Dynamics and Neutron Scattering

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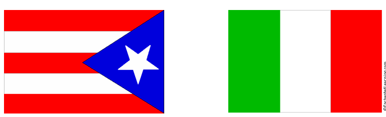
NCNR Summer School on
Methods and Applications of Neutron Spectroscopy

June 25-29, 2007

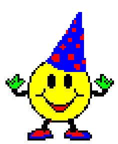
Acknowledgments

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

NIST Center for Neutron Research (NCNR)



Yamali and Antonio

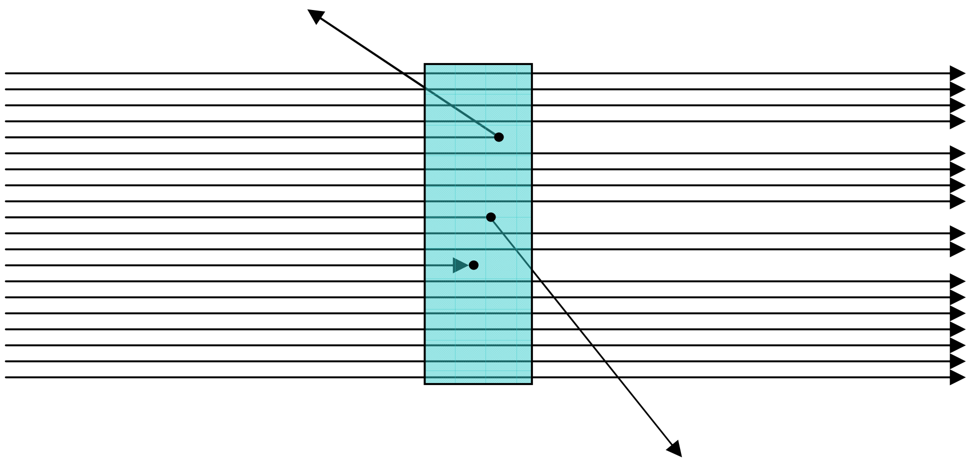


Julie

The three fates of a neutron

Consider a "thin" sample placed in a neutron beam.
("thin" implies almost transparent, no shadowing)

What happens to the neutrons?

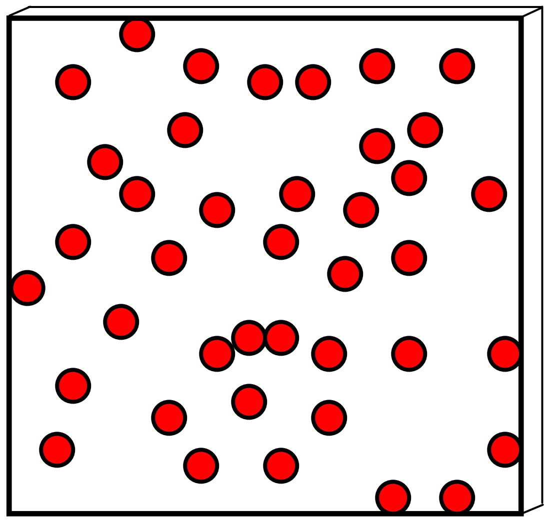


They are transmitted, absorbed, or scattered.

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

Absorption probability (one type of atom)

Consider a "thin" sample in a beam:



- N atoms
- area A
- thickness t
- 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* cross section (barn/atom)

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

1 barn = $10^{-24} cm^2$

Absorption and scattering rates

The "thin" sample is placed in a beam whose current density (or "flux") is ϕ (n/cm^2/s).

Rates of absorption and scattering are as follows:

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

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

Hence the transmission rate is

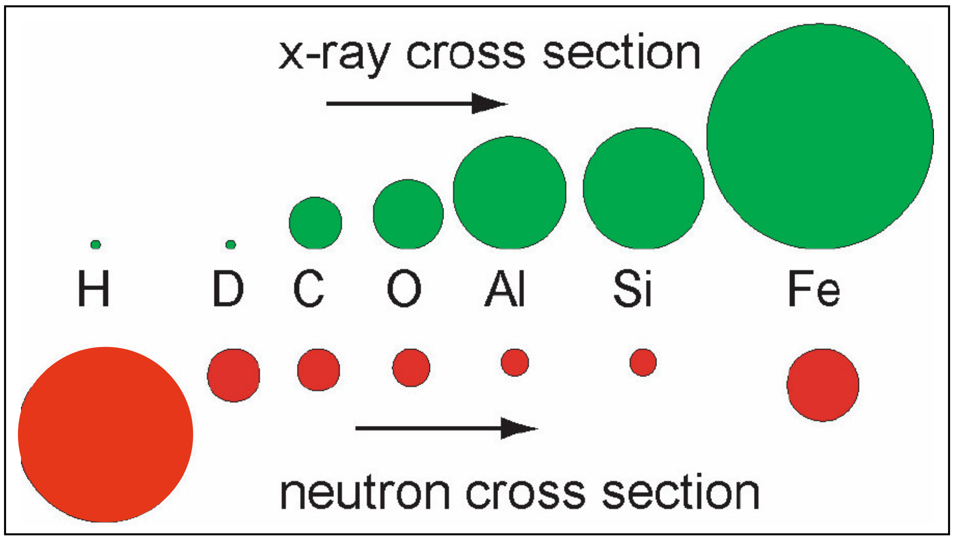
$$I_T = (\Phi A)(1 - \Sigma_T t)$$

More in Appendix

where $\Sigma_T = \Sigma_A + \Sigma_S$ is the <u>total removal cross section.</u>

X-ray and neutron cross sections

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

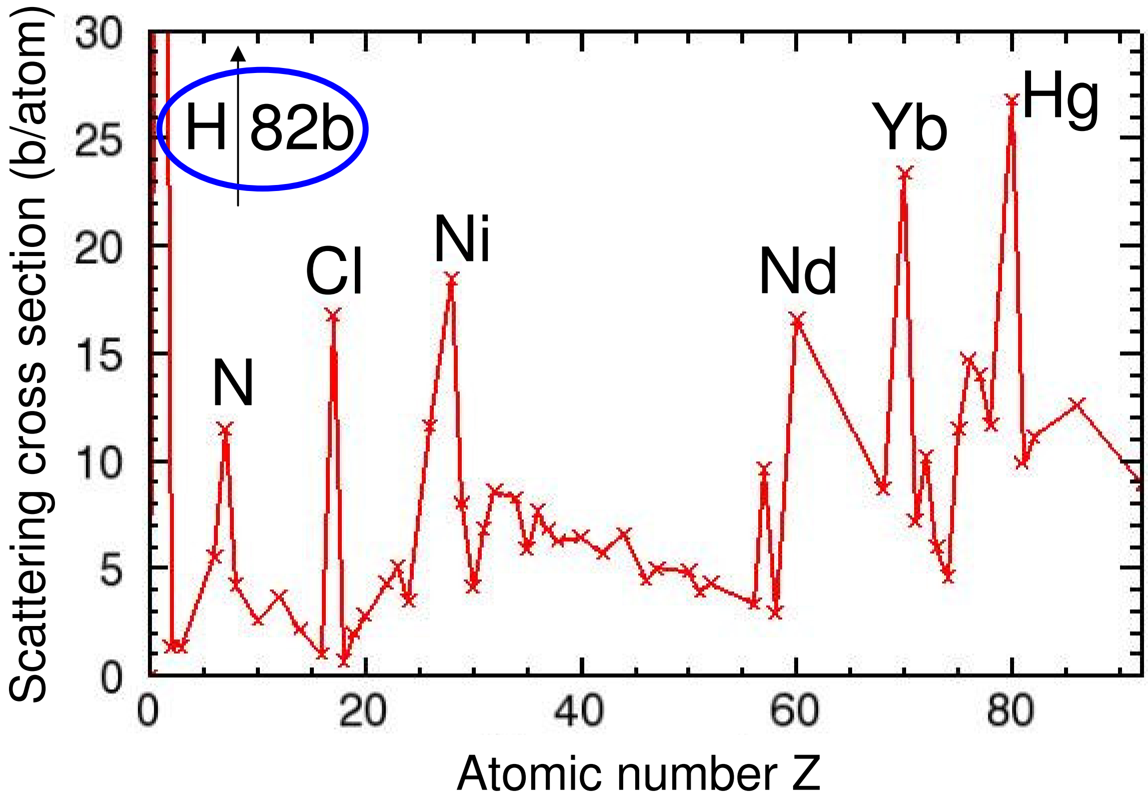


The x-ray scale has been reduced by a factor of ≈1.5 as compared with the neutron scale.

N.B. In this talk we only consider the interaction of neutrons with nuclei. We ignore the magnetic interaction of neutrons with unpaired electrons.

Scattering cross sections

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



More in Appendix

Absorption cross sections

- 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:

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

- The most important exceptions are Cd and Gd.

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

Absorption cross sections

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

N.B. log scale

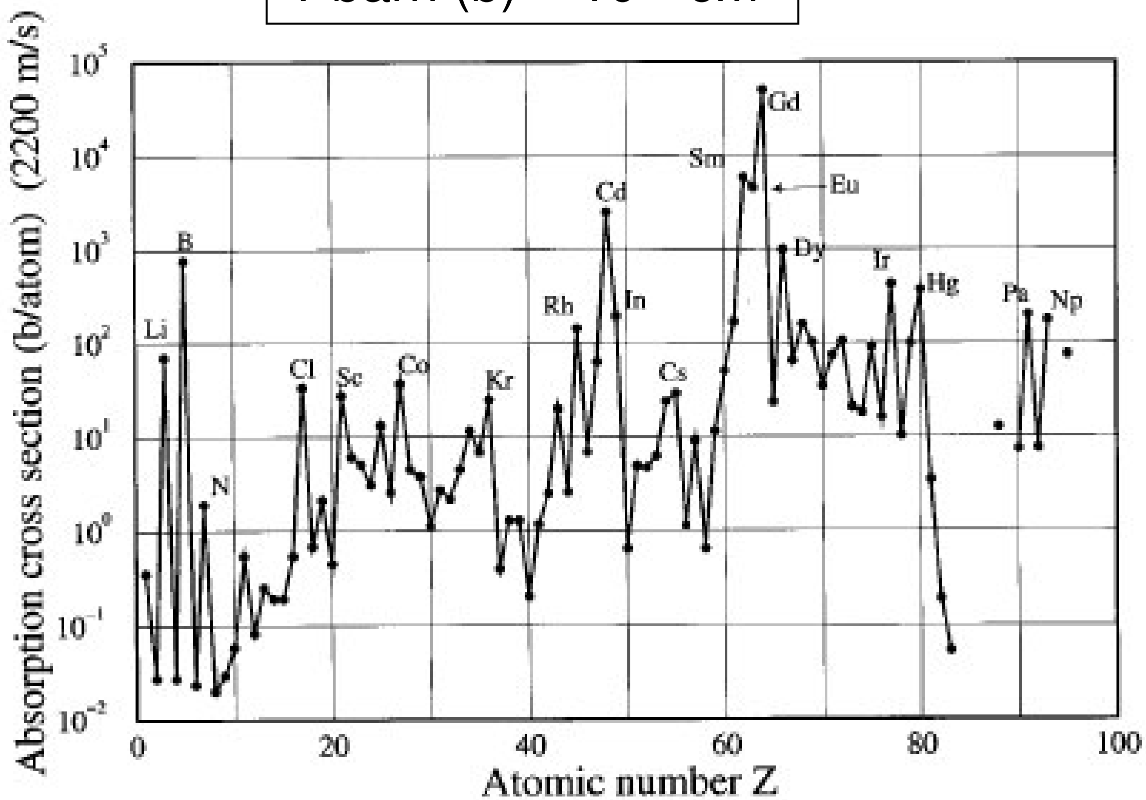


Fig. 8. The absorption cross section for 2200 m/s neutrons for the naturally occurring elements. Notice that the ordinate is plotted on a log scale.

More in Appendix

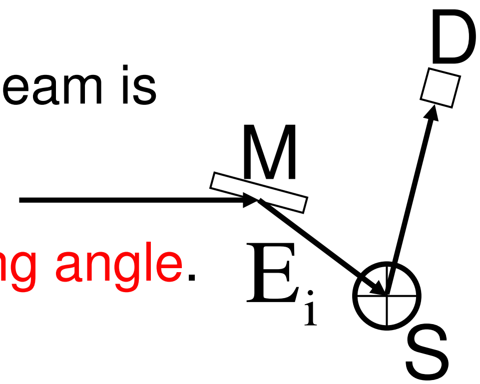
Cross section examples

		0.1 mm water	1 m (dry) air	1 cm aluminum	10 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	1	0.0254
Scattering		5.5%	4.8%	8.5%	0.2%
Absorption		0.0%	0.7%	1.3%	94.6%
Transmission		94.5%	94.5%	90.1%	5.2%

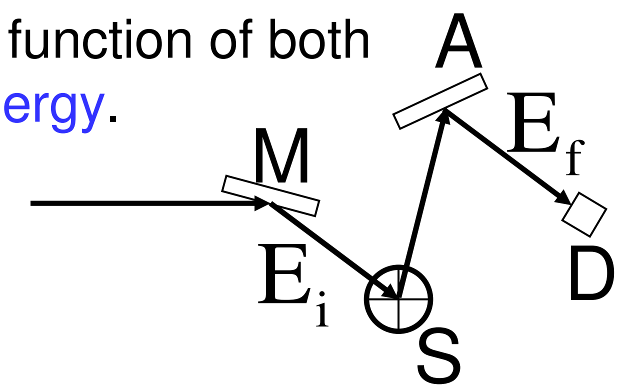
The scattered neutrons

How we look at 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).

We could study the intensity as a function of scattering angle.



We could study the intensity as a function of both scattering angle and scattered energy.



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

Diffraction and Spectroscopy

The Nobel Prize in Physics 1994

“one half to Professor Clifford G. Shull … for the development of the neutron diffraction technique”
“one half 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. In simple terms, Clifford G. Shull has helped answer the question of where atoms "are" and Bertram N. Brockhouse [has helped with] the question of what atoms "do".”

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

Differential cross sections

From before, the total integrated scattering is:

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

Similarly, the measured intensities in diffraction and spectroscopy experiments are related to differential cross sections:

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

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

In turn, the differential cross sections may be related to "scattering functions" (or "structure factors").

When there is one type of atom,

$$\frac{d\sigma}{d\Omega}\left(E_i, 2\theta\right) = \frac{\sigma}{4\pi} S(Q)^{*}$$

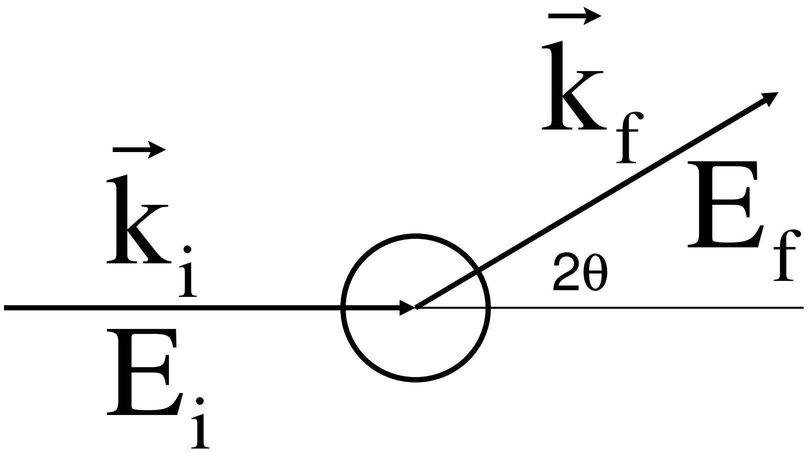
$$\frac{d^2\sigma}{d\Omega dE_f}\left(E_i, 2\theta, E_f\right) = \frac{\sigma}{4\pi\hbar}\frac{k_f}{k_i} S(Q,\omega),$$

ONLY DEPENDS ON THE SAMPLE

but what are Q, ω, 2θ, k_i, k_f, E_i, and E_f?

*(in the static approximation)

Q, ω, 2θ, k_i, k_f, E_i, and E_f



Energy transfer:

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

Wave vector transfer:

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

$$E = \frac{\hbar^2 k^2}{2m} = \frac{1}{2} m v^2$$

(m is neutron mass)

$$k = \frac{2\pi}{\lambda}$$

More in Appendix

Alternative notations

2θ or θ or ϕ

k_i or k_0 or k

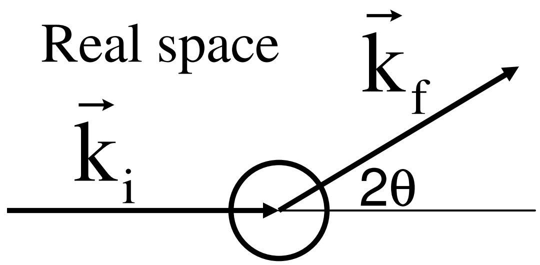
E_i or E_0 or E

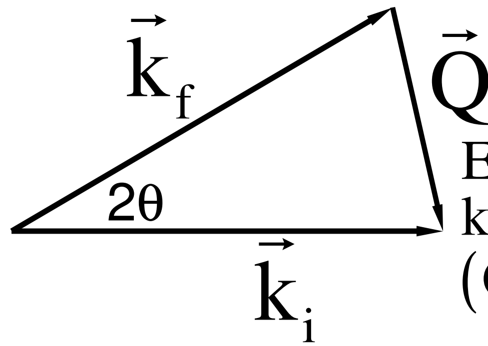
k_f or k′, etc.

Elastic and inelastic scattering

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

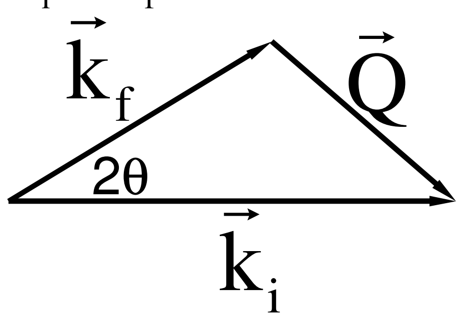
Real space



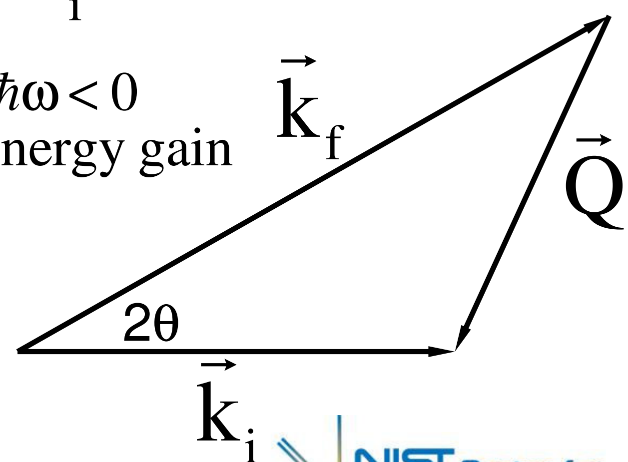


Elastic, $\hbar\omega = 0$
$k_i = k_f$
$(Q = 2k_i \sin\theta)$

Inelastic, $\hbar\omega > 0$
Neutron energy loss
$k_i > k_f$

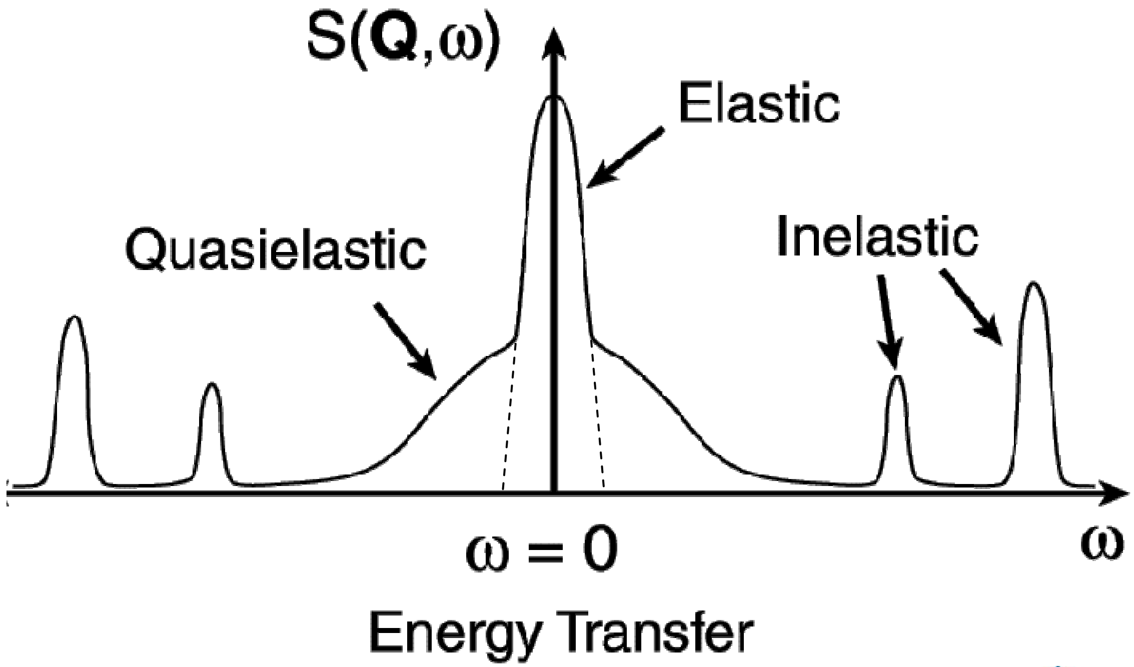


Inelastic, $\hbar\omega < 0$
Neutron energy gain
$k_i < k_f$



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 typically associated with lattice or localized excitations.



The double differential cross section

$$\frac{d^2\sigma}{d\Omega dE_f}(E_i, 2\theta, E_f)\Delta\Omega\Delta E_f,$$

which is proportional to the probability of scattering into solid angle $\Delta\Omega$ and scattered energy window ΔE_f, is directly related to the scattering function S(Q,ω):

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

ONLY DEPENDS ON THE SAMPLE

The scattering function S(Q,ω) only depends on the energy and wave vector transfers Q and ω (rather than on the incident and scattered wave vectors).

Notice that there is no equivalent of the x-ray atomic scattering factor since the neutron interacts with the nucleus. (On the other hand there is a form factor in the magnetic neutron scattering case.)

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.

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.

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).

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:

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

– $S(Q,\omega)$ reflects the collective behavior of the particles (e.g. phonons)

– $S_S(Q,\omega)$ reflects the single particle behavior (e.g. diffusion)

– σ_{inc} and σ_{coh} are "incoherent" and "coherent" scattering cross sections respectively.

Coherent and incoherent scattering

The scattering cross section of an atom is proportional to the square of the strength of its interaction with neutrons (its scattering length), denoted “b”:

$$\sigma = 4\pi b^2$$

For an element with more than one isotope, b depends on the isotope. If the nucleus has nonzero spin b depends on the compound nucleus spin state.

The coherent cross section σ_{coh} reflects the mean scattering length. The incoherent cross section σ_{inc} reflects the variance of the distribution of scattering lengths.

$$\sigma_{coh} = 4\pi\left(\bar{b}\right)^2$$

$$\sigma_{inc} = 4\pi\left[\overline{b^2} - \left(\bar{b}\right)^2\right]$$

The underlying assumption is that there is no correlation between an atom’s position and its isotope and/or spin state.

Coherent and incoherent scattering

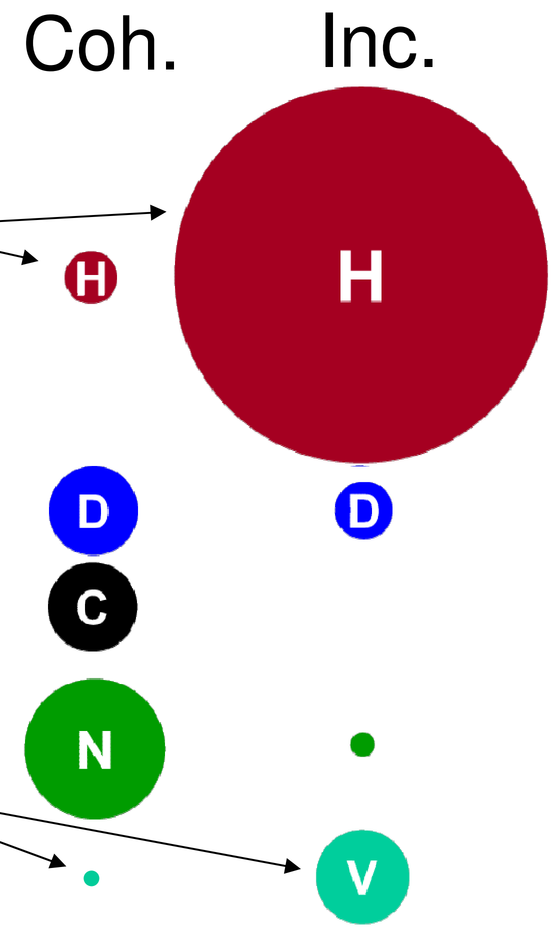
For most elements the coherent cross section dominates.

Hydrogen is a very important exception:

For example, the huge incoherent cross section enables studies of hydrogen diffusion in candidate storage materials

Also selective deuteration enables detailed studies of polymers and biomolecules.

Note too that Vanadium has a significant incoherent cross section and a very small coherent cross section.



The single particle functions

We need to modify some of our earlier statements.

Most neutron spectrometers measure S(Q,ω) and S_S(Q,ω).

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

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

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.

What can one study using n.s.?

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

such as metals, insulators, semiconductors, glasses, magnetic materials, heavy fermions, superconductors, solid and liquid helium, plastic crystals, molecular solids, liquid metals, molten salts, biomolecules, water in confined geometries, polymer systems, micelles, microemulsions, etc etc.

under all sorts of conditions

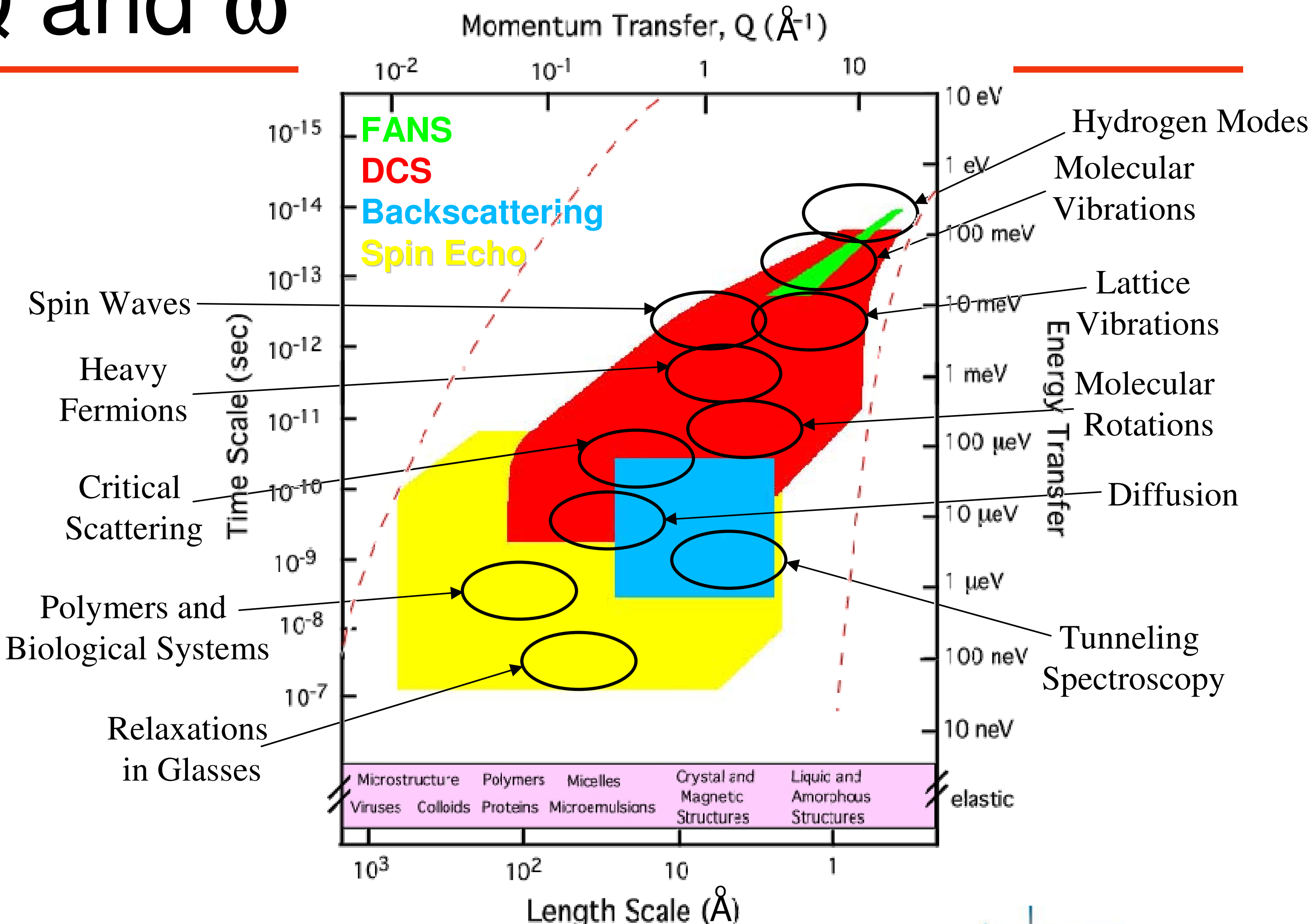
such as (at the NCNR) T ≈50 mK to ≈1900K, P to ≈2.5 GPa, B to ≈11.5T, also strong electric fields, controlled humidity, etc etc.

Provided that

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

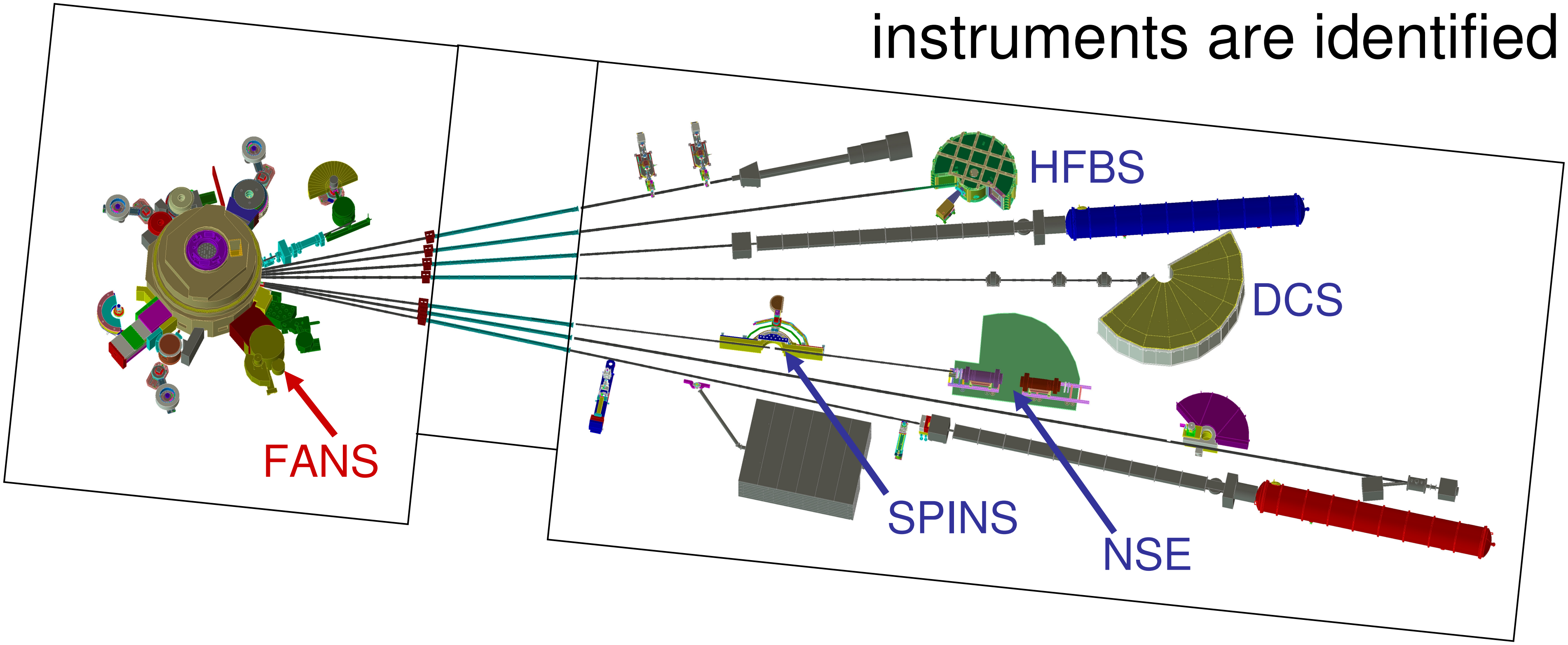
See the NCNR annual reports for additional examples.

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
Hydrogen Modes
Molecular Vibrations
Lattice Vibrations
Molecular Rotations
Diffusion
Tunneling Spectroscopy
Spin Waves
Heavy Fermions
Critical Scattering
Polymers and Biological Systems
Relaxations in Glasses
Microstructure
Polymers
Micelles
Crystal and Magnetic Structures
Liquid and Amorphous Structures
Viruses
Colloids
Proteins
Microemulsions
10^3
10^2
10
1
Length Scale (Å)

NCNR Instruments

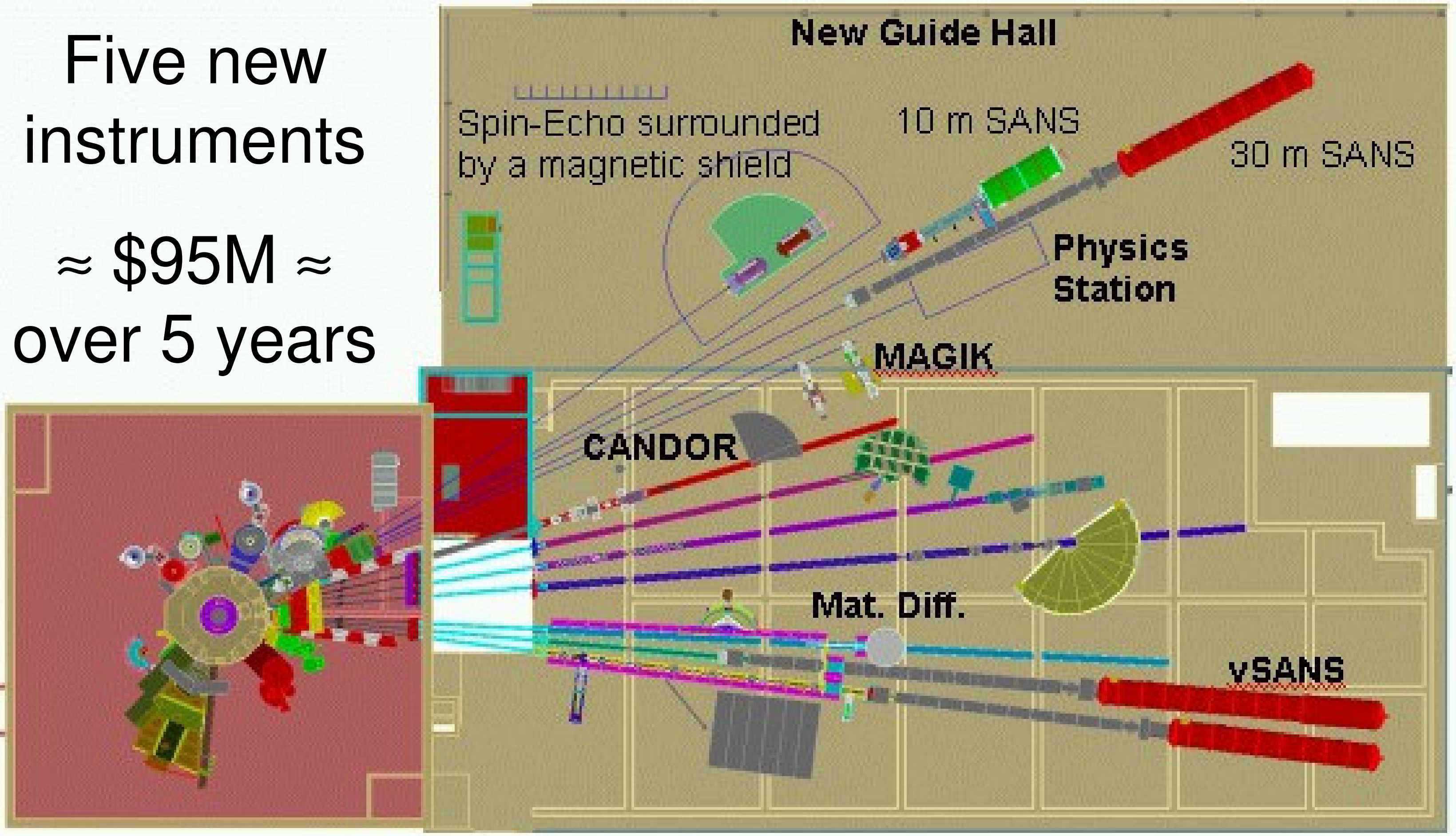
The summer school instruments are identified



The NCNR Expansion Project

Five new instruments

≈ $95M ≈ over 5 years



http://www.ncnr.nist.gov/expansion/

Useful references

R. Pynn, “An Introduction to Neutron Scattering” and “Neutron Scattering for Biomolecular Science” (lecture notes), also “Neutron Scattering: A Primer” (www.mrl.ucsb.edu/~pynn).

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

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

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/.

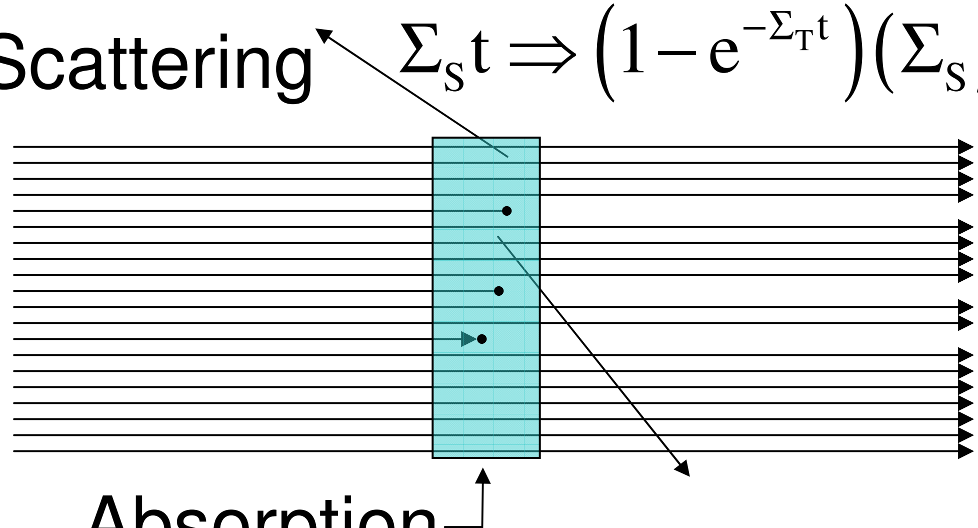
The Appendix

- ❖ Possible fates of a neutron
- ❖ Scattering lengths
- ❖ Penetration depths
- ❖ Exact and approximate relationships
- ❖ Choices of units

Possible fates of a neutron

Scattering, absorption and transmission probabilities for a sample that is "thin" ⇒ "thick"

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



Transmission

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

Absorption

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

Removal cross section

$$\Sigma_T = \Sigma_S + \Sigma_A$$

Scattering lengths

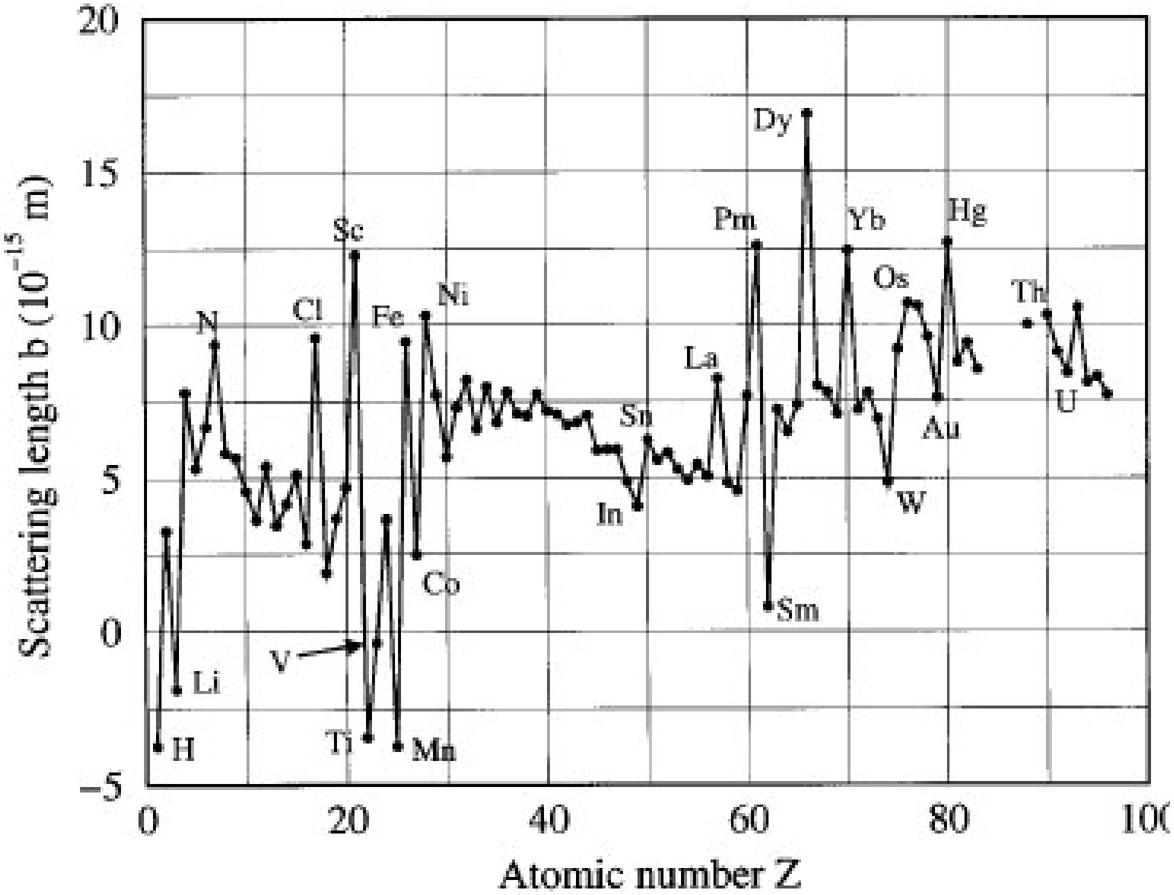
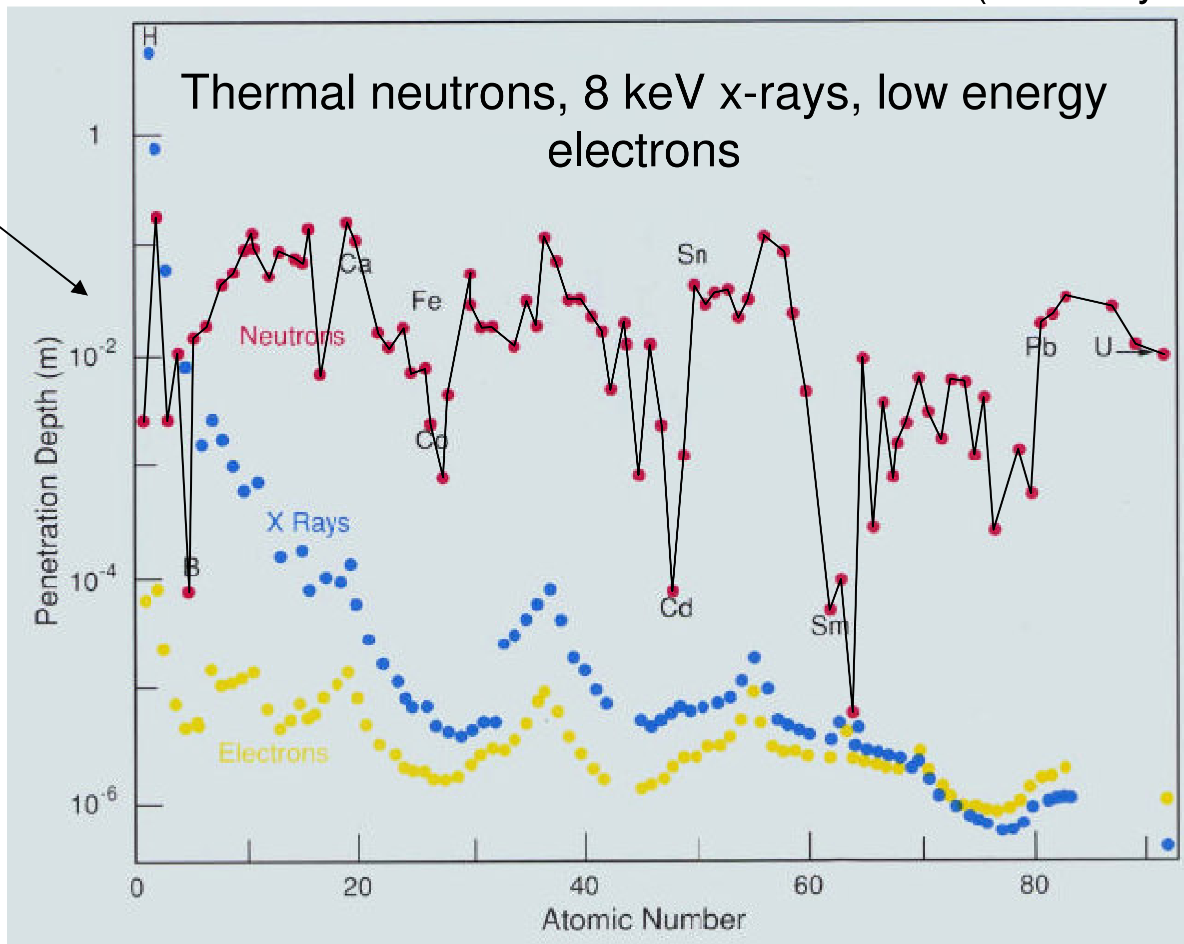


Fig. 7. The real part of the neutron scattering length b for the naturally occurring elements.

Penetration depths

(Courtesy Roger Pynn)

log scale



Exact and approximate relationships

$$\lambda = \frac{h}{mv} = \frac{2\pi}{k} \qquad E = \frac{1}{2}mv^2 = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

$$\lambda(\text{Å}) \approx \frac{4}{v(\text{mm}/\mu\text{s})}$$

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

Choices of units

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

λ	E	v	τ
Å	meV	m/s	ms/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
8.1 cm^{-1}
11.6K
0.023 kcal/mol
0.10 kJ/mol