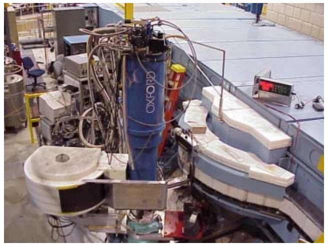
# Choosing the Right Spectrometer




**Peter Gehring**

**NIST Center for Neutron Research**

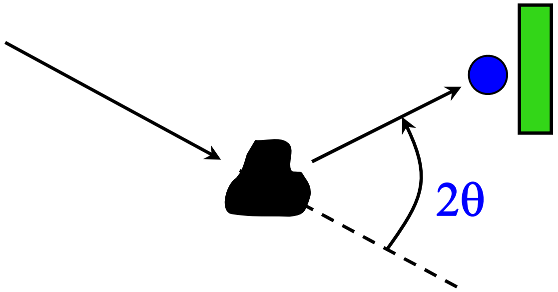


# Main Messages of the Week

(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 ($\hbar\omega$).

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

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




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

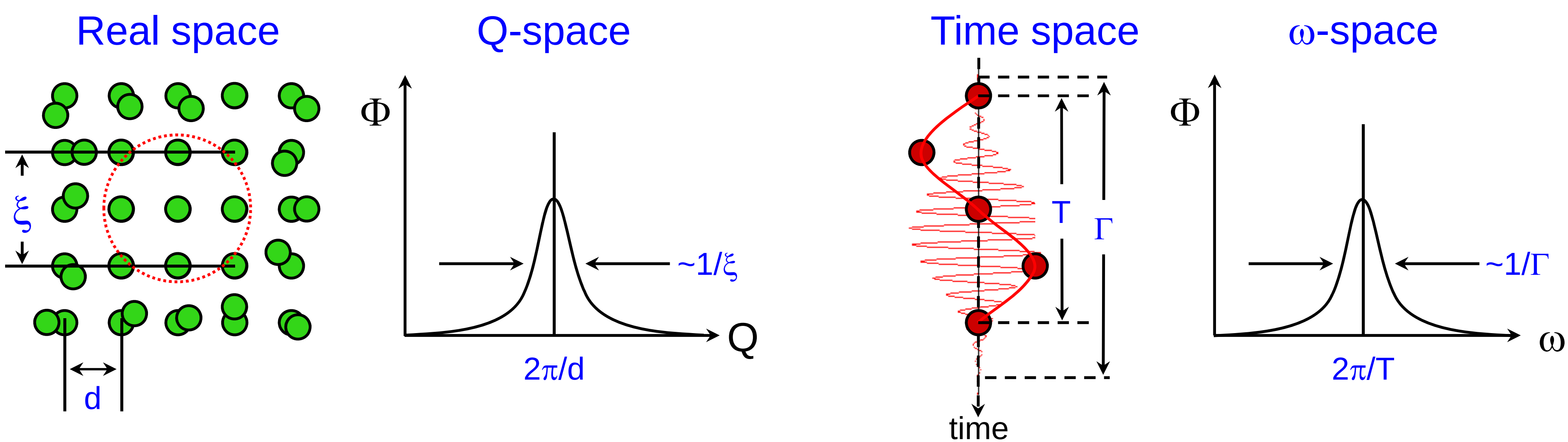
$$\Phi = \mathcal{F}\{\vec{r}_i(t), \vec{r}_j(t), \vec{S}_i(t), \vec{S}_j(t)\}$$

$\Rightarrow$ $\Phi$ 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.

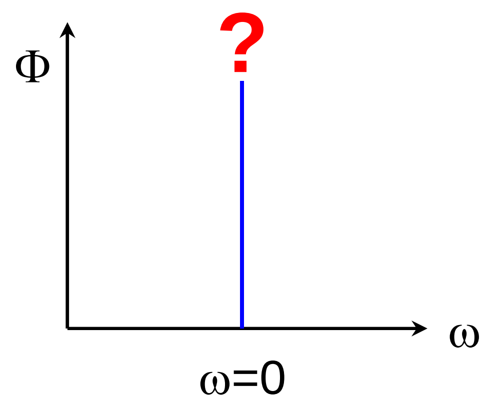
$$\Phi \propto \frac{\partial^2 \sigma}{\partial\Omega\partial\omega} \propto \iint e^{i(\vec{Q}\cdot\vec{r}-\omega t)} G(\vec{r},t)\, d^3\vec{r}\, dt$$



# Pop Quiz!

Question:

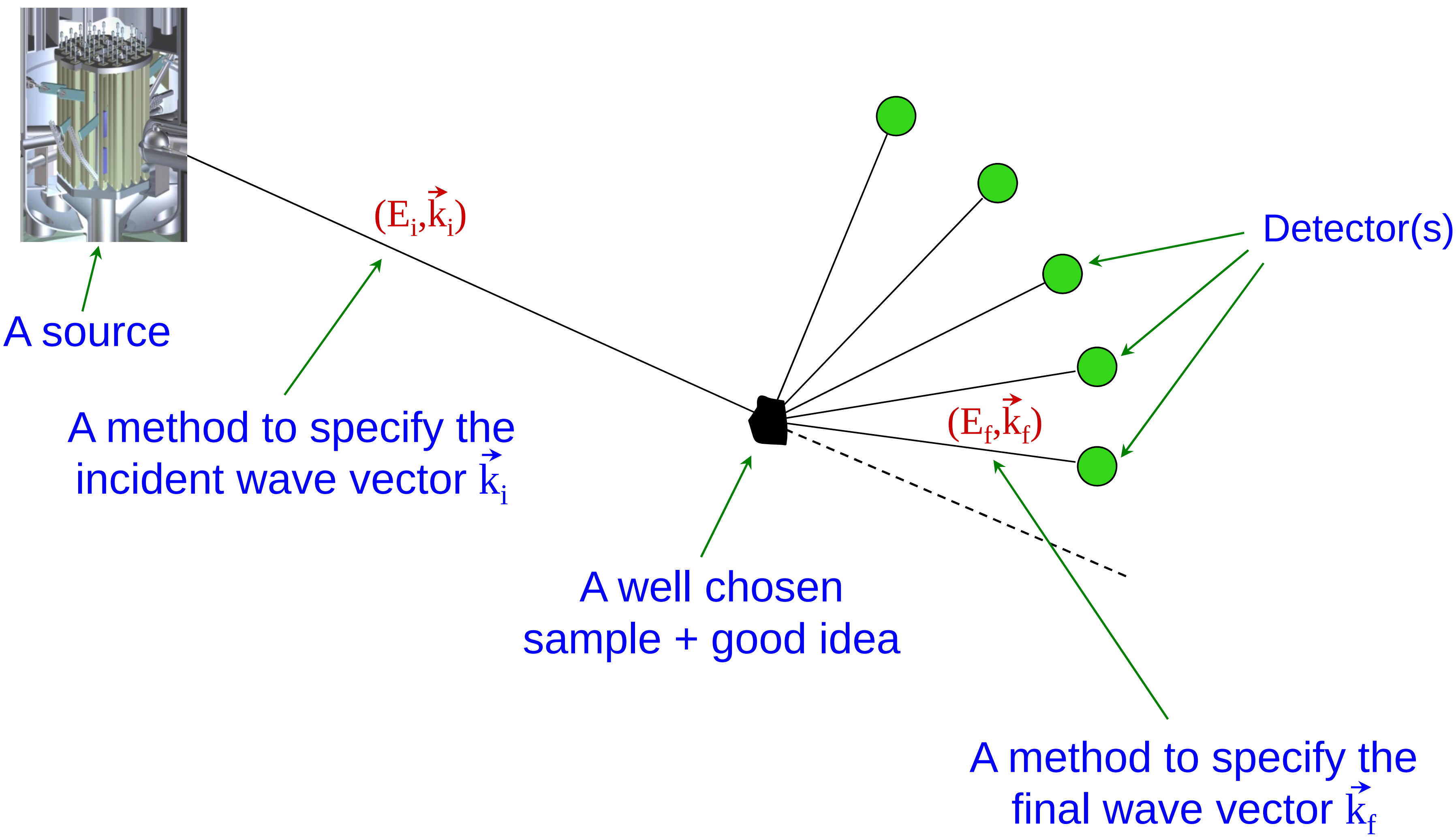
Can one measure elastic scattering from a liquid?




Why? Why not?

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

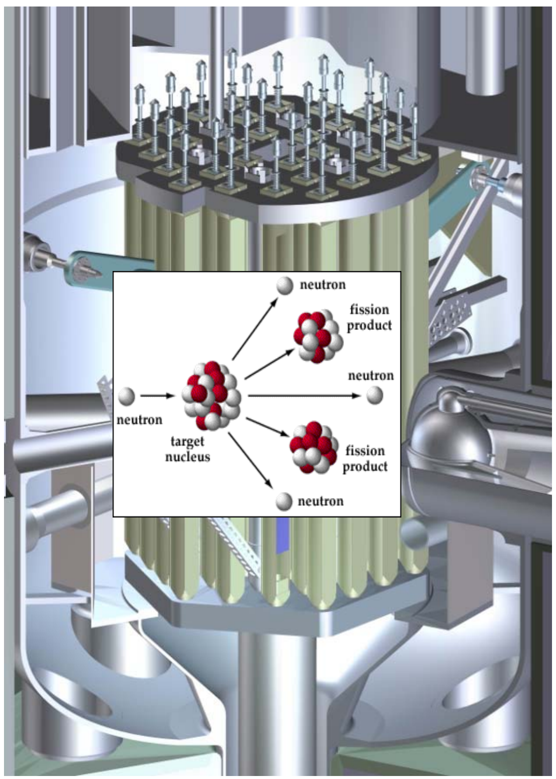
# What is required to do a neutron inelastic scattering experiment?

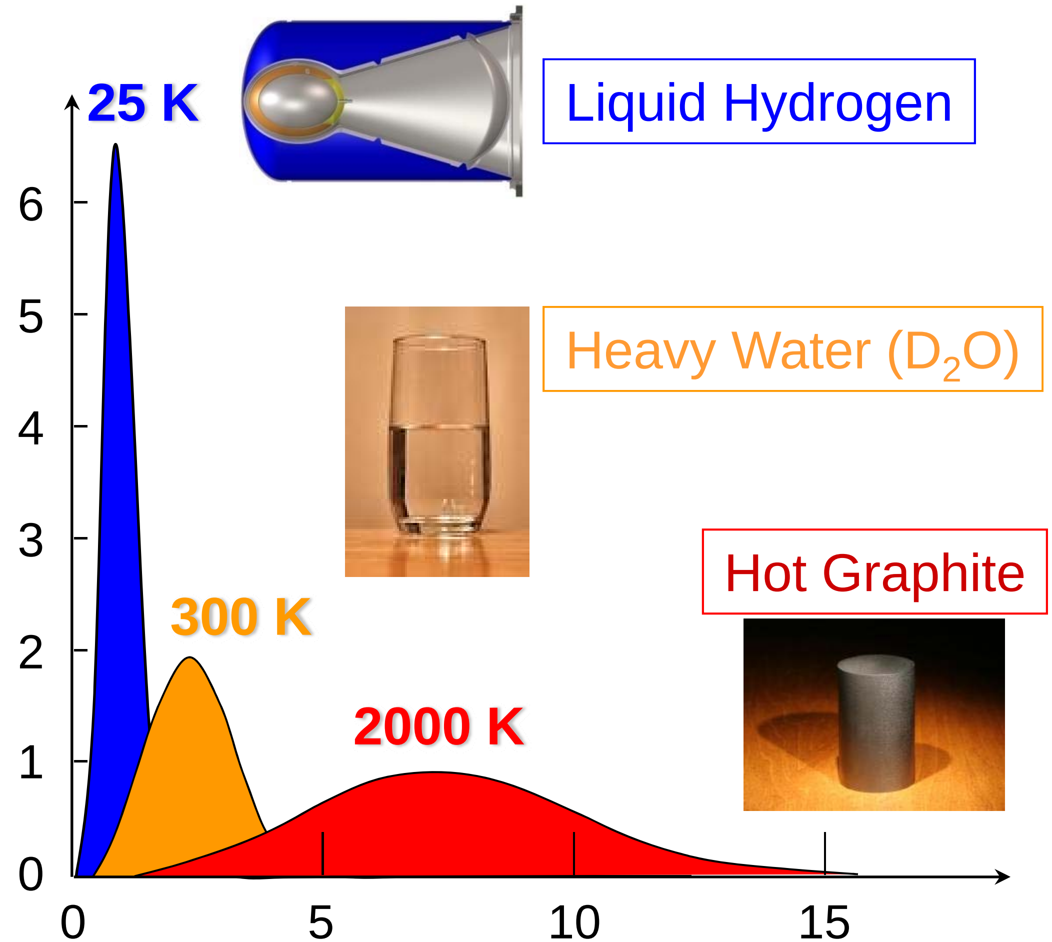


# Neutron Source: Moderation

Maxwellian Distribution

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



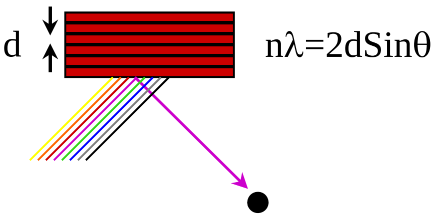

"Fast" neutrons: v = 20,000 km/sec

Neutron velocity *v* (km/sec)

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

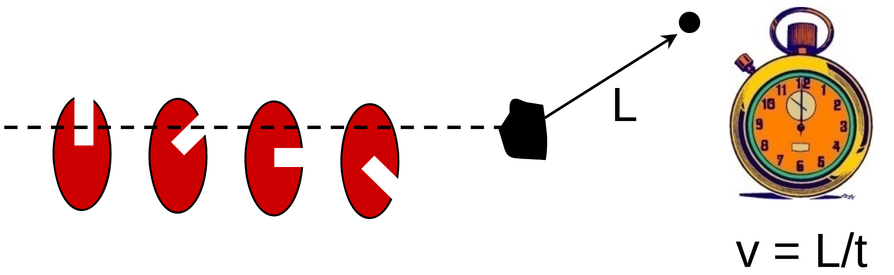
1. Bragg Diffraction

   MACS, SPINS, BT7



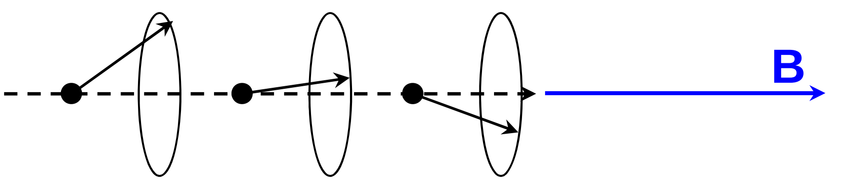

2. Time-of-Flight (TOF)

   DCS

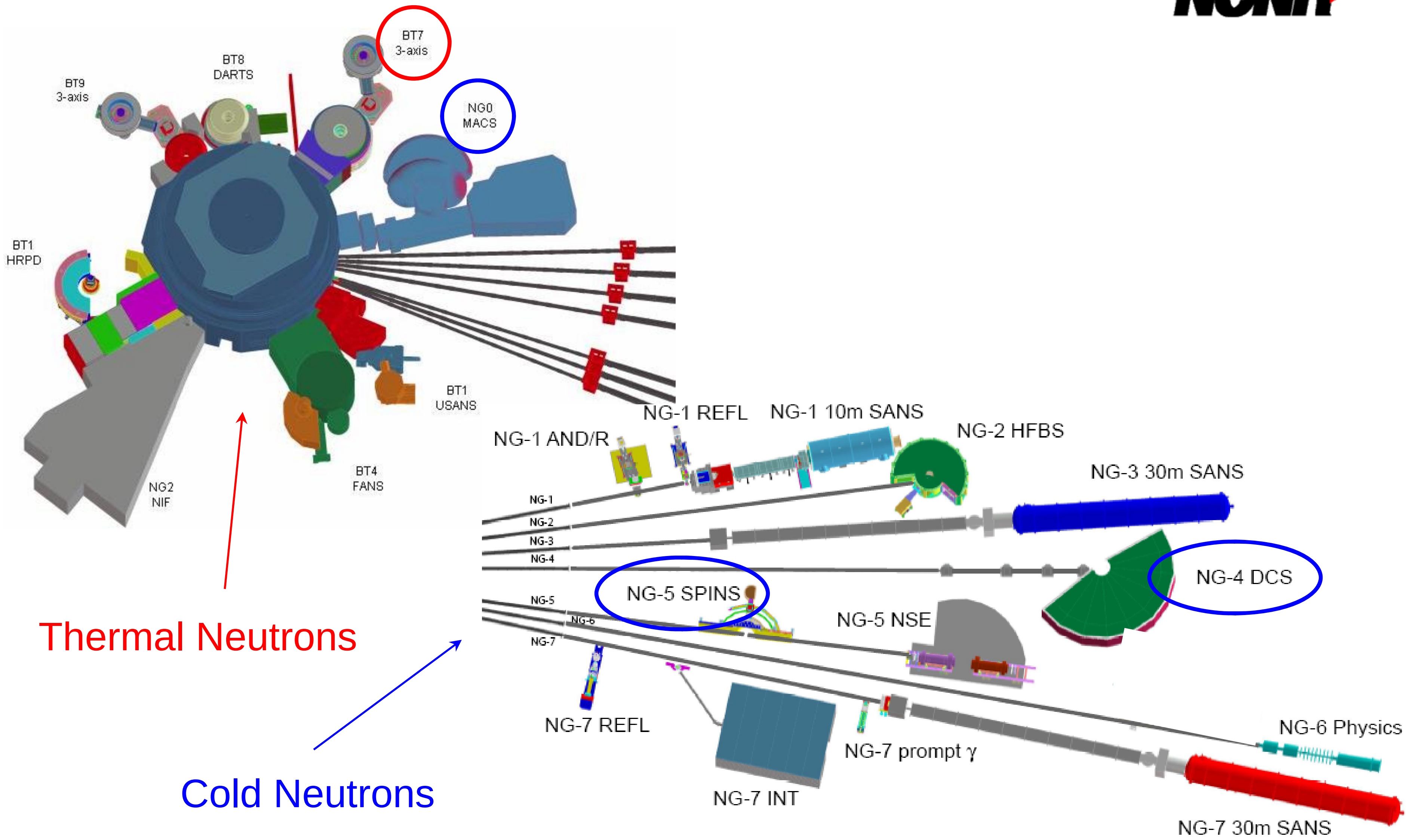



3. Larmor Precession

   NSE



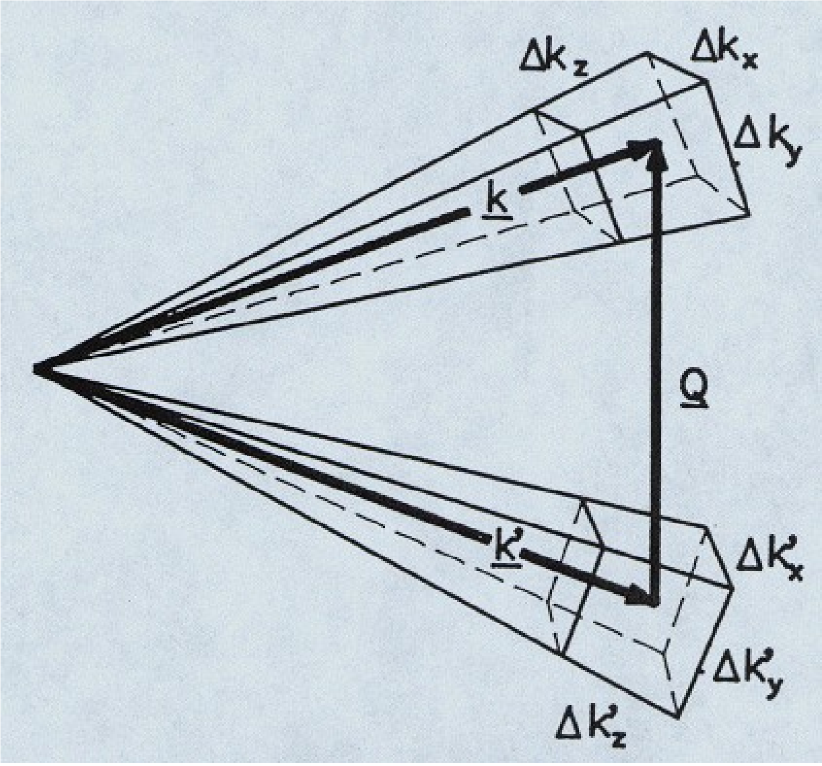
# Why are there so many different spectrometers?



# Why are there so many different spectrometers?

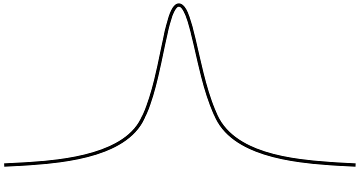
Because neutron scattering is an intensity-limited technique.  Thus detector coverage and resolution MUST be tailored to the science.

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

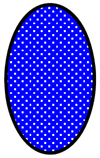



Courtesy of R. Pynn

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

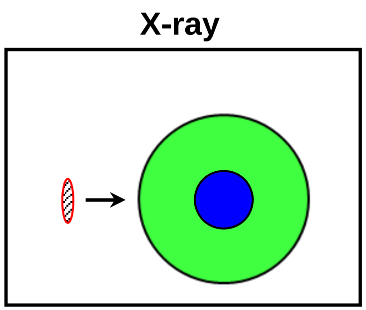


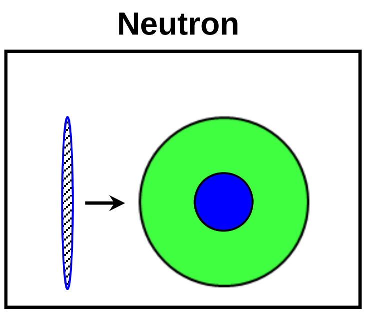
$\propto$

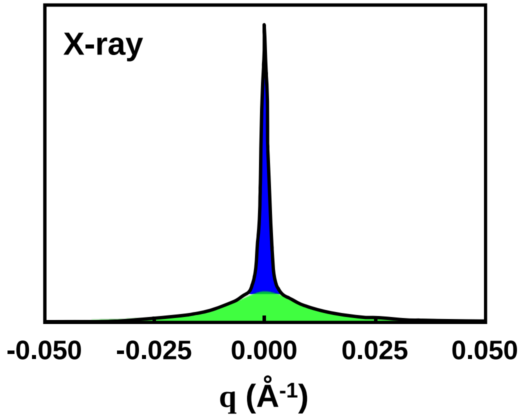


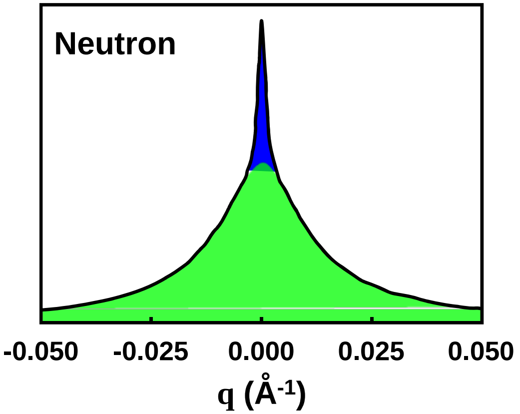
# Q-Resolution Matters!

The "right" resolution depends on what you want to study.



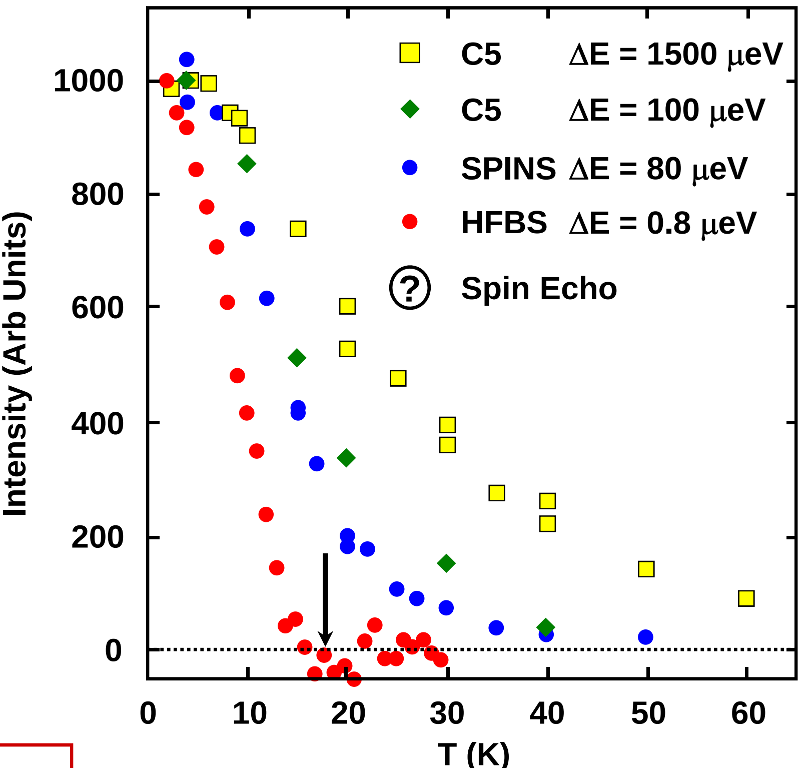
# ħω-Resolution Matters!

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

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

What is $T_N$?

“Elastic” Bragg Peak Intensity

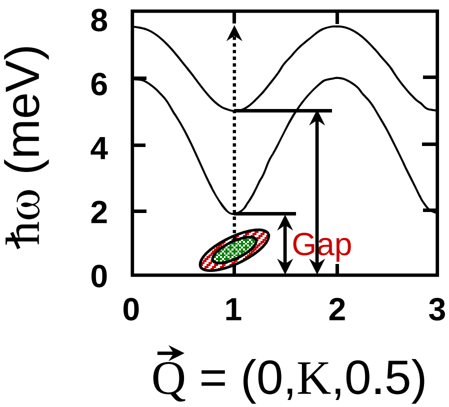


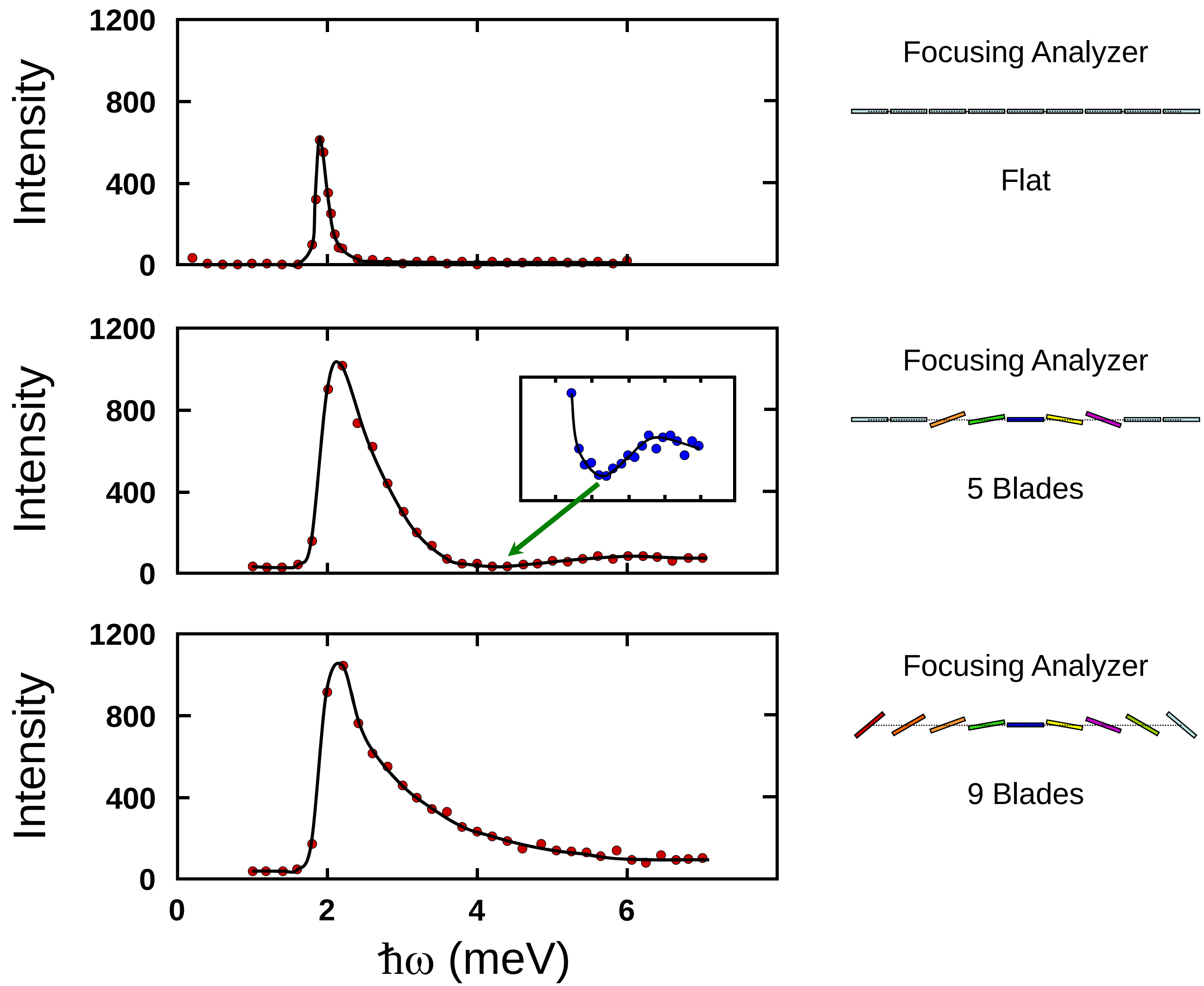

A “fatter” energy resolution integrates over low-energy fluctuations …

# ħω-Resolution Matters!

Another example …

SPINS



# 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)

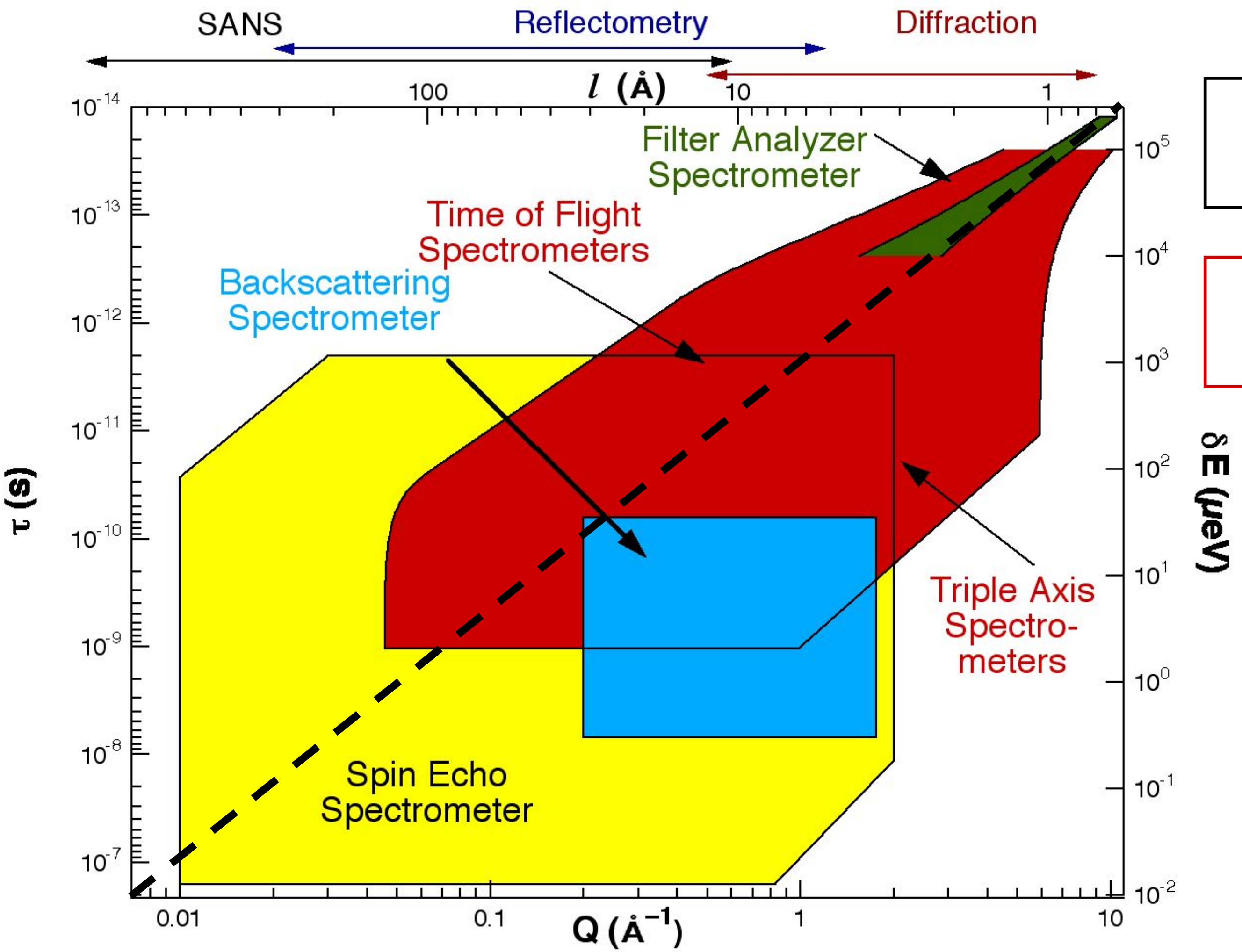
Two additional considerations:

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

2. What momentum resolution ($\Delta Q$) is required?

If all else fails … CALL US!

# 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 BT7 or FANS

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

In between - use DCS, MACS, or SPINS

2. Be certain that the length scales **L** of the relevant motions lie within the range of the spectrometer. For example, recall that $\mathbf{Q} \sim 2\pi/\mathbf{L}$. Then if

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 $\mathbf{Q}$ matter?

Is the expected $\mathbf{Q}$-dependence of the scattering weak?

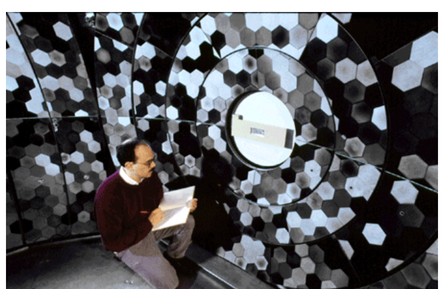
This often means that you want to look at a large region of $\mathbf{Q}$-$\hbar\omega$ space, or that you can sum the data over a large region of $\mathbf{Q}$-$\hbar\omega$ space.

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

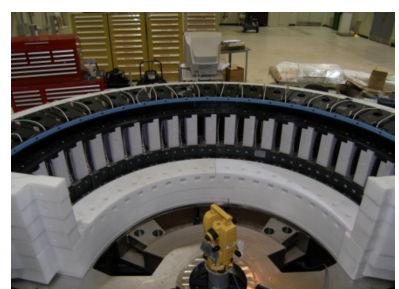
**NO?** Consider 3-axis spectrometers like BT7, SPINS, or MACS.

**DCS**

**HFBS**



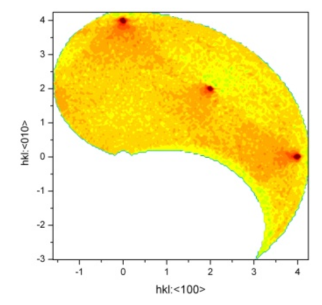
**MACS**



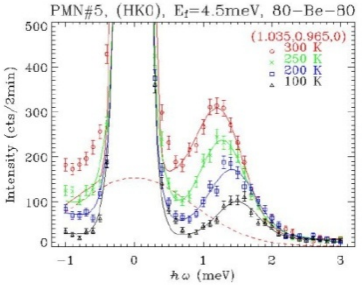
**BT7**

# DCS versus SPINS

DCS – incoherent scattering and/or broad surveys in **Q**-ω




SPINS – coherent scattering and/or limited regions in **Q**-ω



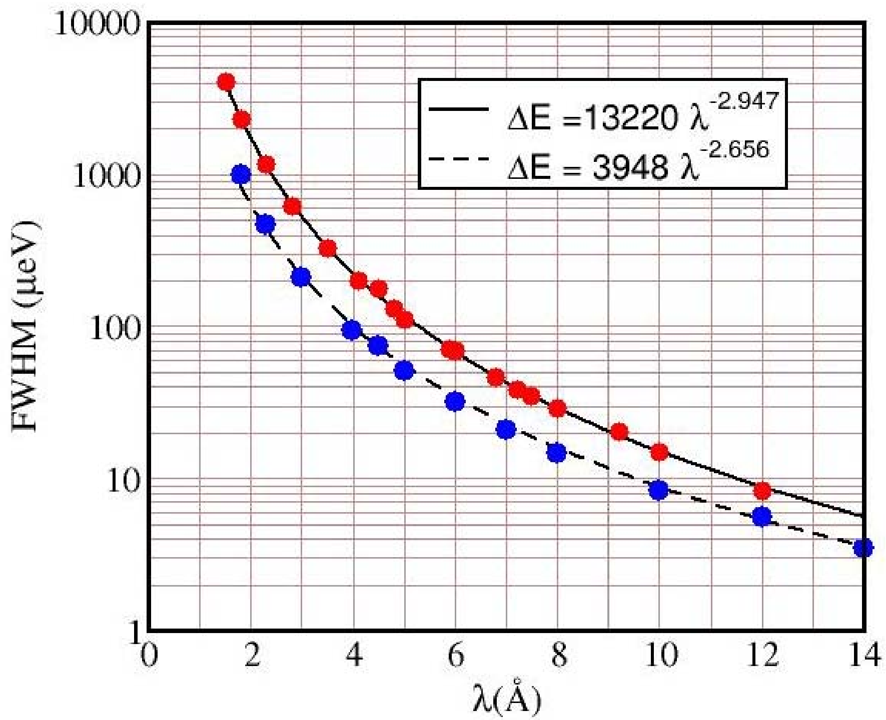

Rules of Thumb: (think carefully before violating)

DCS – systems requiring resolution < 100 μeV

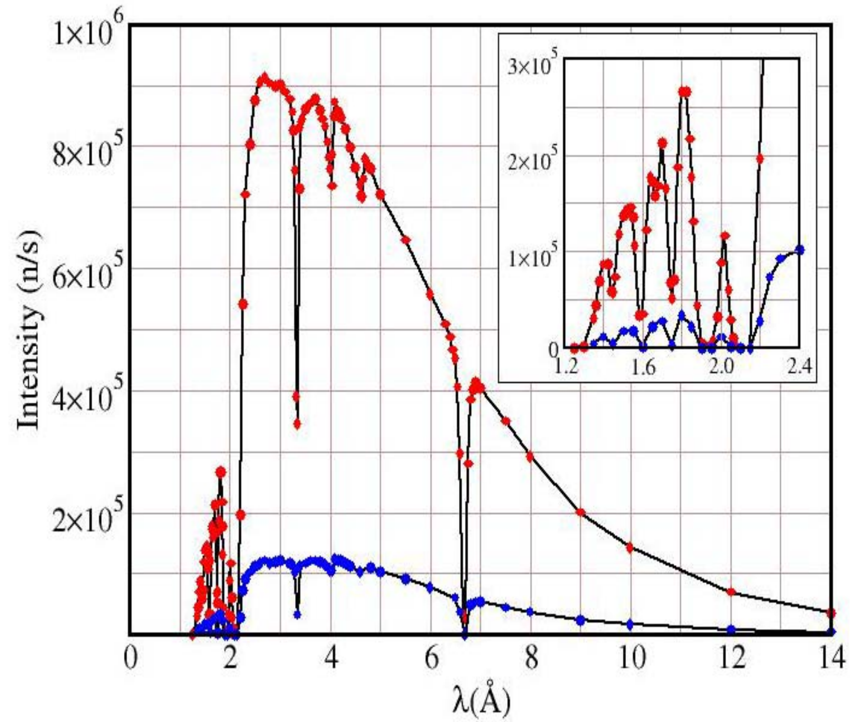
SPINS – single crystals

# Things to consider when choosing DCS

**ΔE**




**I(E)**




Quantities varied

- wavelength λ
- chopper slot widths W

Remember – **Intensity ↓**

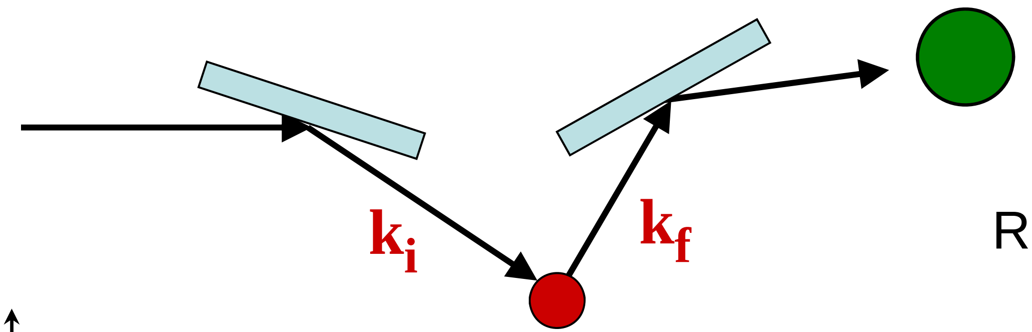
**Resolution ↑**

# Things to consider when choosing SPINS

Triple axis spectrometers are typically used when either -

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

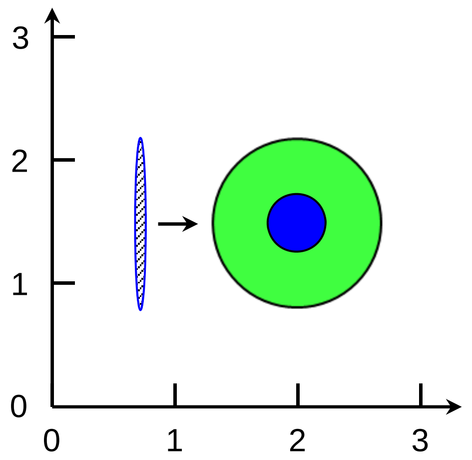
(2) the interesting region of **Q-ω** space is of *limited extent*.




One data point at a time …

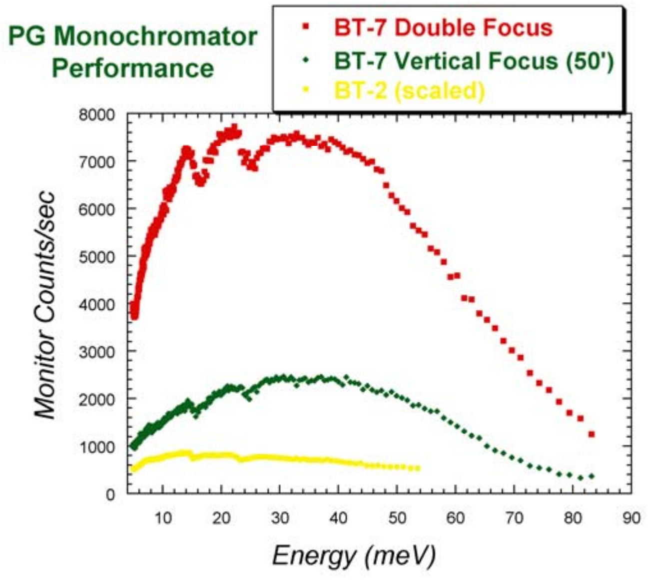
Remember – **Intensity** ↓

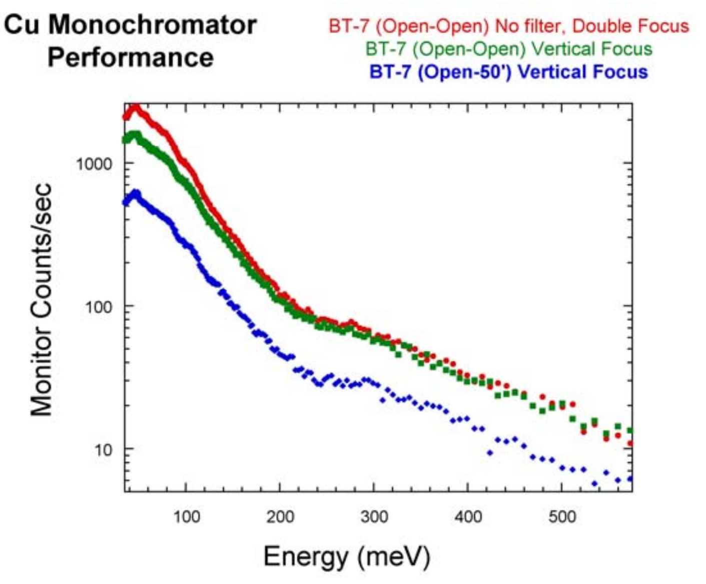
**Resolution** ↑




| 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 |

# Things to consider when choosing BT7



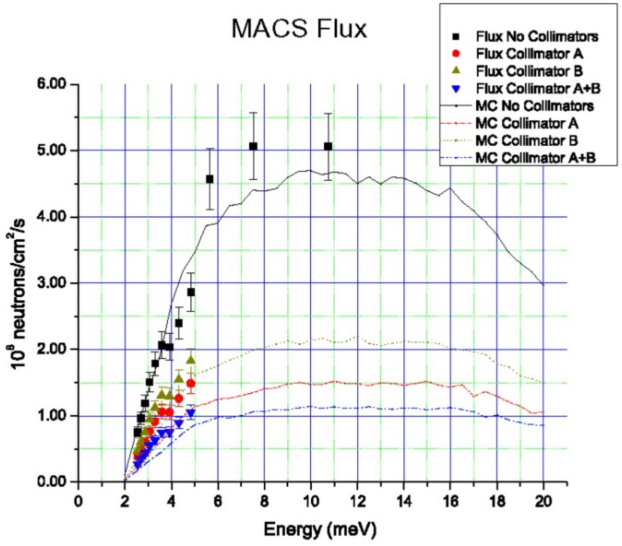




Cu(220) and PG(002) doubly-focusing monochromators provide access to 5 meV < $E_i$ < 500 meV.

Scattering Angle: $0^o < 2\theta < 120^o$

Highest flux thermal triple-axis instrument currently operating.

# Things to consider when choosing MACS




Highest flux cold triple-axis instrument currently operating.

Extremely high flux at sample:
5 x $10^8$ neutrons/$cm^2$-s at
$E_i$=12 meV with open collimators

PG(002) doubly-focusing monochromator provides access to 2.3 meV < $E_i$ < 17 meV. (Cold neutrons)

Energy resolution (FWHM):
0.2 meV < $\delta$E < 1.4 meV.

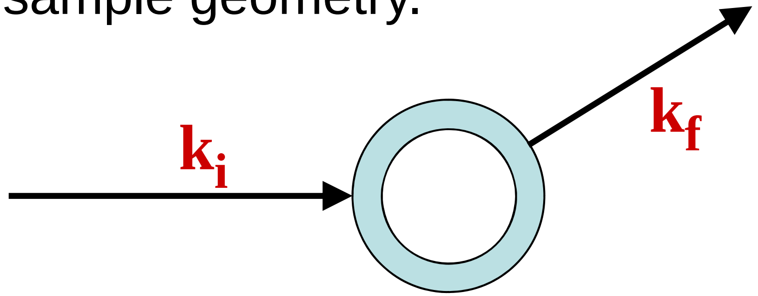
# Sample "design" for triple-axis spectrometers

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

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)

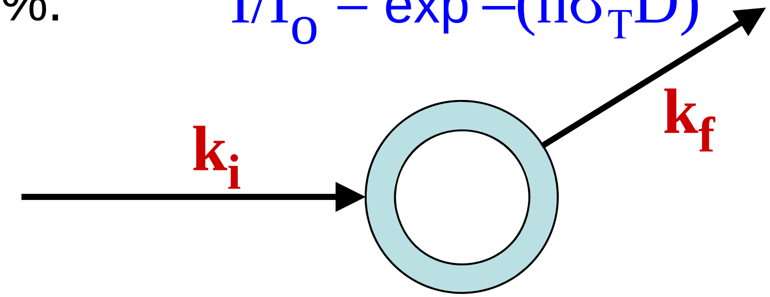
If you have a powder, use cylindrical samples (rather than flat plate).

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

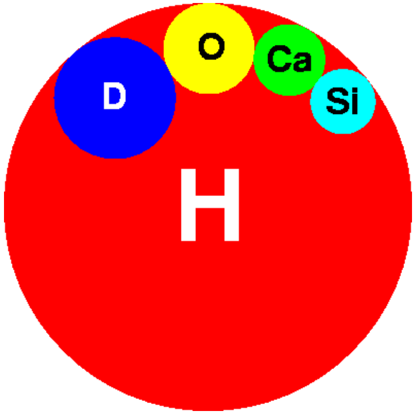


# Sample "design" for DCS

Does the sample contain H?

Remember: Neutrons LOVE H!!

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



# 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

# 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

# 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 –Brian Kirby and Yamali Hernandez

Administrative staff – Julie Keyser

All of the experiment teams

Invited speakers – Feng Ye

**Thanks for coming!**