Choosing the Right Spectrometer

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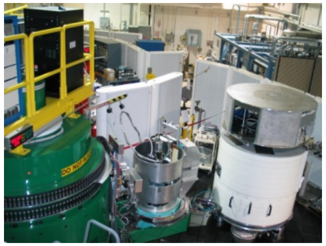
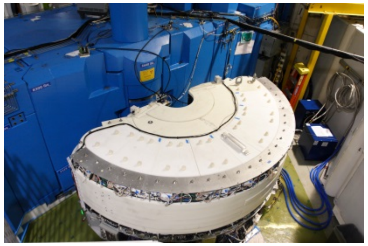
NIST Center for Neutron Research





Review: Main Messages of the Week

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

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

<u>Momentum</u>

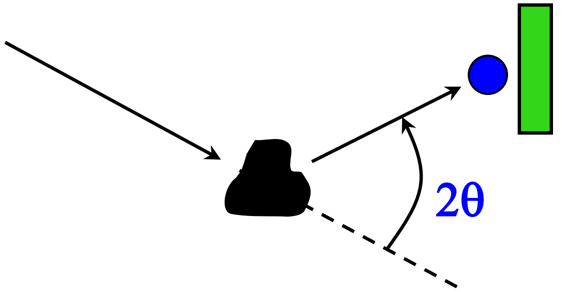
$\hbar k_n = \hbar(2\pi/\lambda_n)$

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

<u>Energy</u>

$\hbar\omega_n = \hbar^2 k_n^{\,2}/2m$

$\hbar\omega = \hbar\omega_i - \hbar\omega_f$



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

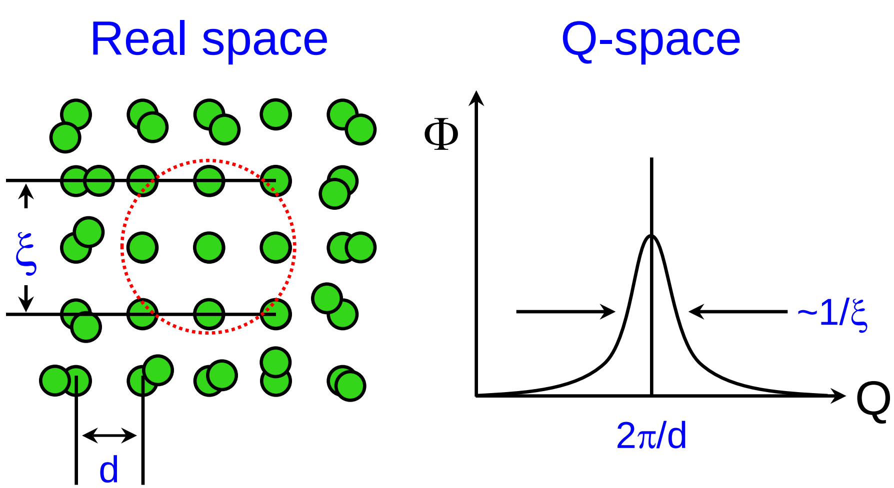
$$\Phi = \mathbb{F}\{\vec{r}_i(t), \vec{r}_j(t), \vec{S}_i(t), \vec{S}_j(t)\}$$

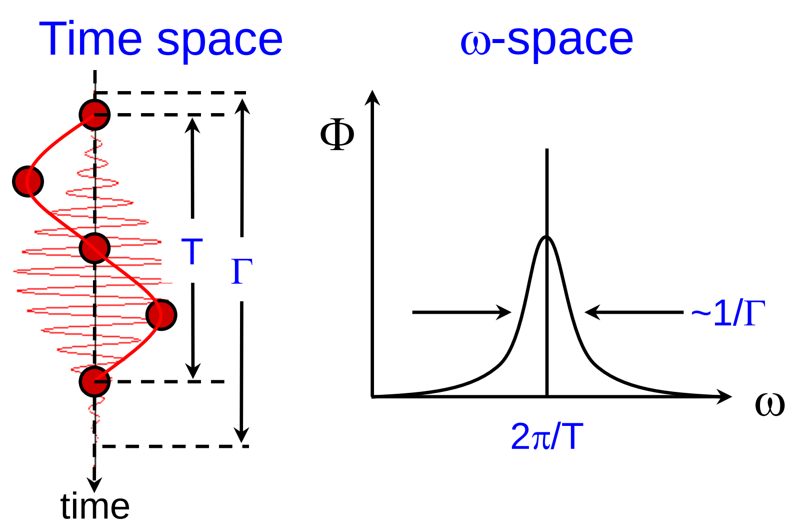
Φ provides information about <u>all</u> of these quantities!

Review: Main Messages of the Week

(3) The scattered neutron flux $\Phi(\vec{Q},\hbar\omega)$ is proportional to the <u>space</u> ($\vec{r}$) and <u>time</u> (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.

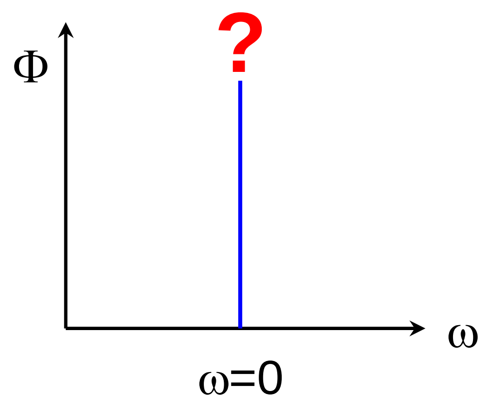
$$\Phi \propto \frac{\partial^2 \sigma}{\partial\Omega\,\partial\omega} \propto \iint e^{i(\vec{Q}\cdot\vec{r}-\omega t)}\, G(\vec{r},t)\, d^3\vec{r}\, dt$$





Pop Quiz!

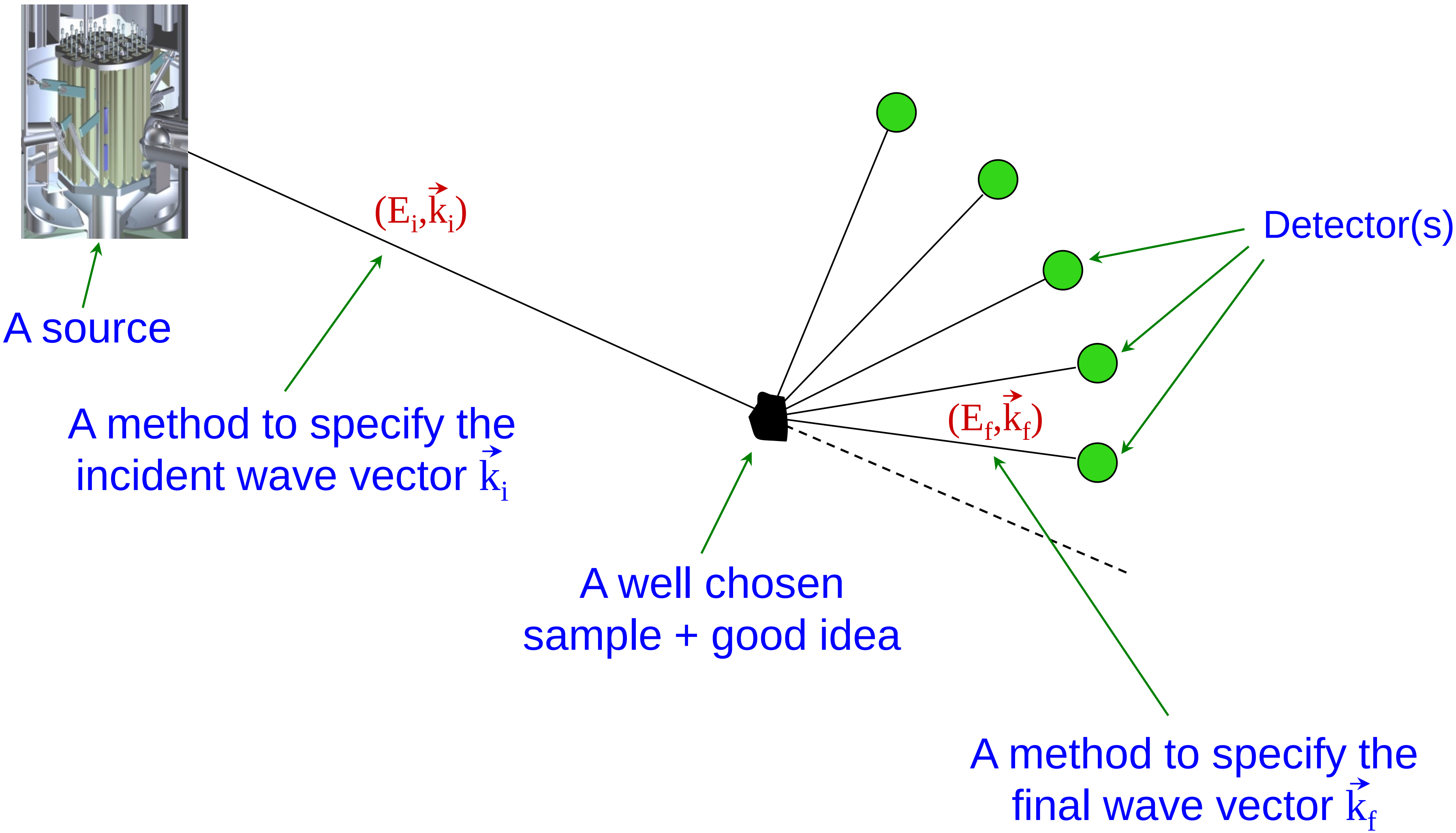
Question: Can one measure elastic scattering from a liquid?



Why? Why not?

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

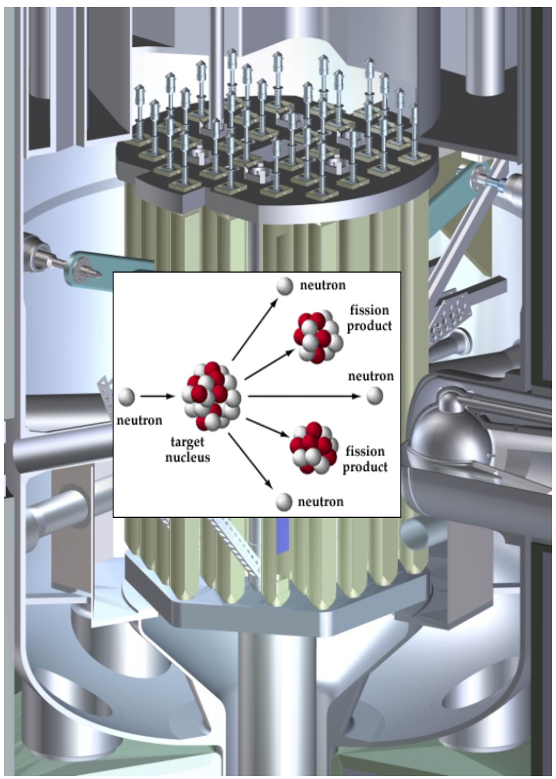
Basics Elements of a Neutron Inelastic Scattering Experiment

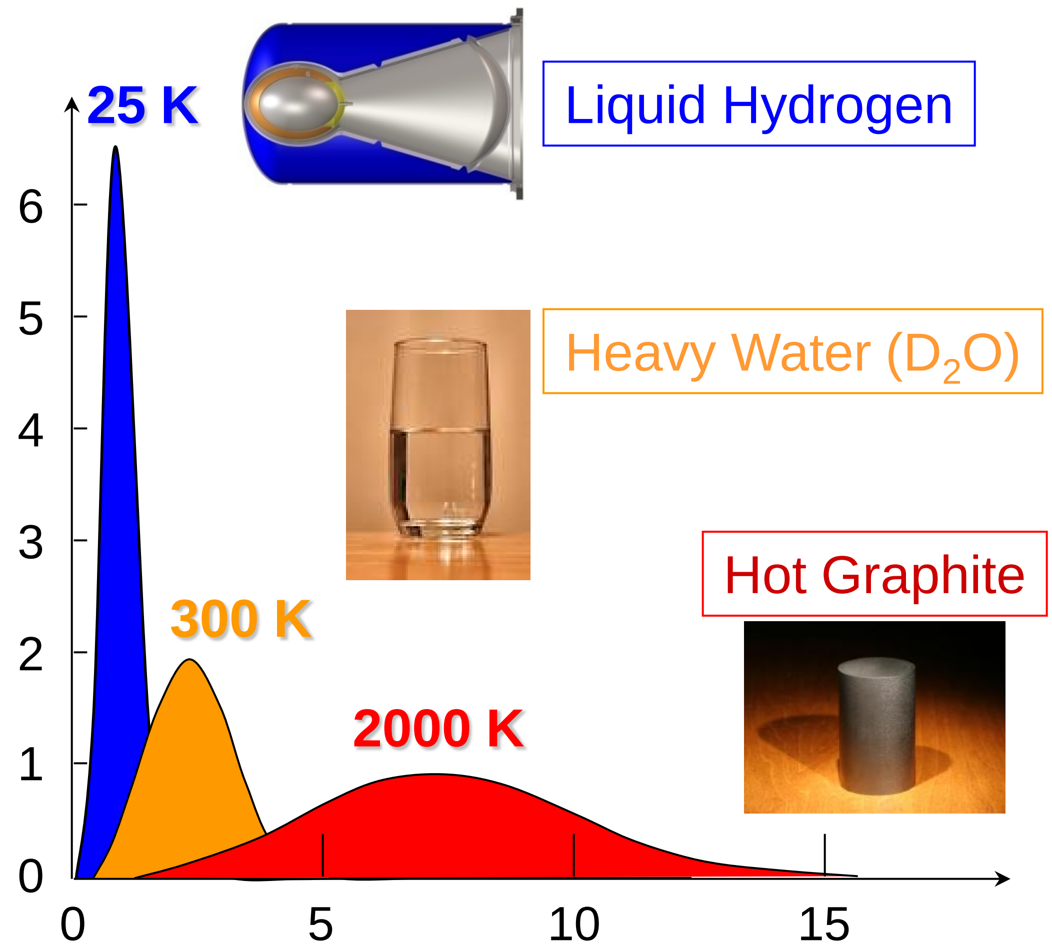


Neutron Source: Moderation

Maxwellian Distribution

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





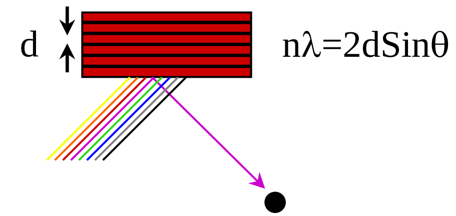
“Fast” neutrons: v = 20,000 km/sec

Neutron velocity *v* (km/sec)

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

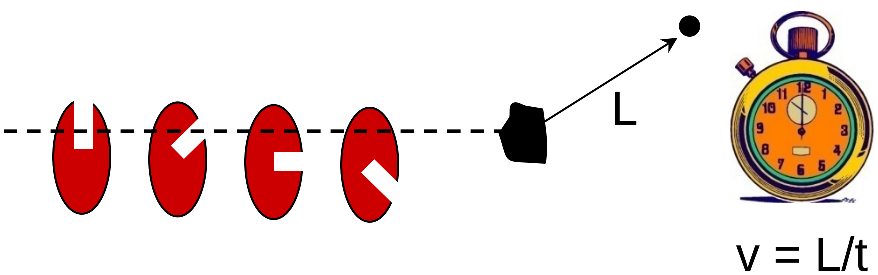
1. Bragg Diffraction

   BT7, SPINS, HFBS



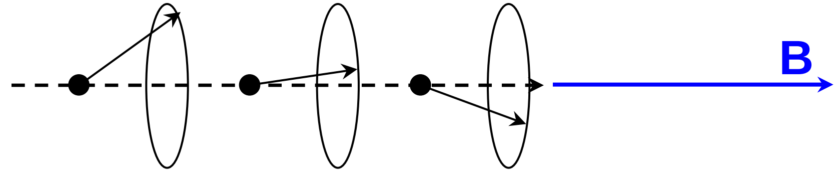
2. Time-of-Flight (TOF)

   DCS, HFBS

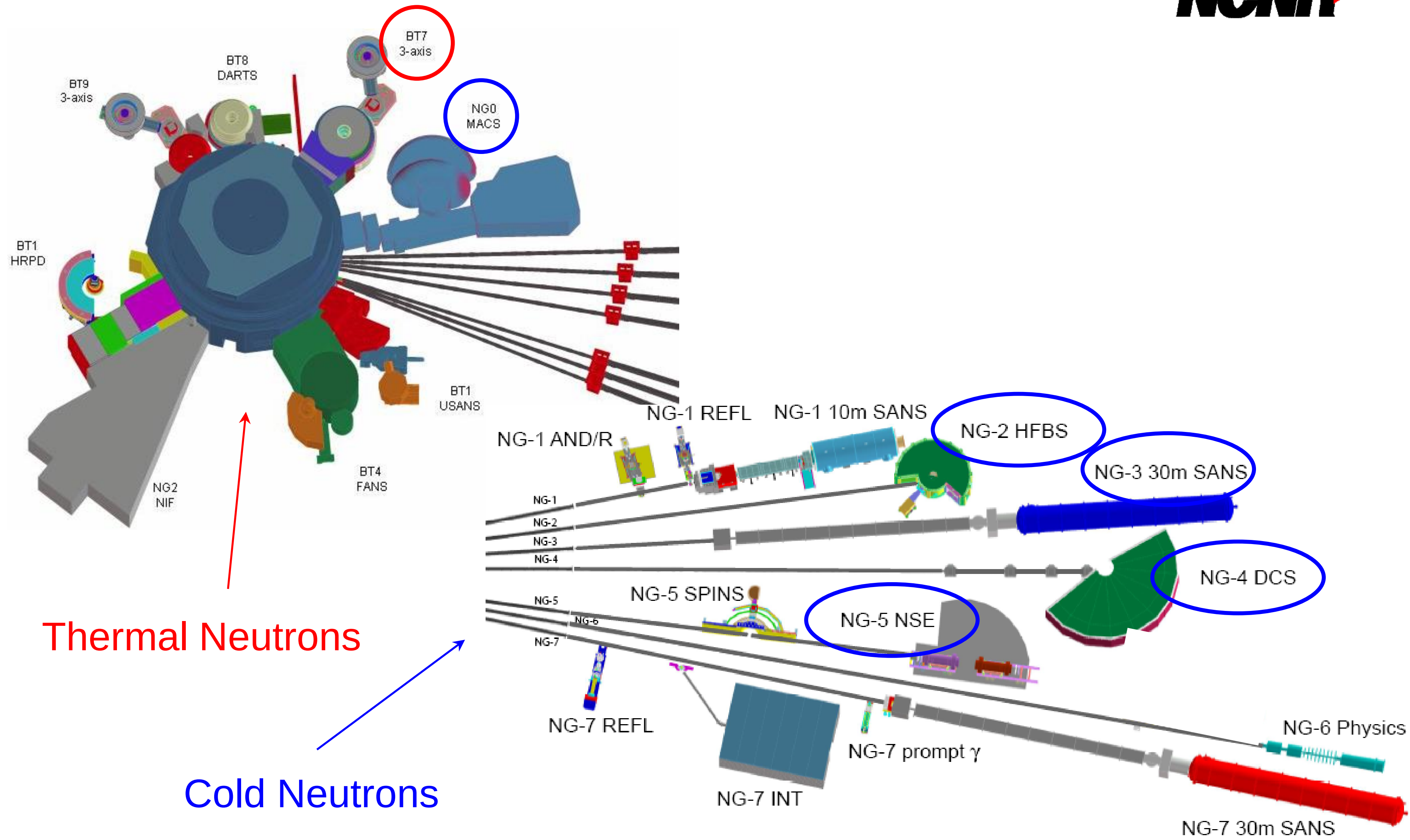


3. Larmor Precession

   NSE



Why So Many Different Spectrometers?

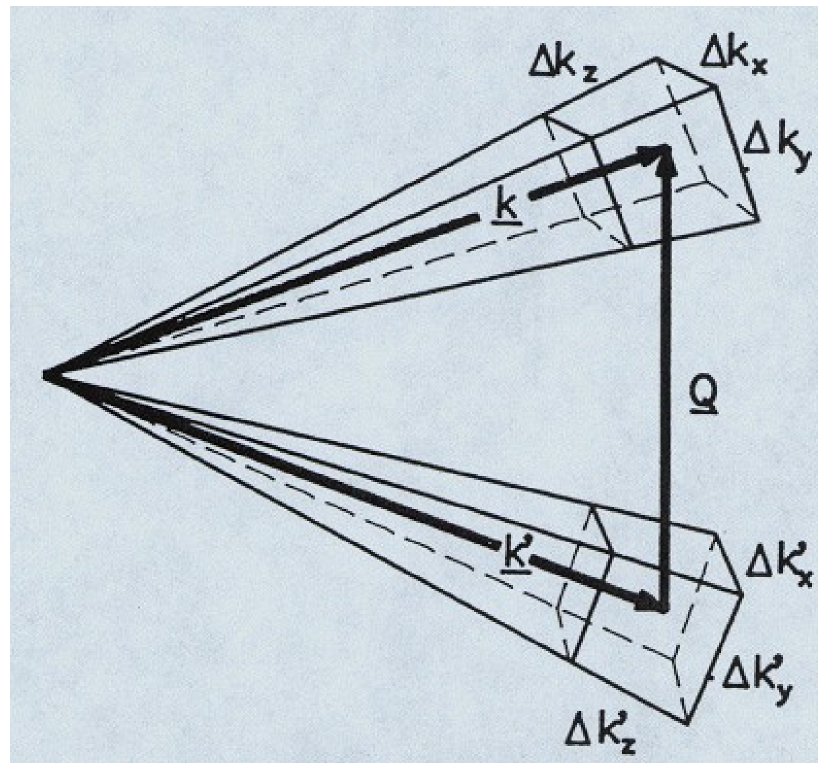


Why So Many Different Spectrometers?

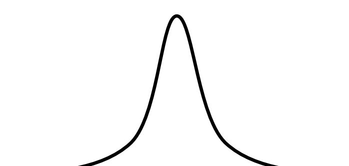
Because neutron scattering is an intensity-limited technique. Thus detector coverage and resolution MUST be tailored to the science.

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

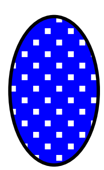
The total signal in a scattering experiment is proportional to the resolution volume → better resolution leads to lower count rates! *Choose carefully* …



Courtesy of R. Pynn

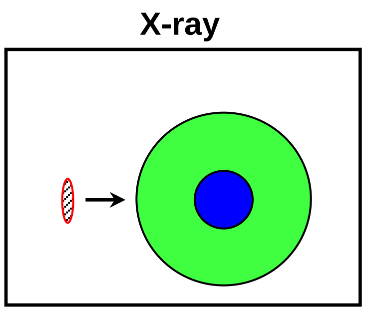


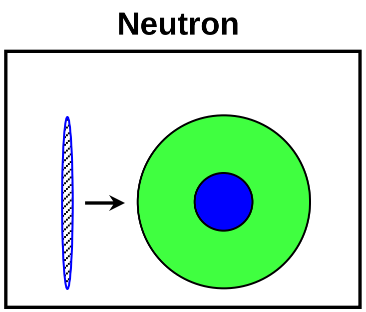
$\propto$

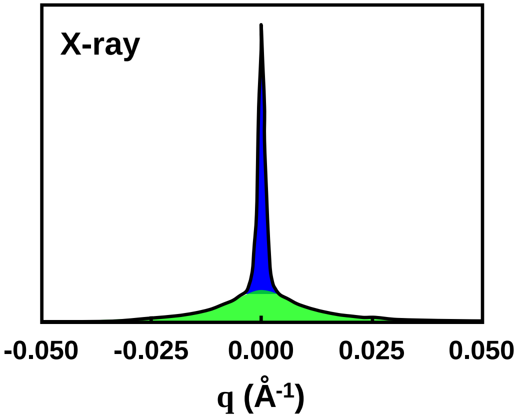


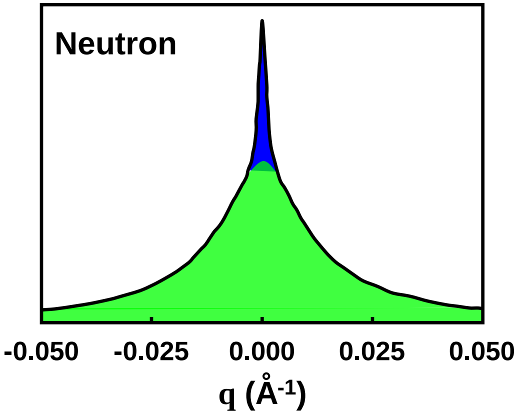
Q-Resolution Matters!

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





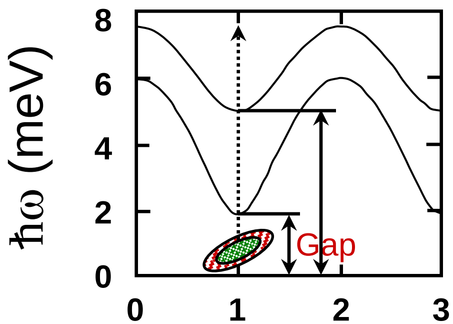




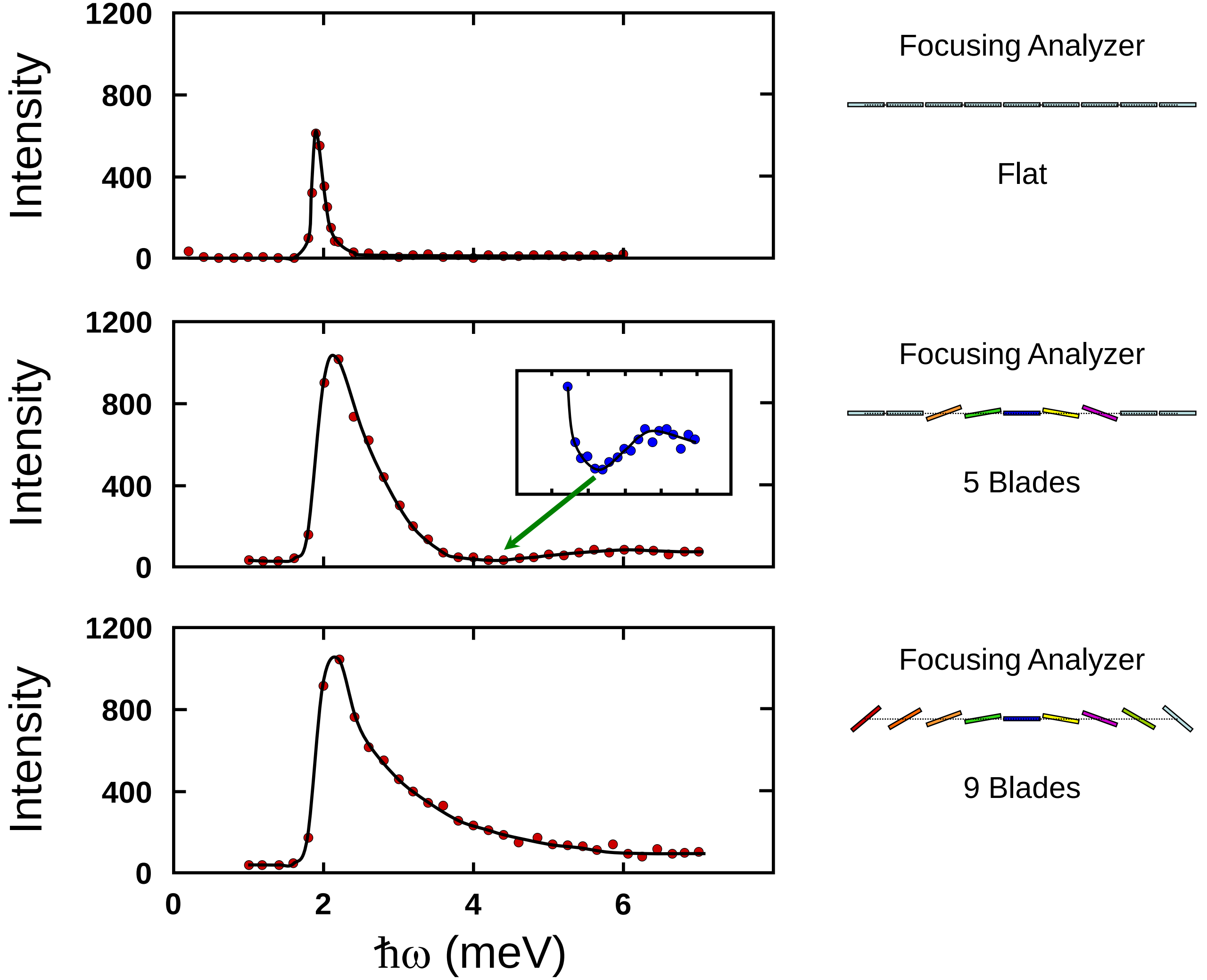
ħω-Resolution Matters!

Another example …

SPINS



$\vec{Q} = (0,K,0.5)$



How do I Choose the Right Spectrometer?

Two basic considerations:

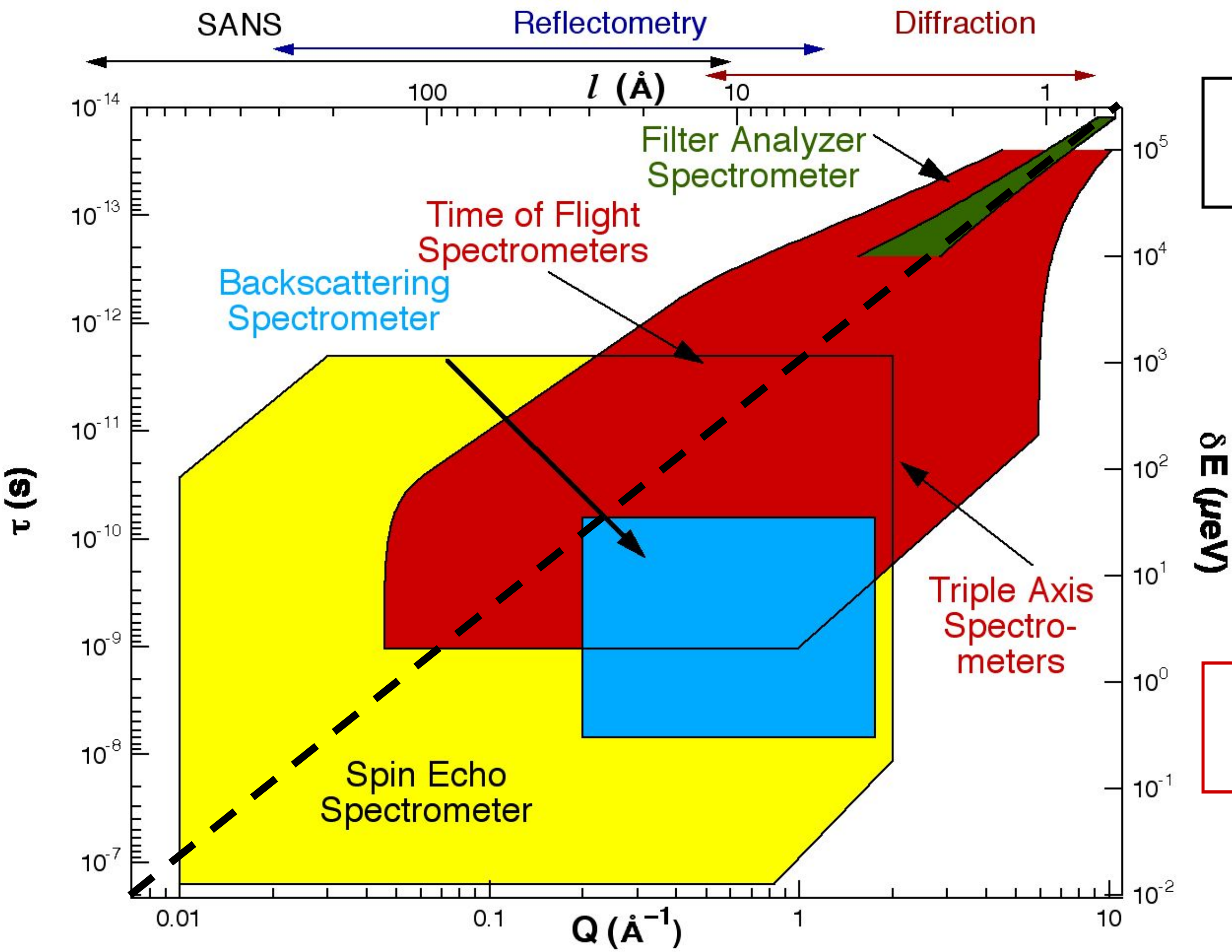
1. What are the time scales ($\hbar\omega$) of interest?
2. What are the length scales (Q) of interest?

(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 a thermal triple-axis spectrometer like BT7.

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

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

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 <u>inversely</u> 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?

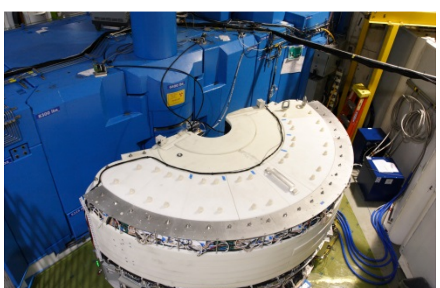
Is the expected **Q**-dependence of the scattering weak?

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.

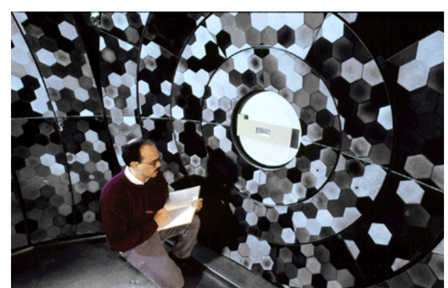
NO? Consider using a triple-axis spectrometer like BT7 or SPINS.

MACS



DCS

HFBS



BT7

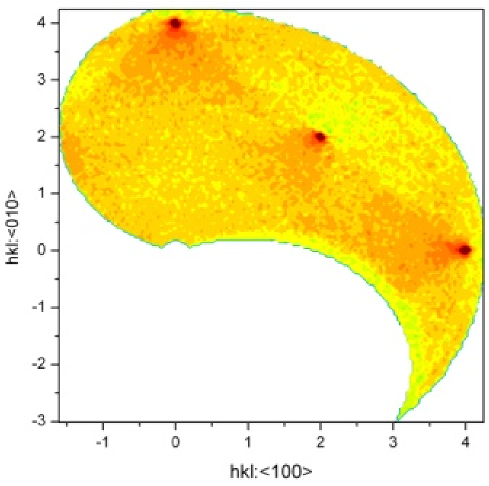
For Example: DCS versus BT7

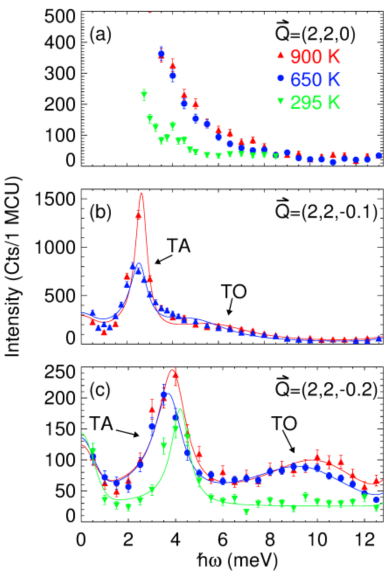
DCS

Incoherent scattering
Broad surveys in **Q-ω**

BT7

Coherent scattering
Limited regions in **Q-ω**





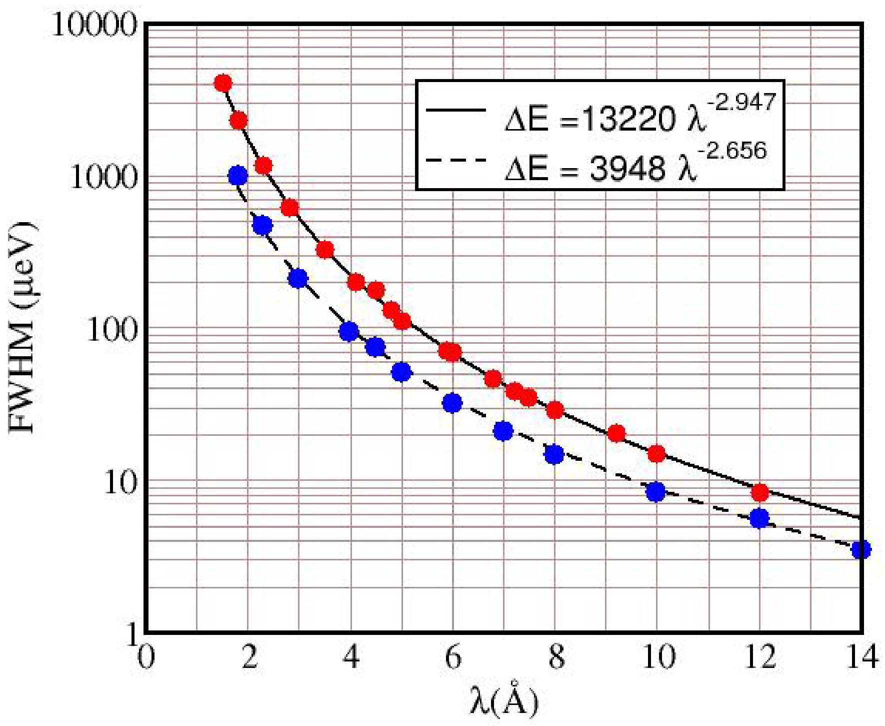
Rules of Thumb: (think carefully before violating)

DCS – systems requiring resolution < 100 μeV

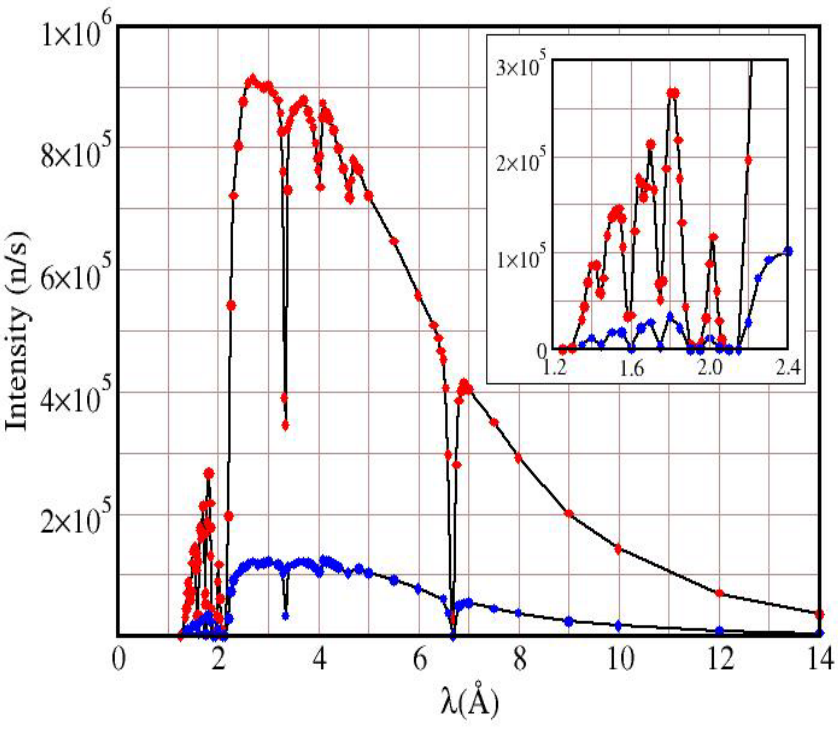
BT7 – single crystals

Things to Consider When Choosing DCS

ΔE



I(E)



Quantities varied

- wavelength λ
- chopper slot widths W

Remember – **Intensity** ↓

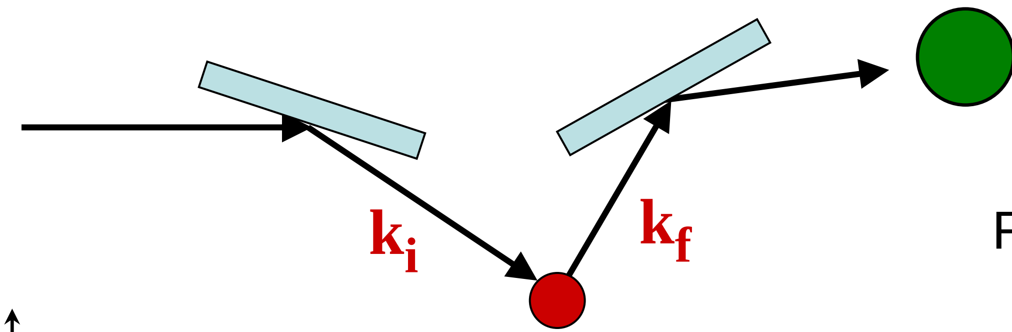
Resolution ↑

Things to Consider When Choosing BT7

Triple axis spectrometers are typically used when either -

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

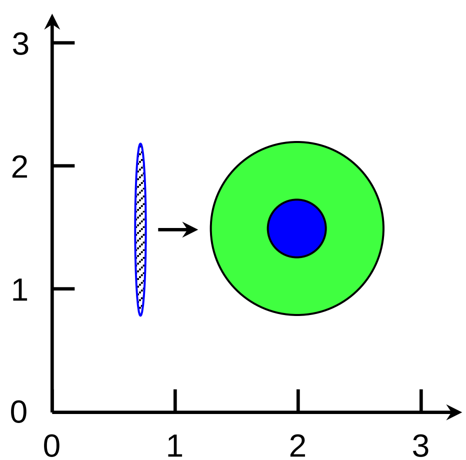
(2) the interesting region of **Q-ω** space is of *limited extent*.



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

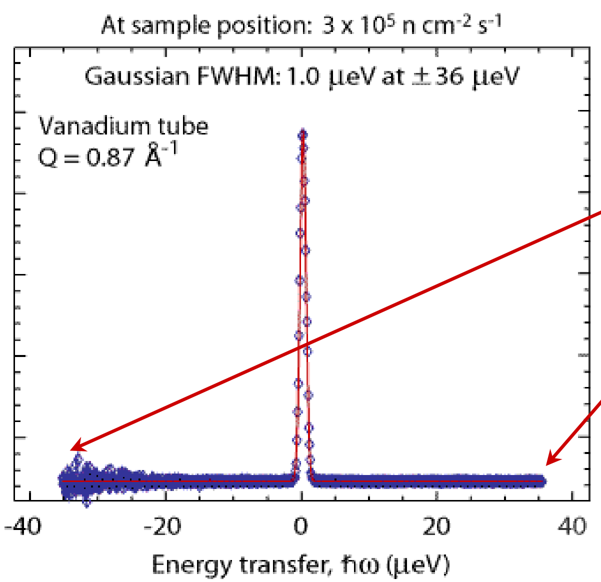
Things to Consider When Choosing HFBS

0.25 Å^{-1} < **Q** < 1.75 Å^{-1}

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

δ**Q** < 0.1 - 0.2 Å^{-1}

Can you live with such coarse Q-resolution?



Do the features of interest lie within this hω-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**) …

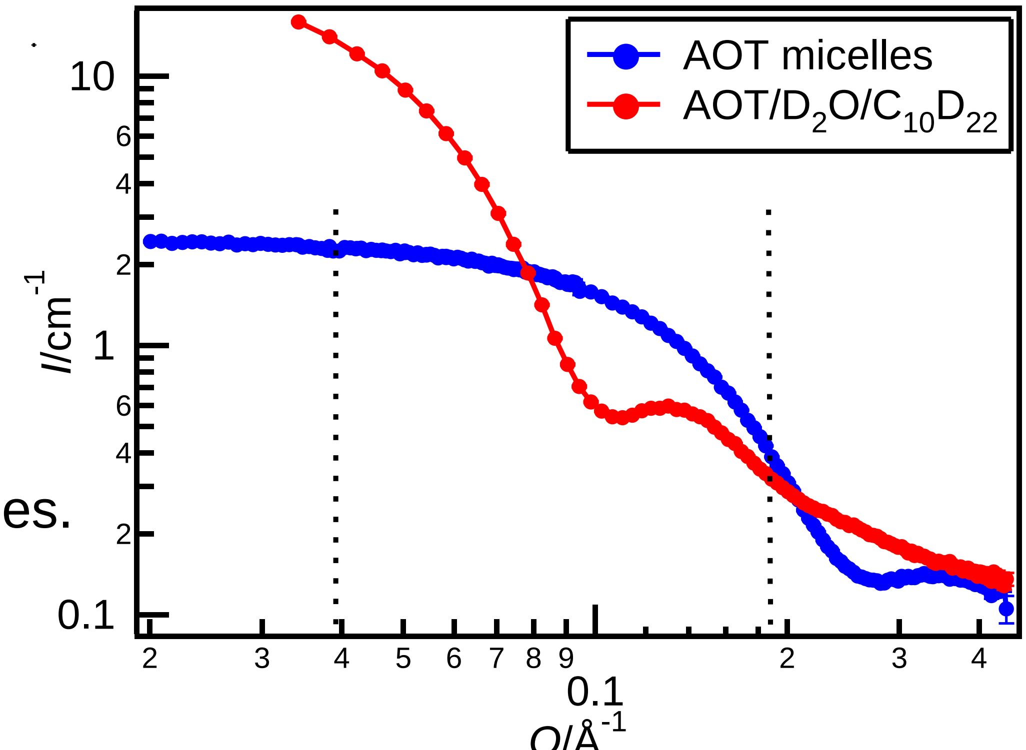
… then use NSE (low **Q**, long times)

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"

NCNR

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" for Triple-Axis Spectrometers

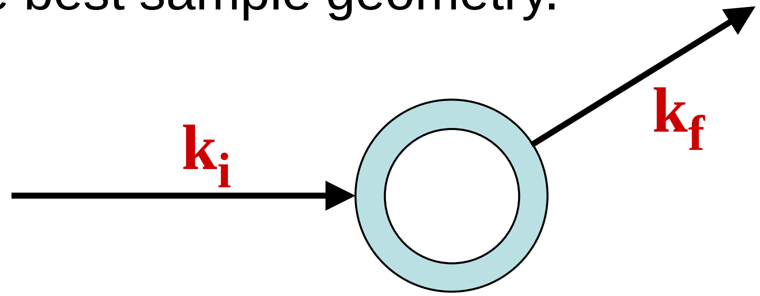
NCNR

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

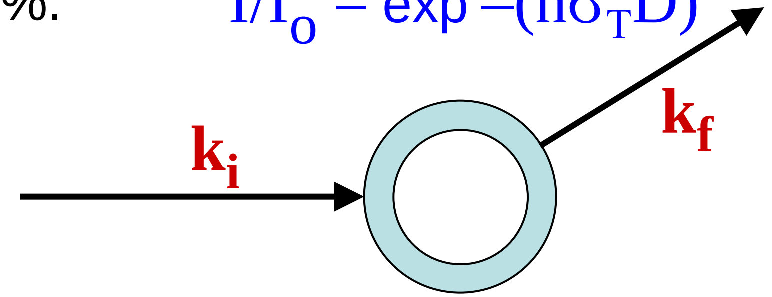
If possible, use cylindrical samples (rather than flat plate)

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

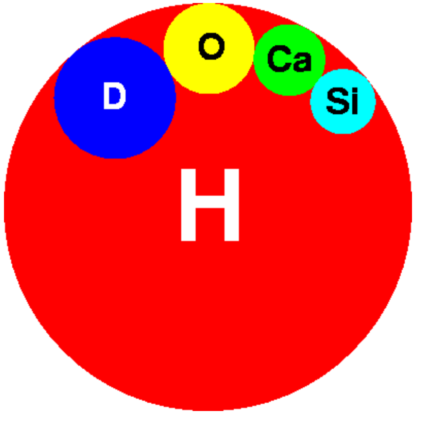


Sample "Design" for DCS and HFBS

Does the sample contain H?

Remember: Neutrons LOVE H!!

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

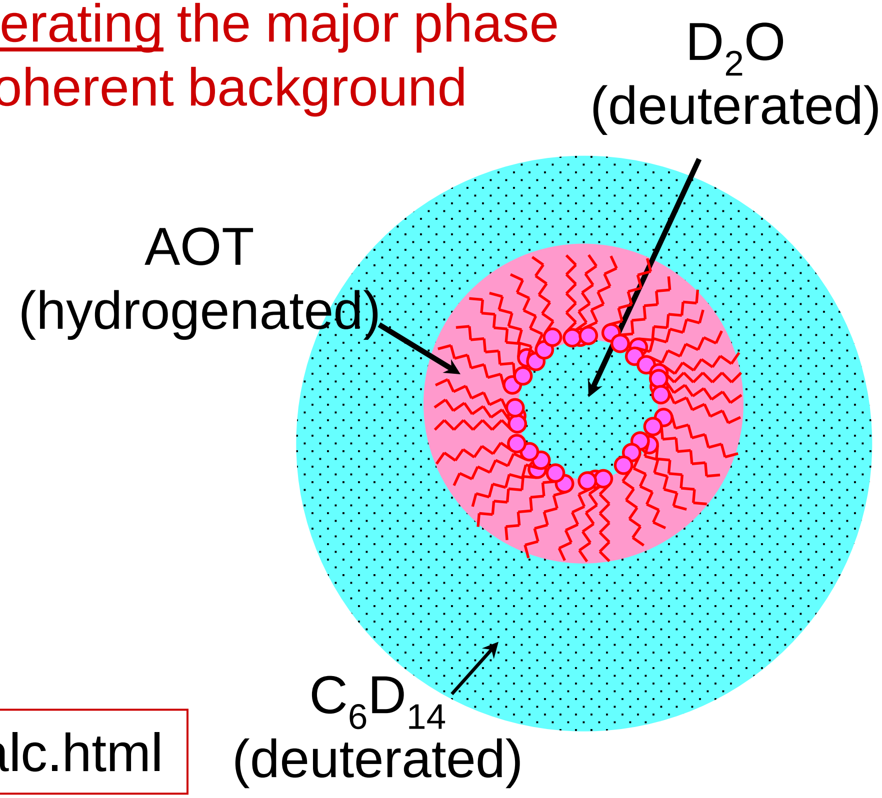


Sample "Design" for NSE

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	10.0×10^{-6} Å^{-2}
SLD solvent	6.1×10^{-6} Å^{-2}



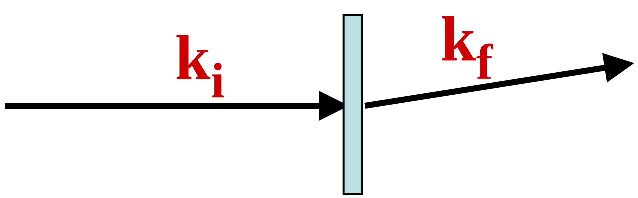
http://www.ncnr.nist.gov/resources/sldcalc.html

Sample "Design" for NSE

Increase the intensity by increasing the amount of sample

→ Fill the beam with sample

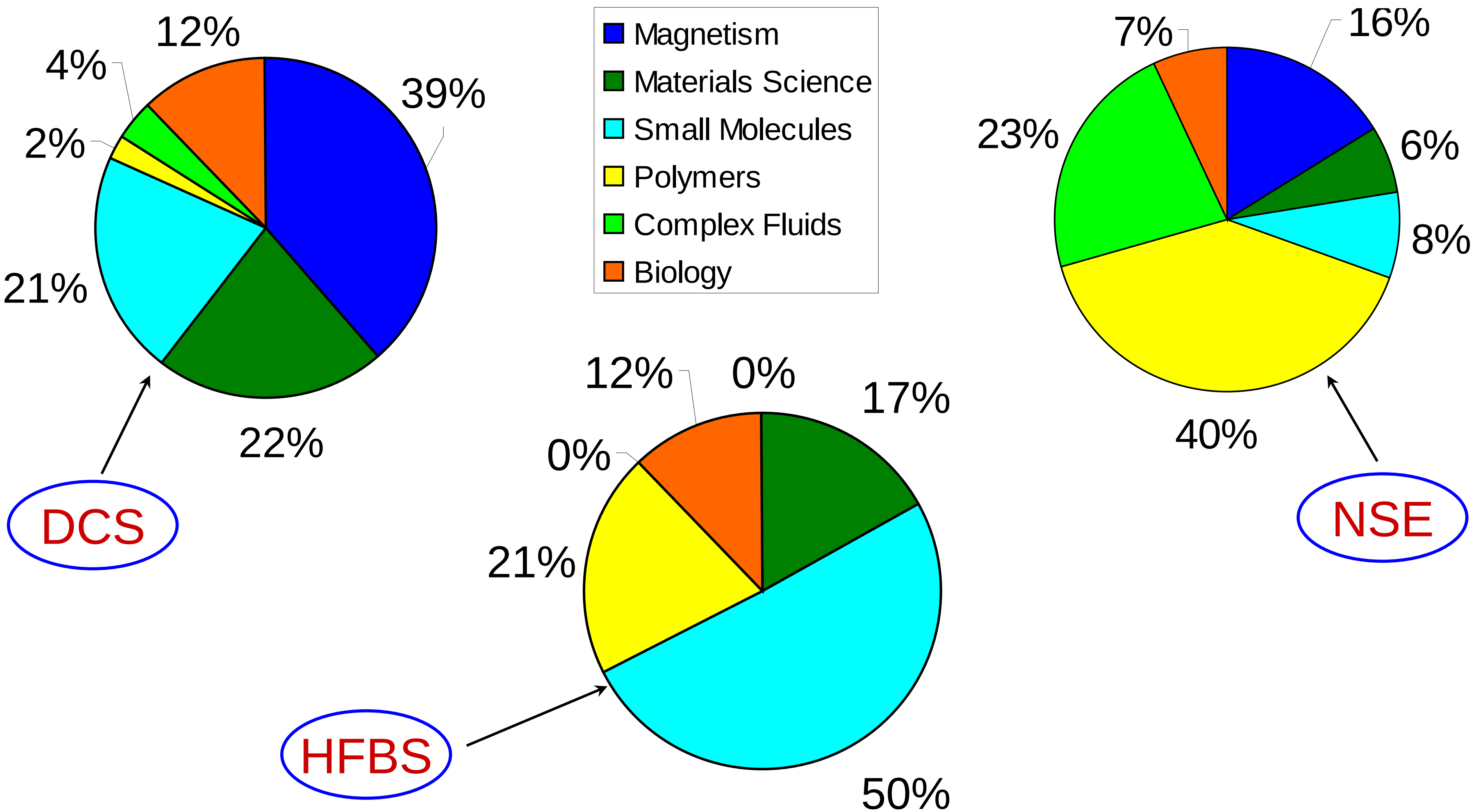
Typically use flat plate samples (at small angles)



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

Rule of thumb - the transmission should be ~70%

Typical Distributions of Science by Instrument



Applying for Beam Time

Access to the neutron scattering instruments that you've used over the past week is merit-based. Open to all qualified users, but subject to an anonymous peer-review of proposals.

Calls for proposals are issued about twice/yr.

Next deadline for new proposals ~ December 2013.

Further information on submitting proposals :

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

Some Summer School Success Stories

2001

2003

Jae-Ho Chung
University Prof.

Vicky Garcia-Sakai
ISIS Staff Scientist

1999

1997

William Ratcliff
NCNR Staff Physicist

Rob Dimeo
NCNR Director

Ok, so you can't win them all …

Acknowledgements

Organizers – Bulent Akgun and Yamali Hernandez

Administrative staff

Experiment teams

Invited speakers

Scatter Well!