

# Choosing the Right Spectrometer



**NCNR** →

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**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

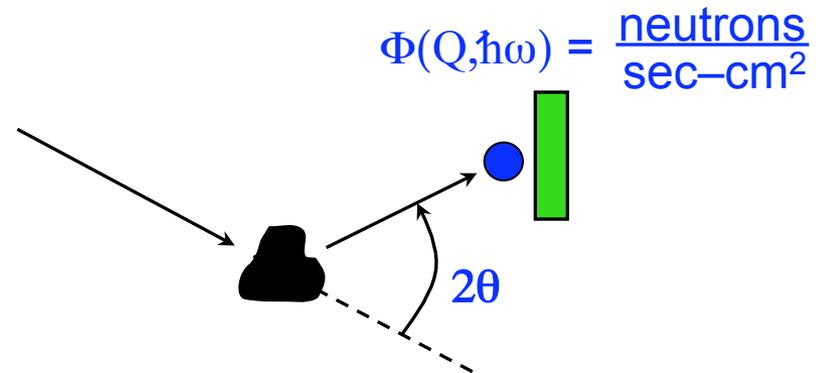
$$\hbar k_n = \hbar(2\pi/\lambda_n)$$

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

## Energy

$$\hbar\omega_n = \hbar^2 k_n^2 / 2m$$

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



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

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



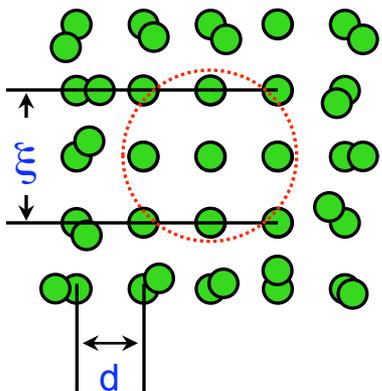
$\Phi$  provides information about all of these quantities!

# Main Messages of the Week

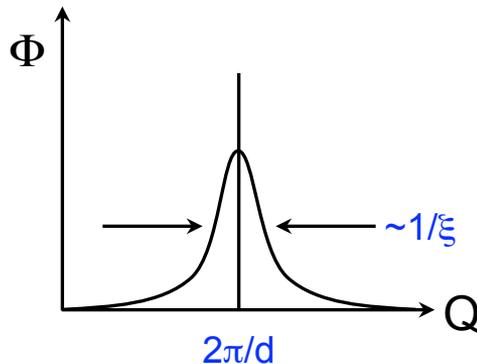
(3) The scattered neutron flux  $\Phi(\vec{Q}, \hbar\omega)$  is proportional to the space ( $\vec{r}$ ) and time (t) Fourier transform of the probability  $G(\vec{r}, t)$  of finding one or two atoms separated by a particular distance at a particular time.

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

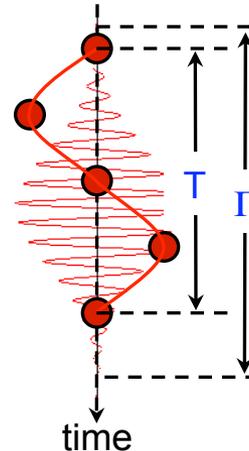
Real space



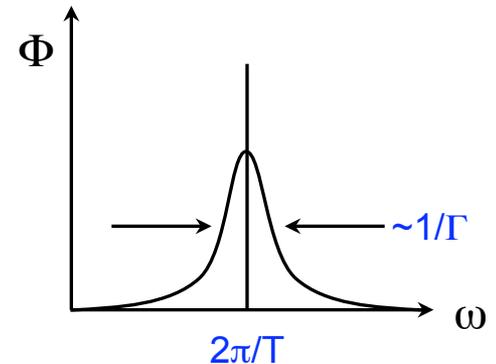
Q-space



Time space



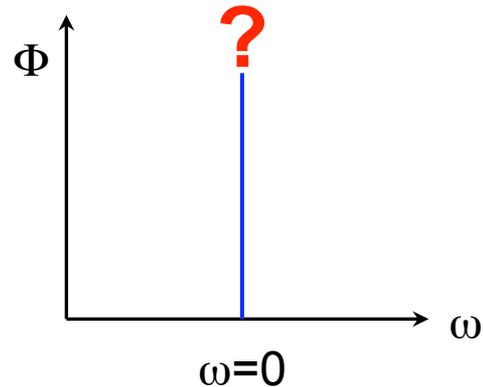
$\omega$ -space



# Pop Quiz!

Question:

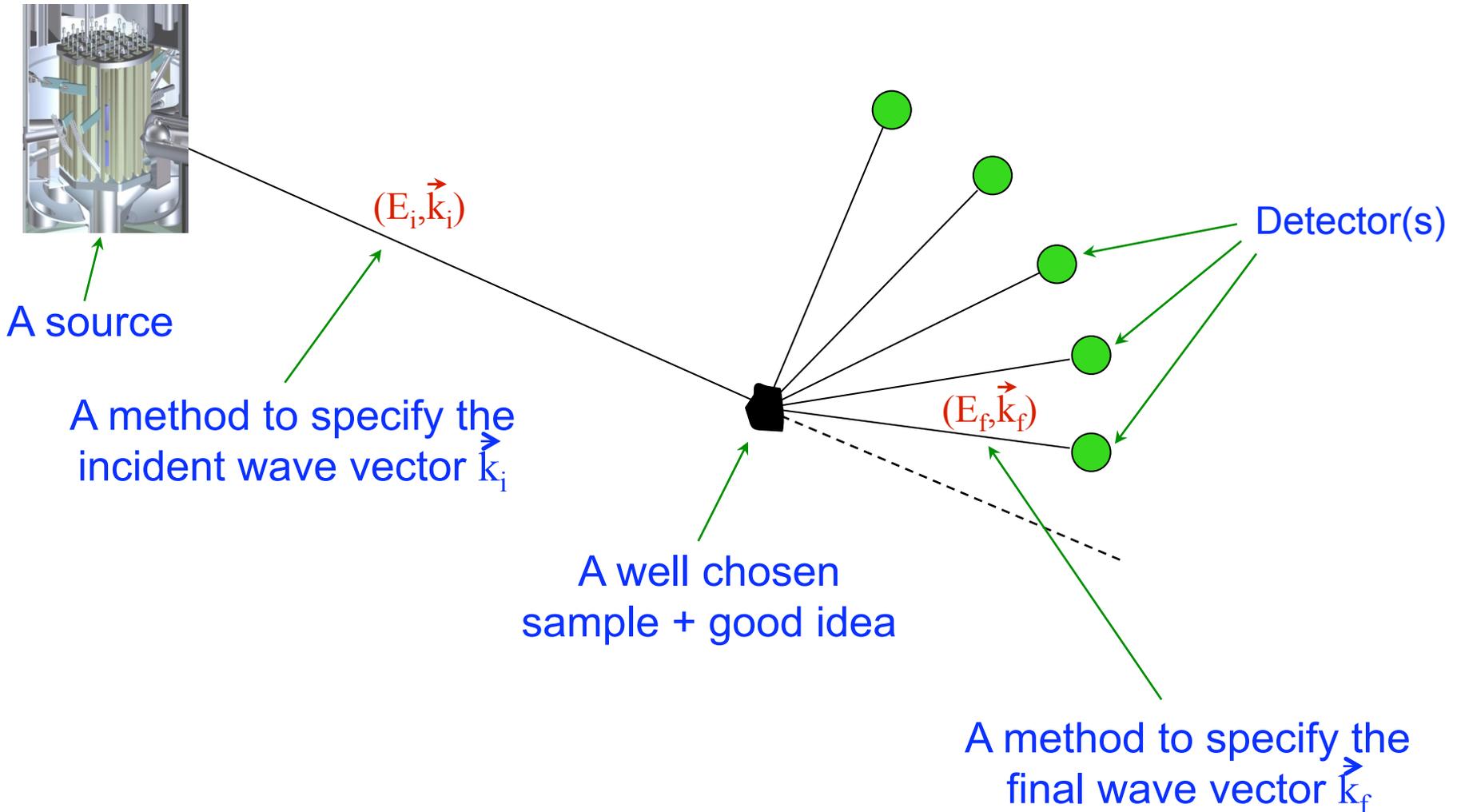
Can one measure elastic scattering from a liquid?



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 an inelastic neutron scattering experiment?

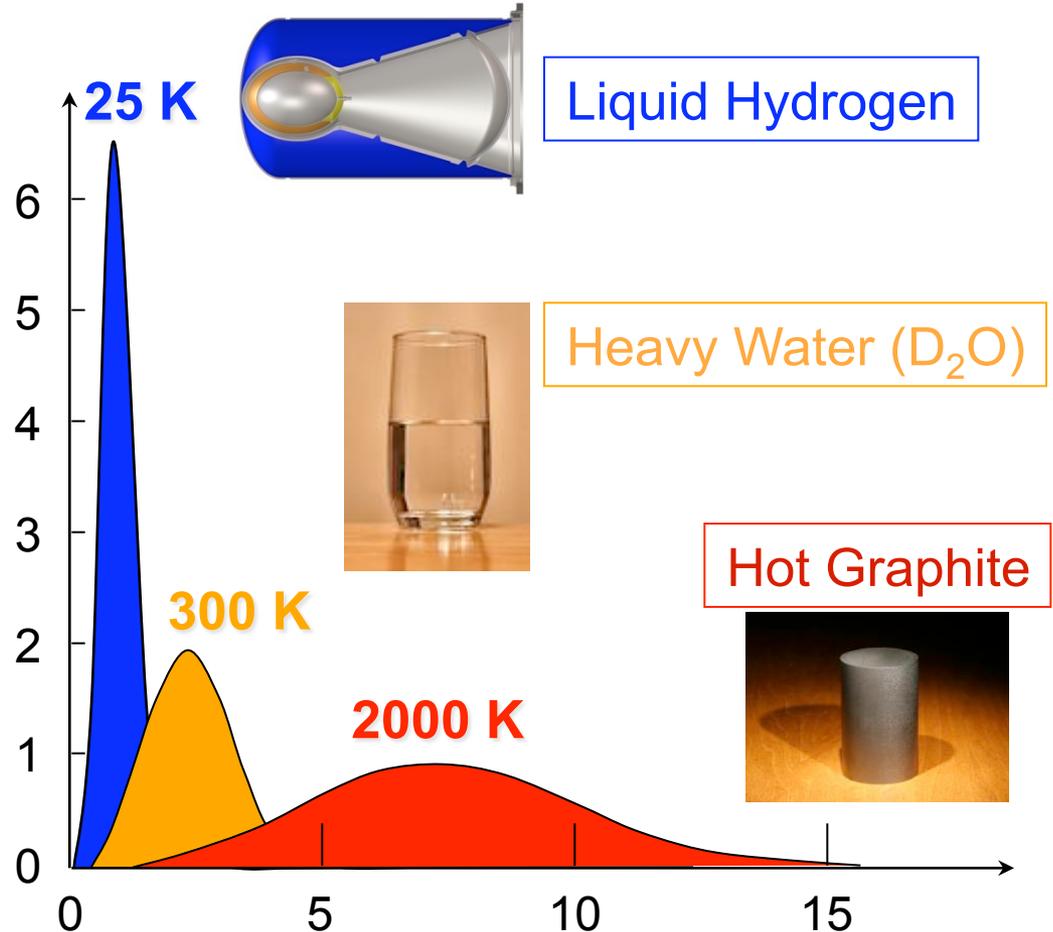
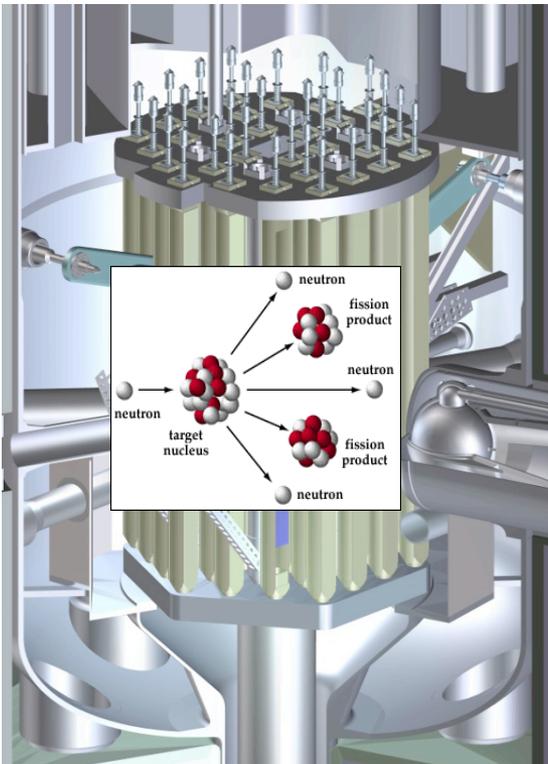


# Neutron Source: Moderation

Maxwellian  
Distribution

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

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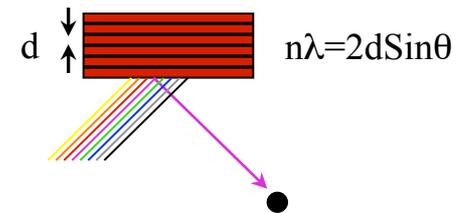
“Fast” neutrons:  $v = 20,000$  km/sec

Neutron velocity  $v$  (km/sec)

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

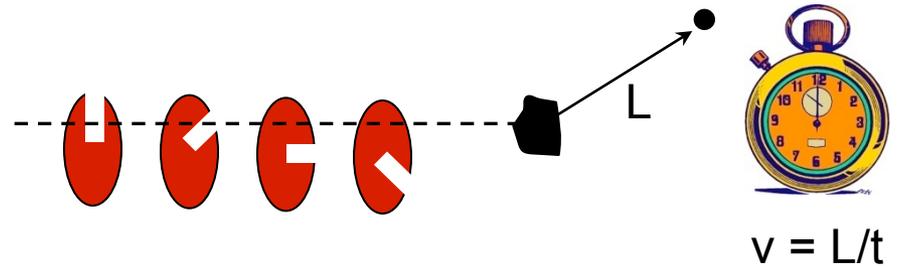
## 1. Bragg Diffraction

SPINS, BT7, Backscattering



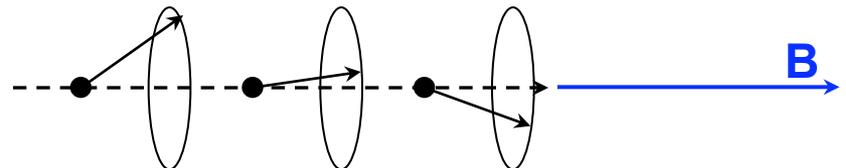
## 2. Time-of-Flight (TOF)

DCS, Backscattering (?)

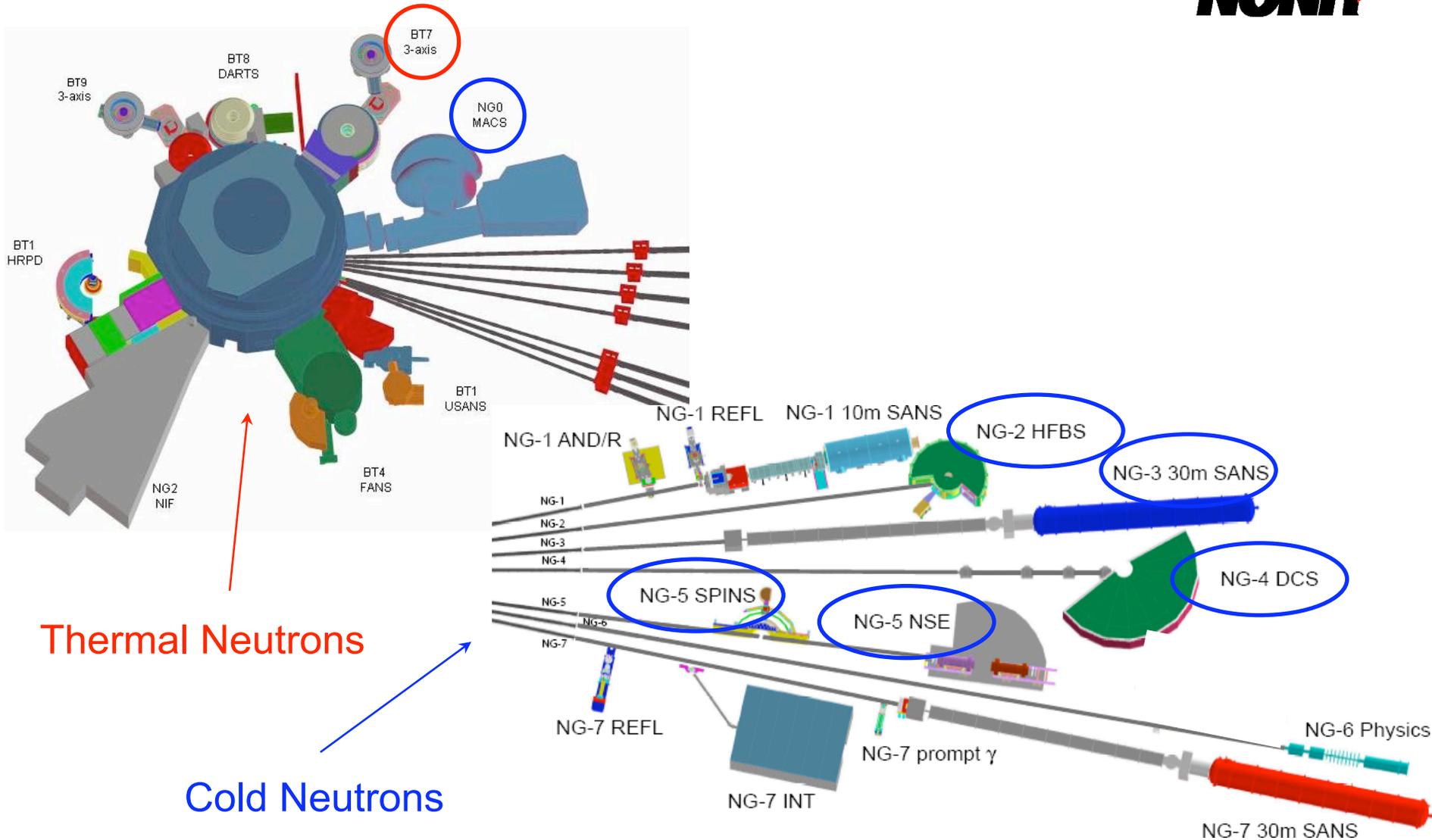


## 3. Larmor Precession

Spin Echo



# Why are there so many different spectrometers?



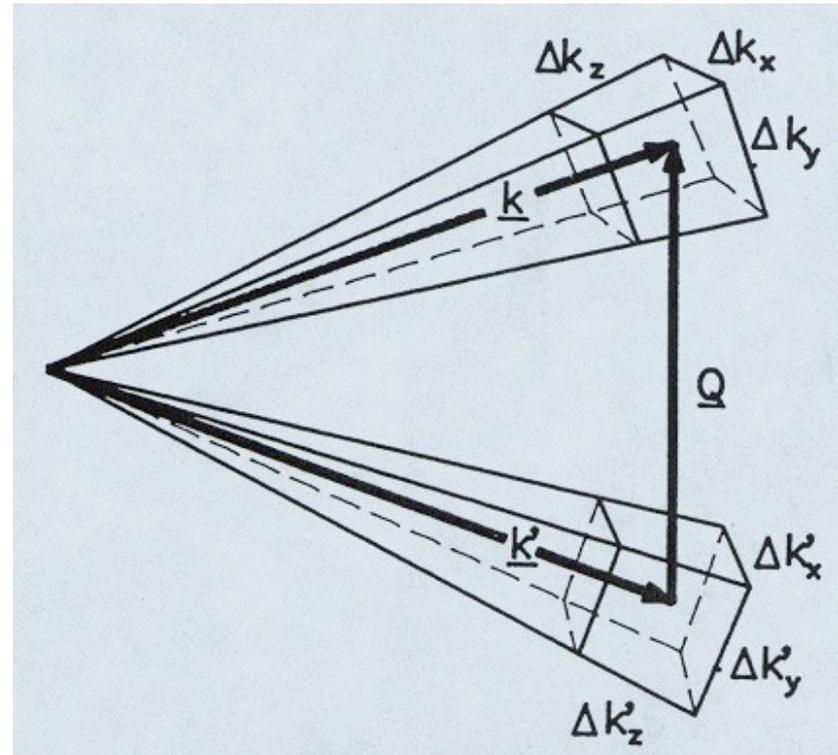
# Why are there so many different spectrometers?



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 certain precision.

The total signal in a scattering experiment is proportional to the resolution volume  $\rightarrow$  better resolution leads to lower count rates! *Choose carefully* ...

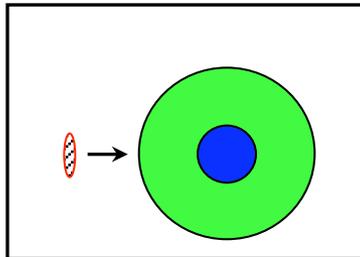


Courtesy of R. Pynn

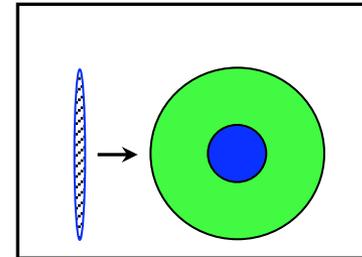
# Q-Resolution Matters!

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

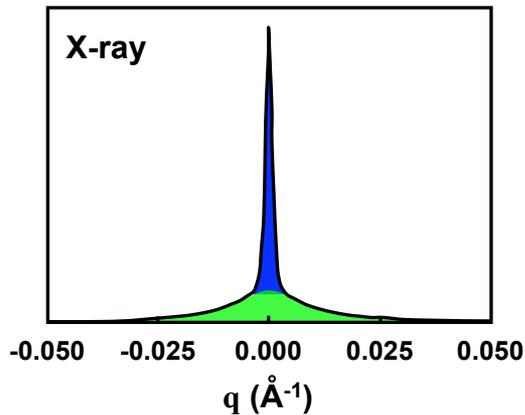
X-ray



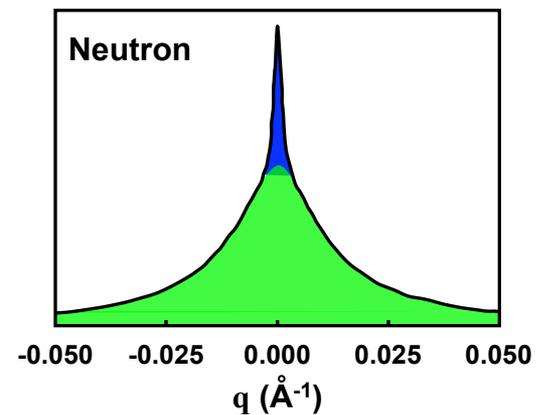
Neutron



X-ray



Neutron



# $\hbar\omega$ -Resolution Matters!

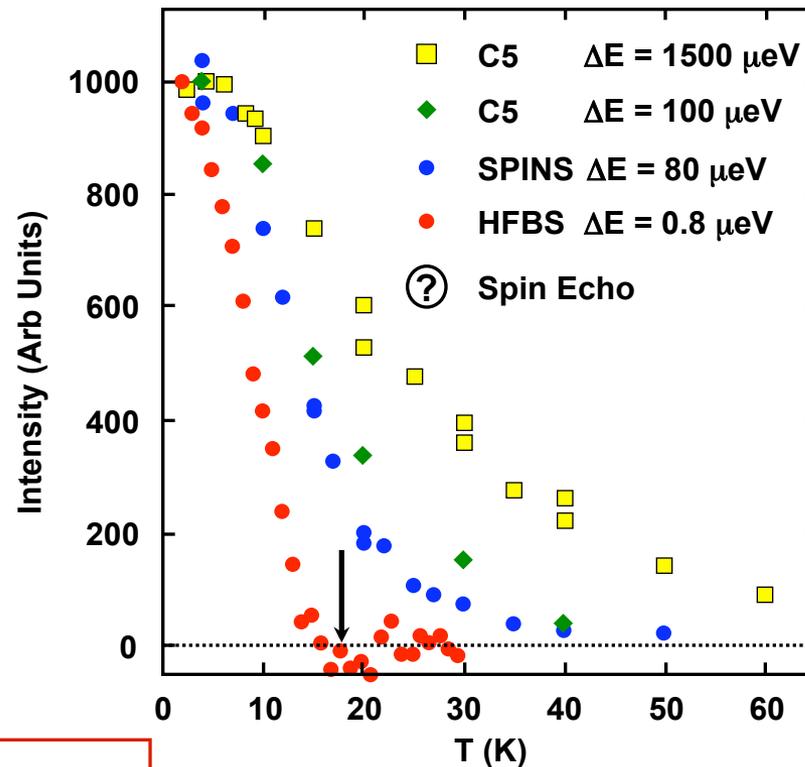
Consider  $\text{YBa}_2\text{Cu}_3\text{O}_{6.35}$   
 $T_c = 18\text{K}$

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

What is  $T_N$ ?

A “fatter” energy resolution  
integrates over low-energy  
fluctuations

“Elastic” Bragg Peak Intensity

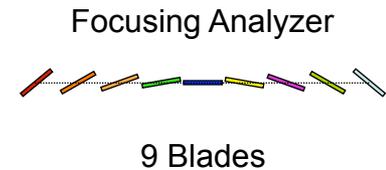
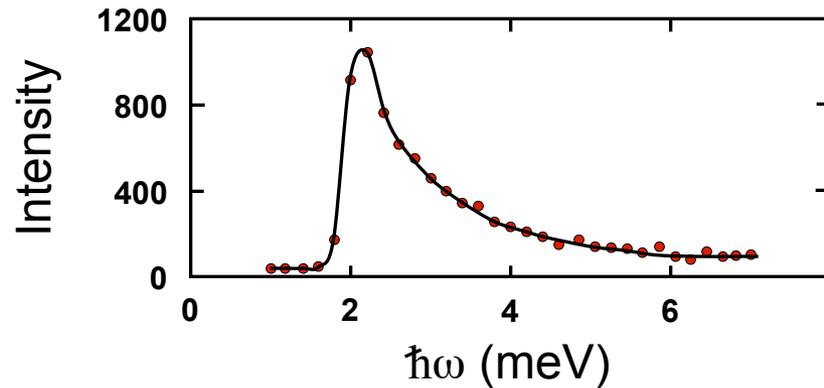
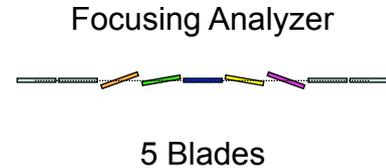
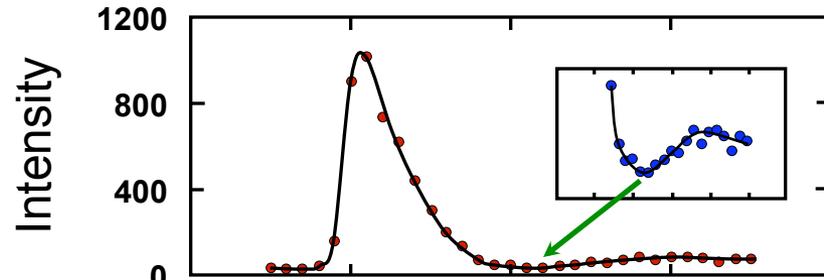
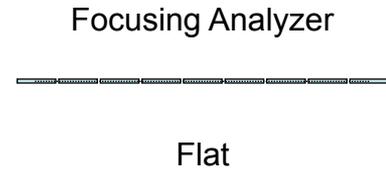
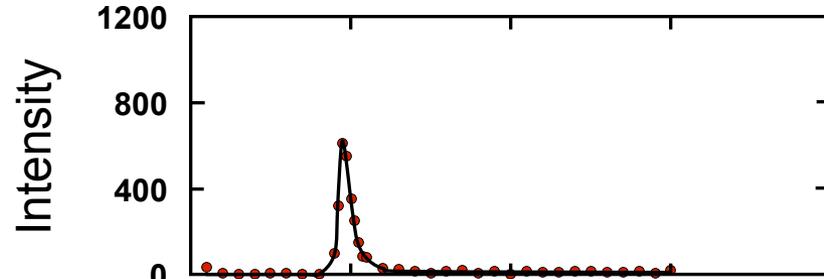
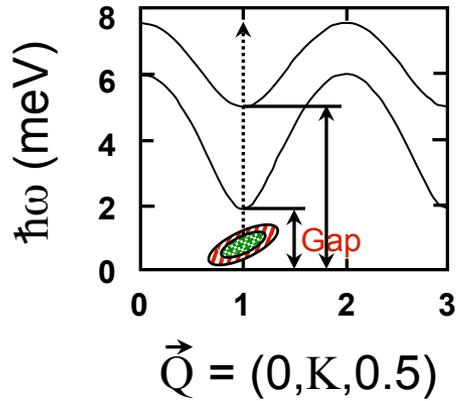


# $\hbar\omega$ -Resolution Matters!



Another example ...

SPINS



# So, how do I choose the right spectrometer?



Two basic considerations:

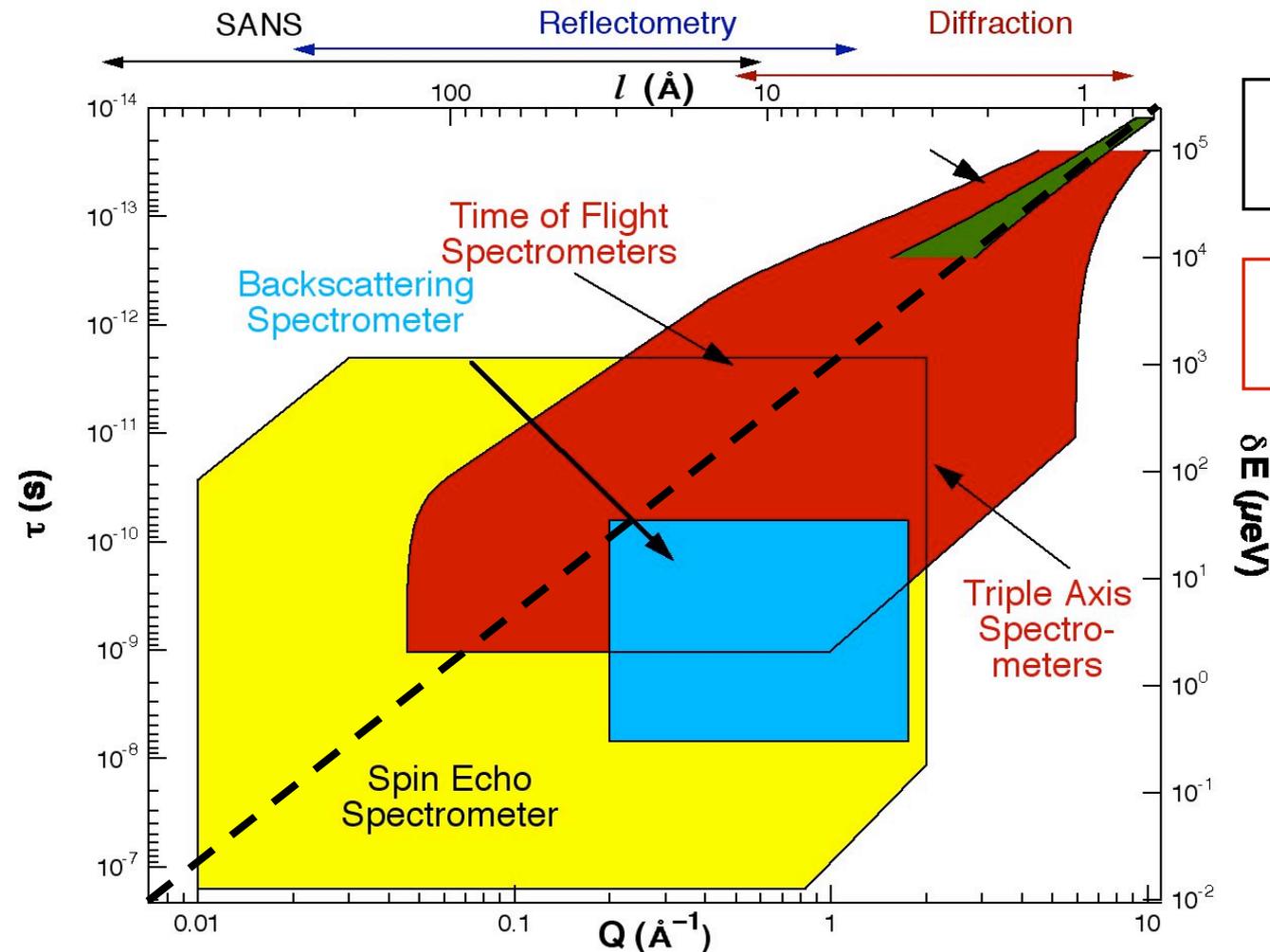
1. What are the **time** scales ( $\hbar\omega$ ) of interest?
2. What are the **length** scales ( $Q$ ) of interest?

(Some spectrometers overlap  $\rightarrow$  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 ( $\Delta Q$ ) is required?

# Different spectrometers cover different regions of phase space



Do you see a pattern here?

Larger “objects” tend to imply slower motions.

# Rules of Thumb



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

$\hbar\omega > 10\text{-}20 \text{ meV}$  - use FANS (or another spectrometer designed for vibrational spectroscopy)

$\hbar\omega < 20\text{-}30 \text{ }\mu\text{eV}$  - use HFBS

**In between** - use DCS (or another cold neutron TOF spectrometer)

2. Be certain that the length scales of the relevant motions lie within the range of the spectrometer.

As a simple example, consider the HFBS instrument. ( $Q \sim 2\pi/L$ )

$$Q_{\min} = 0.25 \text{ \AA}^{-1} \rightarrow L_{\max} \sim 25 \text{ \AA}$$

$$Q_{\max} = 1.75 \text{ \AA}^{-1} \rightarrow L_{\min} \sim 3.5 \text{ \AA}$$

**REMEMBER -  $Q_{\min}$  and  $Q_{\max}$  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.

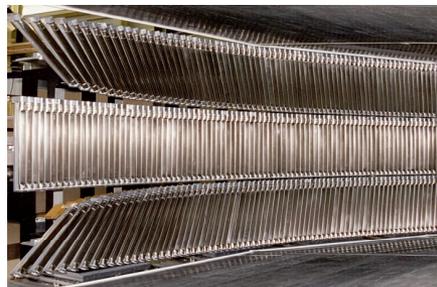
**YES?** Consider instruments with large analyzer areas.

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

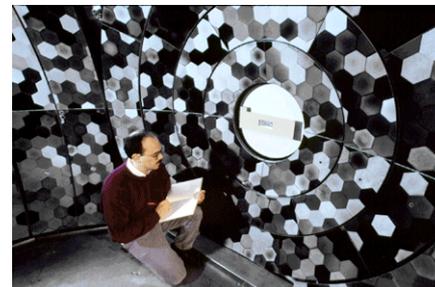
**FANS**



**DCS**



**HFBS**



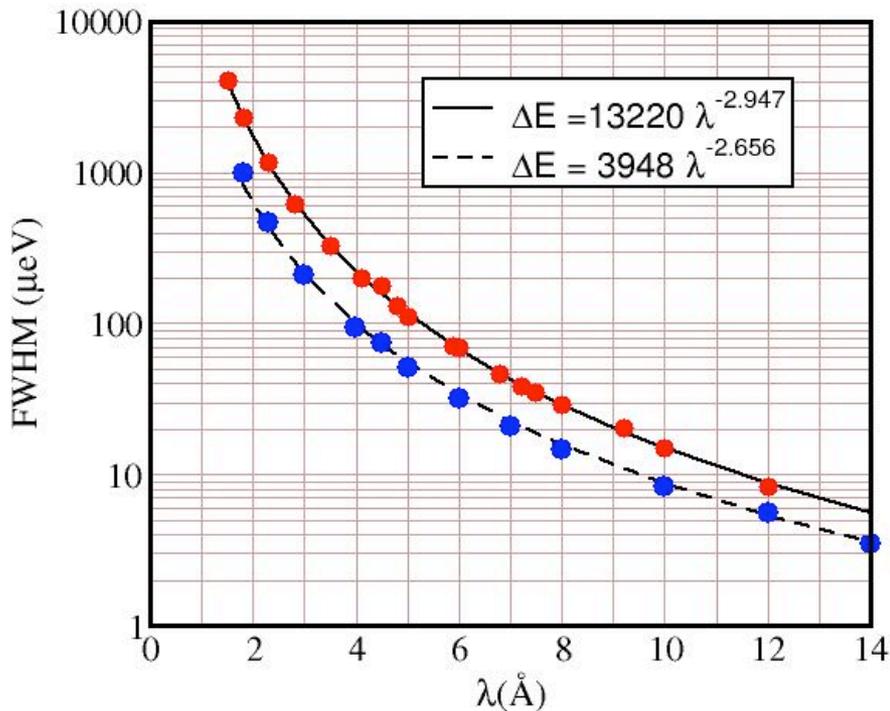
**BT7**



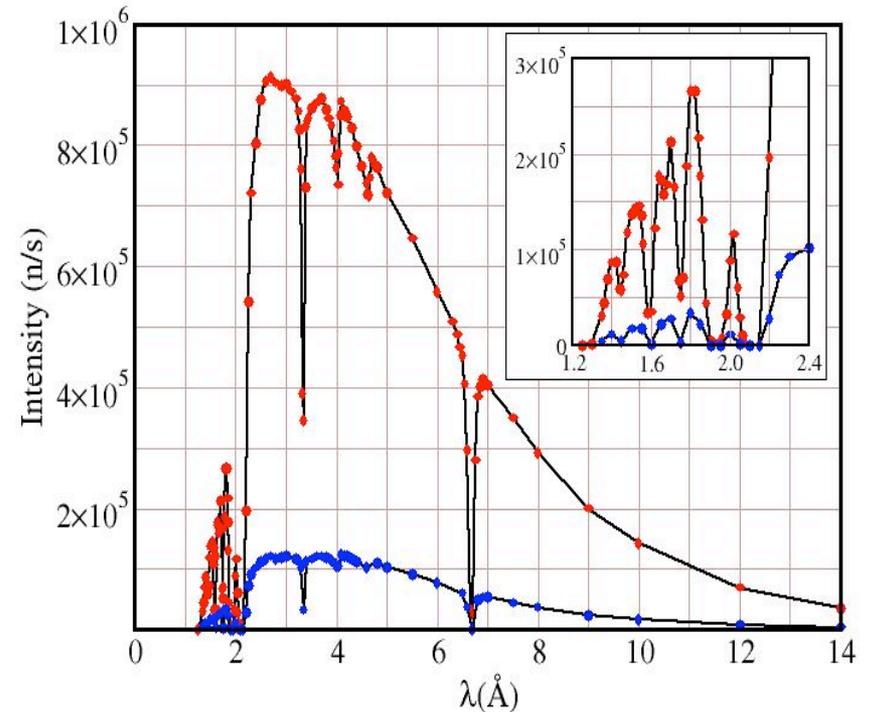
# Things to consider when choosing DCS



$\Delta E$



$I(E)$



Quantities varied

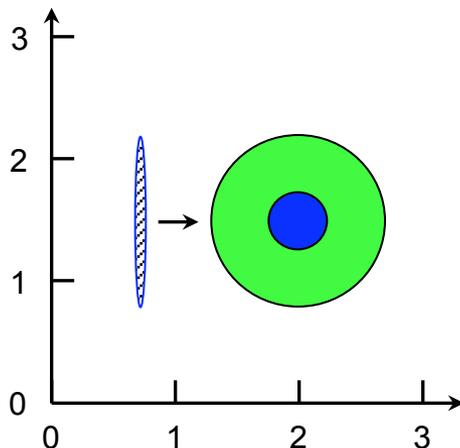
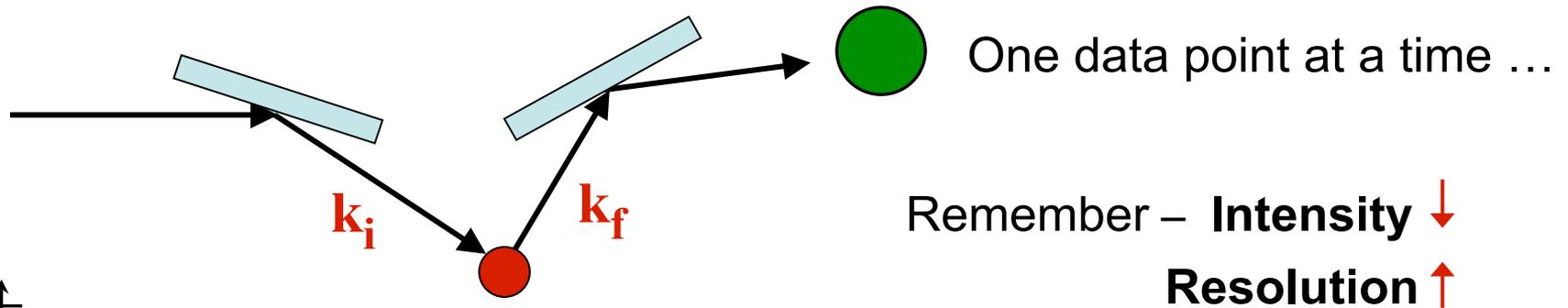
- wavelength  $\lambda$
- chopper slot widths  $W$

Remember – Intensity ↓  
Resolution ↑

# Things to consider when choosing SPINS



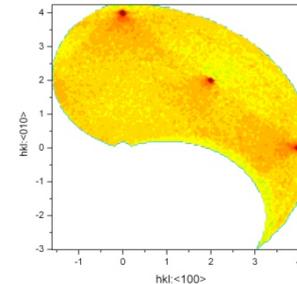
Triple axis spectrometers are typically used when either -  
 (1) the *direction* of  $\mathbf{Q}$  is important or  
 (2) the interesting region of  $\mathbf{Q}$ - $\omega$  space is of *limited extent*.



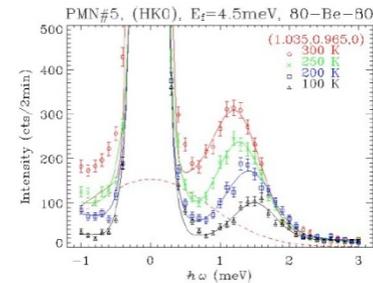
Collimation(')	$\lambda$	rel. signal	FWHM.
55-80-80-80	4 Å	1.00	0.28 meV
55-40-40-40	4 Å	0.24	0.17 meV
69-80-80-80	5 Å	0.26	0.13 meV
84-80-80-80	6.1 Å	0.03	0.05 meV

# DCS versus SPINS

DCS – incoherent scattering,  
broad surveys in  $Q$ - $\omega$



SPINS – coherent scattering,  
limited regions in  $Q$ - $\omega$



Rules of Thumb: (think carefully before violating)

DCS – systems requiring resolution  $< 100 \mu\text{eV}$

SPINS – single crystals

# Things to consider when choosing HFBS

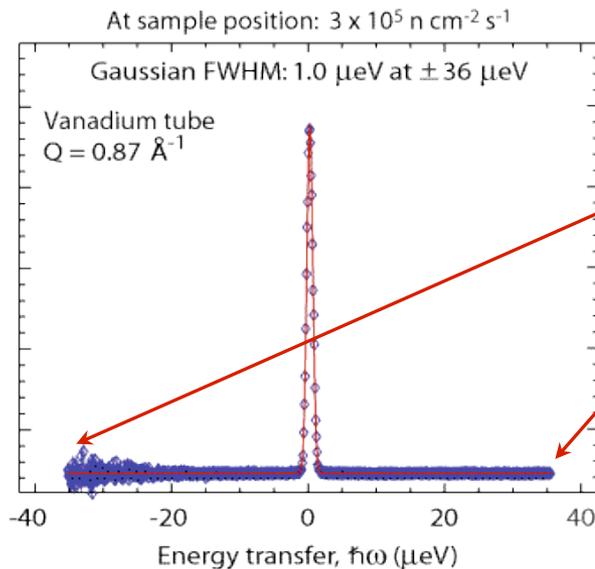


$$0.25 \text{ \AA}^{-1} < Q < 1.75 \text{ \AA}^{-1}$$

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

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

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  $\delta E \sim 1 \text{ \mu eV}$  (or perhaps even better resolution)?

# Things to consider when choosing NSE



If the  $h\omega$ -resolution of backscattering is “not good enough,” or if you are only interested in a “limited” region of  $Q$ -space (typically small  $Q$ )

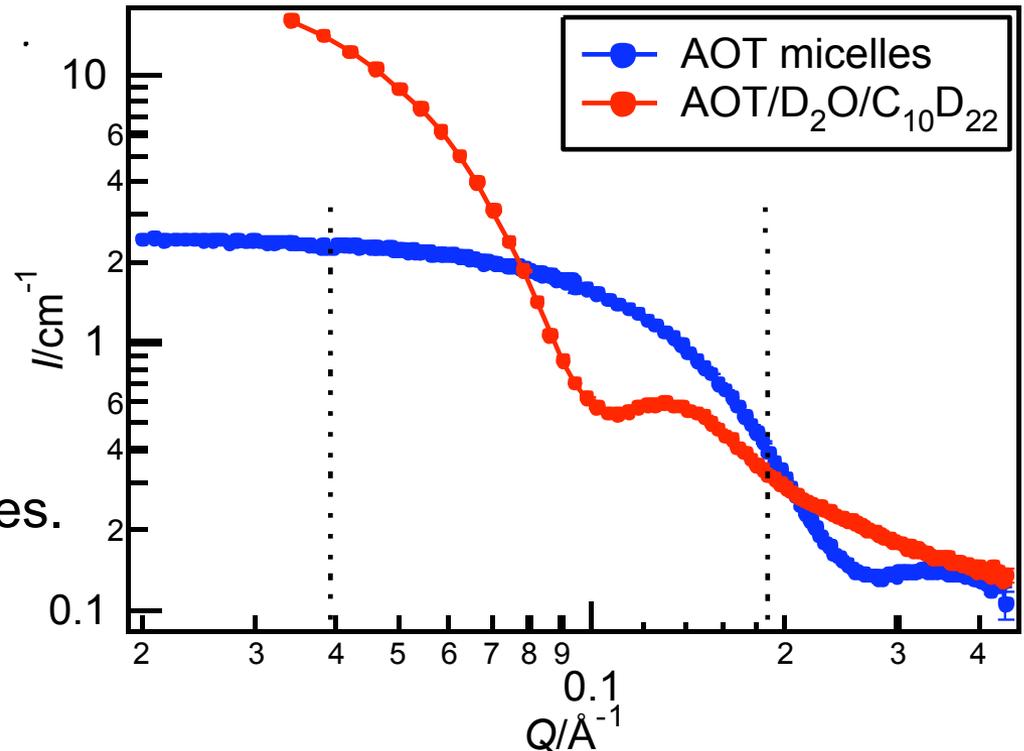
... **... then use NSE (low  $Q$ , long times)**

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.

${}^6\text{Li}$   ${}^{10}\text{B}$   ${}^{113}\text{Cd}$   ${}^{157}\text{Gd}$

For a complete listing go to

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

# Sample “design” for triple-axis spectrometers

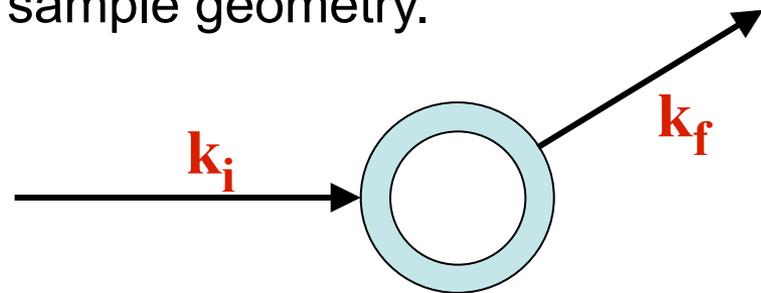


Single crystals yield the most information.

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 10cm)

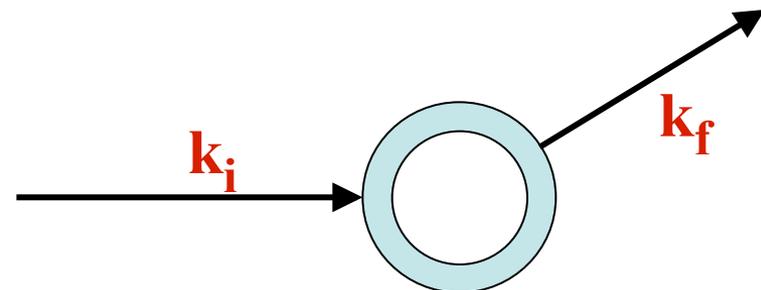
Backscattering: 3 cm x 3 cm

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

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

$$I/I_0 = \exp -(n\sigma_T D)$$

Often annular is the best sample geometry



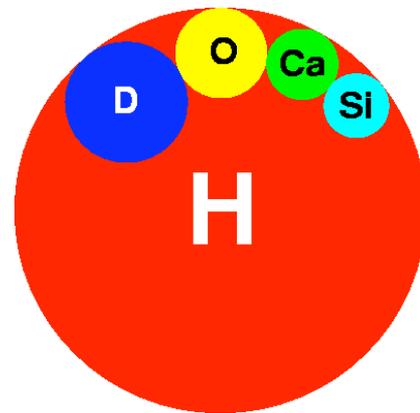
# Sample “design” for DCS and HFBS



Does the sample contain H?

Remember: **Neutrons LOVE H!!**

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



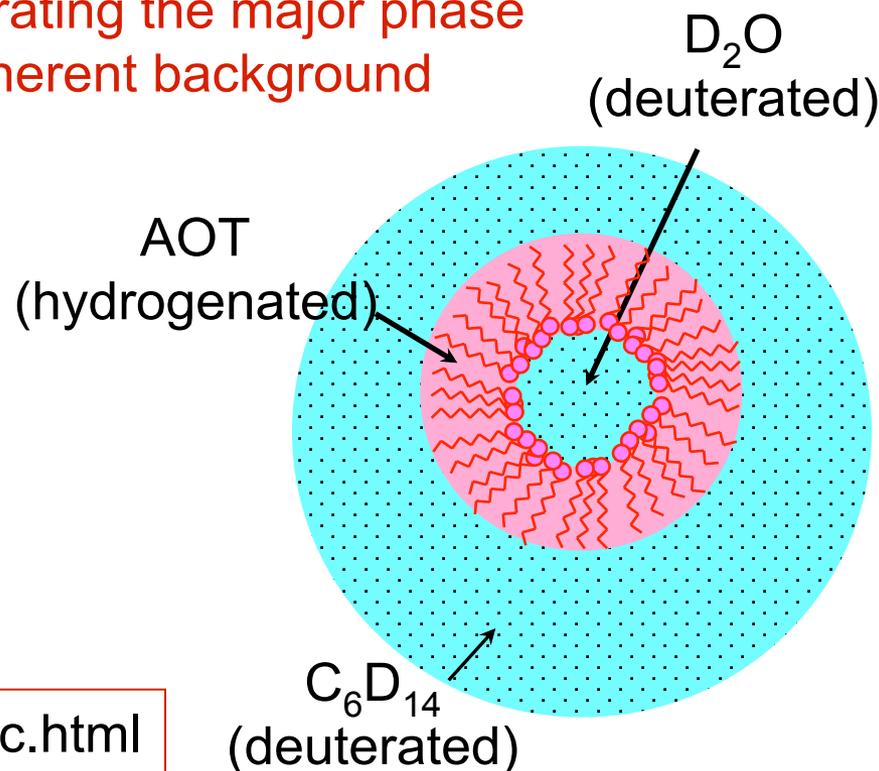
# Sample “design” for NSE



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	$6.4 \times 10^{-6} \text{ \AA}^{-2}$
SLD shell	$1.0 \times 10^{-6} \text{ \AA}^{-2}$
SLD solvent	$6.5 \times 10^{-6} \text{ \AA}^{-2}$



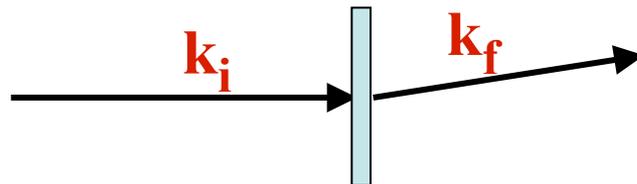
# Sample “design” for NSE



Increase the intensity by increasing the amount of sample

→ Fill the beam with sample

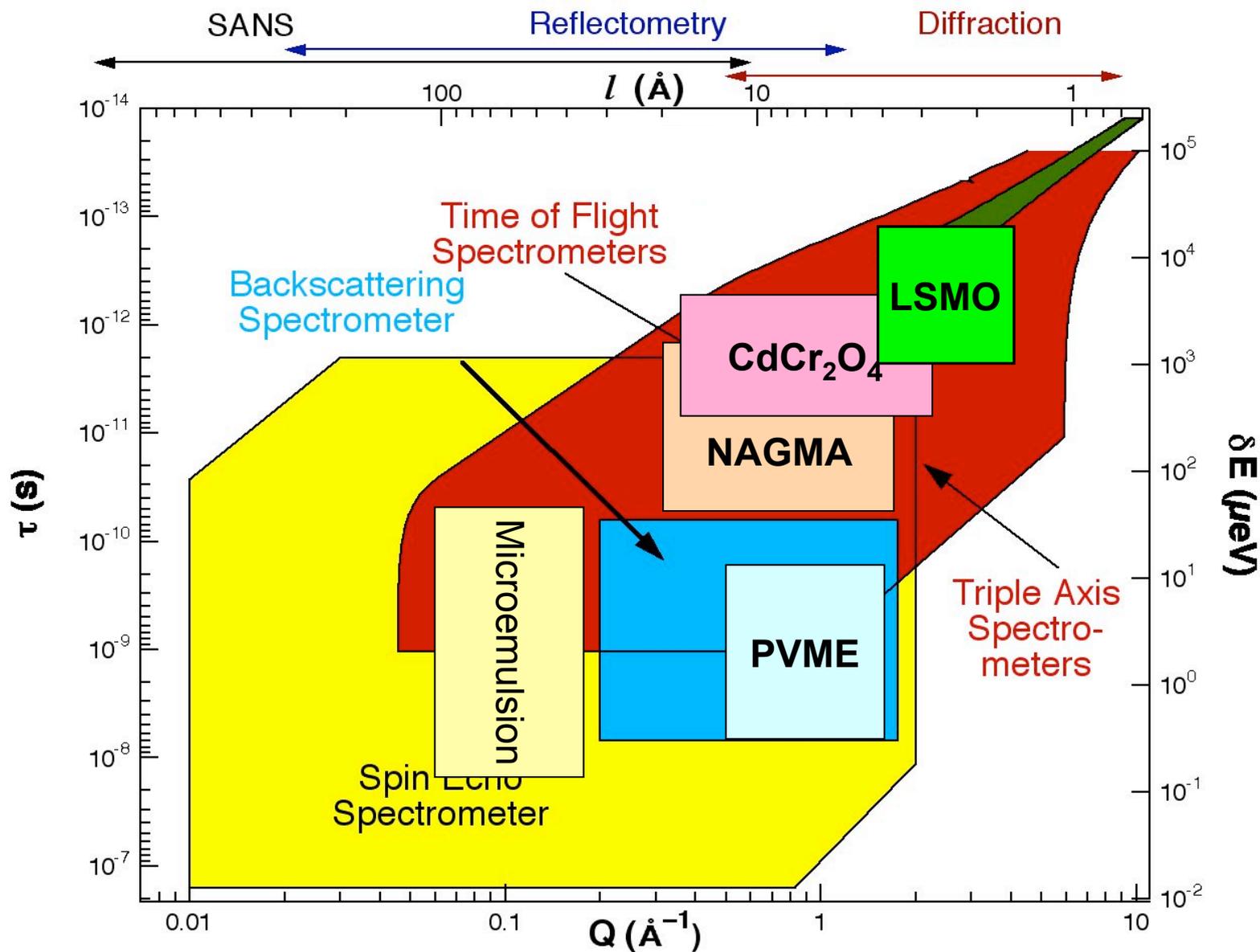
Typically use flat plate samples (at small angles)



$$I/I_0 = \exp -(n\sigma_T D)$$

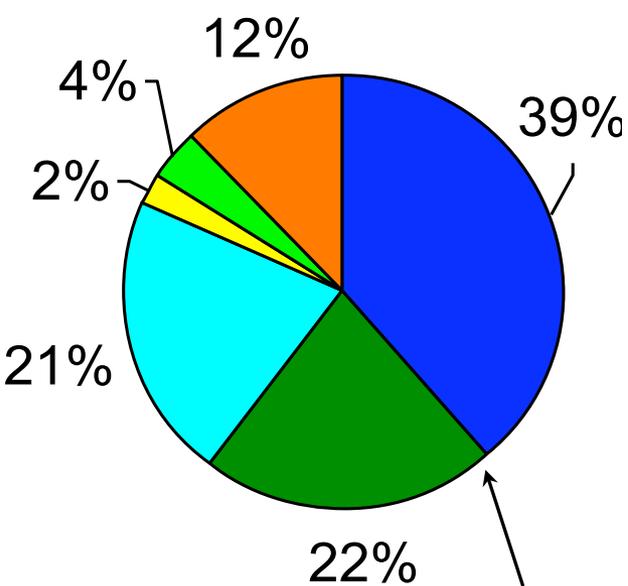
Rule of thumb - the transmission should be ~70%

# Samples from this Summer School

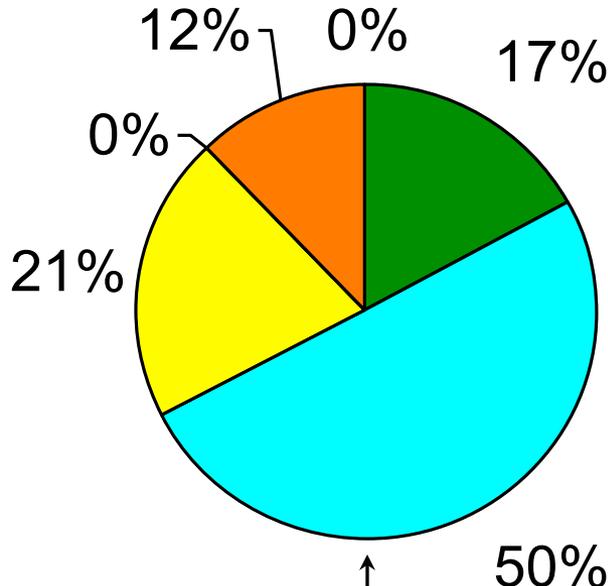


# Types of Science

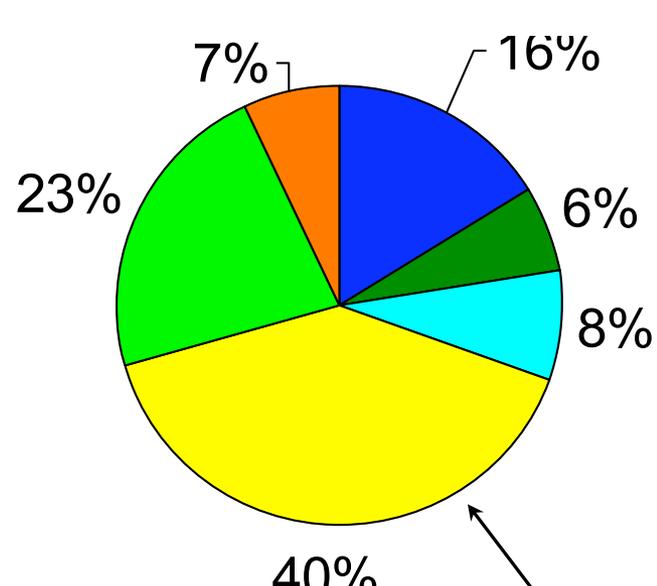
**NCNR** →



DCS



HFBS



NSE

- Magnetism
- Materials Science
- Small Molecules
- Polymers
- Complex Fluids
- Biology

# 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](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 speaker – Feng Ye



**Thanks for coming!**