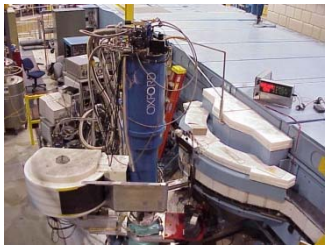
Choosing the Right Spectrometer

NCNR

Peter Gehring
NIST Center for Neutron Research

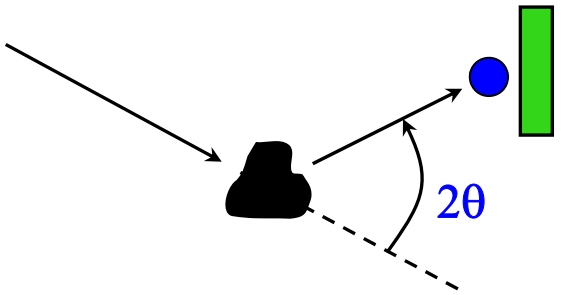


Main Messages of the Week

(1) Neutron scattering experiments measure the flux of neutrons scattered by a sample into a detector as a function of the change in neutron wave vector ($\vec{Q}$) and energy ($\hbar\omega$).

Momentum	Energy
$\hbar k_n = \hbar(2\pi/\lambda_n)$	$\hbar\omega_n = \hbar^2 k_n^2/2m$
$\hbar\vec{Q} = \hbar\vec{k}_i - \hbar\vec{k}_f$	$\hbar\omega = \hbar\omega_i - \hbar\omega_f$

$\Phi(Q,\hbar\omega) = \frac{\text{neutrons}}{\text{sec–cm}^2}$



(2) The expressions for the scattered neutron flux Φ involve the positions and motions of atomic nuclei or unpaired electron spins.

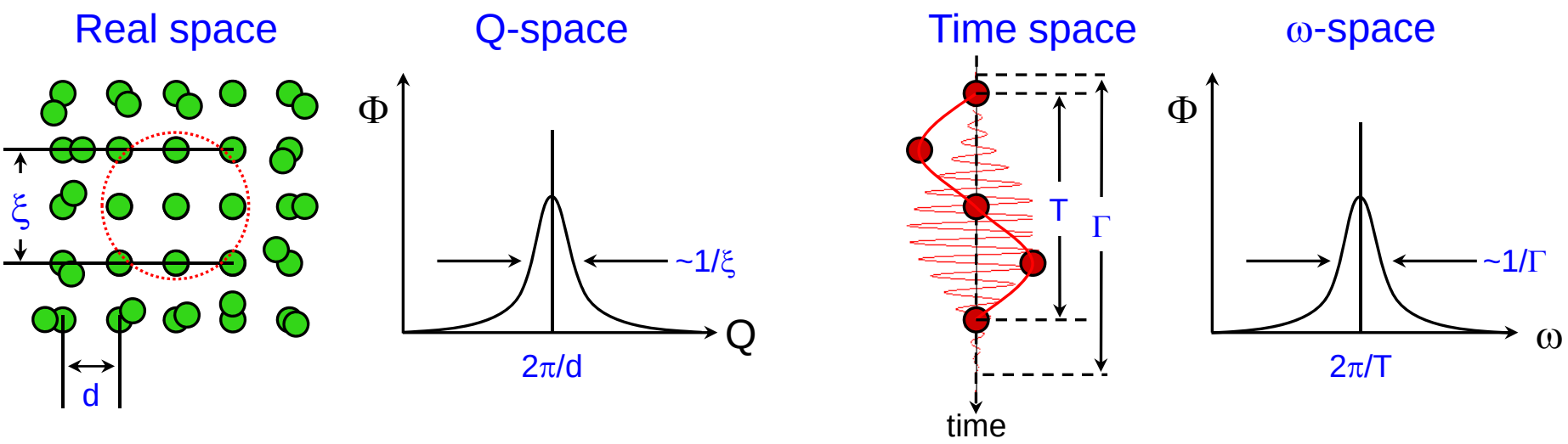
$$\Phi = \mathbb{F}\{\vec{r}_i(t), \vec{r}_j(t), \vec{S}_i(t), \vec{S}_j(t)\}$$

Φ provides information about all of these quantities!

Main Messages of the Week

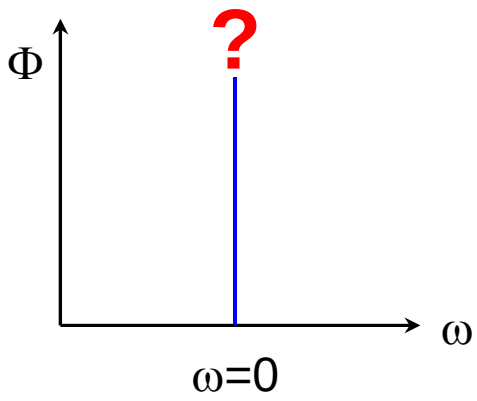
(3) The scattered neutron flux $\Phi(\vec{Q},\hbar\omega)$ is proportional to the space ($\vec{r}$) and time (t) Fourier transform of the <u>probability</u> $G(\vec{r},t)$ of finding one or two atoms separated by a particular distance at a particular time.

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



Pop Quiz!

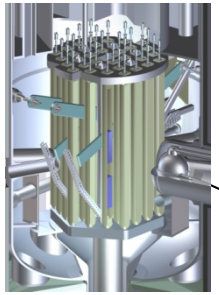
Question: Can one measure elastic scattering from a liquid?



Why? Why not?

Hint: What is the correlation in time of one atom in a liquid with another atom a distance r away?

What is required to do a neutron inelastic scattering experiment?



A source

$(E_i, \vec{k}_i)$

A method to specify the incident wave vector $\vec{k}_i$

Detector(s)

$(E_f, \vec{k}_f)$

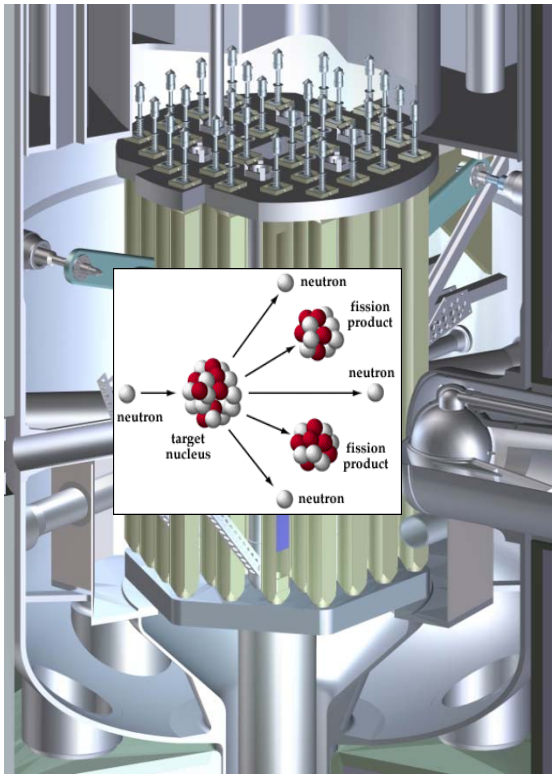
A well chosen sample + good idea

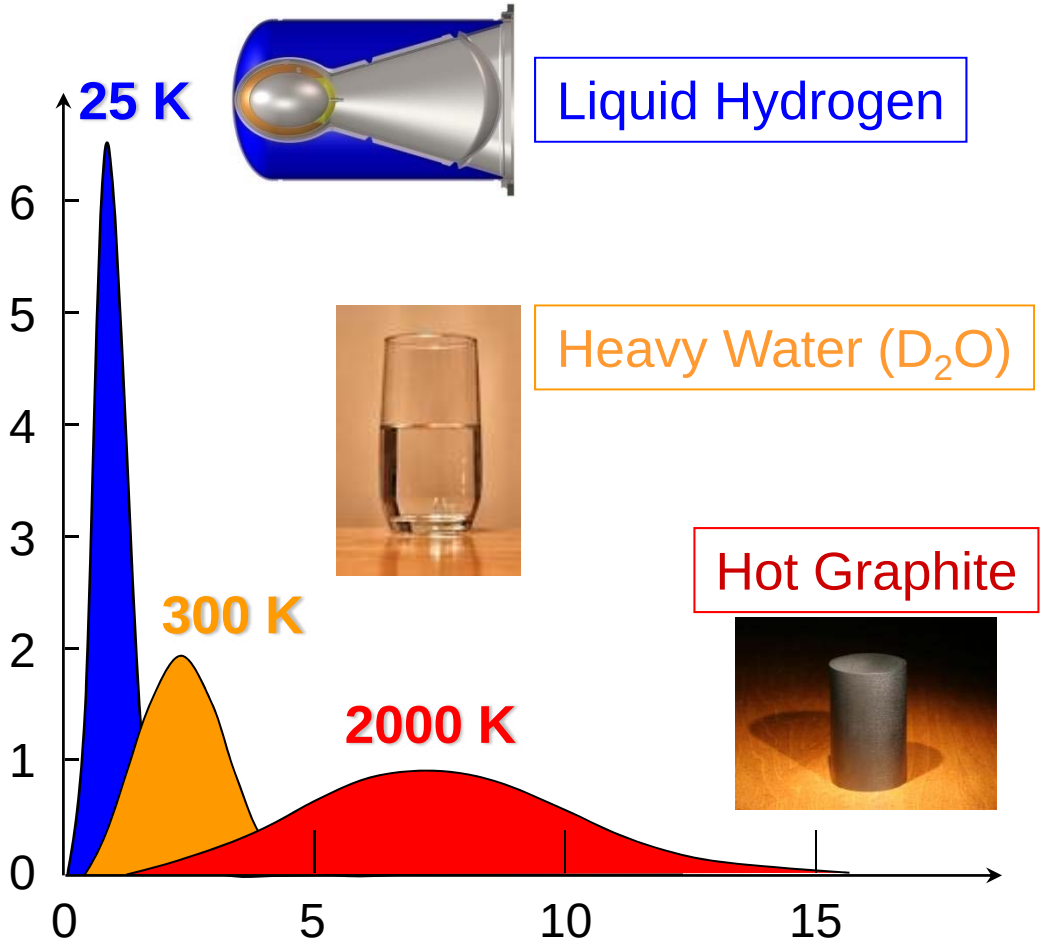
A method to specify the final wave vector $\vec{k}_f$

Neutron Source: Moderation

Maxwellian Distribution

$$\Phi \sim v^3 e^{(-mv^2/2k_BT)}$$



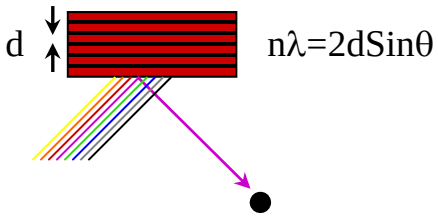


"Fast" neutrons: v = 20,000 km/sec

Methods of specifying and measuring $\vec{k}_i$ and $\vec{k}_f$

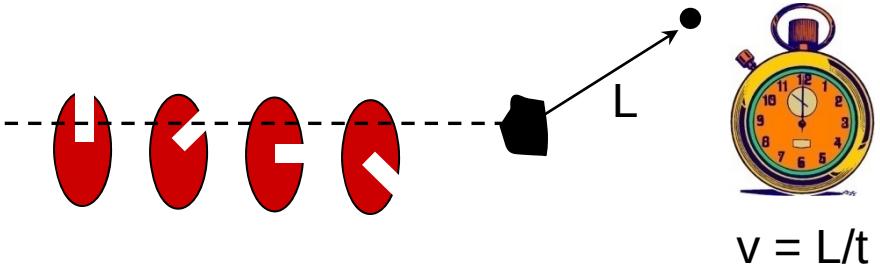
1. Bragg Diffraction

   SPINS, BT7, HFBS



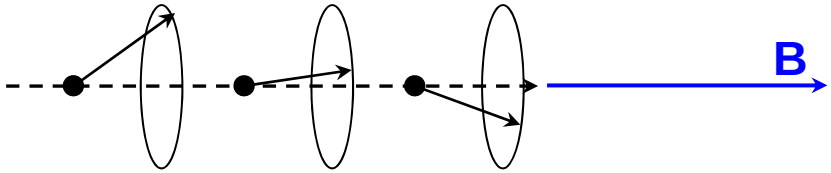
2. Time-of-Flight (TOF)

   SANS, DCS, HFBS (?)

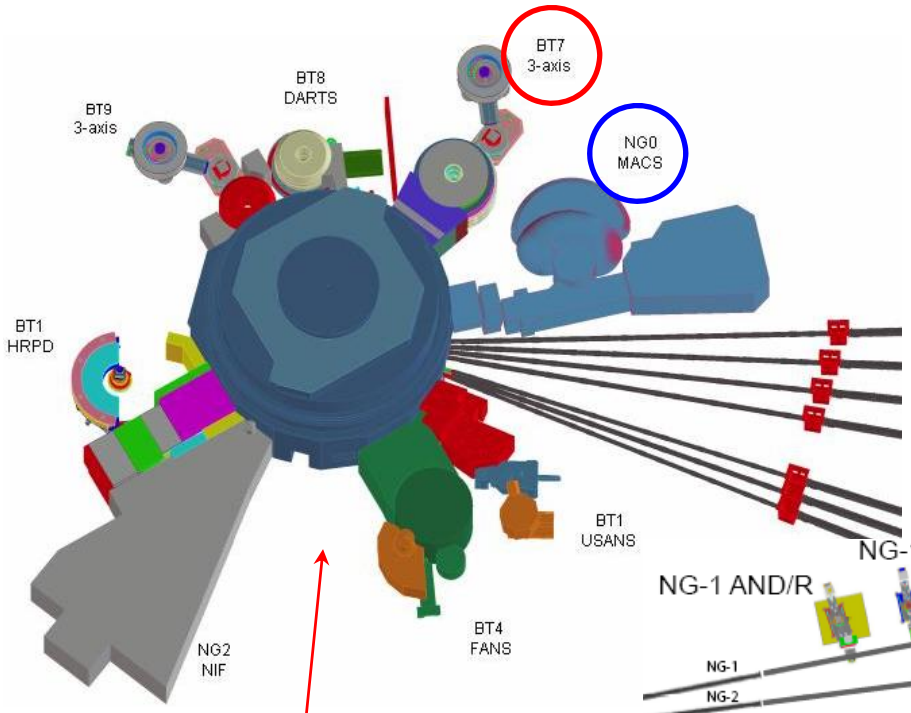


3. Larmor Precession

   NSE

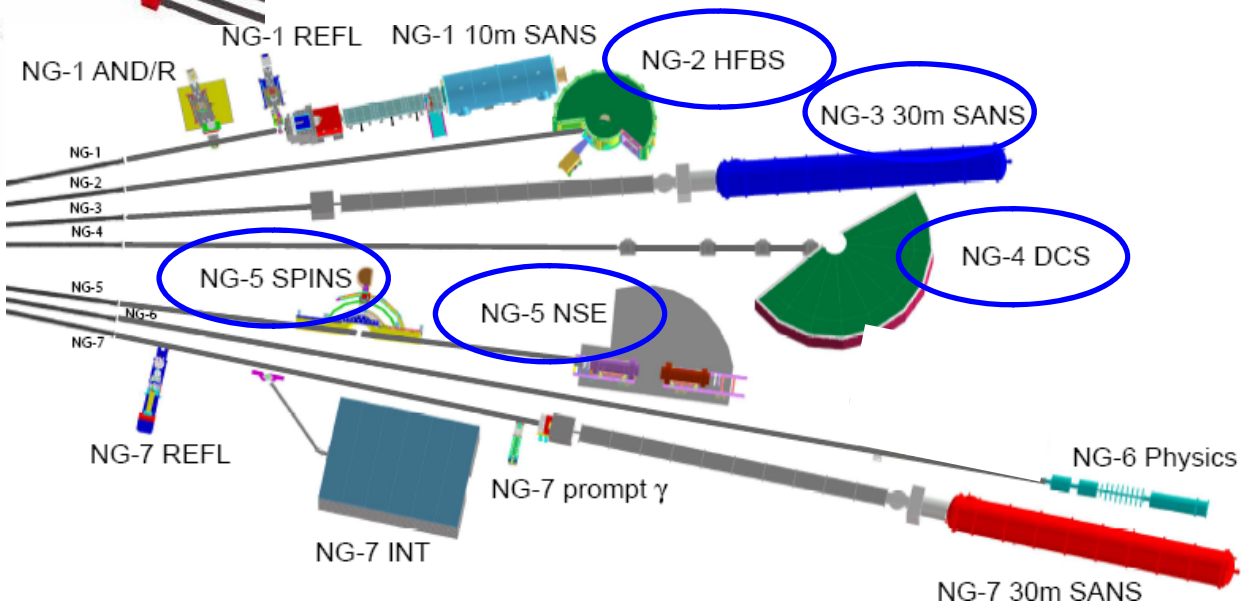


Why are there so many different spectrometers?



Thermal Neutrons

Cold Neutrons

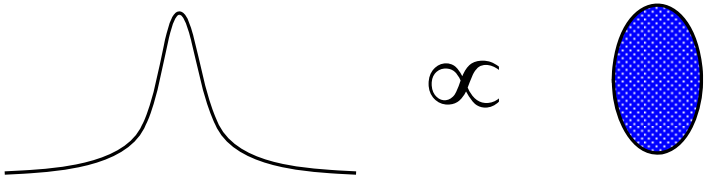


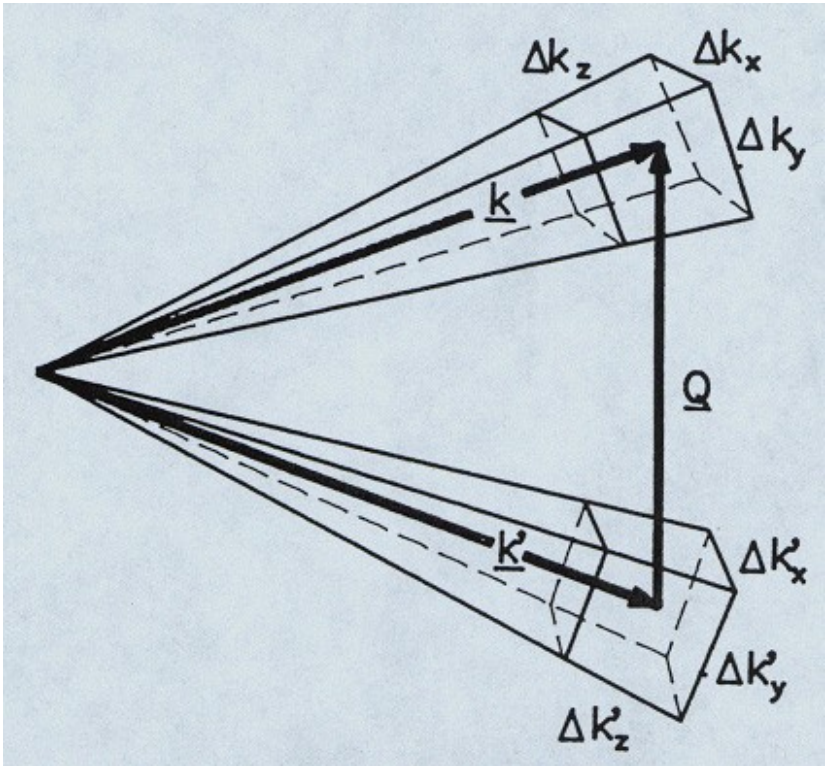
Why are there so many different spectrometers?

Because neutron scattering is an intensity-limited technique. Thus detector coverage and resolution MUST be tailored to the science.

Uncertainties in the neutron wavelength and direction imply **Q** and $\hbar\omega$ can only be defined with a finite precision.

The total signal in a scattering experiment is proportional to the resolution volume → better resolution leads to lower count rates! Choose *carefully* …

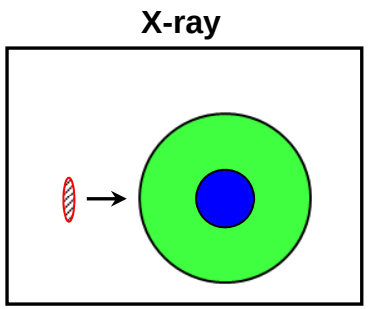


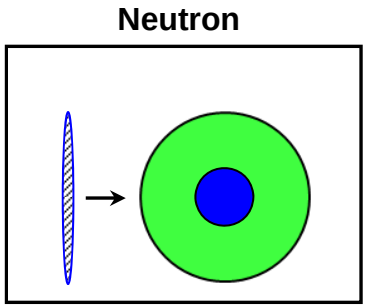


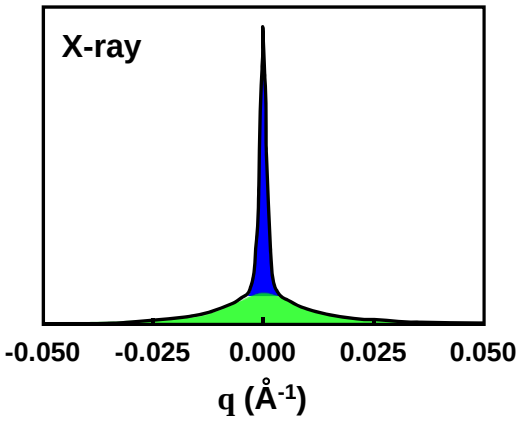
Courtesy of R. Pynn

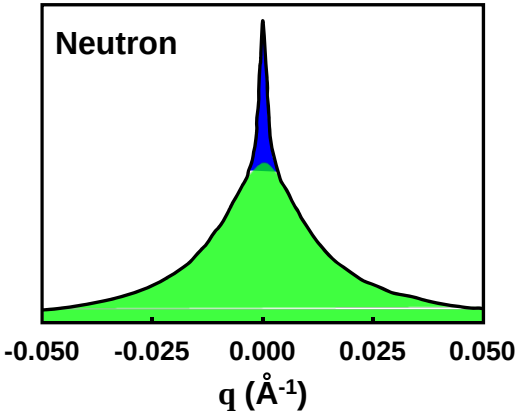
Q-Resolution Matters!

The “right” resolution depends on what you want to study.







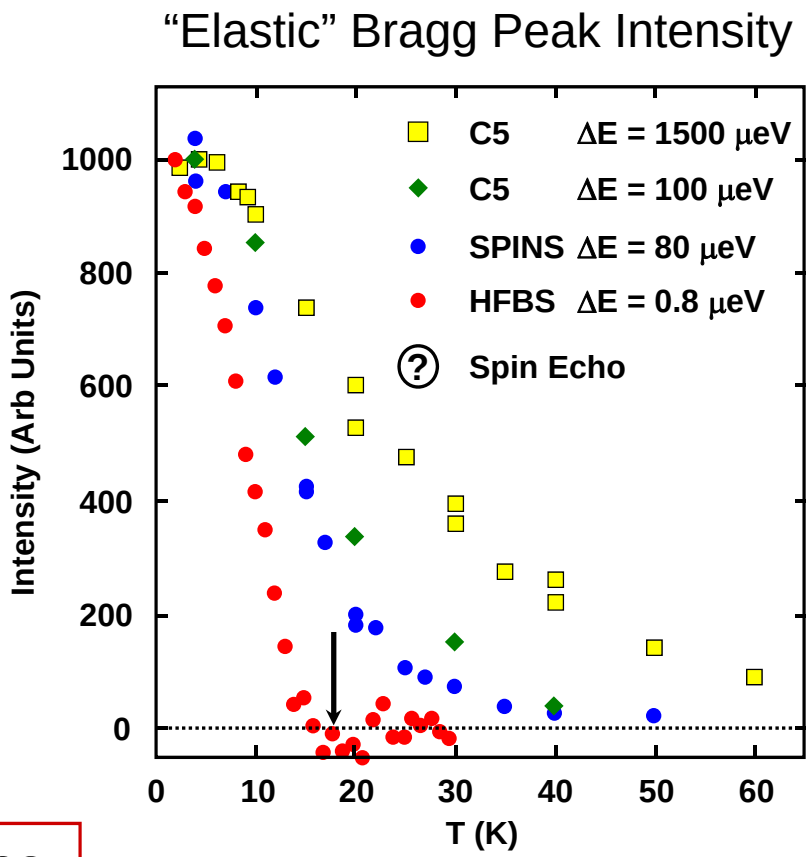


ħω-Resolution Matters!

Consider $YBa_2Cu_3O_{6.35}$ (T_c = 18K)

Magnetic order occurs at Q = (1/2,1/2,2).

What is T_N?

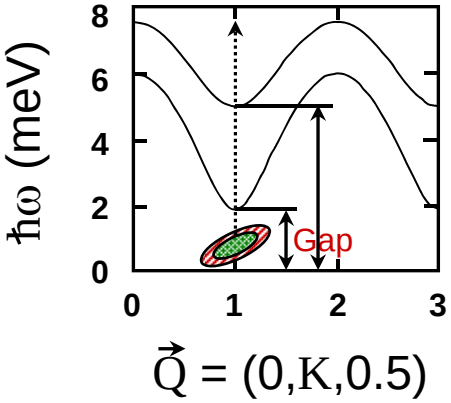


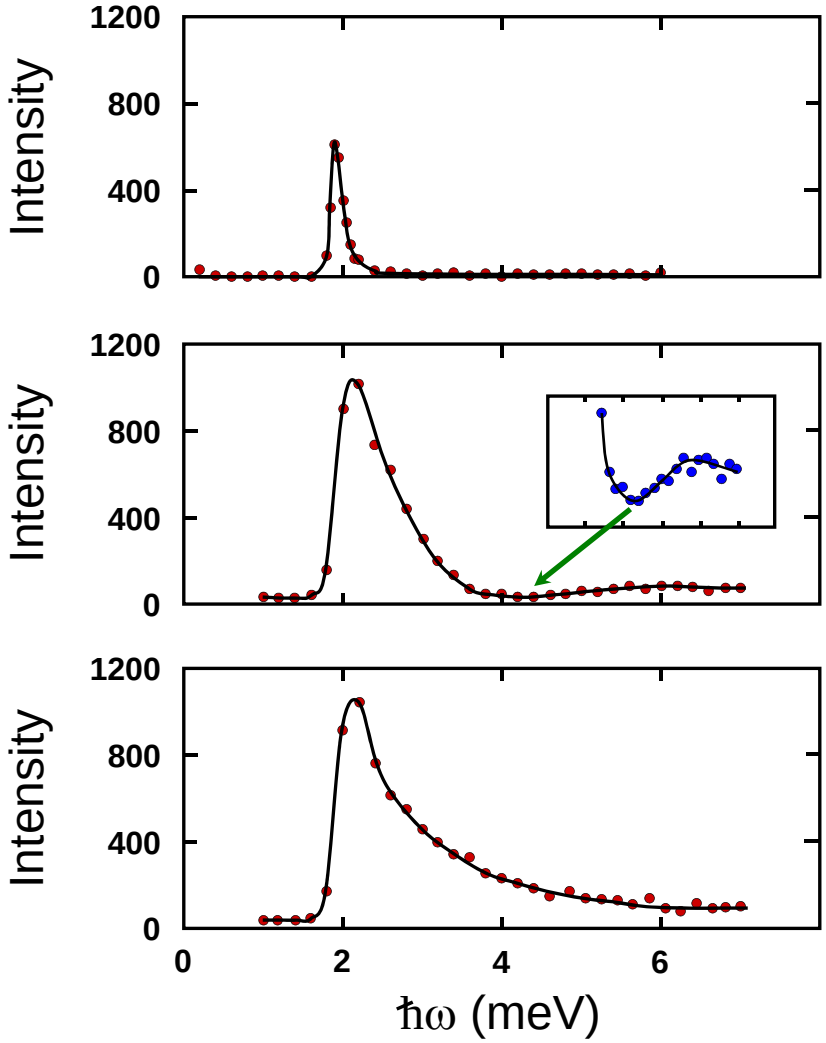
A "fatter" energy resolution integrates over low-energy fluctuations …

ħω-Resolution Matters!

Another example …

SPINS





Focusing Analyzer

Flat

Focusing Analyzer

5 Blades

Focusing Analyzer

9 Blades

OK, how do I choose the right spectrometer?

Two basic considerations:

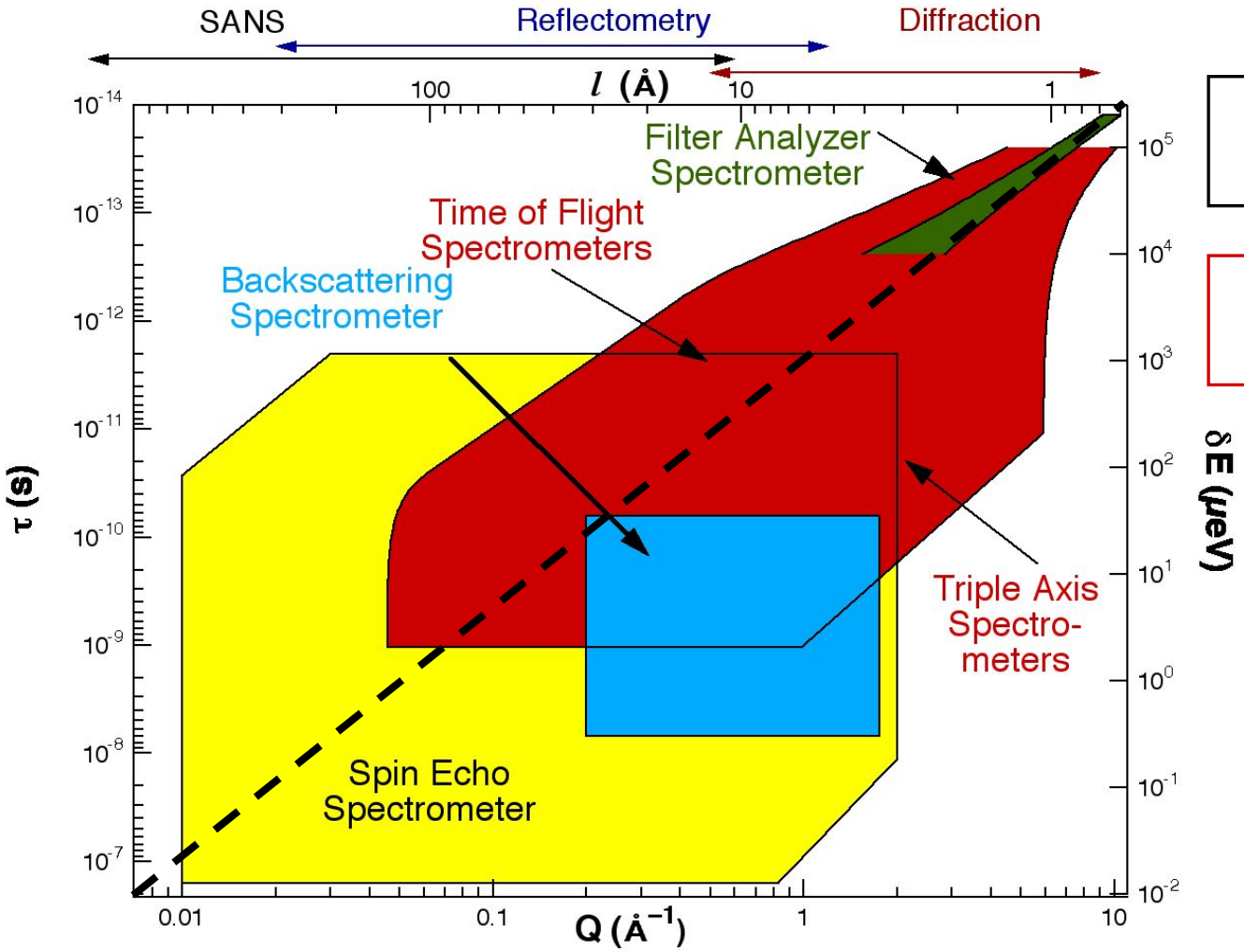
1. What are the time scales ($\hbar\omega$) of interest?
2. What are the length scales (Q) of interest?

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

Two additional considerations:

1. What energy resolution ($\Delta\hbar\omega$) is required?
2. What momentum resolution (ΔQ) is required?

Different spectrometers cover different regions of phase space



Do you see a pattern here?

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?

   $\hbar\omega >$ 10-20 meV - use FANS or a thermal triple-axis spectrometer.

   $\hbar\omega <$ 20-30 μeV - use HFBS or NSE

   In between - use DCS or a cold neutron TAS spectrometer.

2. Be certain 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.

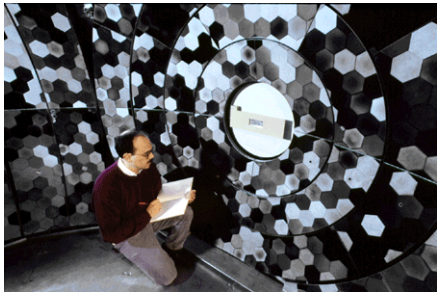
YES? Consider instruments with large analyzer areas.

NO? Consider using a triple-axis spectrometer like BT7 or SPINS.

FANS

DCS

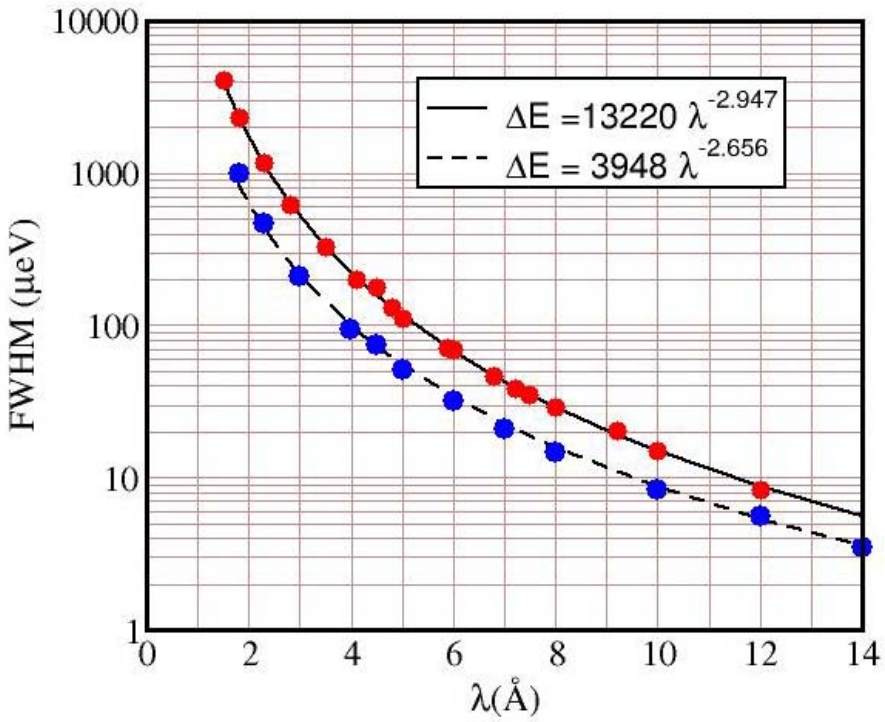
HFBS



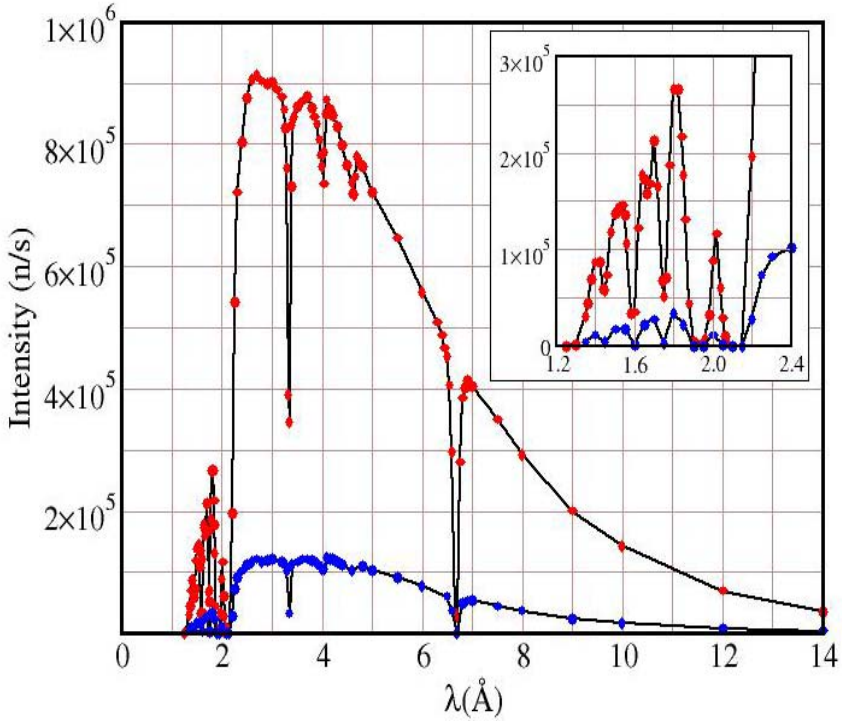
BT7

Things to consider when choosing DCS

ΔE



I(E)



Quantities varied

- wavelength λ
- chopper slot widths W

Remember – **Intensity** ↓

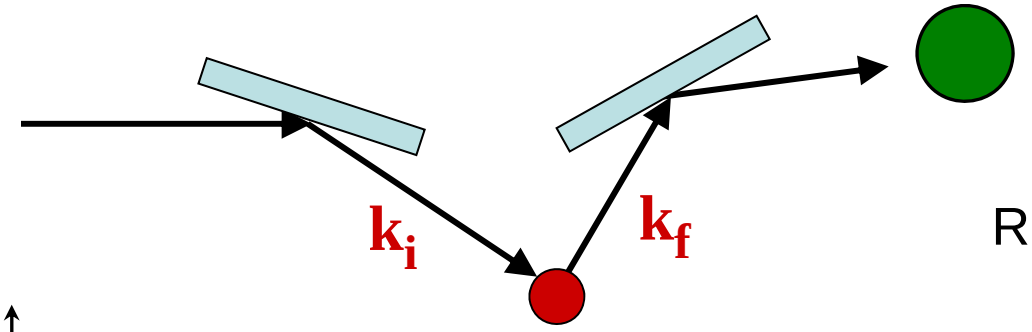
Resolution ↑

Things to consider when choosing SPINS

Triple axis spectrometers are typically used when either -

(1) the *direction* of **Q** is important or

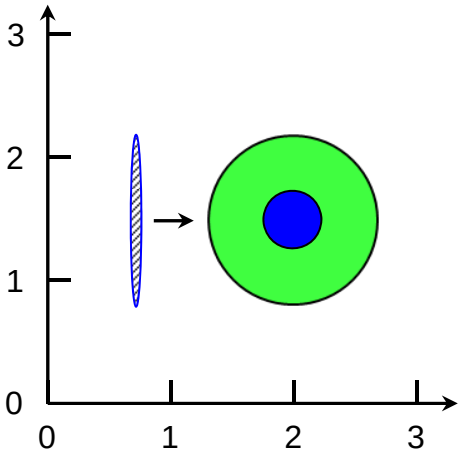
(2) the interesting region of **Q-ω** space is of *limited extent*.



One data point at a time …

Remember – **Intensity** ↓

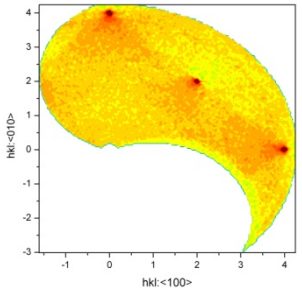
Resolution ↑



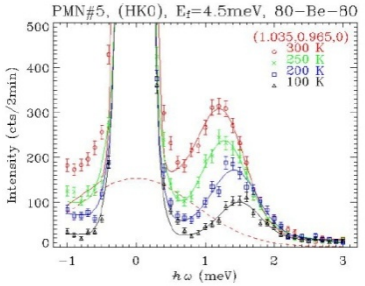
Collimation(')	λ	rel. signal	FWHM .
55-80-80-80	4 Å	1.00	0.28 meV
55-40-40-40	4 Å	0.24	0.17 meV
69-80-80-80	5 Å	0.26	0.13 meV
84-80-80-80	6.1 Å	0.03	0.05 meV

DCS versus SPINS

DCS – incoherent scattering,
broad surveys in **Q-ω**



SPINS – coherent scattering,
limited regions in **Q-ω**



Rules of Thumb: (think carefully before violating)

DCS – systems requiring resolution < 100 μeV

SPINS – single crystals

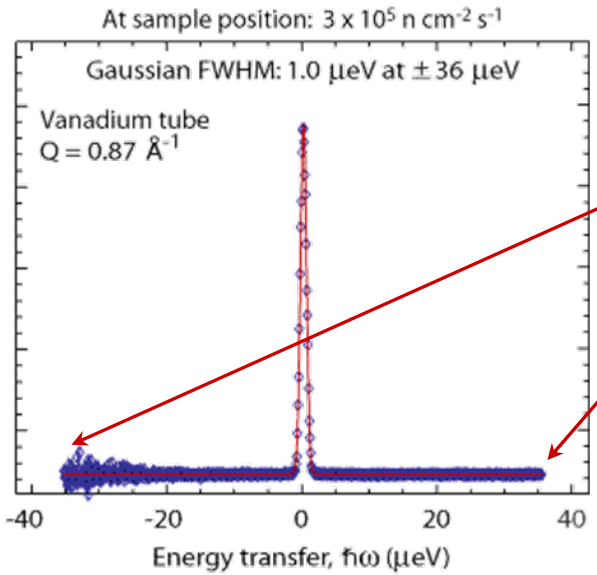
Things to consider when choosing HFBS

$0.25\ \text{Å}^{-1} < \mathbf{Q} < 1.75\ \text{Å}^{-1}$

Do the length scales of interest lie within this Q-range?

$\delta\mathbf{Q} < 0.1 - 0.2\ \text{Å}^{-1}$

Can you live with such coarse Q-resolution?



Do the features of interest lie within this $\hbar\omega$-range?

Do you really require such good energy resolution $\delta E \sim 1\ \mu eV$ (or perhaps even better resolution)?

Things to consider when choosing NSE

If the hω-resolution of backscattering is "not good enough," or if you are only interested in a "limited" region of **Q**-space (typically small **Q**) …

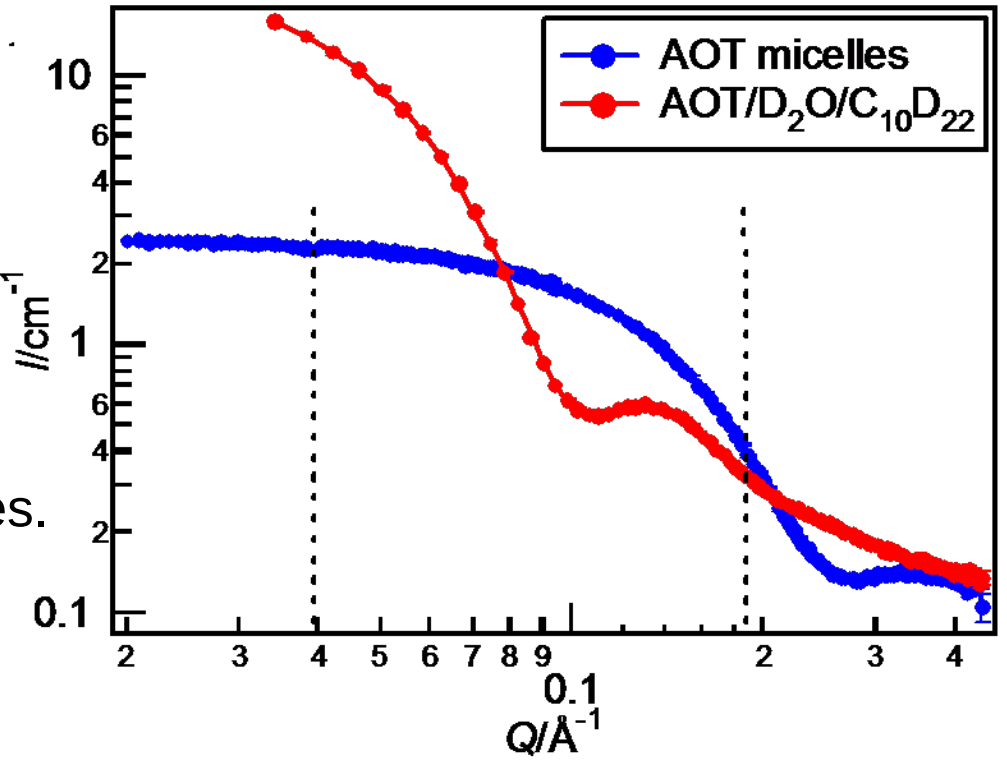
… then use NSE (low **Q**, long times)

These cases typically involve coherent scattering, which tends to peak near

$$Q \sim \frac{2\pi}{\text{relevant length scale}}$$

Remember – slower motions usually imply longer length scales.

Many atoms moving together
→ Coherent scattering



General sample “design”

The most important thing is:

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

The types of things that you might want to know include:

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

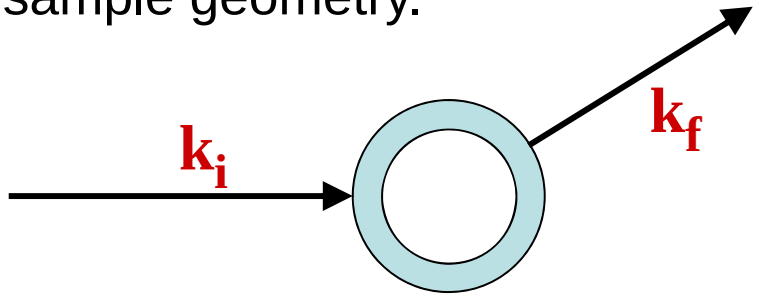
Sample “design” for triple-axis spectrometers

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 on triple-axis spectrometers involve coherent scattering
→ sample should be deuterated (if it contains H at all).

Sample “design” for DCS and HFBS

Increase the intensity by increasing the amount of sample

→ Fill the beam with sample

The maximum beam size is usually given in the instrument description:

DCS: 3 cm x 10 cm (or 1.5 cm x 10 cm)

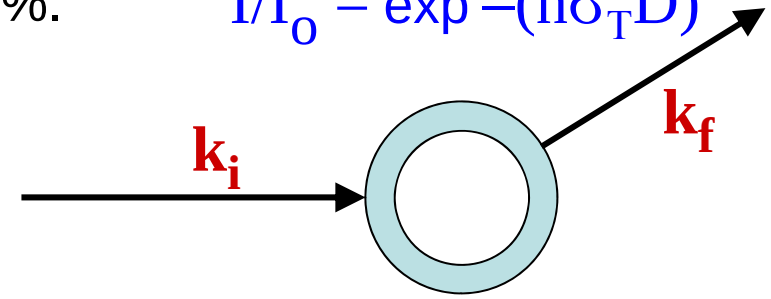
Backscattering: 3 cm x 3 cm

If possible, use cylindrical samples (rather than flat plate)

Remember - for incoherent, quasielastic scattering the transmission of the beam should be ~90%.

$$I/I_o = \exp -(n\sigma_T D)$$

Often annular is the best sample geometry

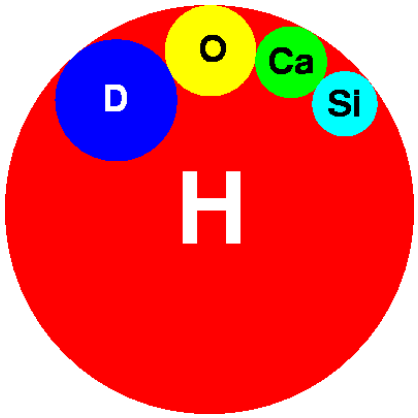


Sample “design” for DCS and HFBS

Does the sample contain H?

Remember: Neutrons LOVE H!!

Create a sample where -
the “interesting” portions are hydrogenated and
the “uninteresting” portions are deuterated.

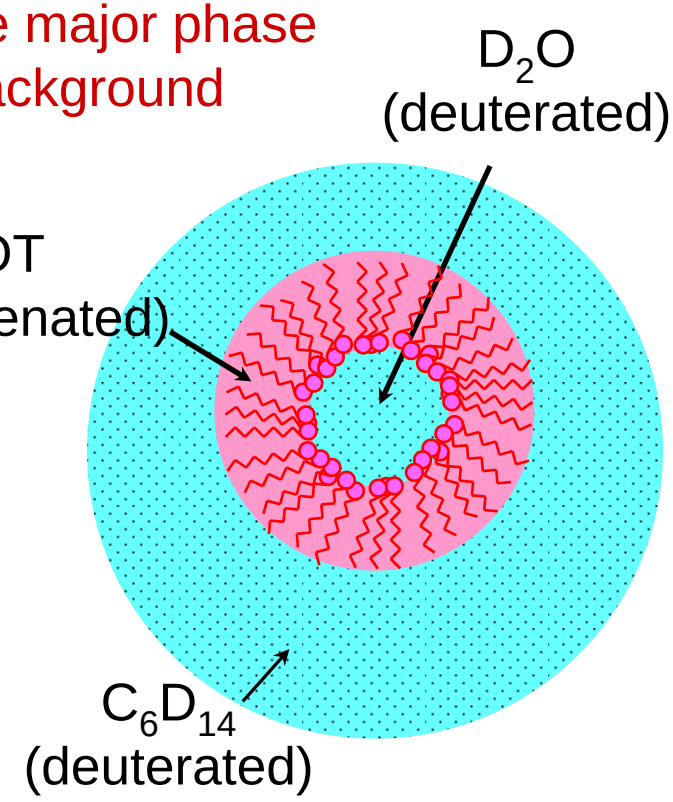


Sample “design” for NSE

Create a sample where the “interesting” portions of the sample have a different SLD than the “uninteresting” portions

Typically this means deuterating the major phase in order to reduce the incoherent background

SLD core	6.4×10^{-6} Å^{-2}
SLD shell	1.0×10^{-6} Å^{-2}
SLD solvent	6.5×10^{-6} Å^{-2}



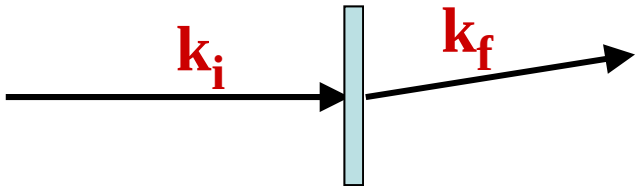
http://www.ncnr.nist.gov/resources/sldcalc.html

Sample “design” for NSE

Increase the intensity by increasing the amount of sample

→ Fill the beam with sample

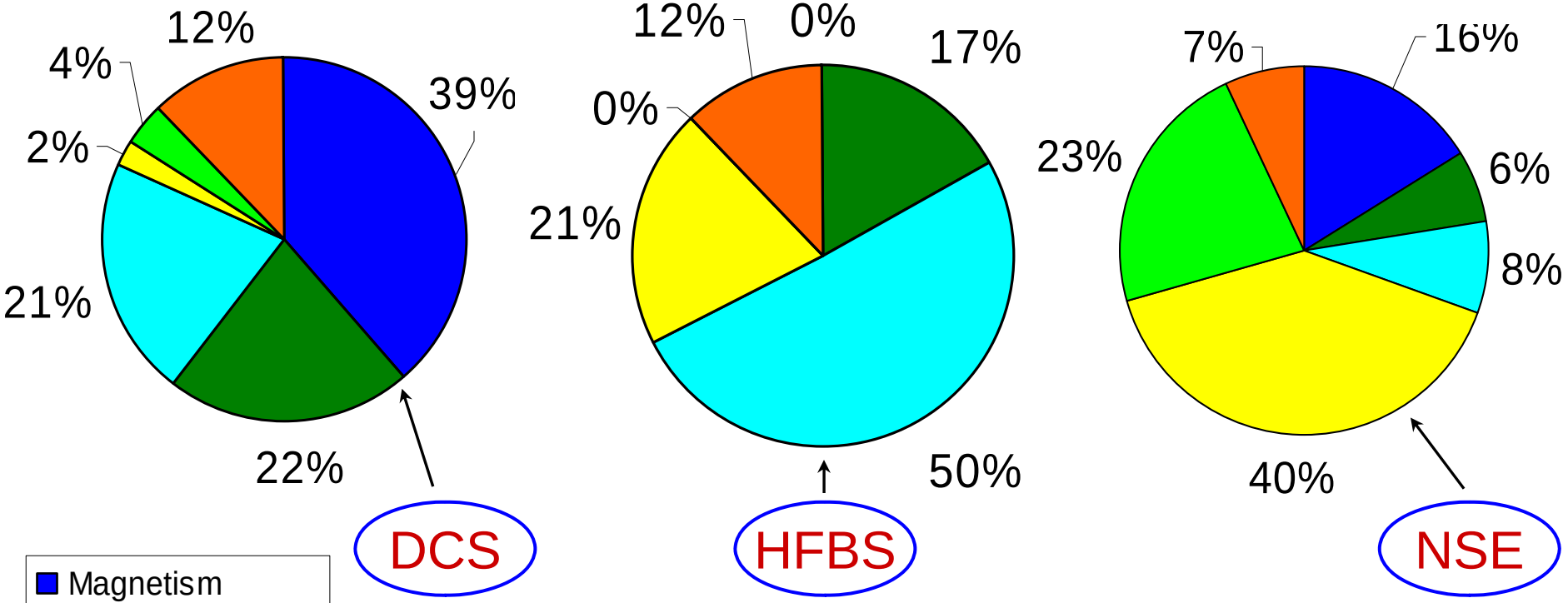
Typically use flat plate samples (at small angles)



$$I/I_o = \exp -(n\sigma_T D)$$

Rule of thumb - the transmission should be ~70%

Types of Science



Applying for beam time

The use of the neutron scattering instrumentation that you've used over the past week is open to all qualified users based on peer-reviewed proposals. Calls for proposals are issued about twice/yr.

The **next deadline** for **new proposals** will be **~ September 2011**.

Further information on submitting proposals can be found at:

http://www.ncnr.nist.gov/programs/CHRNS/CHRNS_prop.html

Some Summer School Success Stories

2001

Jae-Ho Chung
University Prof.

2003

Vicky Garcia-Sakai
ISIS Staff Scientist

1999

William Ratcliff
NCNR Staff Physicist

1997

Rob Dimeo
NCNR Director

Ok, so you can't win them all …

Acknowledgements

Organizers – Yamali Hernandez and Brian Kirby
Administrative staff - Julie Keyser
All of the experiment teams
Invited speakers – Vijay Tirumala and Ramanan Krishnamoorti

Thanks for coming!