Dynamics and Neutron Scattering

John R.D. Copley

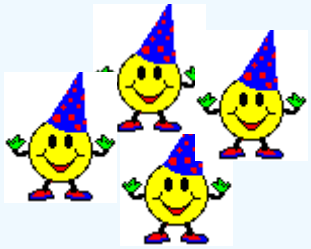
NCNR Neutron Spectroscopy and
Neutron Physics Summer Schools

June 22-26, 2009

Acknowledgments

Center for High Resolution Neutron Scattering (CHRNS)
NSF DMR-0454672

NIST Center for Neutron Research (NCNR)



Yamali and David

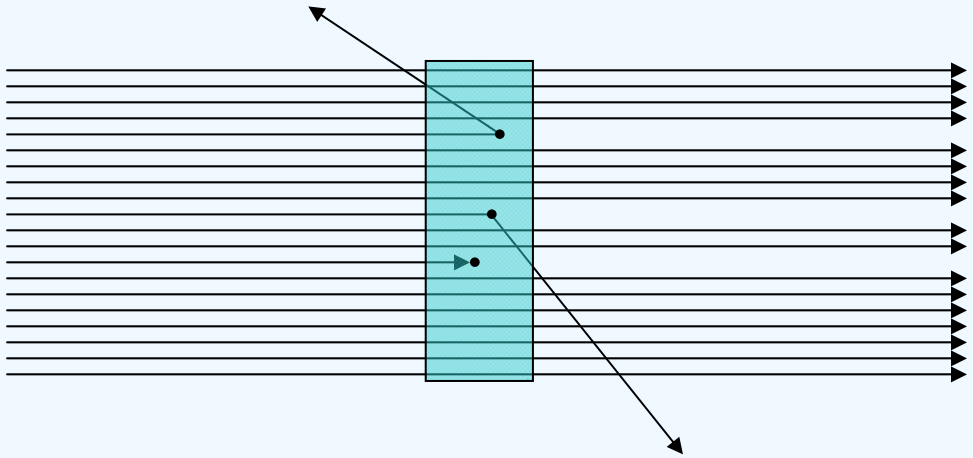
Julie and Mary Ann

Outline

- Cross sections
- Diffraction and spectroscopy
- Elastic and inelastic (and quasielastic) scattering
- Correlation functions
- Single particle motion
- Theoretical expressions
- Samples
- Spectrometers

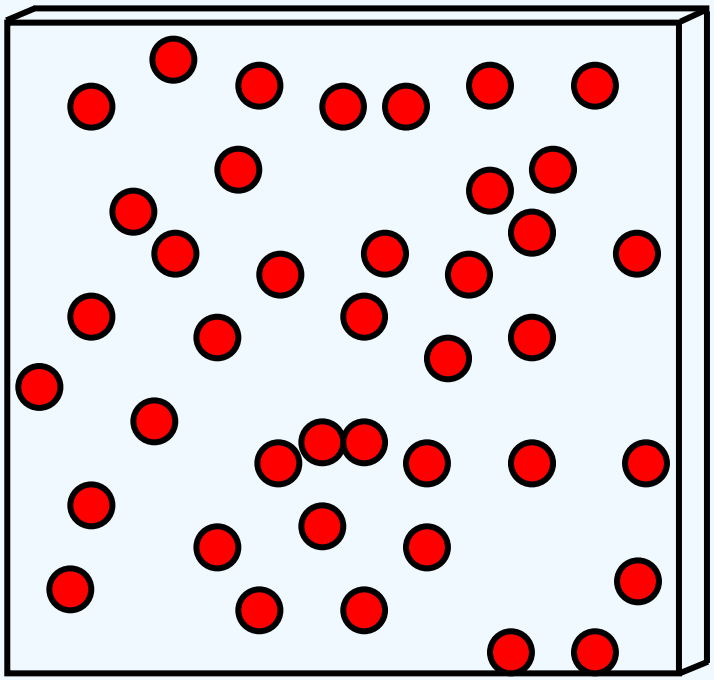
A sample is placed in a beam…

Consider a “thin” sample placed in a neutron beam.
(“thin” implies almost transparent, no shadowing)
The neutrons are transmitted, absorbed, or scattered, with probabilities p_T, p_A and p_S respectively.



$$p_T + p_A + p_S = 1, \quad \text{but what are } p_T,\ p_A \text{ and } p_S\ ?$$

Absorption probability p_A



- N atoms
- sample area A
- sample thickness t
- sample volume V=At
- number density ρ=N/V

$$p_A = \frac{N\sigma_A}{A} = \frac{N\sigma_A t}{V} = \Sigma_A t$$

σ_A is the microscopic absorption cross section (barn/atom)

(1 barn = 10^{-24}cm^2)

$\Sigma_A=\rho\sigma_A$ is the macroscopic absorption cross section (cm^{-1})

Event rates

Our "thin" sample is placed in a beam whose current density (or "flux") is Φ (n/cm^2/s). The current, i.e. the number of neutrons hitting the sample, is $I_0 = \Phi A$ n/s.

The absorption rate is as follows:

$$I_A = I_0 p_A = (\Phi A)(\Sigma_A t) = \Phi V \Sigma_A = \Phi N \sigma_A$$

Similarly the scattering rate is:

$$I_S = I_0 p_S = (\Phi A)(\Sigma_S t) = \Phi V \Sigma_S = \Phi N \sigma_S$$

Hence the transmission rate (n/s) is

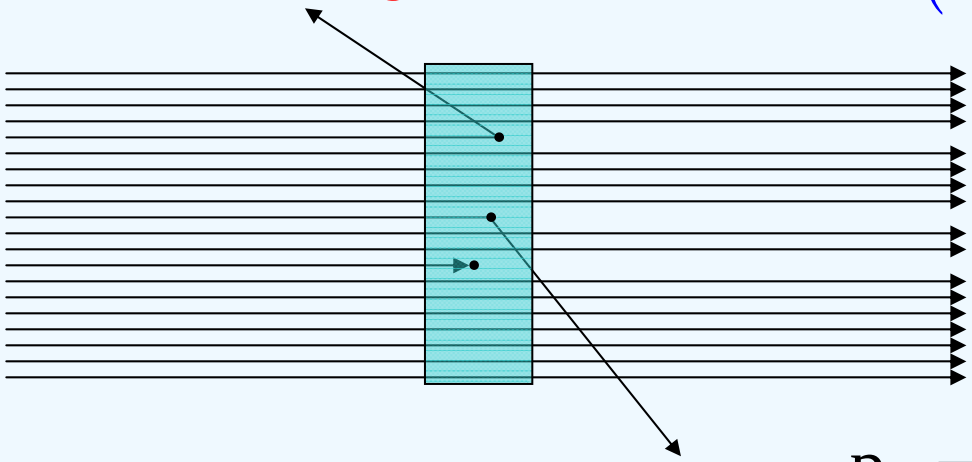
$$I_T = I_0 p_T = I_0 - I_A - I_S = (\Phi A)(1 - \Sigma_T t)$$

where $\Sigma_T = \Sigma_A + \Sigma_S$ is the total removal cross section.

“Not necessarily thin” samples

The scattering, absorption and transmission probabilities for a sample that is “not necessarily thin” are as follows:

Scattering $p_S = \Sigma_S t \rightarrow p_S = \left(1 - e^{-\Sigma_T t}\right)\left(\Sigma_S / \Sigma_T\right)$



(N.B. The scattering may still be followed by absorption, or by additional scattering)

Transmission

$$p_T = \left(1 - \Sigma_S t - \Sigma_A t\right) \Rightarrow p_T = e^{-\Sigma_T t}$$

Absorption

$$p_A = \Sigma_A t \Rightarrow p_A = \left(1 - e^{-\Sigma_T t}\right)\left(\Sigma_A / \Sigma_T\right)$$

Absorption

- As compared with x-ray absorption cross sections, neutron absorption cross sections are generally small.
- Strong absorbers include ^{3}He, ^{6}Li, ^{10}B, ^{113}Cd, ^{135}Xe*, ^{157}Gd.
- For most elements and isotopes the "1/v" law applies:

$$\sigma_{Abs} \propto 1/v \propto \lambda$$

- Important exceptions to the "1/v" law are Cd and Gd.

*http://en.wikipedia.org/wiki/Xenon#Isotopes

(2.6×10^{6} barns)

Absorption cross sections

1 barn (b) = 10^{-24}cm^2

log scale

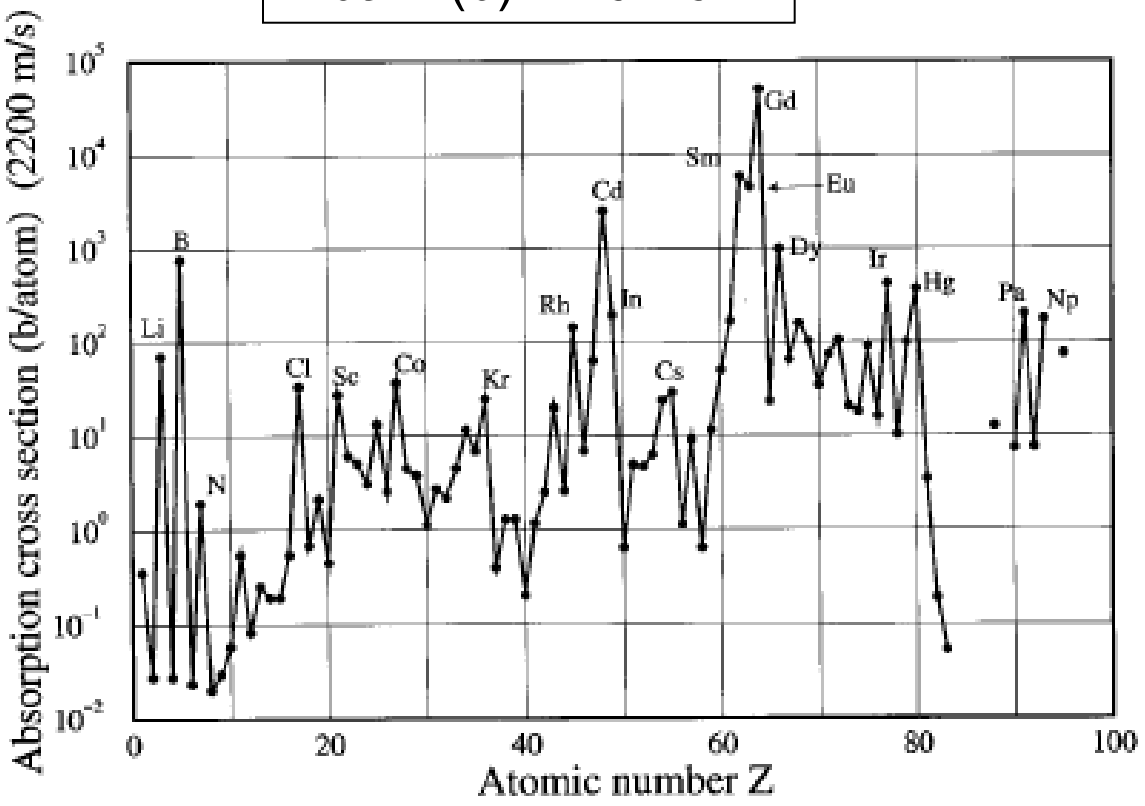
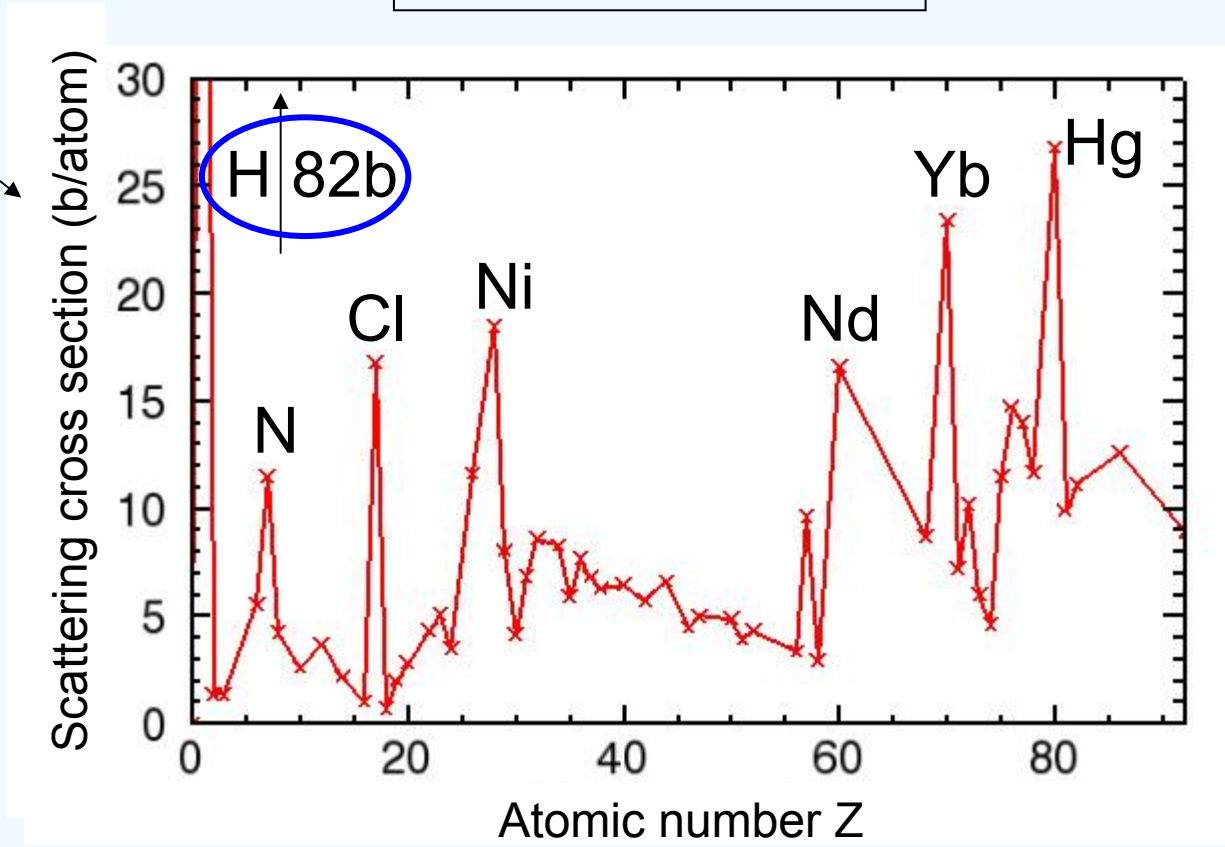


Fig. 8. The absorption cross section for 2200 m/s neutrons for the naturally occurring elements. Notice that the ordinate is plotted on a log scale.

Scattering cross sections

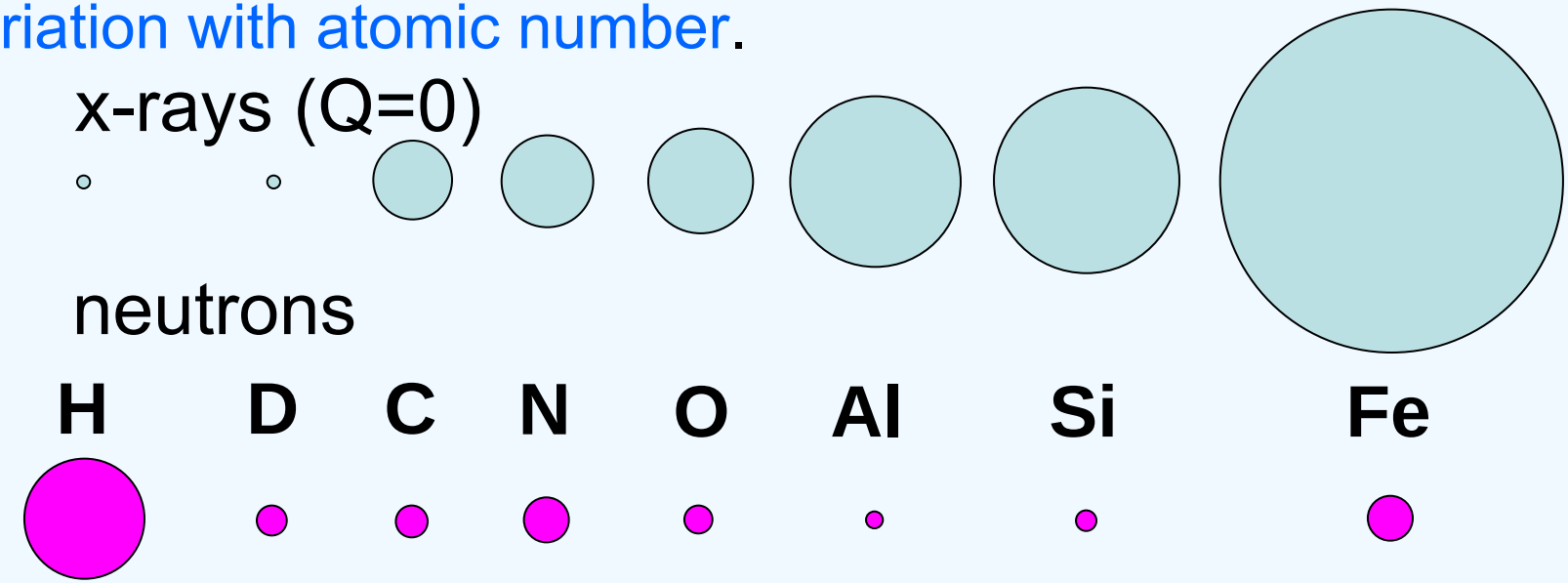
linear scale

1 barn (b) = 10^{-24}cm^2



Comparison with x-rays

As compared with x-ray scattering cross sections, which vary as Z^2, neutron scattering cross sections show little systematic variation with atomic number.

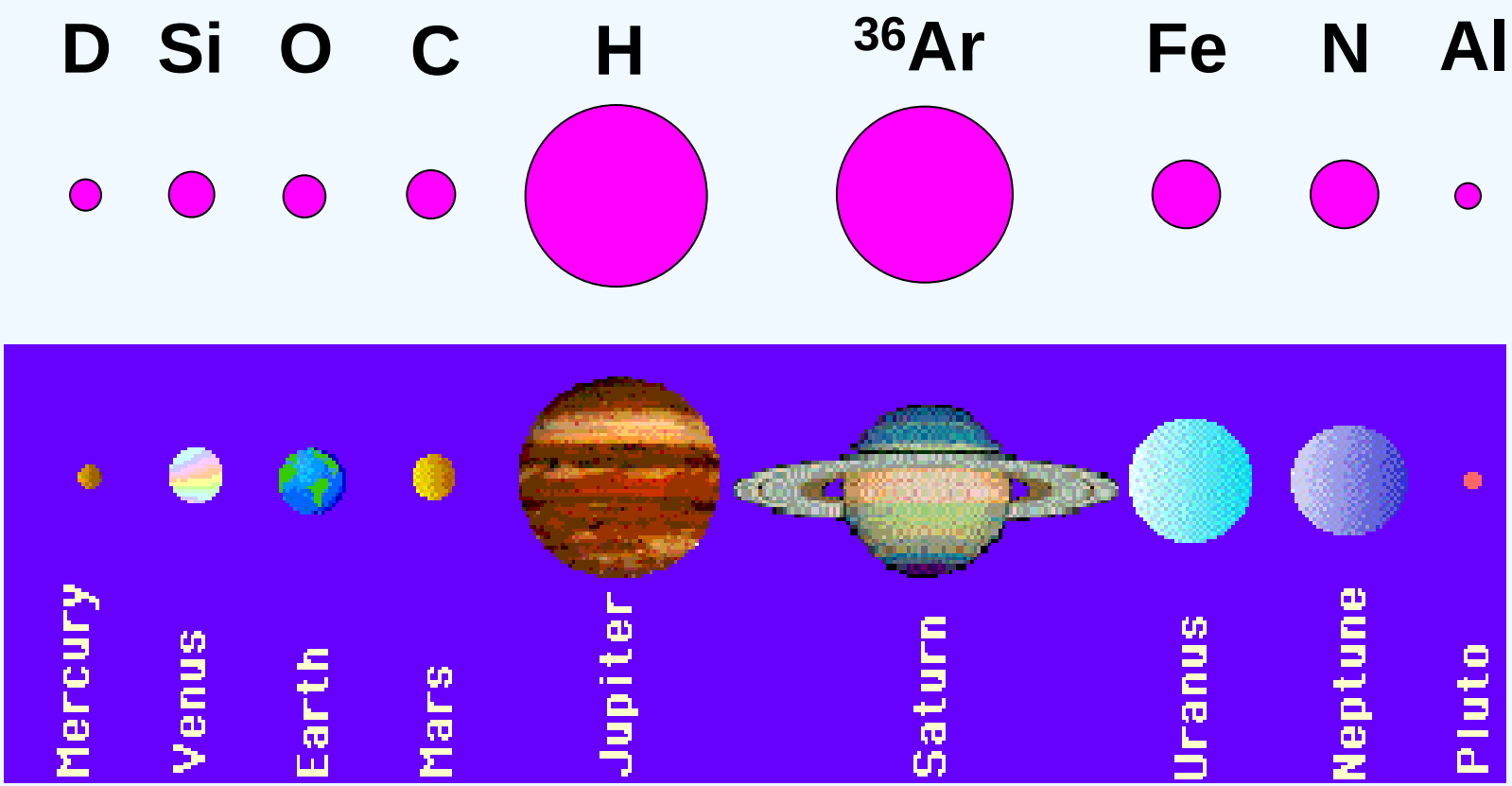


X-ray cross sections vary with Q*; neutron cross sections do not.

(We ignore the neutron's magnetic interaction)

* Q is momentum transfer

The planets


D
Si
O
C
H
36Ar
Fe
N
Al
Mercury
Venus
Earth
Mars
Jupiter
Saturn
Uranus
Neptune
Pluto

Cross section examples

[Using absorption cross sections at 2200 m/s (1.8 Å)]

		0.1 mm water	1 m (dry) air	1 mm aluminum	20 thou cadmium
"Molecule"		H2O	(N2)0.8(O2)0.2	Al	Cd
sigma_s	barn	168.3	20.1	1.5	6.5
sigma_a	barn	0.67	3.04	0.23	2520
sigma_t	barn	168.97	23.14	1.73	2526.5
Density	g/cc	1	0.00117	2.7	8.65
Mol. Wt.		18	28.8	27	112.4
Number density	E24/cc	0.033333	0.000024	0.060000	0.046174
SIGMA_S	cm-1	5.610000	0.000490	0.090000	0.300133
SIGMA_A	cm-1	0.022333	0.000074	0.013800	116.359431
SIGMA_T	cm-1	5.632333	0.000564	0.103800	116.659564
Thickness	cm	0.01	100	0.1	0.0508
Scattering		**5.5%**	**4.8%**	**0.9%**	**0.3%**
Absorption		**0.0%**	**0.7%**	**0.1%**	**99.5%**
Transmission		**94.5%**	**94.5%**	**99.0%**	**0.3%**

The scattered neutrons

Terminology

In a **neutron diffraction** experiment, intensity is measured as a function of scattering angle 2θ, with **no energy analysis**.

In a **neutron spectroscopy** experiment, intensity is measured as a function of both scattering angle 2θ **and energy transfer** $E_i - E_f$.

Elastic scattering is scattering with **no change in energy**.

Inelastic scattering is scattering with **a change in energy**.

(**Quasielastic scattering** is a type of inelastic scattering.)

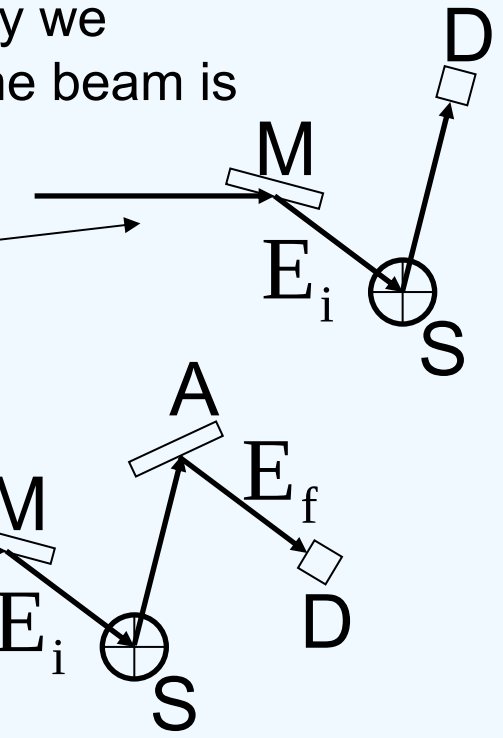
Studying the scattered neutrons

How we study the scattered neutrons depends on several factors including the type of source. For simplicity we assume that the source is continuous and that the beam is ***monochromatic*** (single incident energy E_i).

(a) We could study the intensity as a function of **scattering angle 2θ**.

(b) We could study the intensity as a function of both **scattering angle 2θ and scattered energy E_f**.

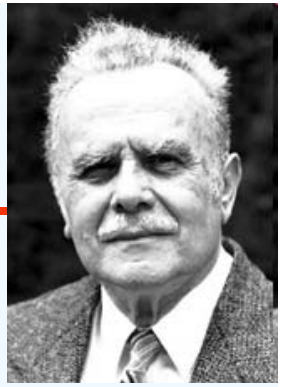
These are examples of **diffraction (no energy analysis)** and **spectroscopy (energy analysis)**.



Elastic scattering: $E_i = E_f$.

Inelastic scattering: $E_i \neq E_f$.

Diffraction and Spectroscopy



The Nobel Prize in Physics 1994

"to Professor Clifford G. Shull .. for the development of the neutron diffraction technique"

"to Professor Bertram N. Brockhouse .. for the development of neutron spectroscopy"

"Both methods are based on the use of neutrons flowing out from a nuclear reactor. When the neutrons bounce against (are scattered by) atoms in the sample being investigated, their *directions* change, depending on the atoms' relative positions. This shows how the atoms are arranged in relation to each other, that is, the structure of the sample. Changes in the neutrons' *velocity,* however, give information on the atoms' movements, e.g. their individual and collective oscillations, that is their dynamics.

... Clifford G. Shull has helped answer the question of **where atoms "are"**

... Bertram N. Brockhouse [has helped with] the question of **what atoms "do"**

http://nobelprize.org/nobel_prizes/physics/laureates/1994/press.html

The single differential cross section

For a "thin" sample, the total integrated scattering is:

$$I_S = \phi N \sigma_S .$$

The measured intensity in a diffraction experiment (on a "thin" sample) is related to the single differential scattering cross section:

$$I_S(E_i, 2\theta) = \phi N \left(\frac{d\sigma}{d\Omega} \right) \Delta\Omega$$

solid angle

When there is one type of atom we obtain, in the static approximation,

$$\frac{d\sigma}{d\Omega}(E_i, 2\theta) = \frac{\sigma_S}{4\pi} S(Q)$$

$(Q = 4\pi \sin\theta / \lambda)$

ONLY DEPENDS ON THE SAMPLE

The single differential cross section is approximately proportional to the "structure factor" $S(Q)$.

Thus the measured intensity is approximately proportional to S(Q).

The double differential cross section

The measured intensity in a spectroscopy experiment is related to the double differential scattering cross section:

$$I_S(E_i, 2\theta, E_f) = \phi N \left(\frac{d^2\sigma}{d\Omega dE_f} \right) \Delta\Omega \Delta E_f .$$

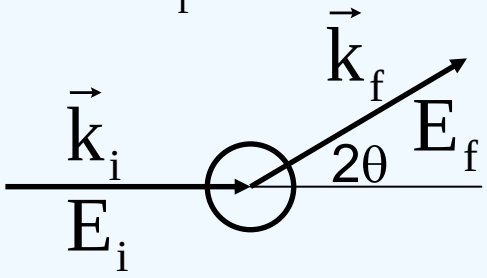
energy window

The double differential cross section is related to the "scattering function"

$$S(Q,\omega)$$

When there is one type of atom, we obtain

$$\frac{d^2\sigma}{d\Omega dE_f}(E_i, 2\theta, E_f) = \frac{\sigma}{4\pi\hbar}\frac{k_f}{k_i} S(Q,\omega),$$



ONLY DEPENDS ON THE SAMPLE

The measured intensity is proportional to $(k_f/k_i)S(Q,\omega)$.

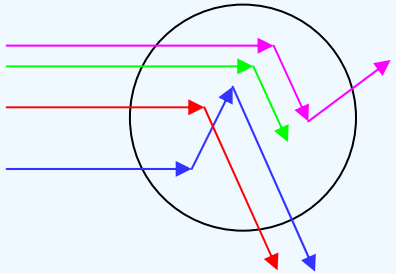
$$\vec{Q} = \vec{k}_i - \vec{k}_f \qquad \hbar\omega = E_i - E_f$$

Caveats

- More than one type of atom

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{1}{\hbar}\frac{k_f}{k_i} b^2 S(Q,\omega) \Rightarrow \frac{d^2\sigma}{d\Omega dE_f} = \frac{1}{\hbar}\frac{k_f}{k_i} \sum_{m,m'} b_m b_{m'} S_{mm'}(Q,\omega)$$

- Multiple scattering and self shielding
- Container scattering and sample attenuation
- Backgrounds
- Resolution
- “Spurions”

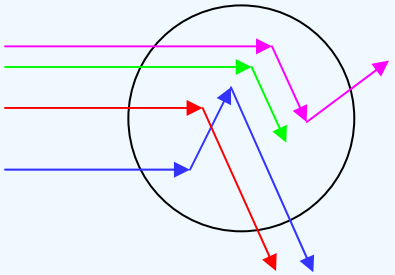


(σ_S varies with E)

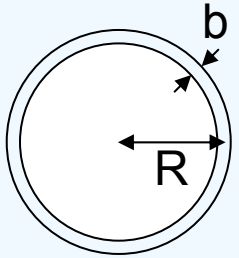
Multiple scattering and self-shielding

For slab geometry self-shielding (SS) depends strongly on orientation; for annular geometry it is almost isotropic

The 90% transmission "rule of thumb" (no absorption)

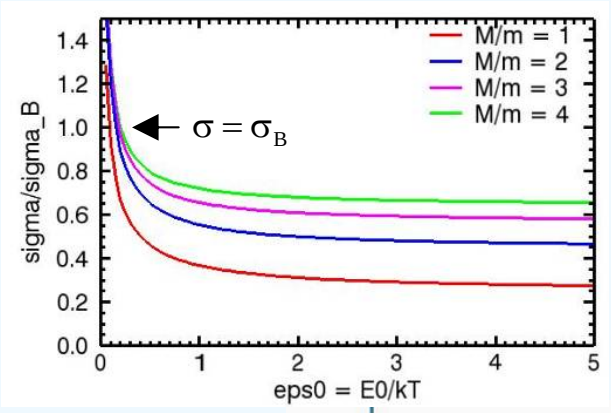


- The "rule" is that if T=90%, S_1=10% and S_m/S_1=10%, and if that is the case multiple scattering (MS) can be neglected.



- The first part is valid for slab geometry, not necessarily valid for other geometries: for example, consider annular geometry with b=0.1 mm and R=10 mm, i.e. b/R = 0.01; if T=90%, S_1=8.5% and $S_m/S_1 \approx 18\%$.

- If indeed S_m/S_1 = 10%, can neglect of MS be justified? What if S_m/S_1 = 15%?



If T is calculated what value should be used for σ_s?

In general σ_s depends on E_i, T, chemistry, morphology etc… See J.R.D. Copley, Neutron News, 18(1), 30 (2007).

An excellent reference for MS/SS is V.F. Sears, Adv. Phys. 24, 1 (1975).

Multiple scattering

Quotes from early papers

"The average of distributions obtained at small angles of scattering (Q<1.4) was taken to be the multiple scattering component, …"

"The thickness of the water films ranged from 0.01 inches (~0.08 M.F.P.) to 0.035 inches (~0.3 M.F.P.) depending on the amount of multiple scattering which could be tolerated. ... Multiple scattering was estimated roughly [ref.] as shown ..."

Quotes from more recent papers

"Sample thicknesses were kept around 0.2 mm to achieve transmissions of ≈ **90 %** and avoid multiple scattering effects."

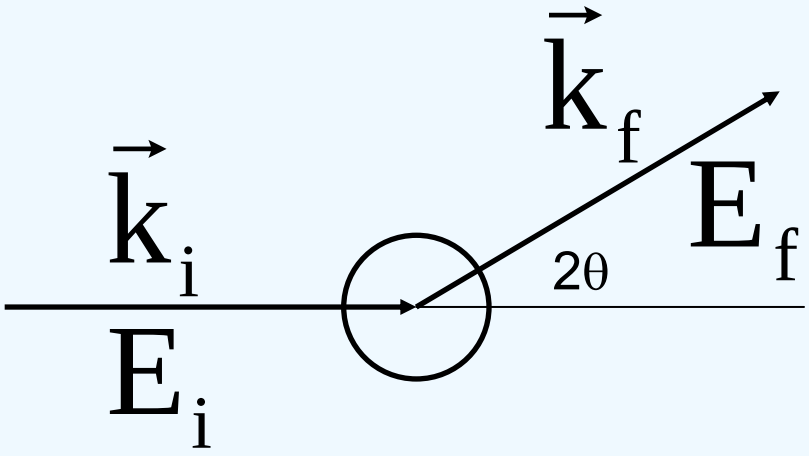
"The sample thickness was chosen to ensure **90%** neutron transmission and thus minimize multiple scattering effects."

"… sample holders chosen to ensure greater than **90%** neutron beam transmission through the sample in order to minimize the effects of multiple scattering …"

"The multiple scattering was minimized using a small thickness for the sample, which was also confirmed by a transmission higher than **0.9**."

"Total neutron scattering from the samples was ~**10%**; thus, multiple scattering was negligible, …"

Q, ω, 2θ, k_i, k_f, E_i, and E_f



Alternative notations

2θ or θ or ϕ

k_i or k_0 or k

E_i or E_0 or E

k_f or k', etc.

$\vec{k}_i$ is the incident neutron wave vector

$\vec{k}_f$ is the scattered neutron wave vector

E_i is the incident neutron energy

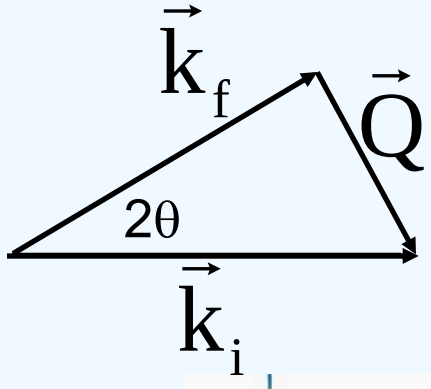
E_f is the scattered neutron energy

$\vec{Q}$ is the wave vector transfer

$\hbar\omega$ is the energy transfer

2θ is the scattering angle

Scattering triangle



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

$$\hbar\omega = E_i - E_f$$

Exact and approximate relationships

$$(1)\quad \lambda = \frac{h}{mv} = \frac{2\pi}{k} \longrightarrow \boxed{\lambda(\text{Å}) \approx 4\tau(\mu s / mm)}$$

$$(2)\quad E = \frac{1}{2}mv^2 = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

$$\boxed{E(meV) \approx 2\left[k\left(\text{Å}^{-1}\right)\right]^2 \approx \frac{82}{\left[\lambda(\text{Å})\right]^2}}$$

Wavelength, energy, velocity, …

A thermal neutron with wavelength 2 Å has energy ≈20 meV and velocity ≈2000 ms^{-1}.

λ	E	v	τ
Å	meV	m/s	μs/mm
1	82	4000	0.25
2	20.5	2000	0.5
4	5.1	1000	1
8	1.3	500	2

1 meV ≈ 0.24×10^{12} c/s (THz)

1.52 ps^{-1}

8.1 cm^{-1}

11.6K

0.023 kcal/mol

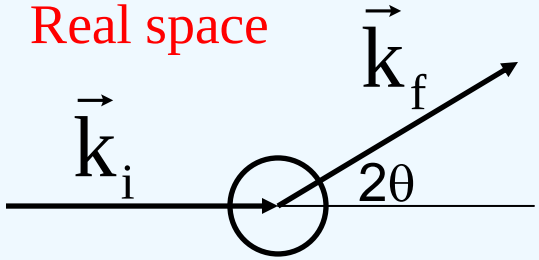
0.10 kJ/mol

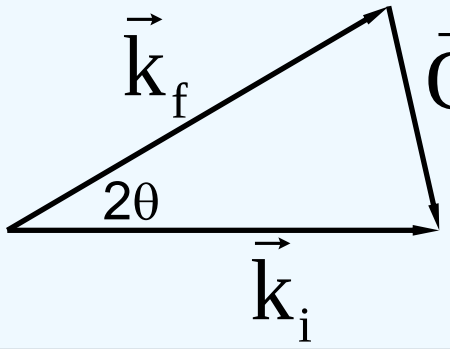
(1Å=0.1nm)

Elastic and inelastic scattering

$$\hbar\omega = E_i - E_f \qquad \vec{Q} = \vec{k}_i - \vec{k}_f$$

Real space





Elastic, $\hbar\omega = 0$

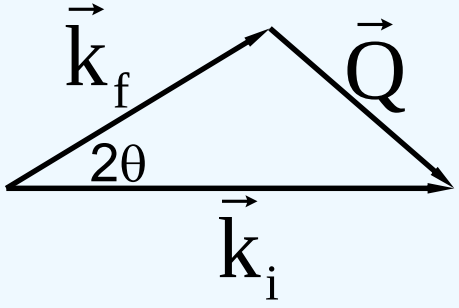
$k_i = k_f$

$(Q = 2k_i \sin\theta)$

Inelastic, $\hbar\omega > 0$

Neutron energy loss

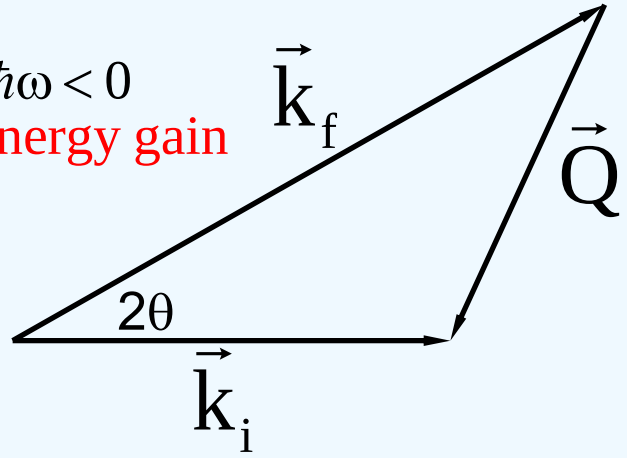
$k_i > k_f$



Inelastic, $\hbar\omega < 0$

Neutron energy gain

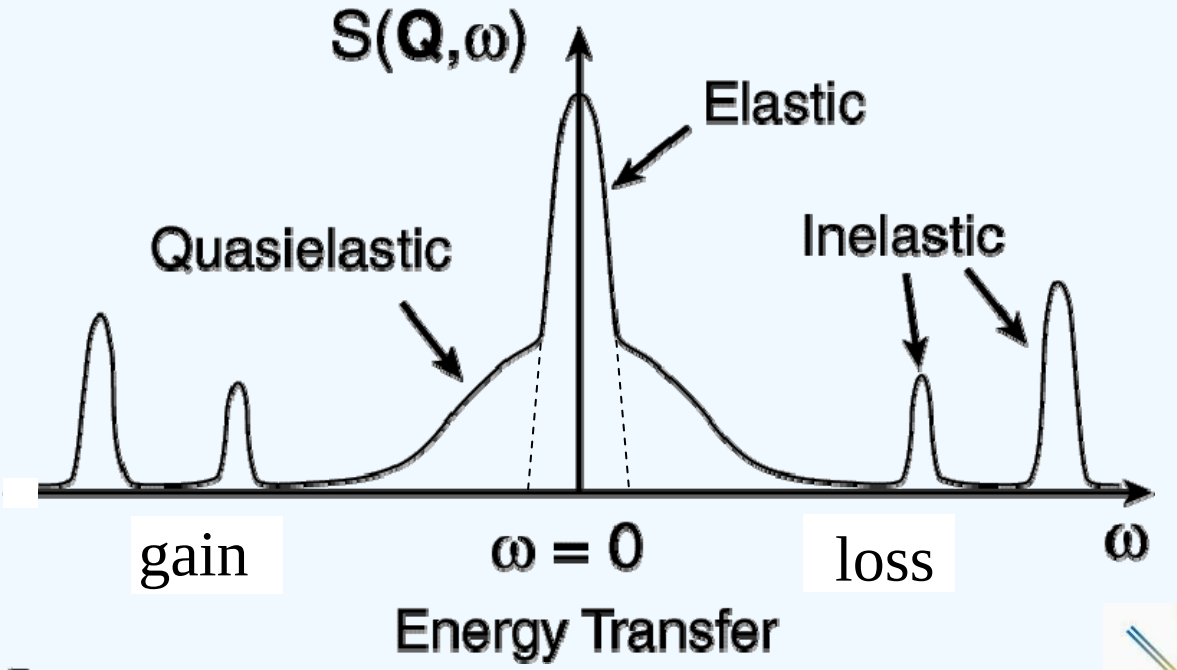
$k_i < k_f$



Quasielastic scattering

Quasielastic scattering is a type of inelastic scattering that is centered at $\omega = 0$, typically associated with diffusive motion, whereas inelastic peaks are usually associated with lattice or localized excitations.

The schematic spectrum shown below is resolution-broadened.



APS Annual Meeting 1955, NYC

MINUTES OF THE 1955 ANNUAL MEETING HELD AT NEW YORK CITY, JANUARY 27–29, 1955

(Corresponding to *Bulletin of the American Physical Society*, Volume 30, No. 1)

M7. Slow Neutron Spectrometry—A New Tool for the Study of Energy Levels in Condensed Systems. B. N. BROCKHOUSE, *Chalk River Laboratories*.—It has long been realized that energy distributions of initially monoenergetic neutrons scattered by molecules or condensed systems would yield important information not otherwise easily accessible to experiment. With high reactor flux and suitable spectrometer design such measurements are now feasible. Monoenergetic neutrons, selected from the *NRX* reactor spectrum by a crystal, are scattered by the specimen and the energy distribution of the scattered neutrons is analyzed by another crystal. A survey of the field has been made and more detailed studies are in progress. The sharp division of incoherent scattering into elastic and inelastic components predicted by theory has been verified with vanadium. In liquid lead, light water, and heavy water a similar division into a "quasi-elastic" component, and an inelastic component which increases with increasing angle, can be made. For coherent scattering the "elastic" component is associated with the peaks in the liquid diffraction pattern. In liquid lead the inelastic component is similar to that of the solid at about the same temperature and angle of scattering. Diffuse magnetic scattering, studied with MnO and Mn_2O_3, and with Cr_2O_3 above and below its Néel temperature, is largely inelastic, the mean energy changes being of the order of the Néel temperatures.

The functions S (Q,ω), I (Q,t), G (r,t)

Most neutron spectrometers measure S(Q,ω) (*).

The quantity I(Q,t), known as the "intermediate scattering function", is the frequency Fourier transform of S(Q,ω):

$$I(\vec{Q},t) = \hbar \int S(\vec{Q},\omega) \exp(i\omega t) d\omega$$

This quantity is typically computed, e.g. in molecular dynamics simulations, for comparison with experiment.
The neutron spin echo technique measures this quantity directly.

The quantity G(r,t), known as the "time-dependent pair correlation function", is the reciprocal space Fourier transform of I(Q,t):

$$G(\vec{r},t) = \frac{1}{(2\pi)^3} \int I(\vec{Q},t) \exp\left(-i\vec{Q}.\vec{r}\right) d\vec{Q}$$

These functions contain detailed information about the collective (pair) dynamics of materials.

(*) sort of

Single particle motion

So far we have implicitly assumed that all atoms of a given element have the same scattering cross section (which is true in the x-ray case).

But what if they don't? This can happen if there is more than one isotope and/or nonzero nuclear spins. In that case there is a second contribution to the double differential cross section. In the simplest case it reads as follows:

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_{coh}}{4\pi\hbar}\frac{k_f}{k_i}S(Q,\omega) + \frac{\sigma_{inc}}{4\pi\hbar}\frac{k_f}{k_i}S_S(Q,\omega)$$

where

- $S(Q,\omega)$ reflects the collective behavior of the particles (e.g. phonons)
- $S_S(Q,\omega)$ reflects the single particle (self) behavior (e.g. diffusion)
- σ_{coh} and σ_{inc} are coherent and incoherent scattering cross sections respectively.

Single particle motion (multi-element)

When there is one type of atom

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_{coh}}{4\pi\hbar}\frac{k_f}{k_i}S(Q,\omega) + \frac{\sigma_{inc}}{4\pi\hbar}\frac{k_f}{k_i}S_S(Q,\omega)$$

More generally

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{1}{\hbar}\frac{k_f}{k_i}\sum_{m,m'} b_m b_{m'} S_{mm'}(Q,\omega) + \frac{1}{\hbar}\frac{k_f}{k_i}\sum_m \frac{\sigma_{inc,m}}{4\pi} S_{S,m}(Q,\omega)$$

Coherent and incoherent scattering

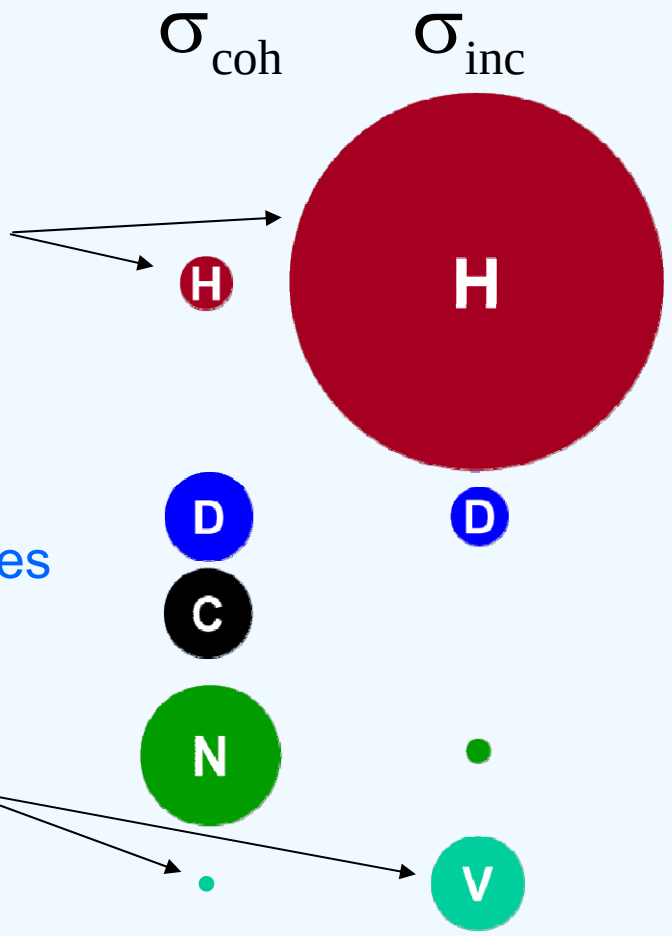
For most elements the coherent cross section dominates.

Hydrogen is a very important exception:

Its huge incoherent cross section enables studies of hydrogen diffusion in a variety of materials, ...

Selective deuteration enables detailed studies of the dynamics of polymers and biomolecules, ...

Vanadium has a significant incoherent cross section and a very small coherent cross section. It is used for instrument calibration/normalization.



The single particle functions

We need to modify some of our earlier statements:

Most neutron spectrometers measure $S(Q,\omega)$ and $S_S(Q,\omega)$ (*).

The quantity $I_S(Q,t)$, is the frequency Fourier transform of $S_S(Q,\omega)$:

$$I_S(\vec{Q},t) = \hbar \int S_S(\vec{Q},\omega) \exp(i\omega t) d\omega$$

This quantity is typically computed, e.g. in molecular dynamics simulations, for comparison with experiment.

The neutron spin echo technique measures $I(Q,t)$ and $I_S(Q,t)$.

The quantity $G_S(r,t)$, known as the "time-dependent self correlation function", is the reciprocal space Fourier transform of $I_S(Q,t)$:

$$G_S(\vec{r},t) = \frac{1}{(2\pi)^3} \int I_S(\vec{Q},t) \exp\left(-i\vec{Q}.\vec{r}\right) d\vec{Q}$$

The self functions contain detailed information about the single particle (self) dynamics of materials.

(*) sort of

Phonons

The one-phonon coherent creation cross section is

$$\left.\frac{d^2\sigma}{d\Omega dE}\right|_{coh}^{cre}(\mathbf{Q},\omega)=\frac{k_f}{k_i}\frac{(2\pi)^3}{V_0}\frac{1}{2N}\sum_{\mathbf{q},j}\left|\sum_{k=1}^{n}\frac{b_k\left[\mathbf{Q}.\mathbf{e}_k(\mathbf{q},j)\right]}{\sqrt{m_k}}e^{-i\mathbf{Q}.\mathbf{R}_k}e^{-W_k}\right|^2\frac{\left\langle n_j(\mathbf{q})+1\right\rangle}{\omega(\mathbf{q},j)}\delta\left(\omega(\mathbf{q},j)-\omega\right)\sum_{\mathbf{G}}\delta(\mathbf{Q}-\mathbf{q}-\mathbf{G})$$

The one-phonon incoherent creation cross section is

$$\left.\frac{d^2\sigma}{d\Omega dE}\right|_{inc}^{cre}(\mathbf{Q},\omega)=\frac{k_f}{k_i}\frac{1}{2N}\sum_{\mathbf{q},j}\sum_{k=1}^{n}\frac{\sigma_{inc,k}}{4\pi}\frac{\left[\mathbf{Q}.\mathbf{e}_k(\mathbf{q},j)\right]^2}{m_k}e^{-2W_k}\frac{\left\langle n_j(\mathbf{q})+1\right\rangle}{\omega(\mathbf{q},j)}\delta\left(\omega(\mathbf{q},j)-\omega\right)$$

This is sometimes considerably simplified:

$$\frac{d^2\sigma}{d\Omega dE}\propto\frac{k_f}{k_i}\frac{Q^2}{\omega}e^{-2W}\left[n(\omega)+1\right]g(\omega)$$

Constrained molecules

$$S(Q,\omega) = S_V(Q,\omega) \otimes S_T(Q,\omega) \otimes S_R(Q,\omega)$$

The vibrational motion is written as a Debye-Waller factor: $S_V(Q,\omega) = e^{-\frac{1}{3}Q^2\langle u^2\rangle}\delta(\omega)$

The translational motion is assumed to be random jump diffusion (Singwi-Sjőlander model: see Bée, eq. 5.101):

$$S_T(Q,\omega) = \frac{1}{\pi}\frac{\Gamma_T(Q)}{\omega^2 + \left[\Gamma_T(Q)\right]^2} \quad \text{with} \quad \Gamma_T(Q) = \frac{D_T Q^2}{1 + D_T Q^2 \tau_0}$$

The rotational motion is assumed to be random diffusion on a sphere (Sears model: see Bée, eq. 6.16):

$$S_R(Q,\omega) = j_0^2(Qa)\delta(\omega) + \frac{1}{\pi}\sum_{\ell=1}^{\infty}(2\ell+1)j_\ell^2(Qa)\frac{\ell(\ell+1)D_R}{\omega^2 + \left[\ell(\ell+1)D_R\right]^2}$$

The result (neglecting $\ell > 1$), is a sum of two Lorentzians:

$$S_{inc}(Q,\omega) = e^{-\frac{1}{3}Q^2\langle u^2\rangle}\left\{ j_0^2(Qa)\frac{1}{\pi}\frac{\Gamma_T(Q)}{\omega^2 + \left[\Gamma_T(Q)\right]^2} + 3j_1^2(Qa)\frac{1}{\pi}\frac{\Gamma_R(Q)+\Gamma_T(Q)}{\omega^2 + \left[\Gamma_R(Q)+\Gamma_T(Q)\right]^2}\right\}$$

What can one study using neutrons?

Single particle and/or collective motions in all sorts of materials

such as metals, insulators, semiconductors, glasses, magnetic materials, superconductors, helium, plastic crystals, molecular solids, molten salts, biomolecules, water in confined geometries, polymers, micelles, microemulsions, …

under all sorts of conditions

such as T from ≈100 mK to ≈1600K; P to ≈2.5 GPa; B to ≈11.5T; E to 6 kV; controlled humidity, etc., etc.,

provided that

- the length and time scales (Q and ω ranges) and the desired instrumental resolution are consistent with instrumental capabilities
- the scattering (and absorption) cross sections are acceptable
- the quantity of material is sufficient

See the NCNR annual reports (on the Web) for examples.

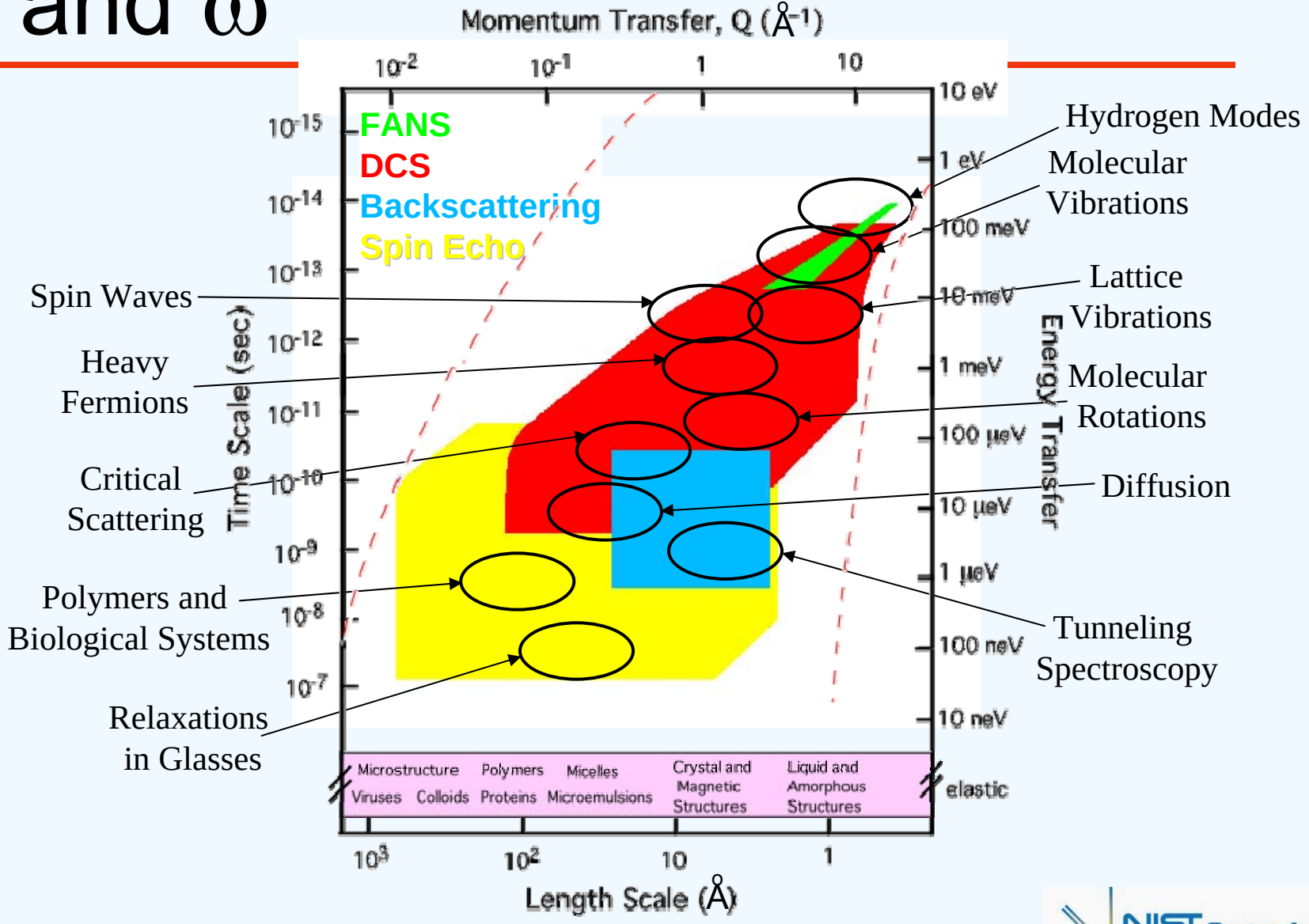
Matching time scales

← (slow) —— S(Q,ω) —— (fast) →

Resolution ↕

	delta-function peak	Narrow peak	Medium width peak	Broad peak	Flat back-ground
Low resn. (broad)	(Elastic)	**Elastic**	**Elastic**	**Match**	(Flat)
Med. resn. (medium)	(Elastic)	**Elastic**	**Match**	**Flat**	(Flat)
High resn. (narrow)	(Elastic)	**Match**	**Flat**	**Flat**	(Flat)

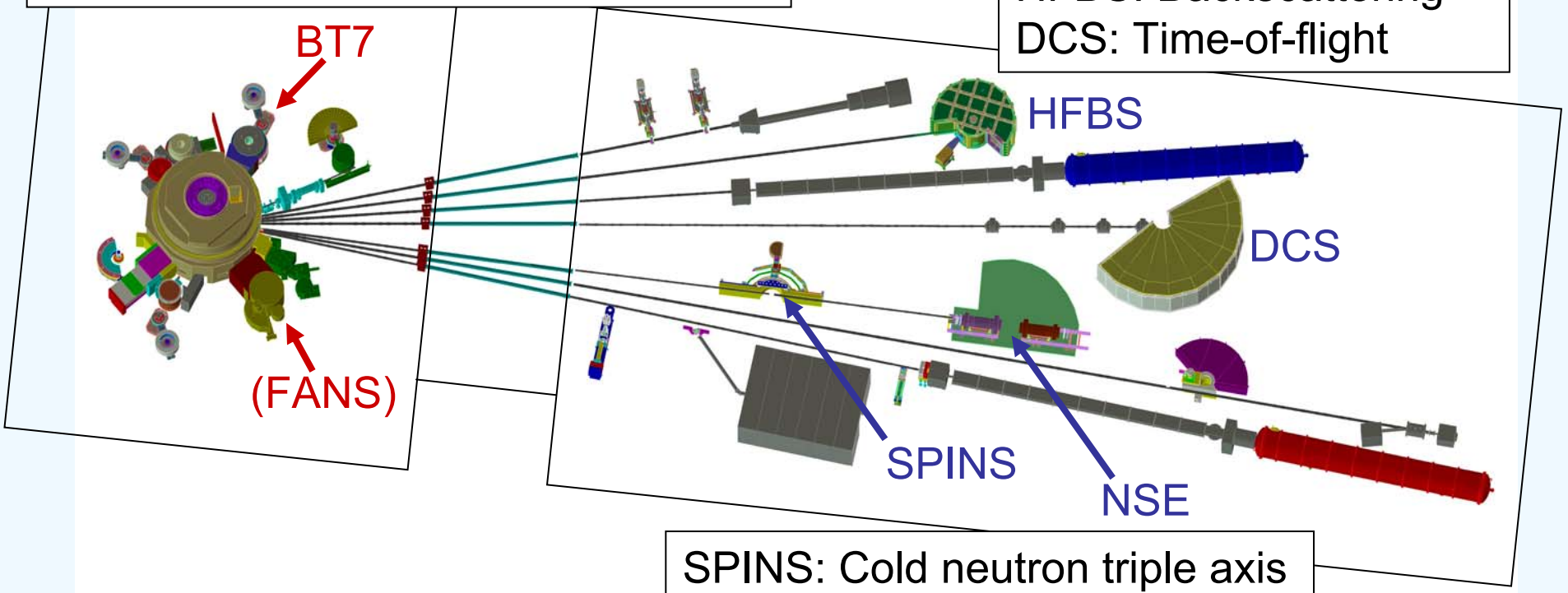
Q and ω


Momentum Transfer, Q (Å⁻¹)
10⁻²
10⁻¹
1
10
FANS
DCS
Backscattering
Spin Echo
Time Scale (sec)
10⁻¹⁵
10⁻¹⁴
10⁻¹³
10⁻¹²
10⁻¹¹
10⁻¹⁰
10⁻⁹
10⁻⁸
10⁻⁷
Energy Transfer
10 eV
1 eV
100 meV
10 meV
1 meV
100 μeV
10 μeV
1 μeV
100 neV
10 neV
elastic
Microstructure
Viruses
Colloids
Polymers
Proteins
Micelles
Microemulsions
Crystal and Magnetic Structures
Liquid and Amorphous Structures
10³
10²
10
1
Length Scale (Å)
Hydrogen Modes
Molecular Vibrations
Lattice Vibrations
Molecular Rotations
Diffusion
Tunneling Spectroscopy
Spin Waves
Heavy Fermions
Critical Scattering
Polymers and Biological Systems
Relaxations in Glasses

Summer school spectrometers

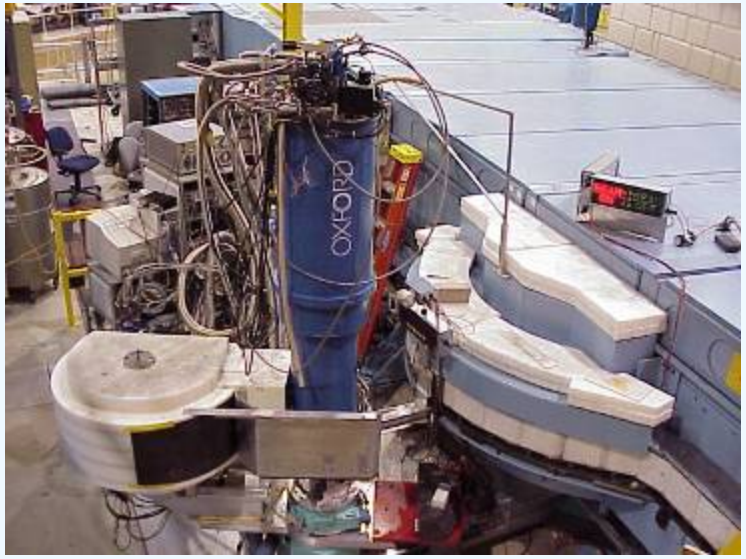
BT7: Thermal neutron triple axis
(FANS: Filter analyzer spectrometer)

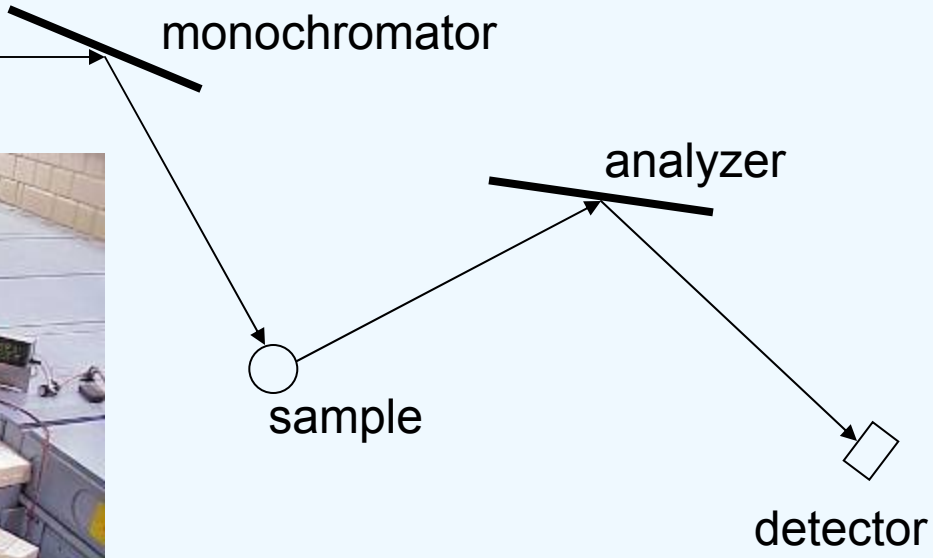
HFBS: Backscattering
DCS: Time-of-flight



SPINS: Cold neutron triple axis
NSE: Neutron spin echo

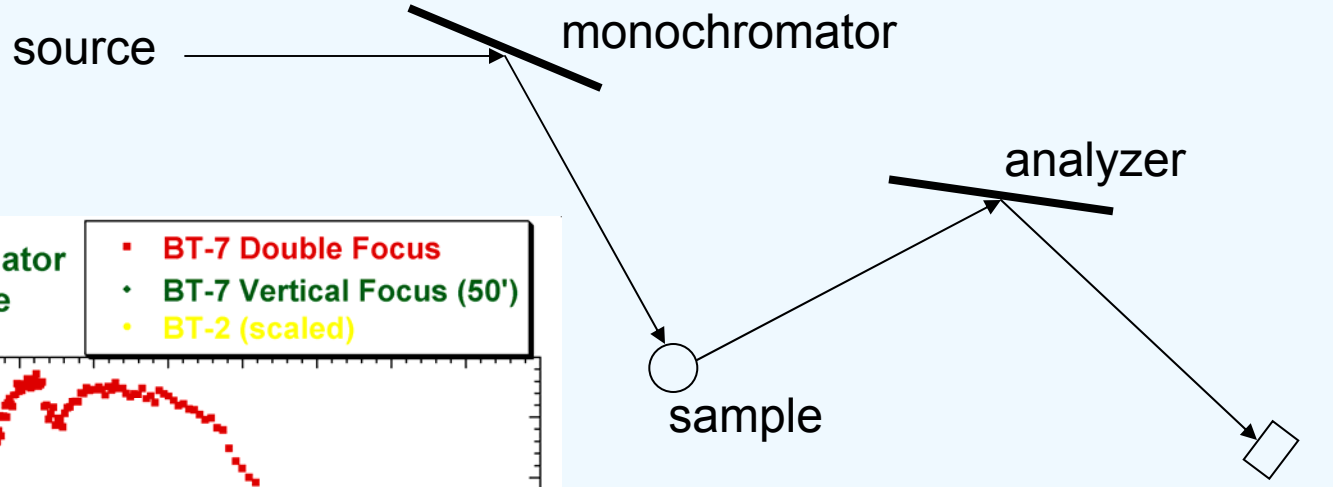
Cold triple axis spectrometer

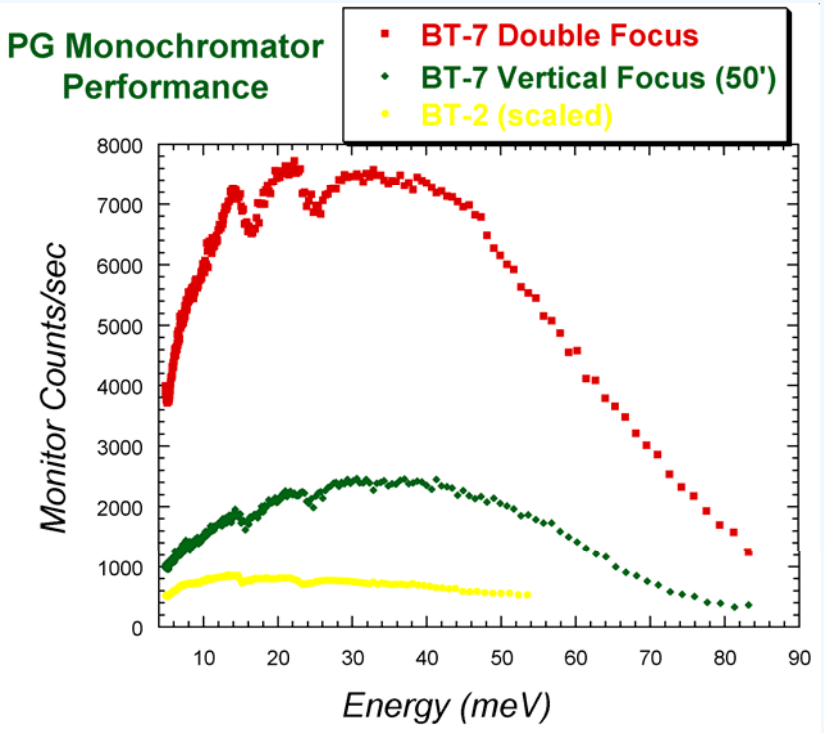




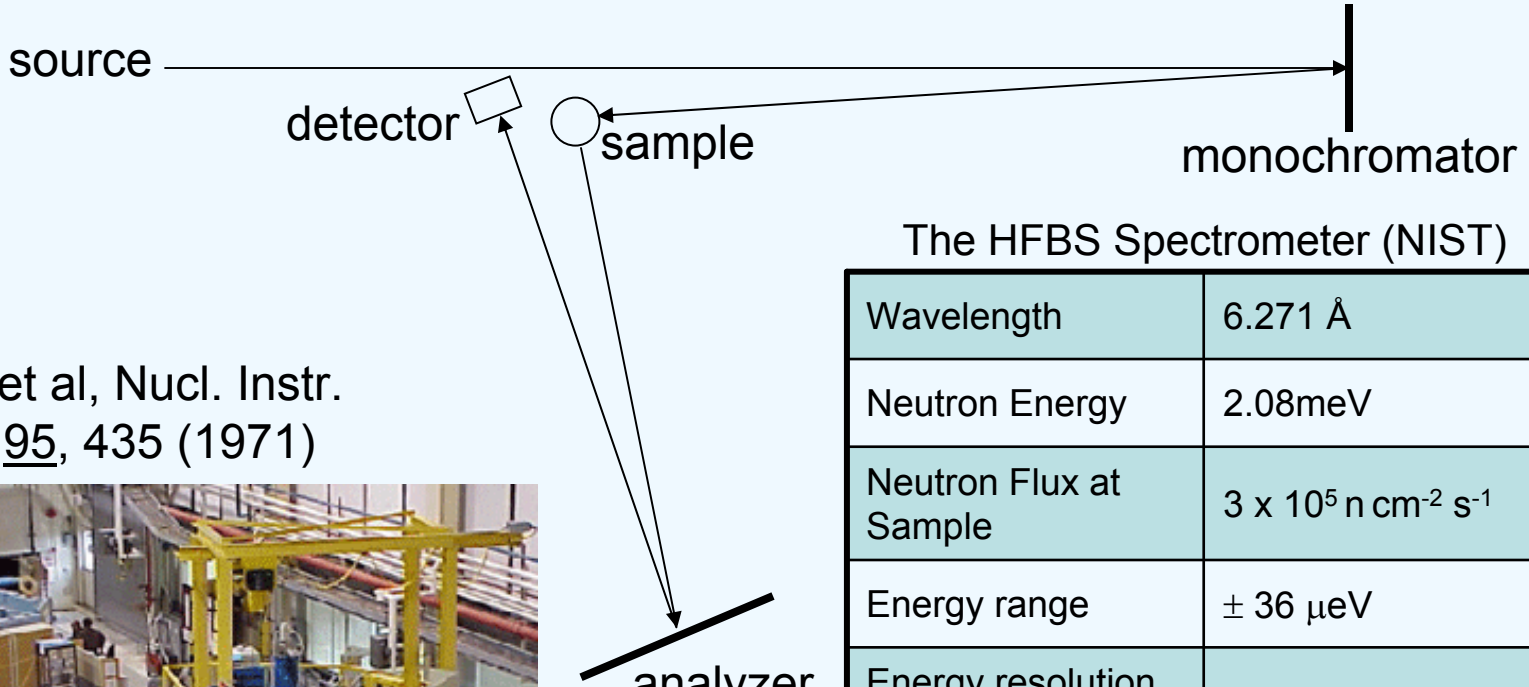
The "SPINS" spectrometer at NIST
Incident energy 14 ~ 2 meV (2.4 ~ 6.1 Å)
Flux at sample: 3.9×10^6 n/cm^2/s at 4 Å.
Resolution: from 0.02 to 1.0 meV

Thermal triple axis spectrometer

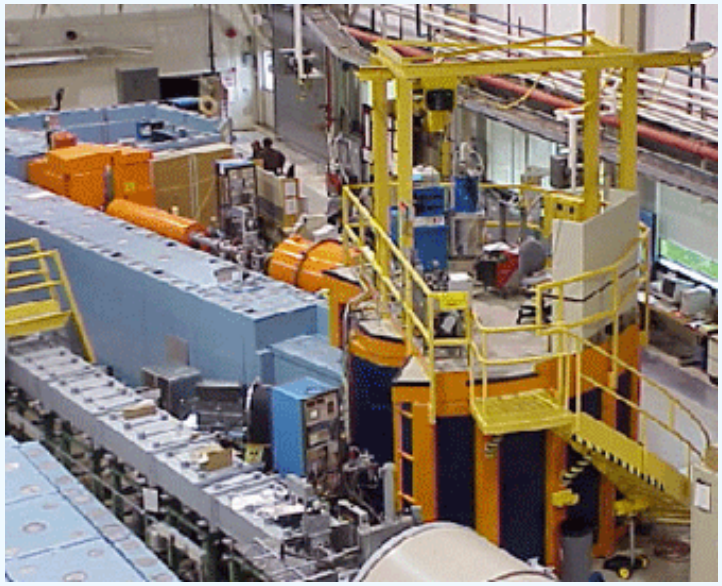




Backscattering spectrometer



M. Birr et al, Nucl. Instr. Meth. 95, 435 (1971)

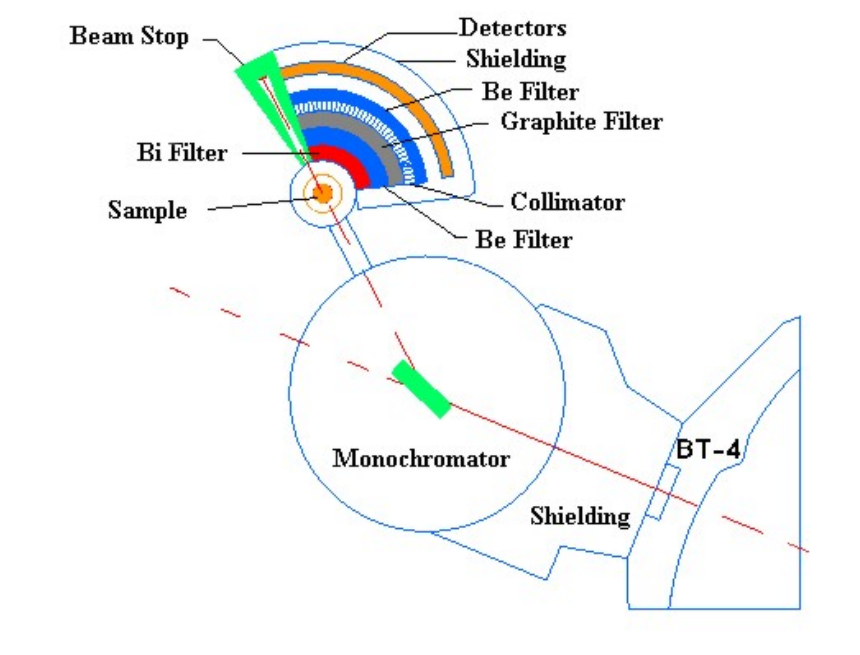


The HFBS Spectrometer (NIST)

Wavelength	6.271 Å
Neutron Energy	2.08meV
Neutron Flux at Sample	3×10^5 n cm^{-2} s^{-1}
Energy range	± 36 μeV
Energy resolution at ± 36 μeV	About 1 μeV
Analyzer Span	165°
Q range	0.25 $Å^{-1}$ – 1.75 $Å^{-1}$

A. Meyer, et al, Rev. Sci. Instrum., **74**, 2759 (2003).

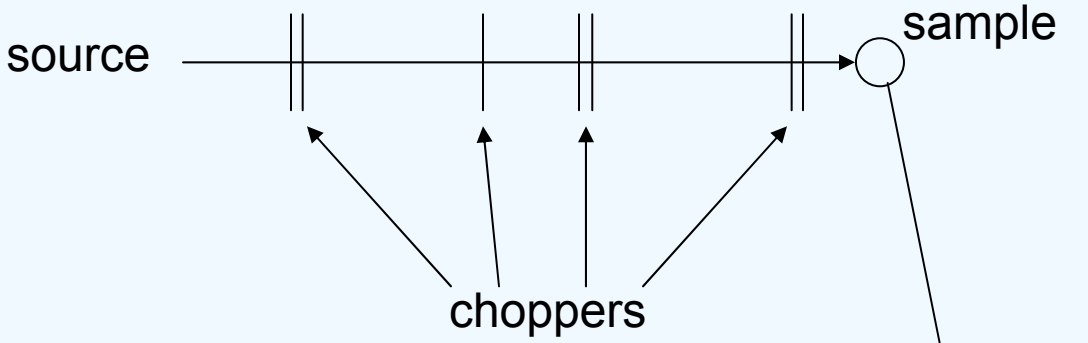
Filter analyzer spectrometer



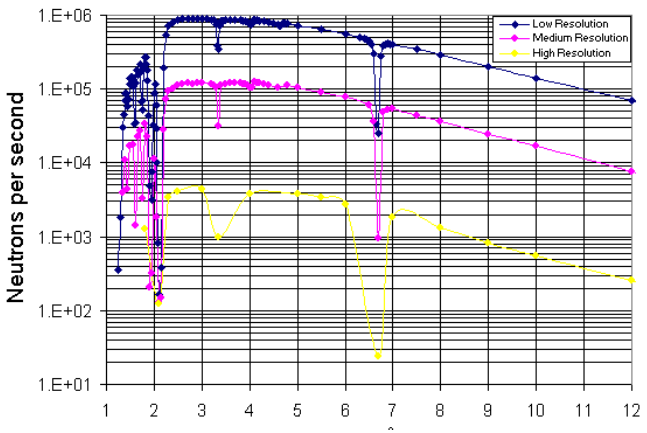
- Energy transfer range 5 - 250 meV.
- Resolution ~1.1 meV at low energies (determined by the filter cutoff).
- Resolution at high energies determined by the monochromator

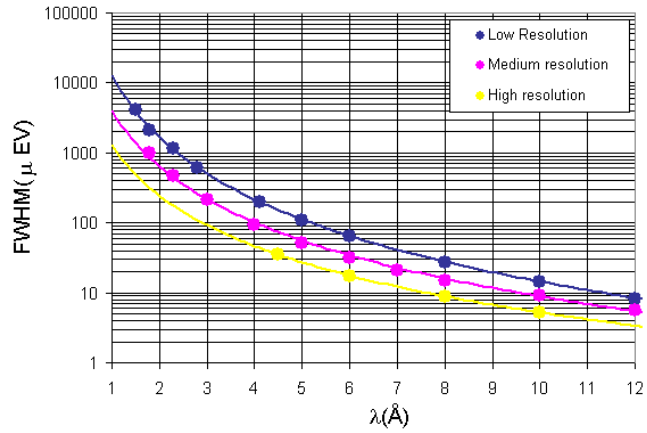
- Detector coverage 9% of 4π.
- Incident beam cross-section 30 mm x 70 mm.
- Minimum sample mass 10 mg for a hydrocarbon sample.

Time-of-flight spectrometer



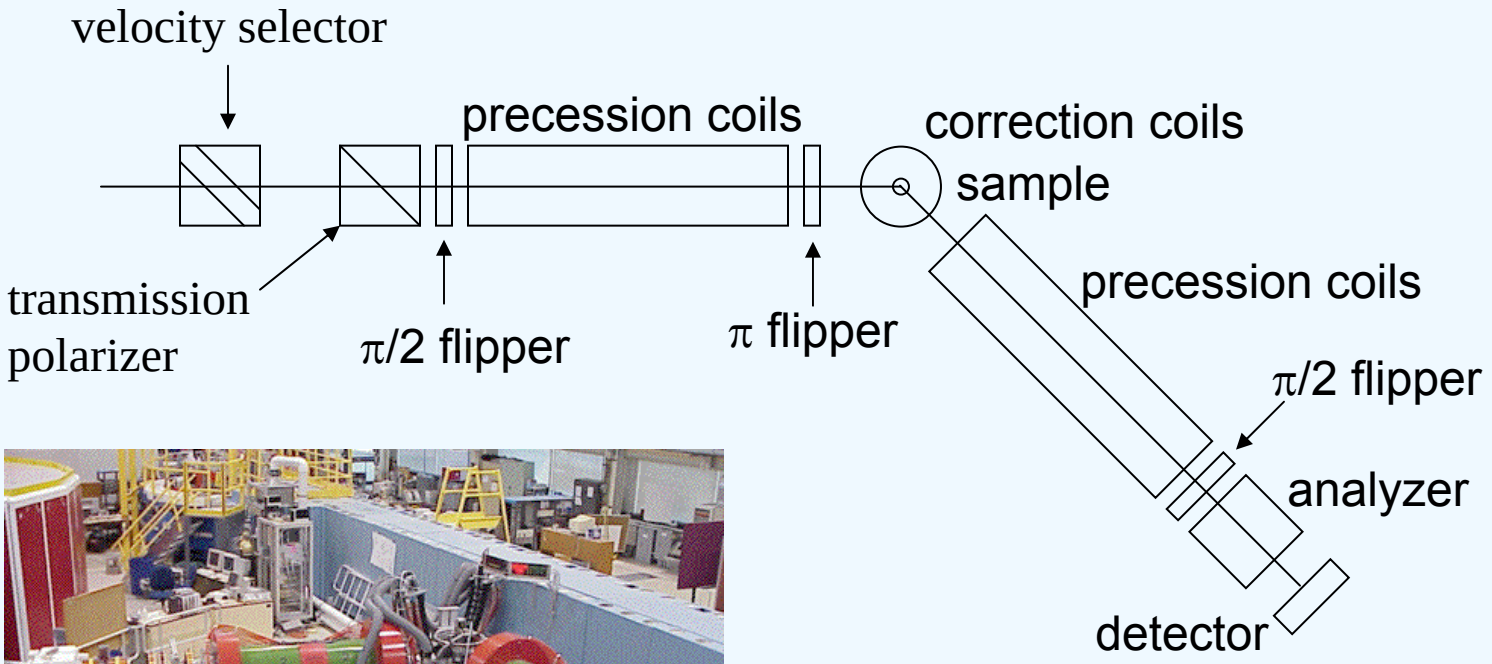
The Disk Chopper Spectrometer (NIST)

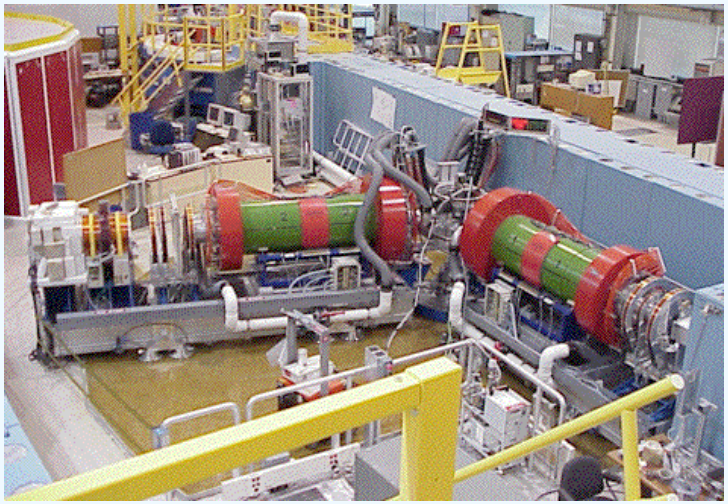




J.R.D. Copley and J.C. Cook, Chem. Phys. 292, 477 (2003)
J.R.D. Copley, C.M. Brown, Y. Qiu, Neutron News 20 (2) 29 (2009)

Spin echo spectrometer





NSE measures I(Q,t) for times t between ≈5 ps and 100-400 ns.

(http://www.ncnr.nist.gov/instruments/nse/)

After D.A. Neumann and B. Hammouda, J. Res. NIST 98, 89 (1993)

Concluding remarks

Neutron spectroscopy is a powerful technique with applications in a variety of fields, but available fluxes are relatively low (generally much lower than for neutron diffraction or SANS), and relatively large samples are needed.

Selective deuteration allows the experimenter to highlight interesting fragments of molecules.

The magnetic interaction provides unique information about magnetic materials.

The NCNR has several spectrometers that collectively cover important ranges in distance and time.

COME AND SEE FOR YOURSELVES!!!

Useful references (1)

G. L. Squires, “Introduction to the Theory of Thermal Neutron Scattering”, Dover Publications (1996) (ISBN 048669447), and references therein.

S. W. Lovesey, “Theory of Thermal Neutron Scattering from Condensed Matter”, Clarendon Press, Oxford (1984).

G. Shirane, S. M. Shapiro, and J. M. Tranquada, “Neutron Scattering With a Triple-Axis Spectrometer”, Cambridge University Press, Cambridge (2002).

M. Bée, “Quasielastic neutron scattering”, Adam Hilger, Bristol and Philadelphia (1988).

For detailed information about scattering and absorption cross sections, see:

V.F. Sears, Neut. News 3 (3) 26 (1992);

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

Useful references (2)

R. Pynn, “An Introduction to Neutron Scattering” and “Neutron Scattering for Biomolecular Science” (lecture notes, possibly “out of print”)

R. Pynn, “Neutron Scattering: A Primer”, Los Alamos Science (1990)

R. Pynn, “Neutron Scattering—A Non-destructive Microscope for Seeing Inside Matter”, the 2nd of 3 free downloads at http://www.springer.com/materials/characterization+%26+evaluation/book/978-0-387-09415-1?detailsPage=samplePages

Neutron Applications in Earth, Energy and Environmental Sciences
Series: Neutron Scattering Applications and Techniques , Vol.
Liang, Liyuan; Rinaldi, Romano; Schober, Helmut (Eds.)
2009, XVIII, 638 p. 35 illus., Hardcover

The bottom line

"Neutron Scattering
is an excellent way
to study dynamics."

(D.A. Neumann, 2001)