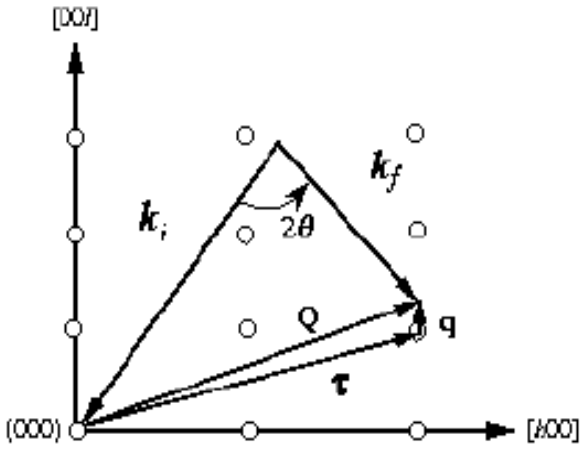


Conservation of Momentum and Energy

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

$$\Delta E = \frac{\hbar^2 k_i^2}{2m} - \frac{\hbar^2 k_f^2}{2m}$$

$$\mathbf{Q}_C = \tau + \mathbf{q}$$



Other Probes

$$E_{neutron}(meV) = 2.0719k^2 = 81.7968/\lambda^2$$

$$E_{photon}(keV) = 2.0k = 12.4/\lambda$$

$$E_{electron}(eV) = 3.8k^2 = 150/\lambda^2$$

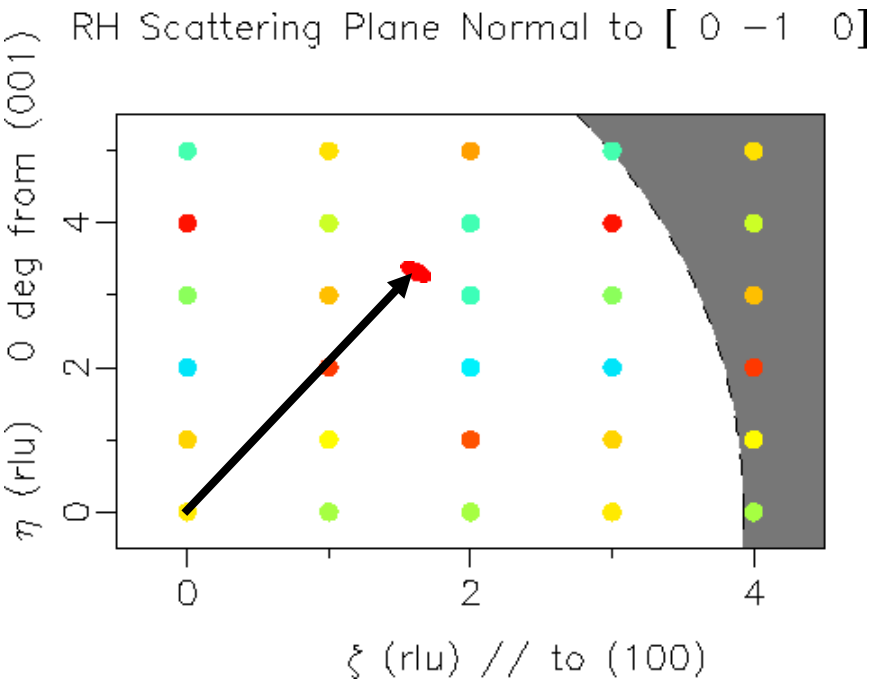
$$1\,meV = 11.6\,K \quad (k_BT)$$

$$1\,meV = 8.06\,cm^{-1} \quad (E/hc)$$

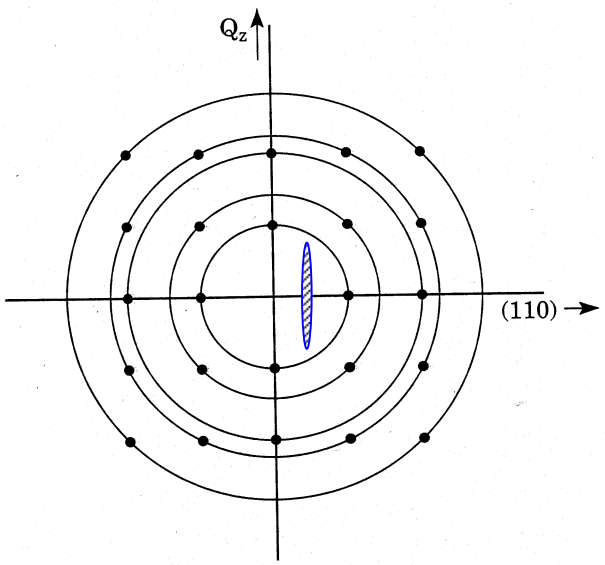
$$1\,meV = 0.2418\,THz \quad (E/h)$$

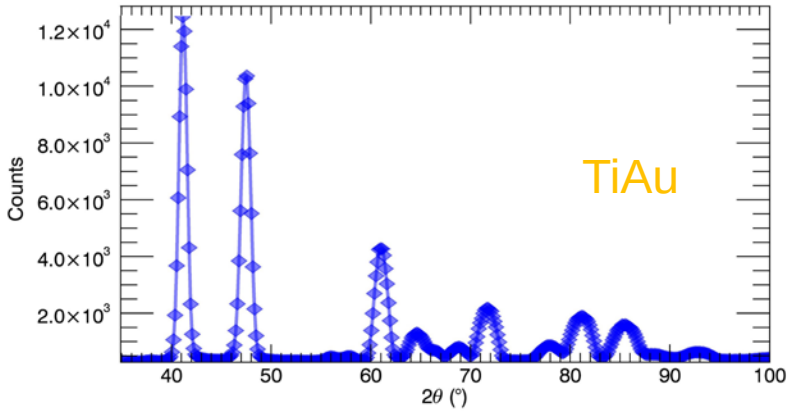
$$1\,meV/\mu_B = 17.3\,T \quad (E/\mu_B)$$

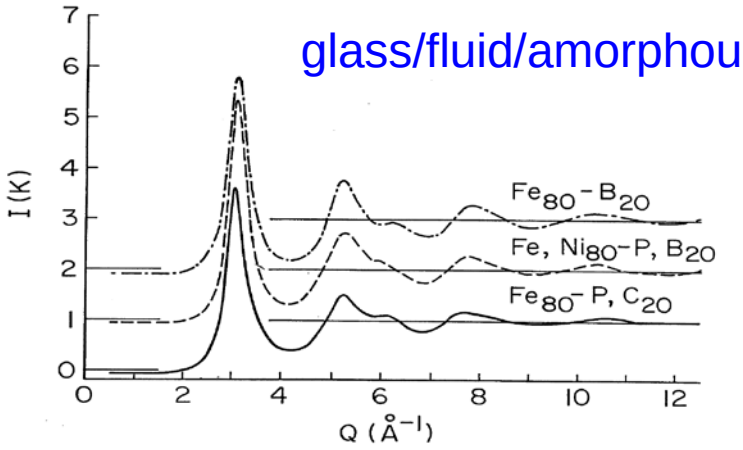
Reciprocal Space for Thermal Neutrons



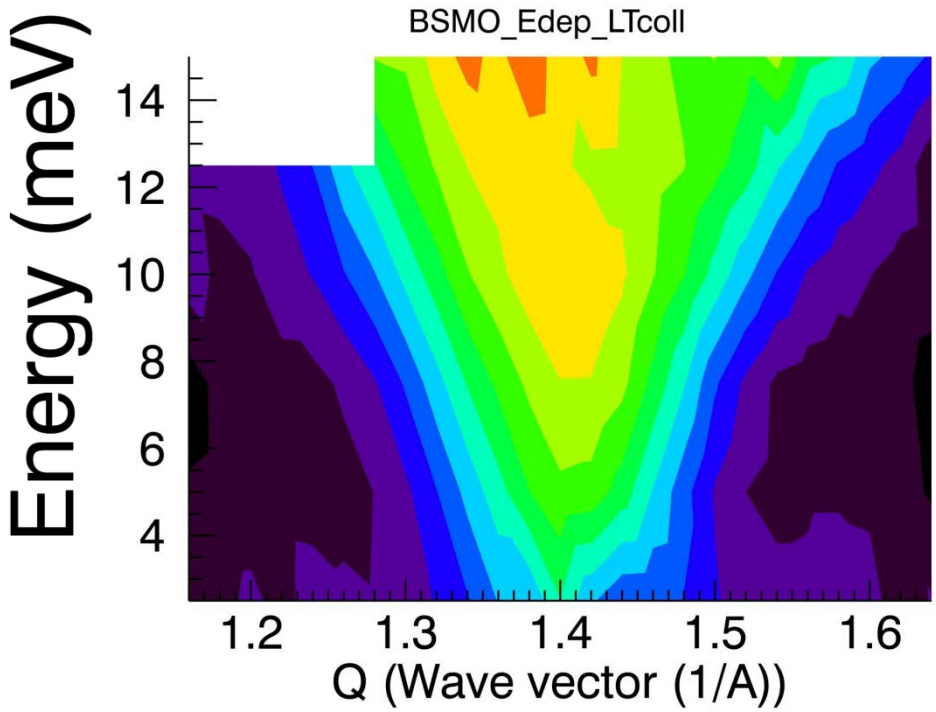
Reciprocal Space for Powder

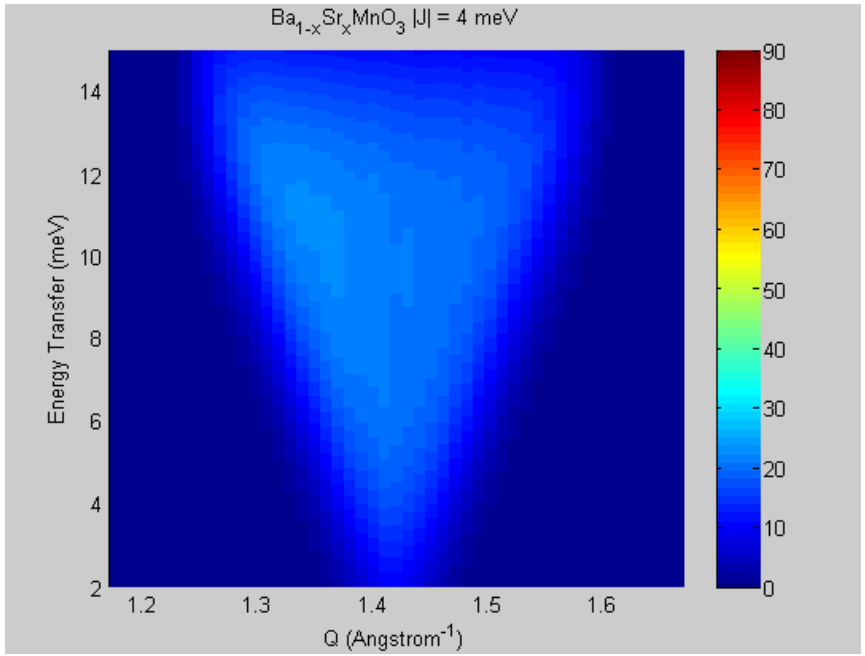






Ground State Inelastic Magnetic Scattering





2.6 K

BT-7

Q (Wave vector (1/A))

Inelastic Spectrometers

	Thermal triple-axis instruments (BT-7) (BT-4)	1 meV
	Cold neutron triple-axis instrument (MACS) (SPINS)	
*S(**Q**,E)*	Disk chopper time-of-flight spectrometer (DCS) (FANS)	250 μeV
	High flux backscattering spectrometer (HFBS)	1 μeV
*S(**Q**,t)*	Spin-echo spectrometer (NSE)	δt → ~50 neV

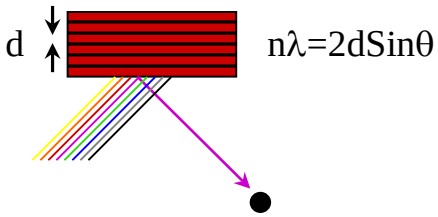
Remember – **Intensity** ↓

Resolution ↑

All these different spectrometers are designed differently to optimize intensity and resolution for different measurement requirements

Crystal Spectrometers: Specifying $\vec{k}_i$ and $\vec{k}_f$

1. Bragg Diffraction



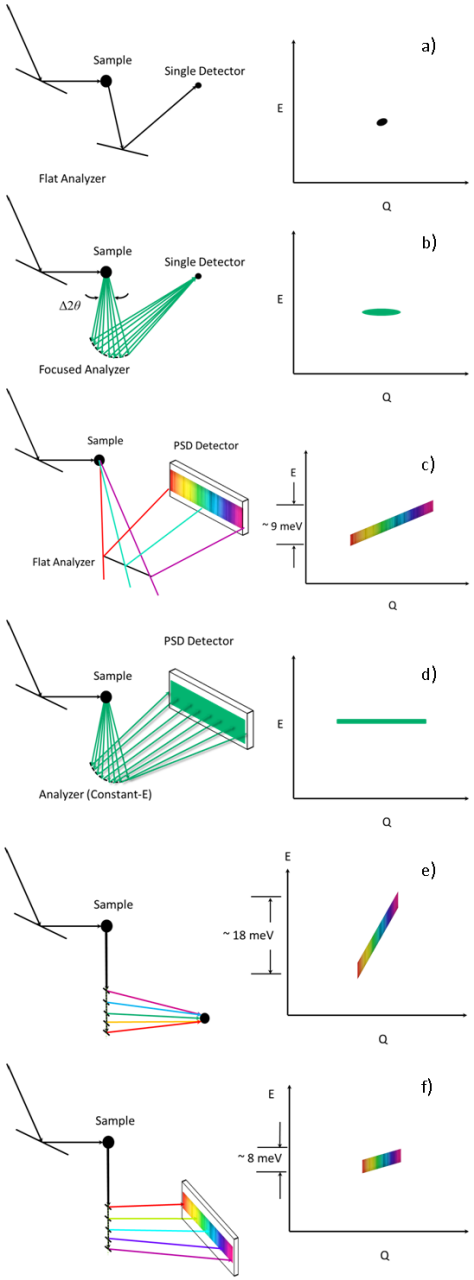
BT7, MACS, HFBS

S(***Q***,*E*)

SPINS (Cold Triple Axis)
BT-4 (Thermal Triple Axis and Filter Analyzer Spectrometer)
BT-1 (High Resolution Powder Diffractometer)
BT-8 (Residual Stress Diffractometer)

BT-7 Inelastic Scattering

Six Inelastic Analyzer Modes of Operation

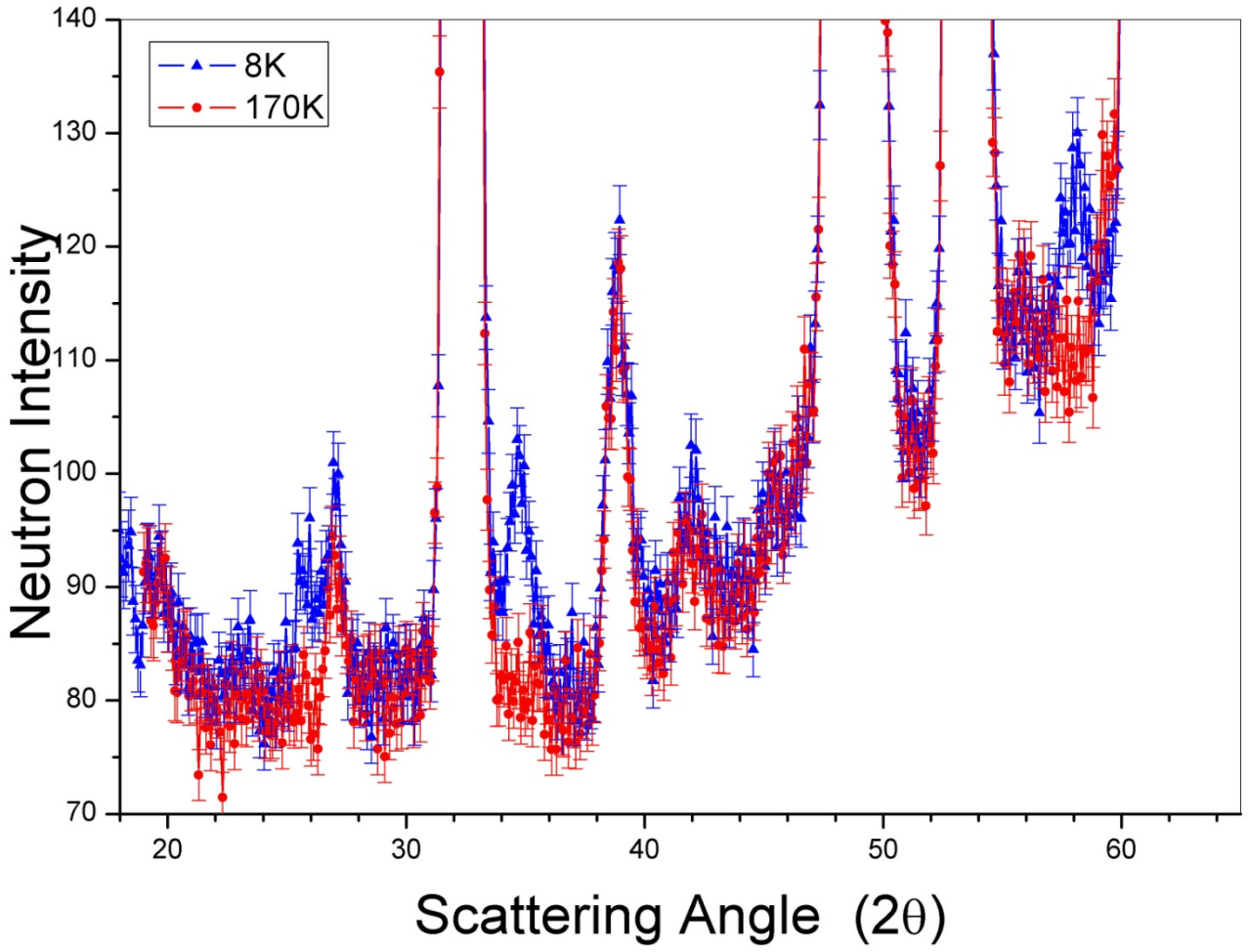


https://www.ncnr.nist.gov/instruments/bt7_new/

Journal of Research of NIST **117**, 61-79 (2012)

Magnetic Scattering from La(O,F)FeAs

PSD or
BT-7



C. de la Cruz, Q. Huang, J. W. Lynn, J. Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and P. Dai,
Nature **453**, 899 (2008).

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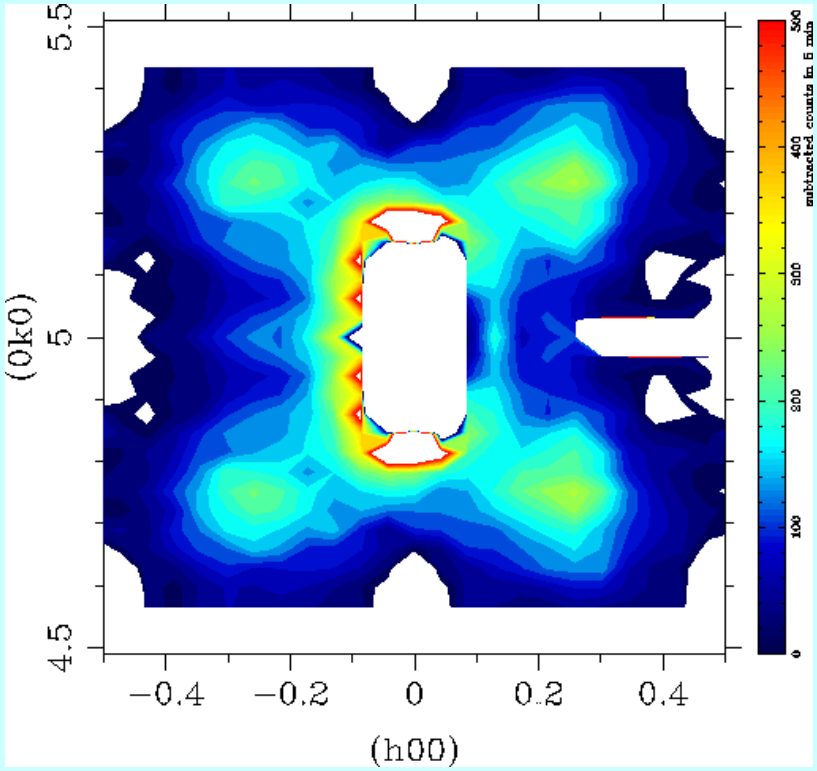
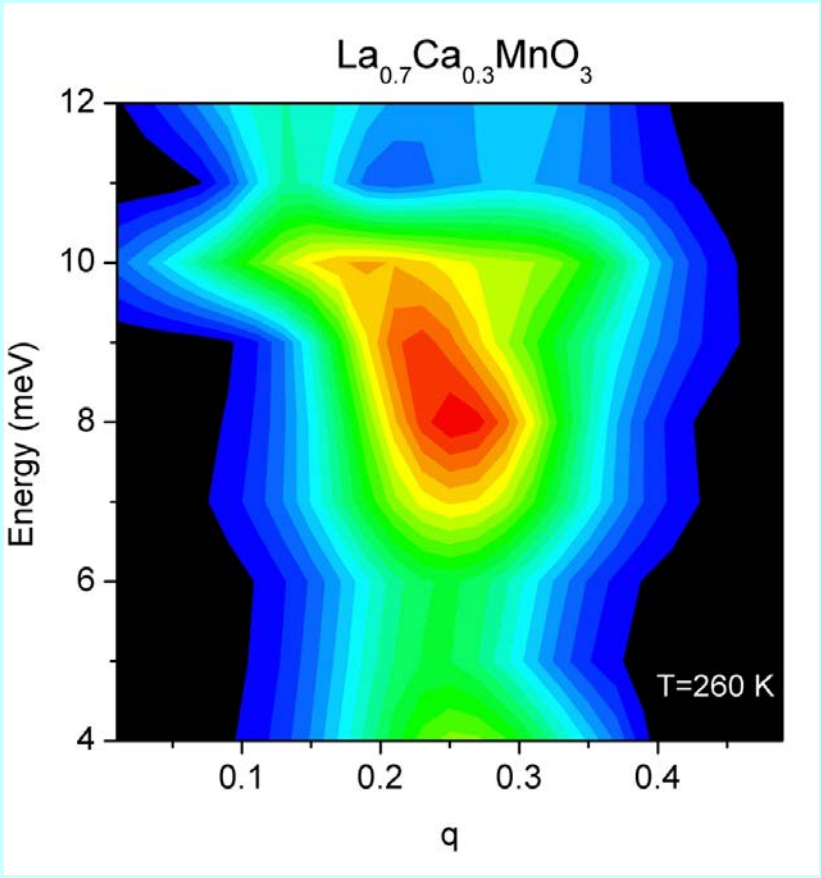
Polaron Dynamics in CMR $La_{0.7}Ca_{0.3}MnO_3$





J. W. Lynn, D. N. Argyriou, Y. Ren, Y. Chen, Y. M. Mukovskii, and D. A. Shulyatev, Phys. Rev. B**76**, 014437 (2007)

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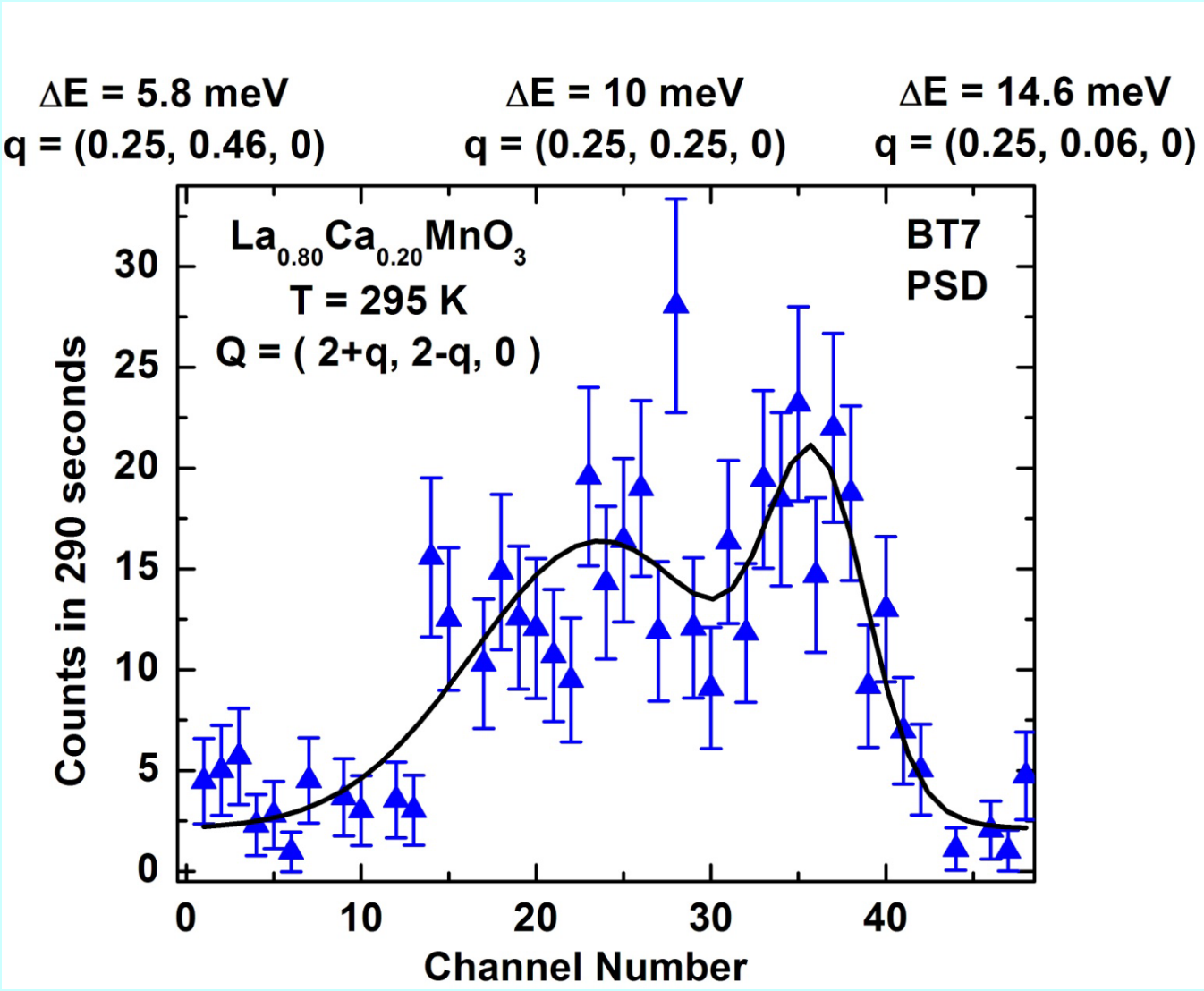
T dependence

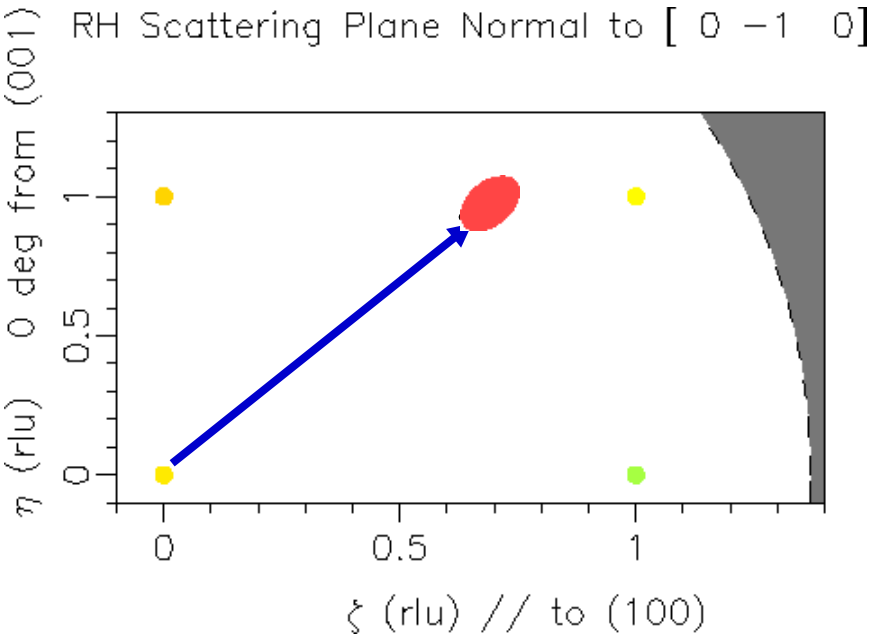
BT-7 using the PSD



Energy Resolution for Crystal Spectrometers

- $E = C(2\pi/\lambda)^2$
- $\Delta E = C' / \lambda^3 \, \delta\lambda$
- Cold Neutrons → higher resolution

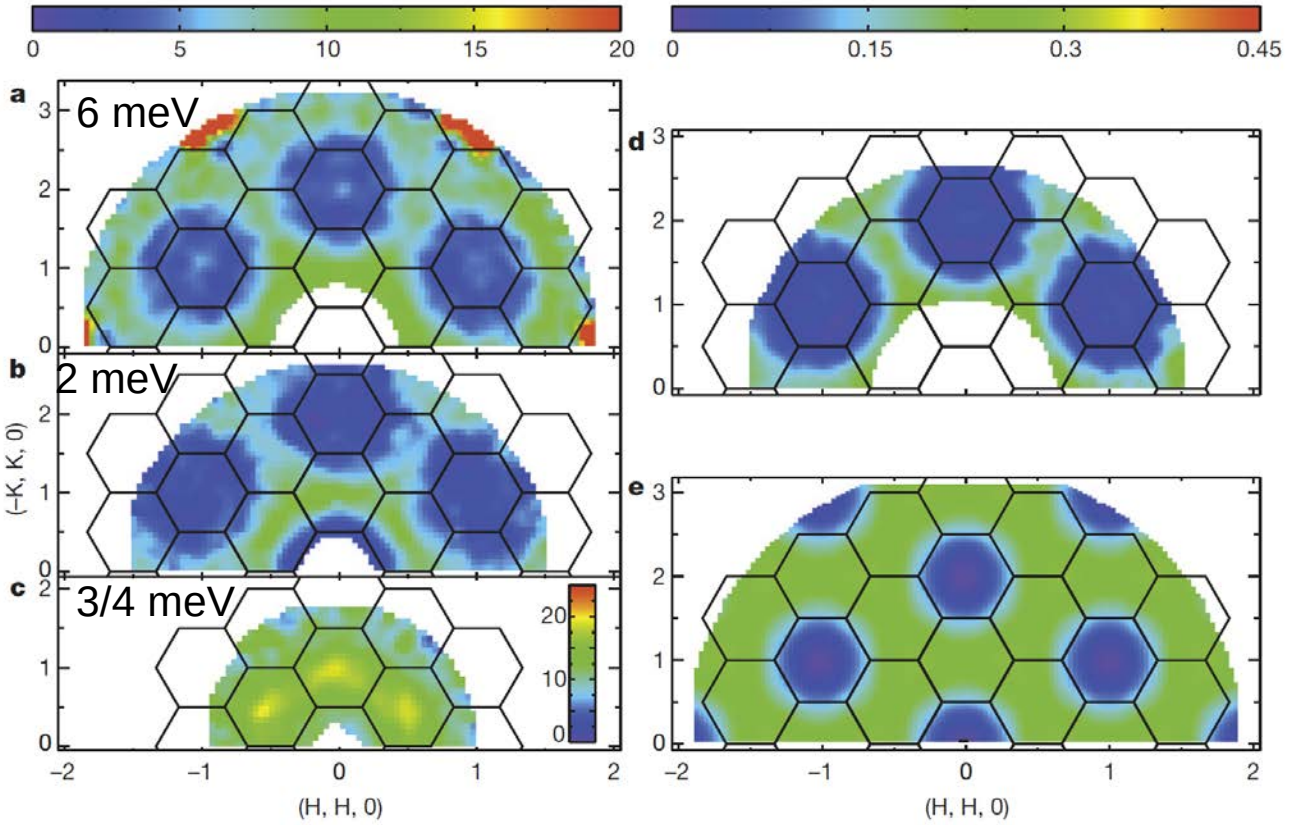
Reciprocal Space for Cold Neutrons



MACS twenty points at a time; high flux horizontal focused monochromator

Spin Liquid Scattering in $ZnCu_3(OD)_6C_{l2}$

T = 1.6 K



MACS

Tian-Heng Han, Joel S. Helton, Shaoyan Chu, Daniel G. Nocera, Jose A. Rodriguez-Rivera, Collin Broholm, and Young S. Lee, Nature **492**, 406 (2012).

Perfect Resolution Backscattering

$$\lambda_i = 2d_M \sin(\theta_M)$$

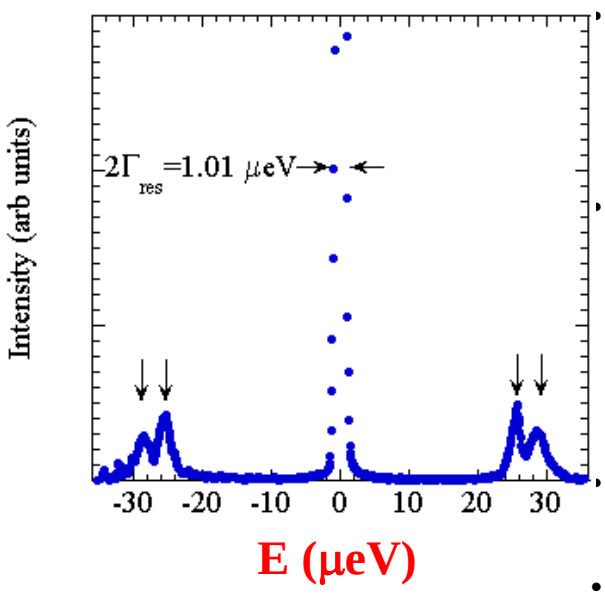
Note: Scattering angle = 2θ

$$\Delta\lambda = 2d_M \cos(\theta_M)\Delta\theta_M$$

Thermal TA	1,000 μeV
Cold TA	200 μeV
HFBS	1 μeV

HFBS

Quantum Rotational Tunneling in Toluene: A Measurement using HFBS



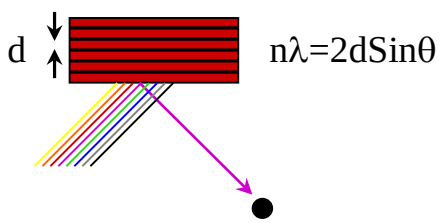
- Motion of methyl groups (CH_3) in toluene ($C_6H_5CH_3$)
- Inelastic peaks correspond to tunneling through a potential barrier: a classically forbidden motion!
- Tunneling rate ~6 GHz
- Presence of two inelastic peaks on the energy loss side and two peaks on the energy gain side indicates two inequivalent sites for molecules in the solid

Methods of Specifying and Measuring $\vec{k}_i$ and $\vec{k}_f$

1. Bragg Diffraction (Crystal Spectrometers)

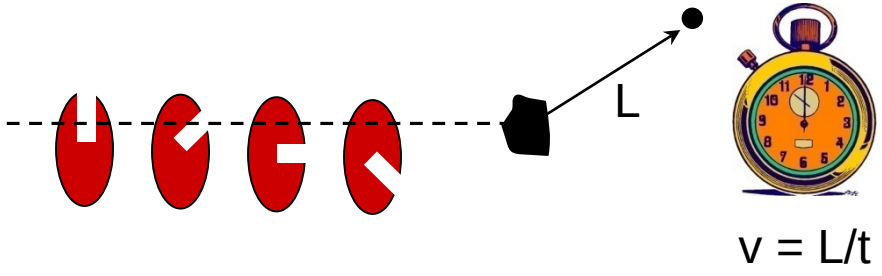
   BT7, MACS, HFBS

   $S(\boldsymbol{Q},E)$

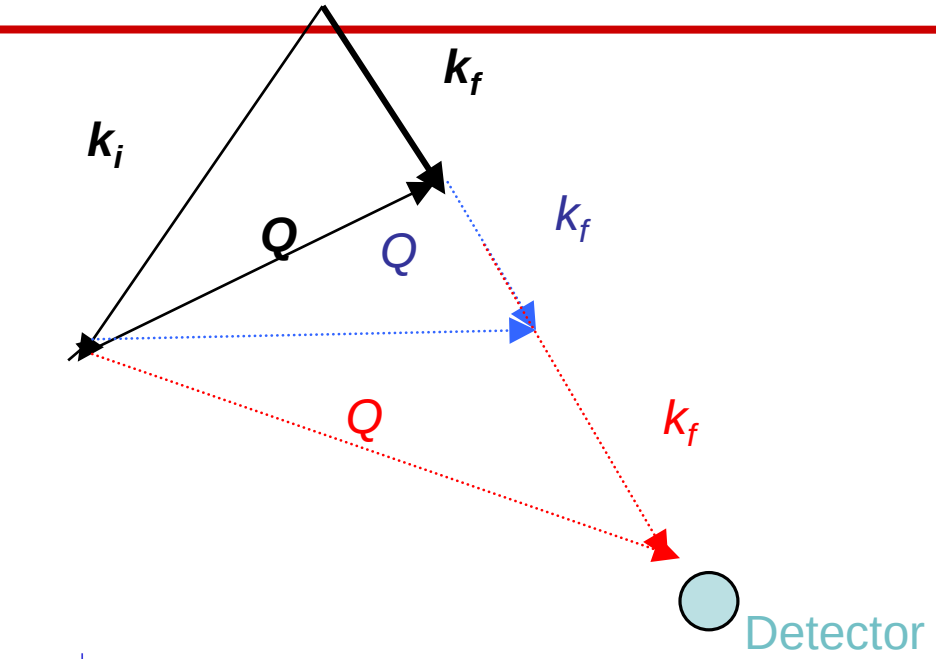


2. Time-of-Flight (TOF)

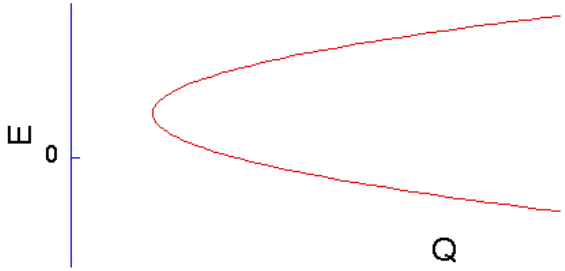
   DCS $S(\boldsymbol{Q},E)$



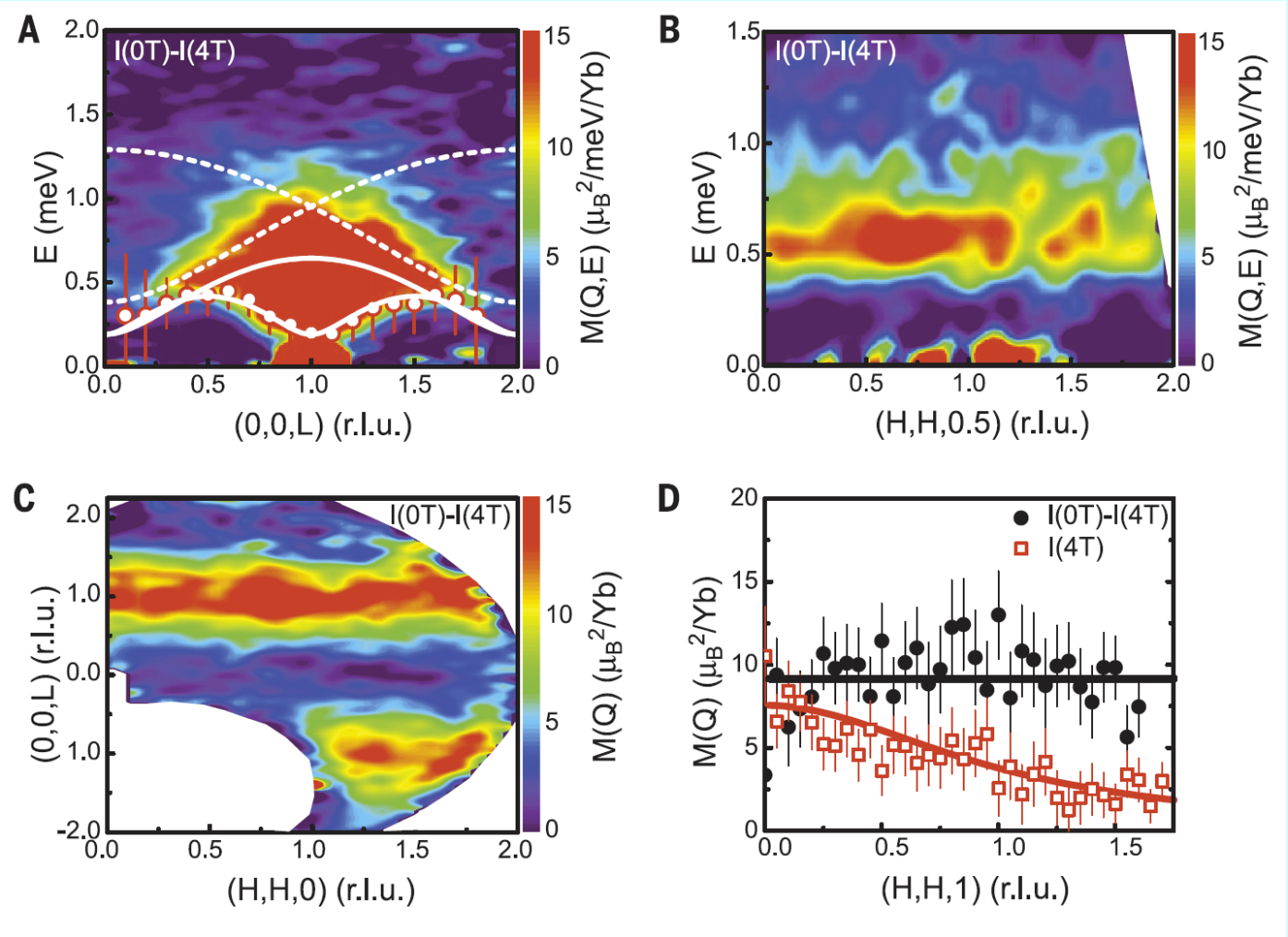
Disk Chopper Spectrometer



913 Detectors
333 Hz Repetition Rate



Fractional Spin Excitations in Yb_2Pt_2Pb



L. S. Wu, W. J. Gannon, I. A. Zaliznyak, A. M. Tsvelik, M. Brockmann, J.-S. Caux, M. S. Kim, Y. Qiu, J. R. D. Copley, G. Ehlers, A. Podlesnyak, M. C. Aronson, Science **352**, 1690 (2016).

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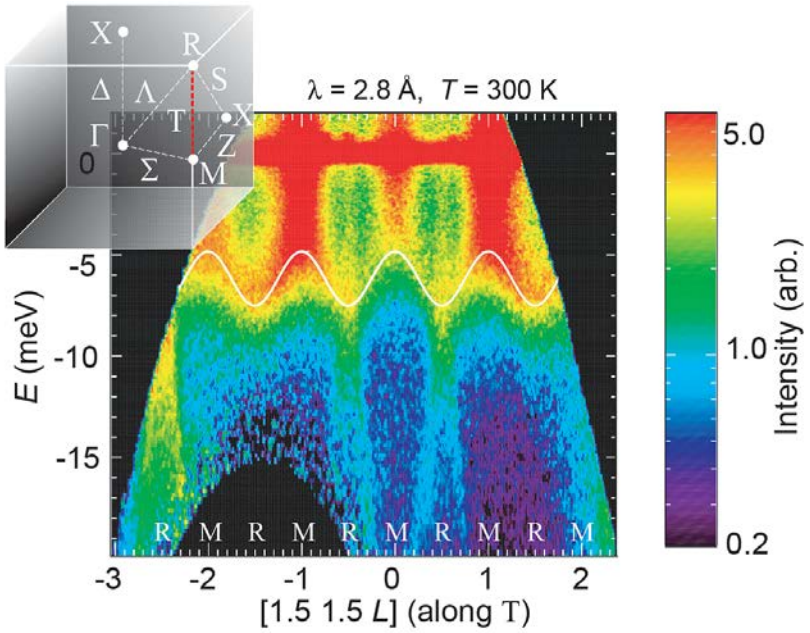
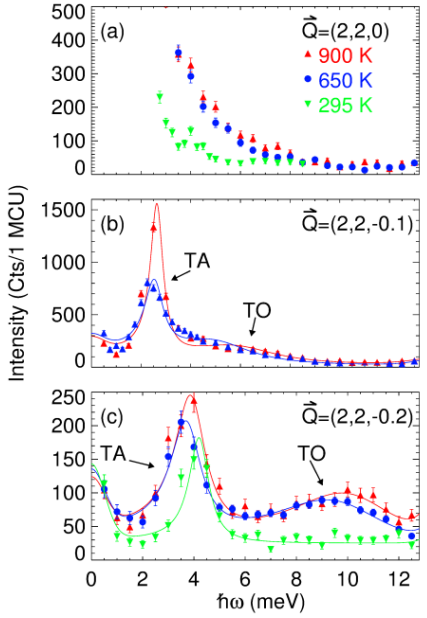
Example: DCS versus BT7

DCS Broad surveys in **Q-ω**



BT7 Limited regions in **Q-ω**



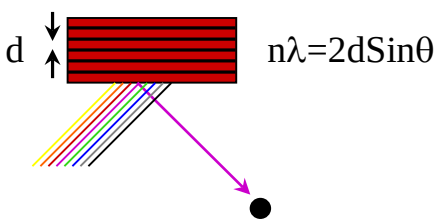
Rules of Thumb: (think carefully before violating)

DCS, MACS – systems requiring resolution < 400 μeV

BT7 – single crystals (or diffraction)

Methods of Specifying and Measuring $\vec{k}_i$ and $\vec{k}_f$

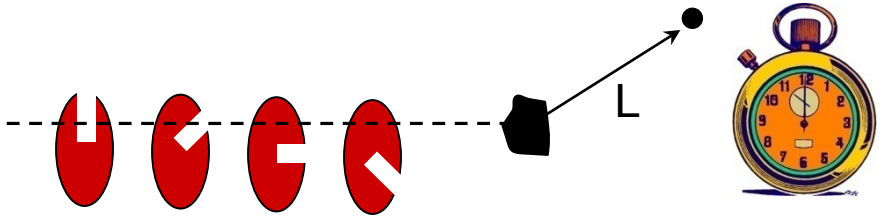
1. Bragg Diffraction (Crystal Spectrometers)



BT7, MACS, HFBS

S(***Q***,*E*)

2. Time-of-Flight (TOF)



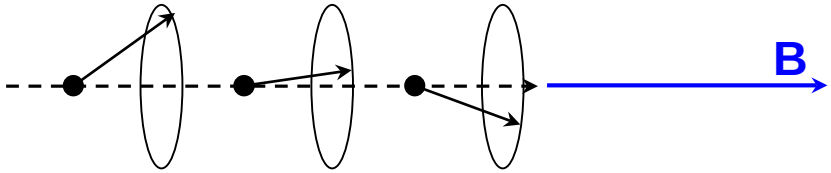
v = L/t

DCS, HFBS S(***Q***,*E*)

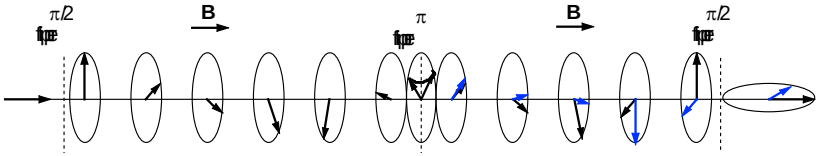
"TOF" Larmor Precession

NSE

S(***Q***,*t*)



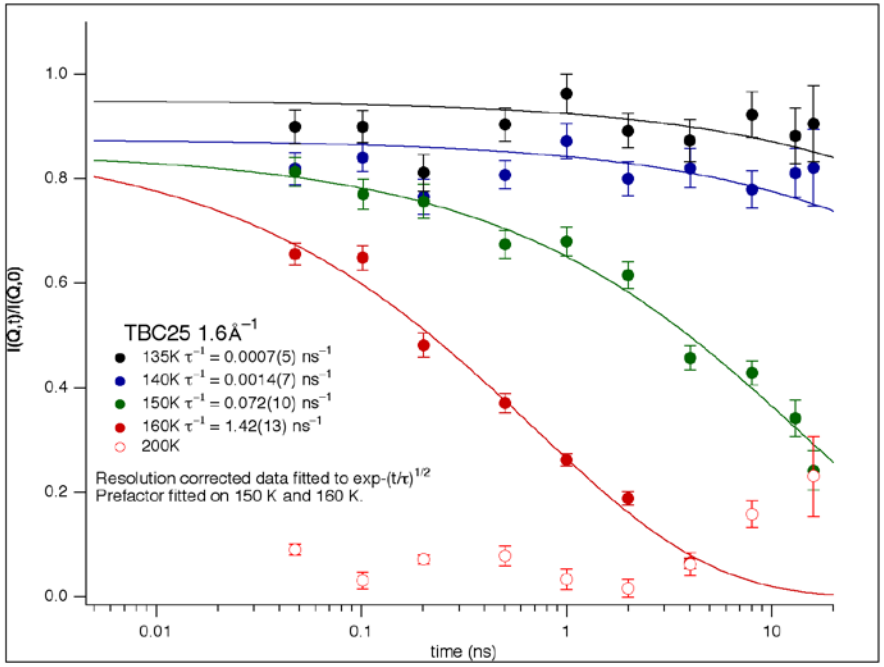
Spin Echo Spectrometer



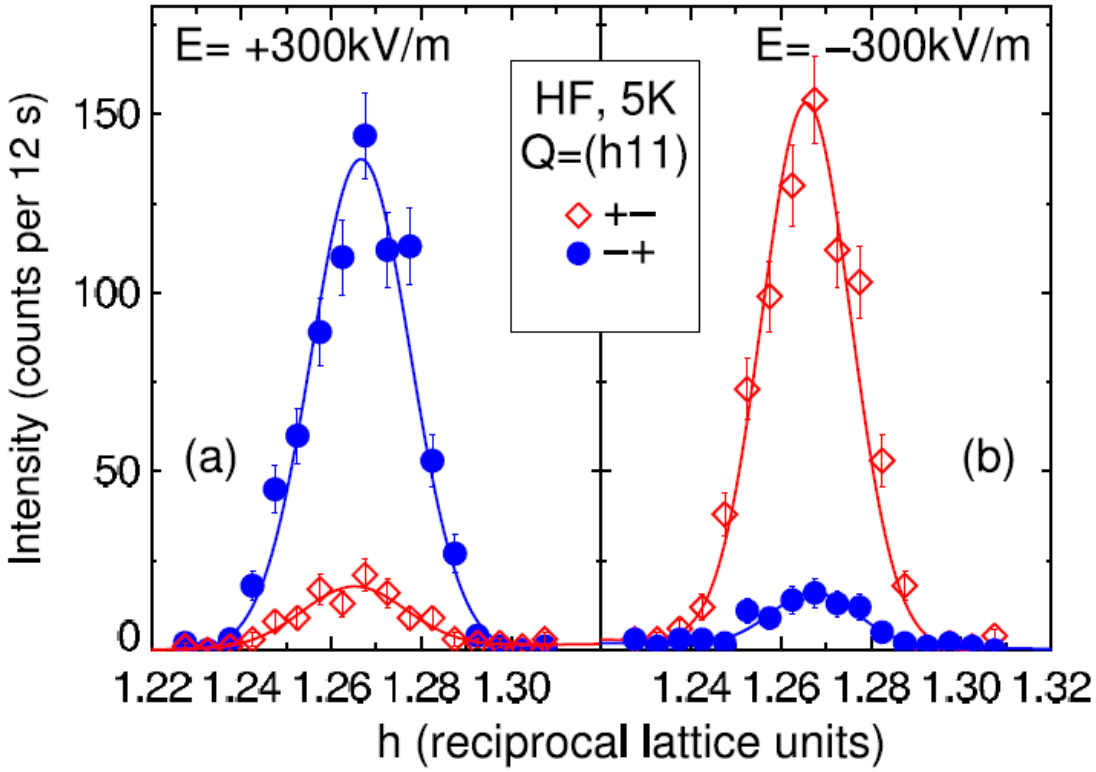
$$t = \frac{L}{v}$$

$$\phi = \omega t = \frac{\gamma B L}{v}$$

Spin Echo Data



Polarized Neutron Scattering Data (BT7, MACS)



Coupled Magnetic and Ferroelectric Hysteresis in Multiferroic $Ni_3V_2O_8$, I. Cabrera, M. Kenzelmann, G. Lawes, Y. Chen, W. C. Chen, R. Erwin, T. R. Gentile, J. B. Leao, J. W. Lynn, N. Rogado, R. J. Cava, and C. Broholm, Phys. Rev. Lett. 103, 087201 (2009).

How do I Choose the Right Spectrometer?

Two basic considerations:

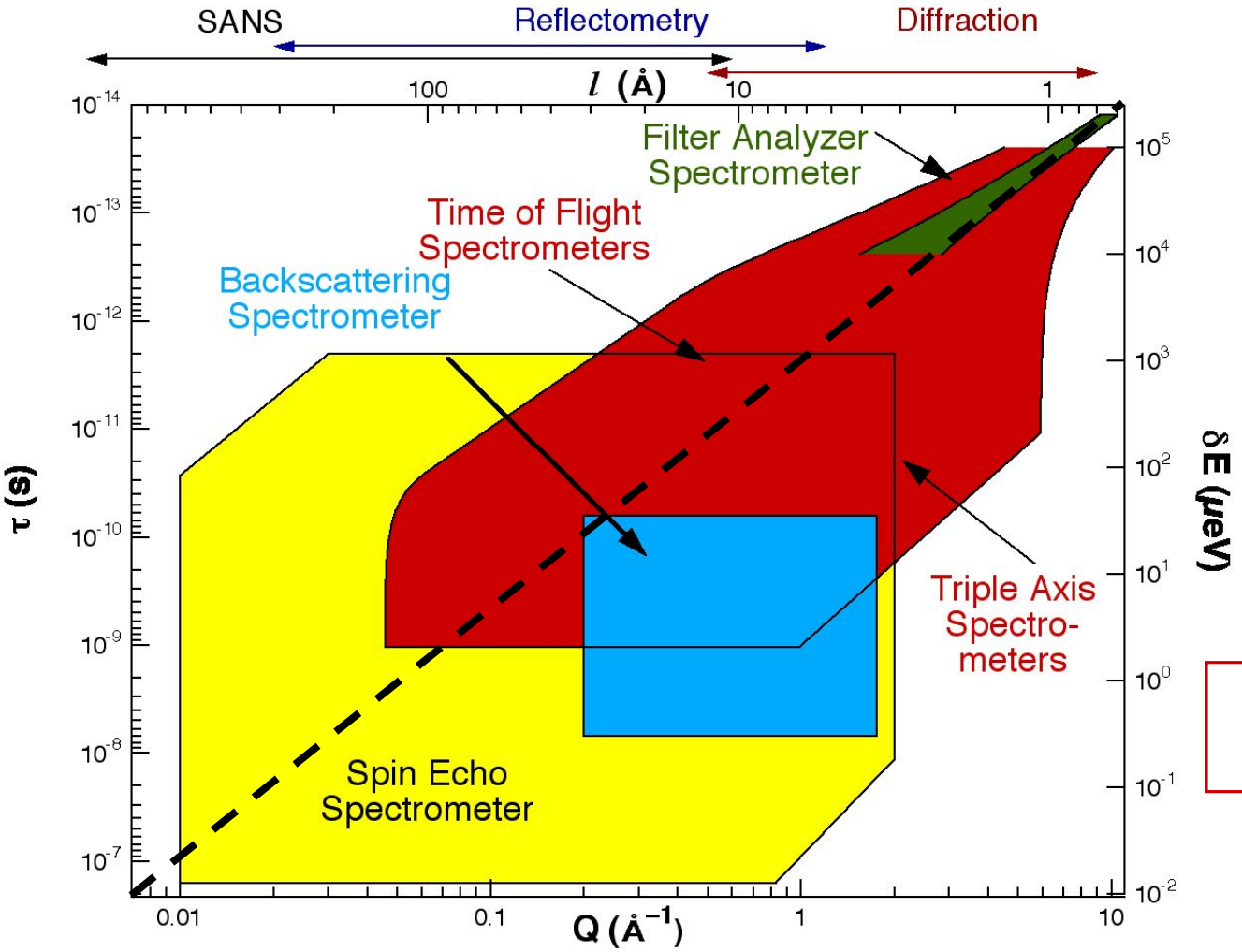
1. What are the time scales (E) of interest?
2. What are the length scales (Q) of interest?

(Some spectrometers overlap →
the choice may boil down to one of resolution)

Two additional considerations:

1. What energy resolution (ΔE) is required?
2. What momentum resolution (ΔQ [or $\Delta \mathbf{Q}$]) is required?

Different Spectrometers Cover Different Regions of Phase Space



Larger “objects” tend to exhibit slower motions.

Rules of Thumb

1. What are the energies ($\hbar\omega$), i.e. time scales ($\Delta t \sim 1/\omega$), of interest?

   $\hbar\omega >$ 1-100 meV - use a thermal triple-axis spectrometer like BT7.

   $\hbar\omega <$ 30 μeV - use HFBS or NSE.

   In between - use MACS or DCS or a cold-neutron triple-axis spectrometer like SPINS.

2. Make sure that the length scales **L** of the relevant motions lie within the range of the spectrometer. For example, consider the HFBS. ($\mathbf{Q} \sim 2\pi/\mathbf{L}$)

$$\mathbf{Q}_{min} = 0.25\ \text{Å}^{-1} \rightarrow \mathbf{L}_{max} \sim 25\ \text{Å}$$
$$\mathbf{Q}_{max} = 1.75\ \text{Å}^{-1} \rightarrow \mathbf{L}_{min} \sim 3.5\ \text{Å}$$

REMEMBER - $\mathbf{Q}_{min}$ and $\mathbf{Q}_{max}$ are inversely proportional to the incident neutron wavelength

More Rules of Thumb

Is your sample polycrystalline or amorphous?

Does ONLY the magnitude (not the direction) of **Q** matter?

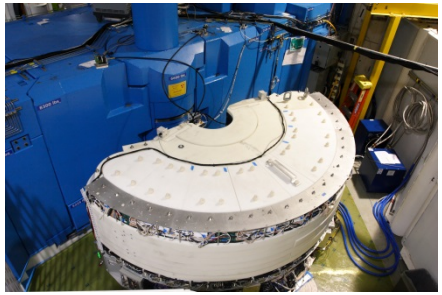
Is the expected **Q**-dependence of the scattering weak?

This often means that you want to look at a large region of **Q**-$\hbar\omega$ space, or that you can sum the data over a large region of **Q**-$\hbar\omega$ space.

YES? Consider instruments with large analyzer areas.

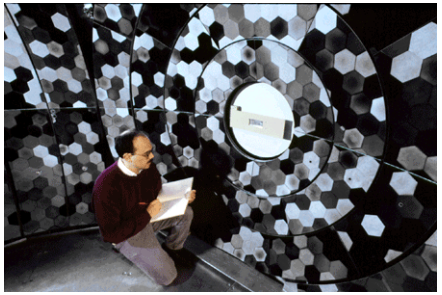
NO? Consider using BT7, SPINS, or NSE.

MACS



DCS

HFBS



BT7

General Sample “Design”

Know as much about your sample as possible!!
(Beamtime costs ~ $5000/day!!)

Other considerations:
What’s the structure (in a general sense)?
Are there any phase transitions (or a glass transition)?
What isotopes are present?
Supplementary data from other measurements …

Magnetization vs T

Muon spin relaxation

X-ray data

Specific heat vs T

Raman spectroscopy

General Sample “Design”

Try to avoid isotopes that are strongly absorbing.

^{6}Li ^{10}B ^{113}Cd ^{157}Gd

For a complete listing go to

http://www.ncnr.nist.gov/resources/n-lengths

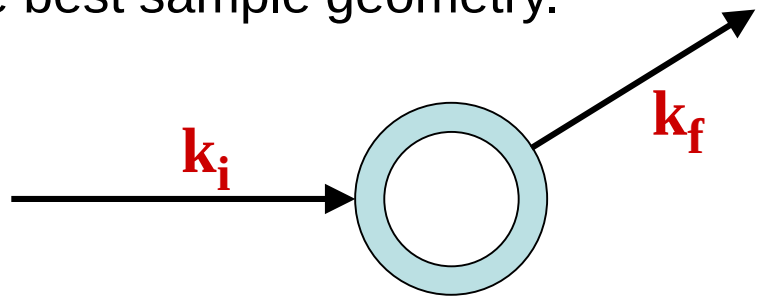
Sample “Design”

Single crystals yield the most information.

Increase the intensity by increasing the amount of sample.

If you have a powder, use a cylindrical container (rather than flat plate).

Annular may be the best sample geometry.



Almost all experiments of collective excitations involve coherent scattering
→ If sample contains H it should be deuterated (D).

Acknowledgements

Organizers – Yamali Hernandez & Alex Grutter

Administrative staff
Experiment teams
Invited speakers

Enjoy the Science!