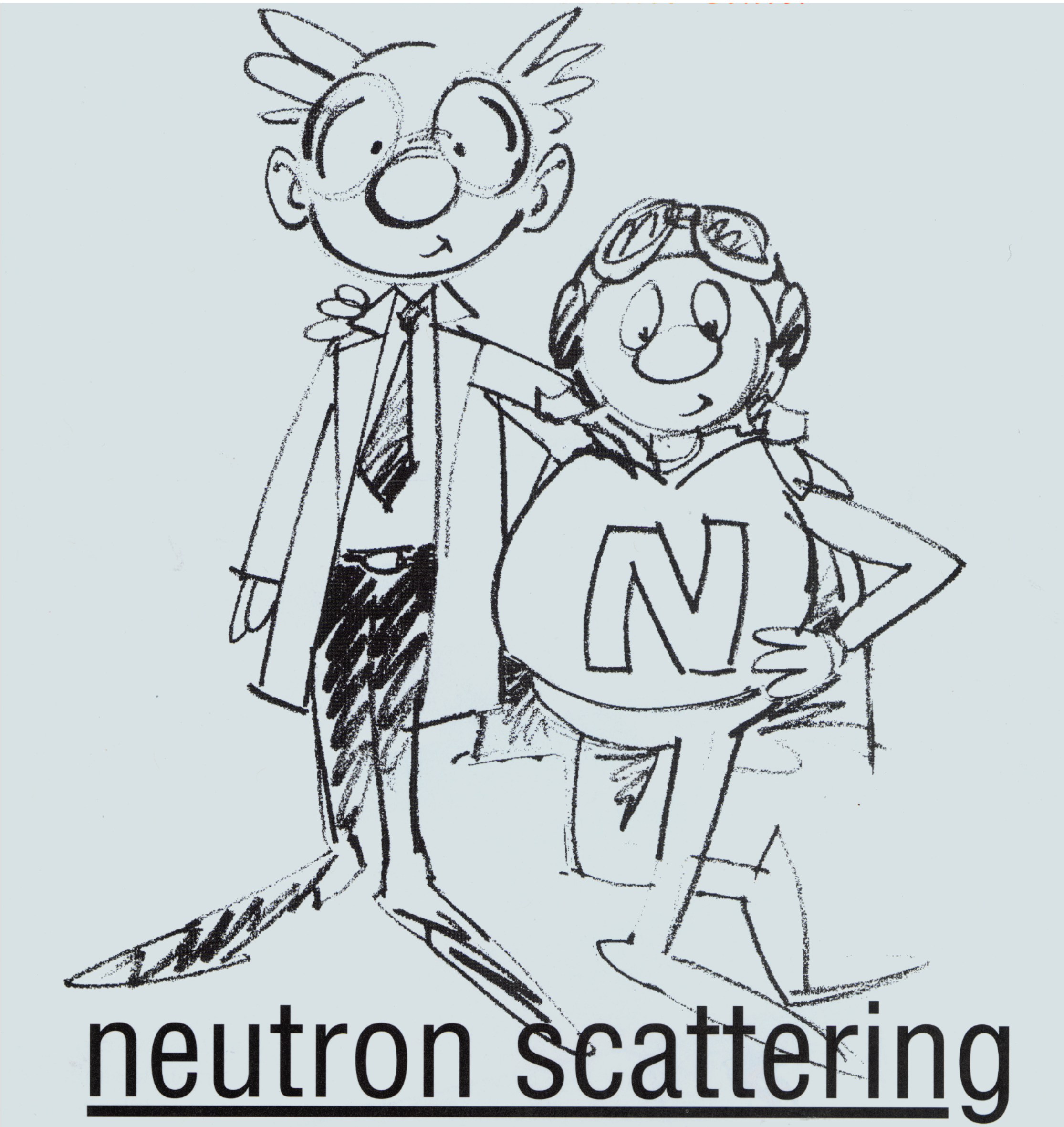

Nuclear Scattering of Neutrons

by

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Overview

Introduction and theory of neutron scattering

- Advantages/disadvantages of neutrons for scattering measurements
- Neutron properties
- Comparison with other structural probes
- Definition of scattering cross sections
- Fermi pseudopotential
- Elastic scattering and definition of the structure factor, S(Q)
- Coherent & incoherent scattering
- References

Why do Neutron Scattering?

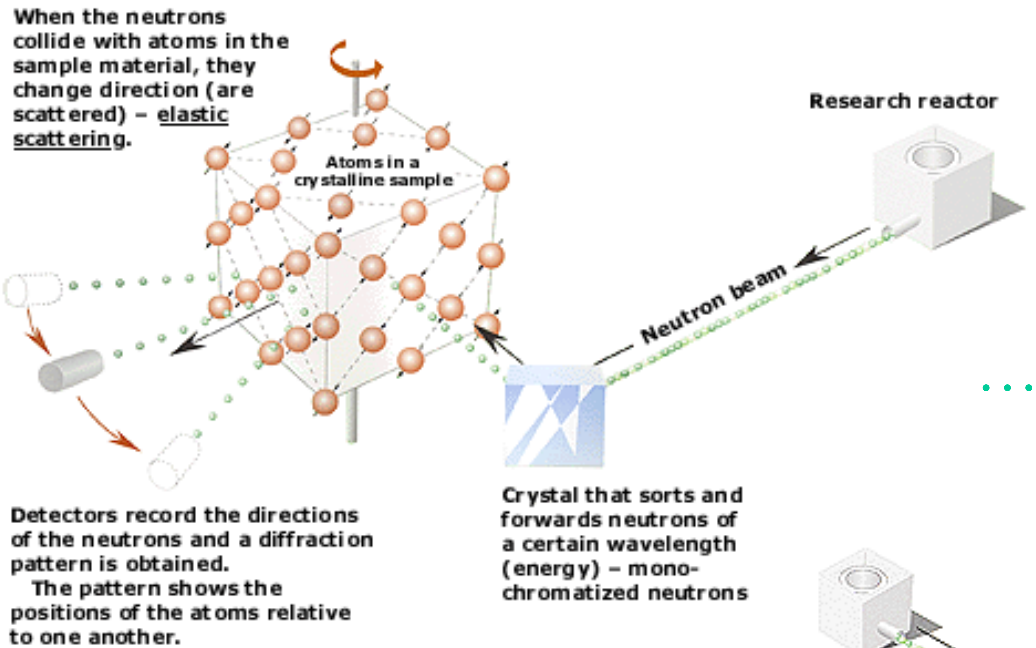
- To determine the positions and motions of atoms in condensed matter
  - 1994 Nobel Prize to Shull and Brockhouse cited these areas
    (see http://www.nobel.se/physics/educational/poster/1994/neutrons.html)

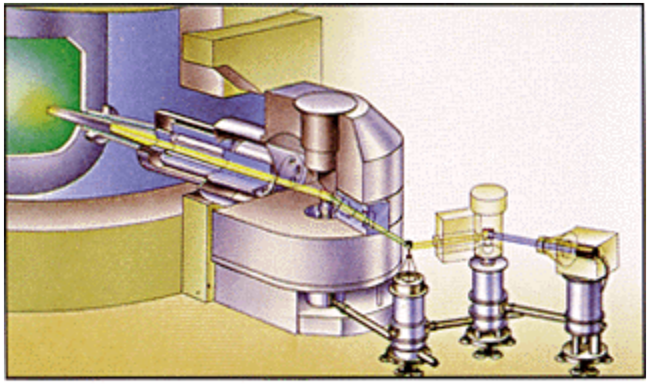
- Neutron advantages:
  - Wavelength comparable with interatomic spacings
  - Kinetic energy comparable with that of atoms in a solid
  - Penetrating => bulk properties are measured & sample can be contained
  - Weak interaction with matter aids interpretation of scattering data
  - Isotopic sensitivity allows contrast variation
  - Neutron magnetic moment couples to ***B*** **=>** neutron "sees" unpaired electron spins

- Neutron Disadvantages
  - Neutron sources are weak => low signals, need for large samples etc
  - Some elements (e.g. Cd, B, Gd) absorb strongly
  - Kinematic restrictions (can't access all energy & momentum transfers)

The 1994 Nobel Prize in Physics – Shull & Brockhouse

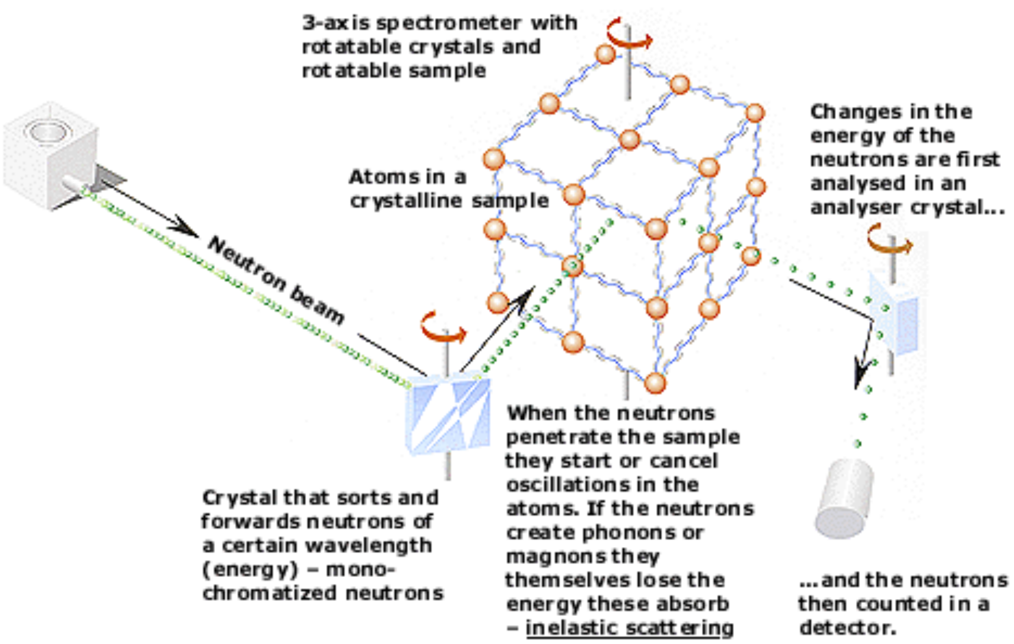
Neutrons show where the atoms are….





3-axis spectrometer

…and what the atoms do.



The Neutron has Both Particle-Like and Wave-Like Properties

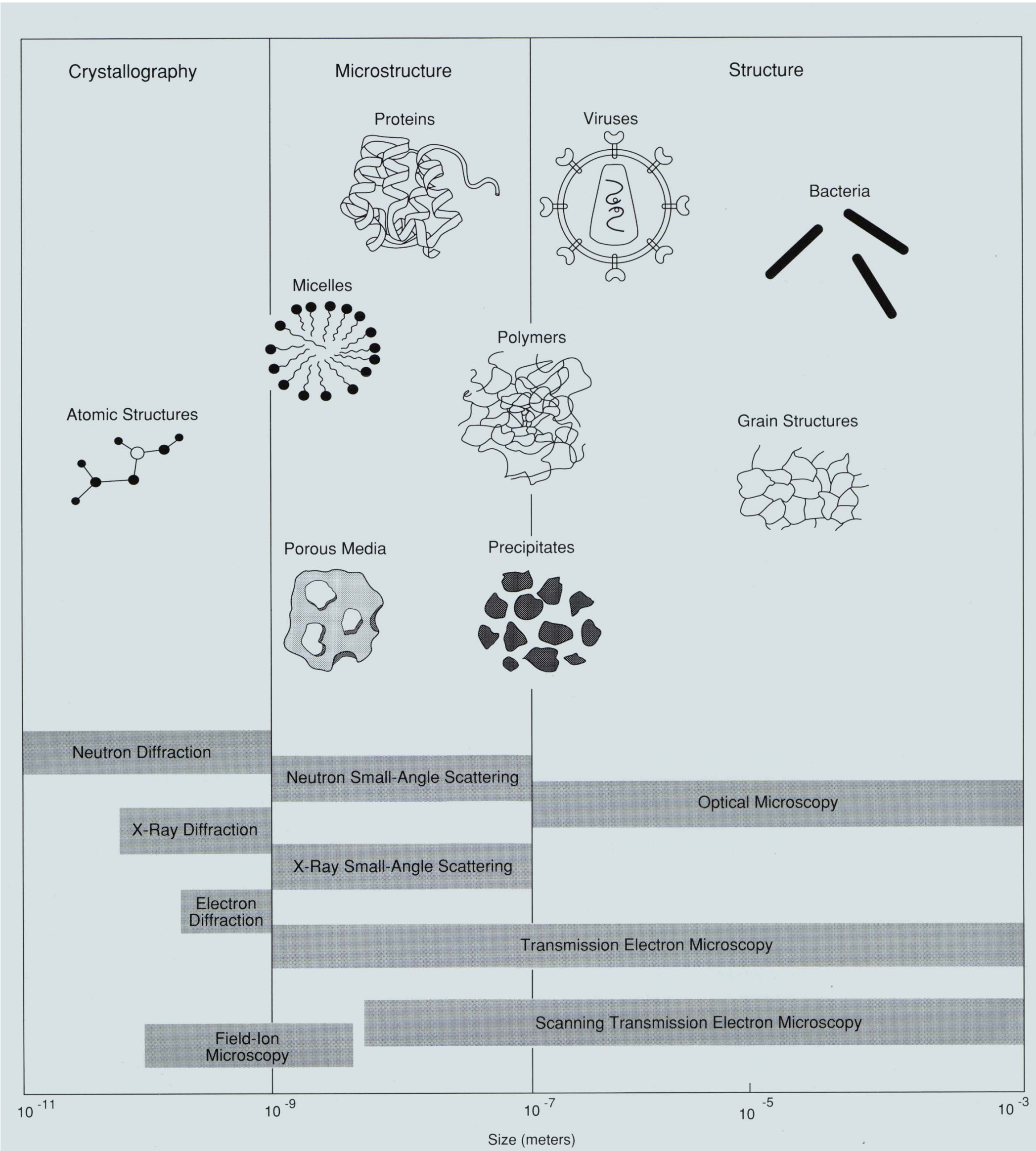
- Mass: $m_n = 1.675 \times 10^{-27}$ kg
- Charge = 0; Spin = ½
- Magnetic dipole moment: $\mu_n = - 1.913\ m_N$
- Nuclear magneton: $\mu_N = eh/4\pi m_p = 5.051 \times 10^{-27}\ J\ T^{-1}$
- Velocity (v), kinetic energy (E), wavevector (k), wavelength (λ), temperature (T).
- $E = m_n v^2/2 = k_B T = (hk/2\pi)^2/2m_n$; $k = 2\ \pi/\lambda = m_n v/(h/2\pi)$

	Energy (meV)	**Temp (K)**	**Wavelength (nm)**
Cold	**0.1 – 10**	**1 – 120**	**0.4 – 3**
Thermal	**5 – 100**	**60 – 1000**	**0.1 – 0.4**
Hot	**100 – 500**	**1000 – 6000**	**0.04 – 0.1**

λ (nm) = 395.6 / v (m/s)

E (meV) = 0.02072 k^2 (k in nm^{-1})

Comparison of Structural Probes



Note that scattering methods provide statistically averaged information on structure rather than real-space pictures of particular instances

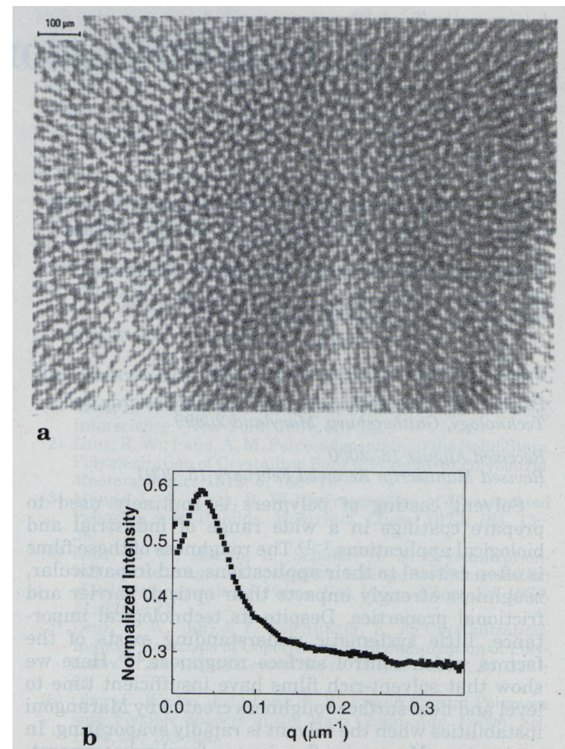


Figure 2. (a) Optical micrograph of PS-200 spin cast at 7500 rpm using THF (P_{vp} = 0.215 bar). (b) One-dimensional Fourier transform of central (isotropic) region of optical micrograph.

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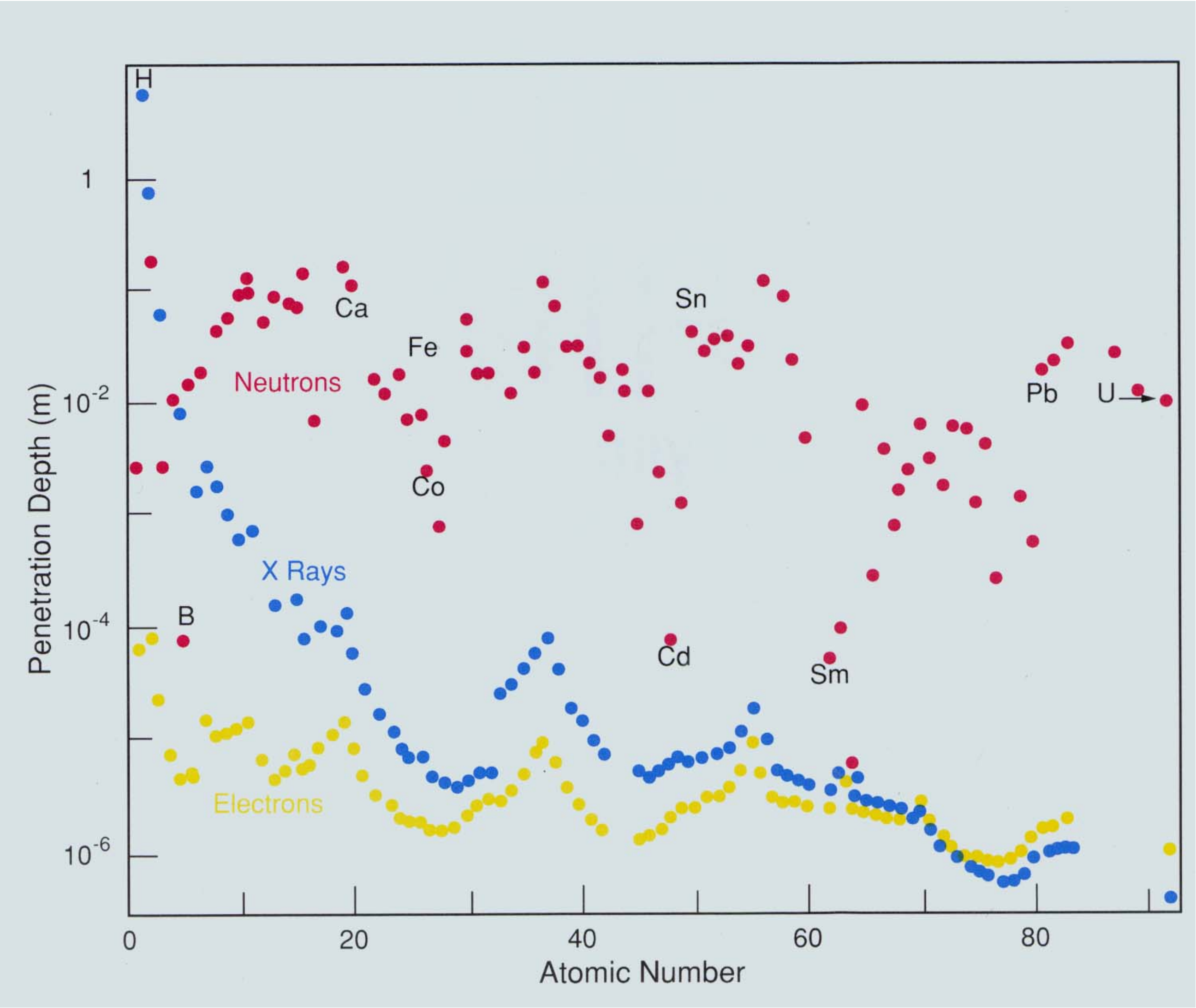
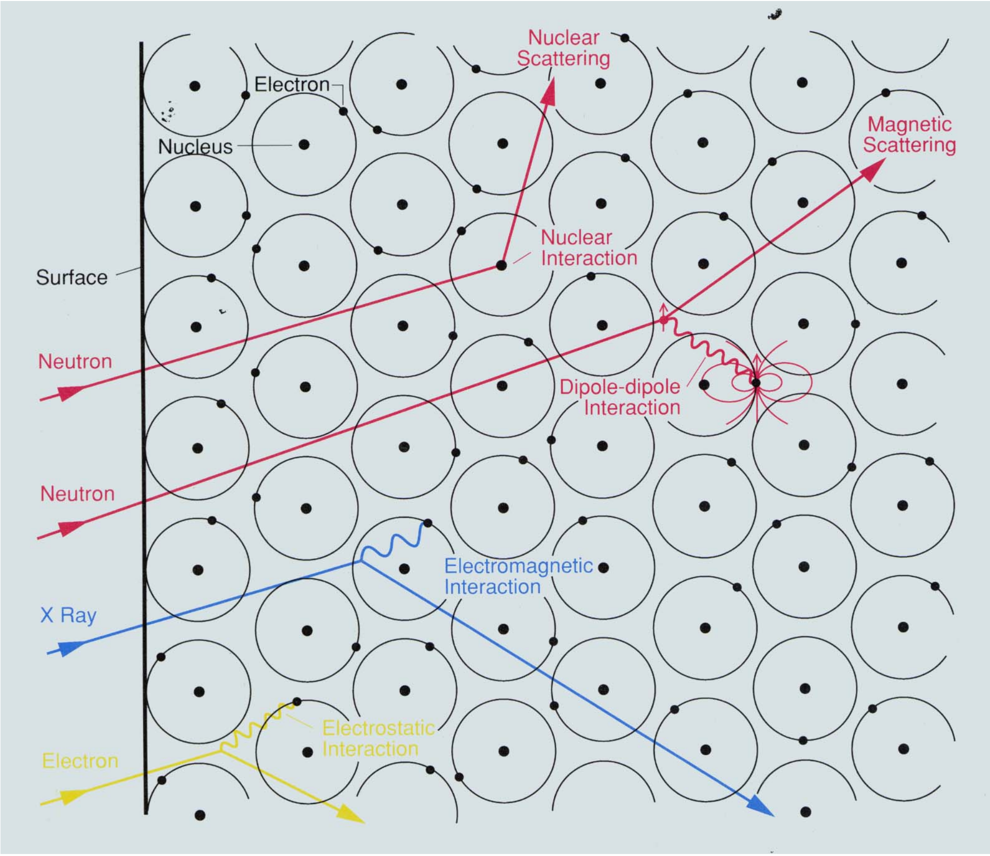
Thermal Neutrons, 8 keV X-Rays & Low Energy Electrons:- Absorption by Matter



Note for neutrons:

- H/D difference
- Cd, B, Sm
- no systematic A dependence

Interaction Mechanisms

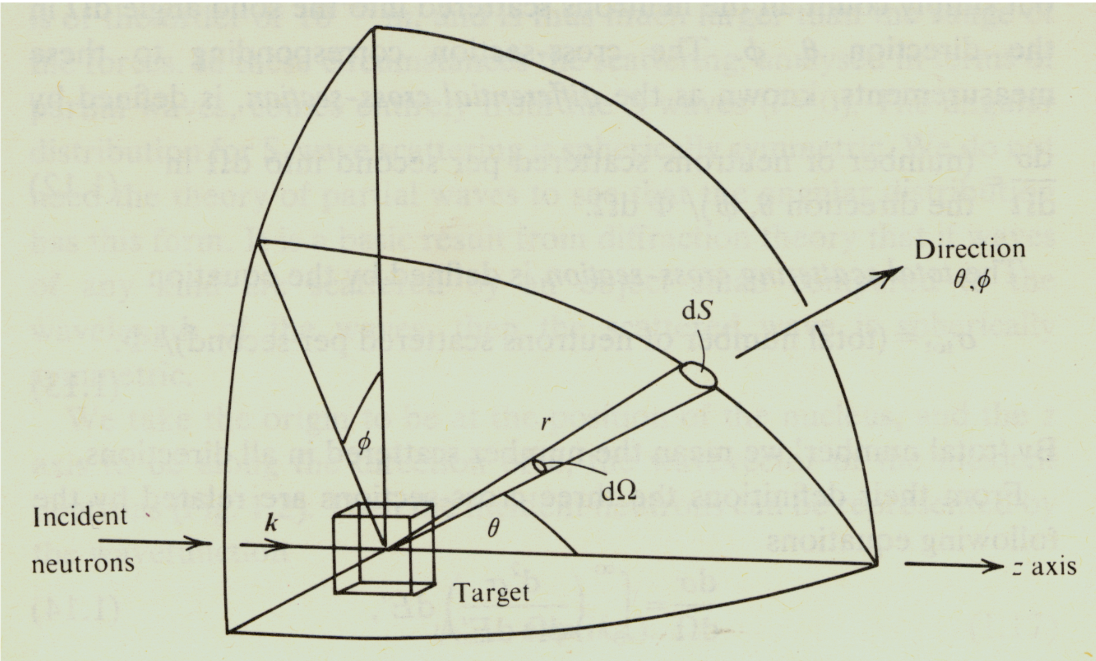


- Neutrons interact with atomic nuclei via very short range (~fm) forces.
- Neutrons also interact with unpaired electrons via a magnetic dipole interaction.

Brightness & Fluxes for Neutron & X-Ray Sources

	Brightness *(s^{-1} m^{-2} $ster^{-1}$)*	*dE/E* *(%)*	*Divergence* *($mrad^2$)*	*Flux* *(s^{-1} m^{-2})*
Neutrons	10^{15}	2	10 x 10	10^{11}
Rotating Anode	10^{16}	3	0.5 x 10	5×10^{10}
Bending Magnet	10^{24}	0.01	0.1 x 5	5×10^{17}
Wiggler	10^{26}	0.01	0.1 x 1	10^{19}
Undulator (APS)	10^{33}	0.01	0.01 x 0.1	10^{24}

Cross Sections

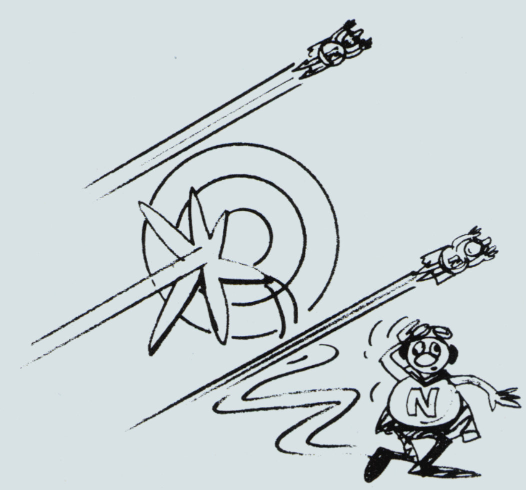


$$\Phi = \text{number of incident neutrons per cm}^2 \text{ per second}$$

$$\sigma = \text{total number of neutrons scattered per second} / \Phi$$

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into d}\Omega}{\Phi \text{ d}\Omega}$$

$$\frac{d^2\sigma}{d\Omega dE} = \frac{\text{number of neutrons scattered per second into d}\Omega \text{ \& dE}}{\Phi \text{ d}\Omega \text{ dE}}$$



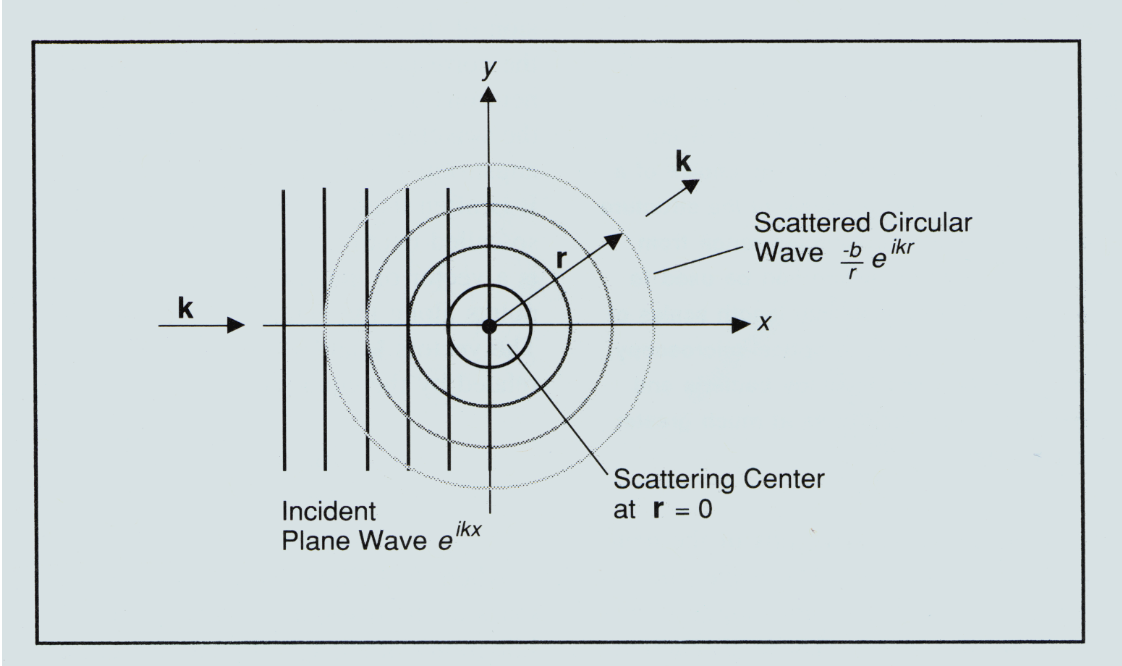
cross section

The effective area presented by a nucleus to an incident neutron. One unit for cross section is the barn, as in "can't hit the side of a barn!"

σ measured in barns:
1 barn = 10^{-24} cm^2

Attenuation = exp(-Nσt)
N = # of atoms/unit volume
t = thickness

Scattering by a Single (fixed) Nucleus



- range of nuclear force (~ 1fm) is << neutron wavelength so scattering is "point-like"
- energy of neutron is too small to change energy of nucleus & neutron cannot transfer KE to a fixed nucleus => scattering is elastic
- we consider only scattering far from nuclear resonances where neutron absorption is negligible

If v is the velocity of the neutron (same before and after scattering), the number of neutrons passing through an area dS per second after scattering is:

$$v\, dS\, |\psi_{scat}|^2 = v\, dS\, b^2/r^2 = v\, b^2\, d\Omega$$

Since the number of incident neutrons passing through unit areas is: $\Phi = v|\psi_{incident}|^2 = v$

$$\frac{d\sigma}{d\Omega} = \frac{v\, b^2\, d\Omega}{\Phi d\Omega} = b^2 \qquad \text{so } \sigma_{total} = 4\pi b^2 \qquad \text{(note units)}$$

Adding up Neutrons Scattered by Many Nuclei

At a nucleus located at $\vec{R}_i$ the incident wave is $e^{i\vec{k}_0.\vec{R}_i}$

so the scattered wave is $\psi_{scat} = \sum e^{i\vec{k}_0.\vec{R}_i} \left[\frac{-b_i}{|\vec{r} - \vec{R}_i|} e^{i\vec{k}'.(\vec{r}-\vec{R}_i)} \right]$

$$\therefore \frac{d\sigma}{d\Omega} = \frac{v dS |\psi_{scat}|^2}{v d\Omega} = \frac{dS}{d\Omega} \left| b_i e^{i\vec{k}'.\vec{r}} \sum \frac{1}{|\vec{r} - \vec{R}_i|} e^{i(\vec{k}_0-\vec{k}').\vec{R}_i} \right|^2$$

If we measure far enough away so that $r >> R_i$ we can use $d\Omega = dS/r^2$ to get

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} b_i b_j e^{i(\vec{k}_0-\vec{k}').(\vec{R}_i-\vec{R}_j)} = \sum_{i,j} b_i b_j e^{-i\vec{Q}.(\vec{R}_i-\vec{R}_j)}$$

where the wavevector transfer Q is defined by $\vec{Q} = \vec{k}' - \vec{k}_0$

Coherent and Incoherent Scattering

The scattering length, b_i , depends on the nuclear isotope, spin relative to the neutron & nuclear eigenstate. For a single nucleus:

$$b_i = \langle b \rangle + \delta b_i \quad \text{where } \delta b_i \text{ averages to zero}$$

$$b_i b_j = \langle b \rangle^2 + \langle b \rangle (\delta b_i + \delta b_j) + \delta b_i \delta b_j$$

$$\text{but } \langle \delta b \rangle = 0 \text{ and } \langle \delta b_i \delta b_j \rangle \text{ vanishes unless } i = j$$

$$\langle \delta b_i^2 \rangle = \langle b_i - \langle b \rangle \rangle^2 = \langle b^2 \rangle - \langle b \rangle^2$$

$$\therefore \frac{d\sigma}{d\Omega} = \langle b \rangle^2 \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} + (\langle b^2 \rangle - \langle b \rangle^2) N$$

Coherent Scattering
(scattering depends on the direction & magnitude of **Q**)

Incoherent Scattering
(scattering is uniform in all directions)

Note: N = number of atoms in scattering system

Nuclear Spin Incoherent Scattering

Consider a single isotope with spin I. The spin of the nucleus - neutron system can be $(I+1/2)$ or $(I-1/2)$.

The number of states with spin $(I+1/2)$ is $2(I+1/2)+1=2I+2$

The number of states with spin $(I-1/2)$ is $2(I-1/2)+1=2I$

If the neutrons and the nuclear spins are unpolarized, each spin state has the same *a priori* probability.

The frequency of occurence of b^+ state is $f^+=(2\mathrm{I}+2)/(4\mathrm{I}+2)$

The frequency of occurence of b^- state is $f^-=(2\mathrm{I})/(4\mathrm{I}+2)$

Thus $\langle b\rangle=\dfrac{1}{2I+1}\left[(I+1)b^+ + Ib^-\right]$ and $\langle \mathrm{b}^2\rangle=\dfrac{1}{2I+1}\left[(I+1)(b^+)^2+I(b^-)^2\right]$

Values of s_{coh} and s_{inc}

Nuclide	s_{coh}	s_{inc}	Nuclide	s_{coh}	s_{inc}
^{1}H	1.8	80.2	V	0.02	5.0
^{2}H	5.6	2.0	Fe	11.5	0.4
C	5.6	0.0	Co	1.0	5.2
O	4.2	0.0	Cu	7.5	0.5
Al	1.5	0.0	^{36}Ar	24.9	0.0

- Difference between H and D used in experiments with soft matter (contrast variation)
- Al used for windows
- V used for sample containers in diffraction experiments and as calibration for energy resolution
- Fe and Co have nuclear cross sections similar to the values of their magnetic cross sections
- Find scattering cross sections at the NIST web site at:

  http://webster.ncnr.nist.gov/resources/n-lengths/

Coherent Elastic Scattering measures the Structure Factor S(Q) I.e. correlations of atomic positions

$$\frac{d\sigma}{d\Omega} = \langle b \rangle^2 N.S(\vec{Q})$$ for an assembly of similar atoms where $$S(\vec{Q}) = \frac{1}{N}\left\langle \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} \right\rangle_{\text{ensemble}}$$

Now $\sum_i e^{-i\vec{Q}.\vec{R}_i} = \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \sum_i \delta(\vec{r} - \vec{R}_i) = \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \rho_N(\vec{r})$ where ρ_N is the nuclear number density

so
$$S(\vec{Q}) = \frac{1}{N}\left\langle \left| \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \rho_N(\vec{r}) \right|^2 \right\rangle$$

or $S(\vec{Q}) = \frac{1}{N}\int d\vec{r}' \int d\vec{r}.e^{-i\vec{Q}.(\vec{r}-\vec{r}')} \langle \rho_N(\vec{r}) \rho_N(\vec{r}') \rangle = \frac{1}{N}\int d\vec{R} \int d\vec{r} e^{-i\vec{Q}.\vec{R}} \langle \rho_N(\vec{r}) \rho_N(\vec{r} - \vec{R}) \rangle$

ie
$$S(\vec{Q}) = 1 + \int d\vec{R}.\{g(\vec{R}) - \bar{\rho}\}.e^{-i\vec{Q}.\vec{R}}$$

where $$g(\vec{R}) = \sum_{i \neq 0} \langle \delta(\vec{R} - \vec{R}_i + \vec{R}_0) \rangle$$ is a function of $\vec{R}$ only.

g(R) is known as the **static pair correlation function**. It gives the probability that there is an atom, i, at distance R from the origin of a coordinate system, given that there is also a (different) atom at the origin of the coordinate system at the same instant in time.

S(Q) and g(r) for Simple Liquids

- Note that S(Q) and g(r)/r both tend to unity at large values of their arguments
- The peaks in g(r) represent atoms in “coordination shells”
- g(r) is expected to be zero for r < particle diameter – ripples are truncation errors from Fourier transform of S(Q)

Fig. 5.1 The structure factor $S(\kappa)$ for ^{36}Ar at 85 K. The curve through the experimental points is obtained from a molecular dynamics calculation of Verlet based on a Lennard-Jones potential. (After Yarnell *et al.*, 1973.)

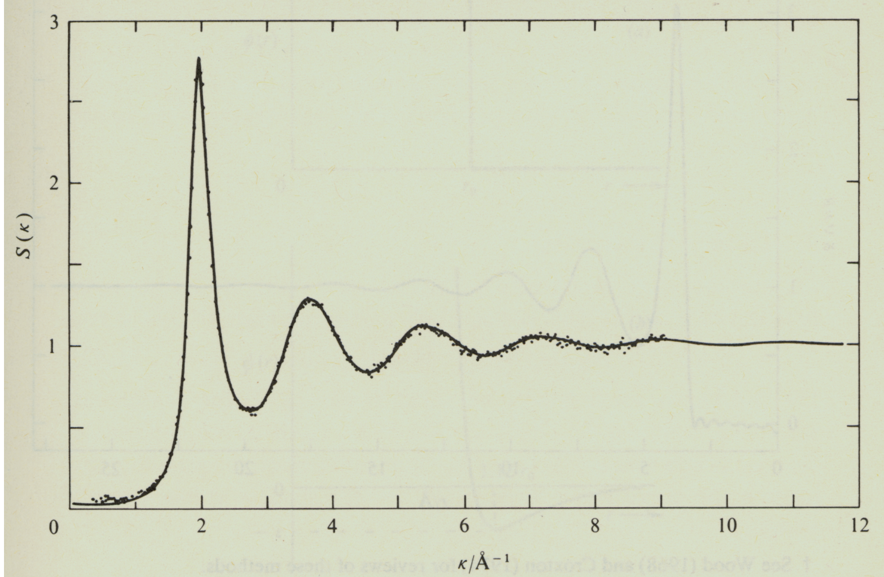
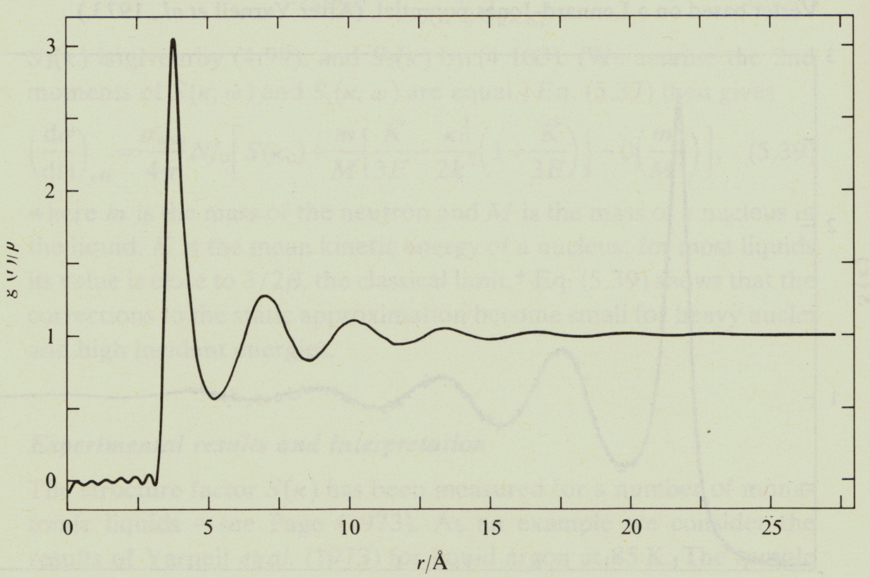


Fig. 5.2 The pair-distribution function $g(r)$ obtained from the experimental results in Fig. 5.1. The mean number density is $\rho = 2.13 \times 10^{28}$ atoms m^{-3}. (After Yarnell *et al.*, 1973.)

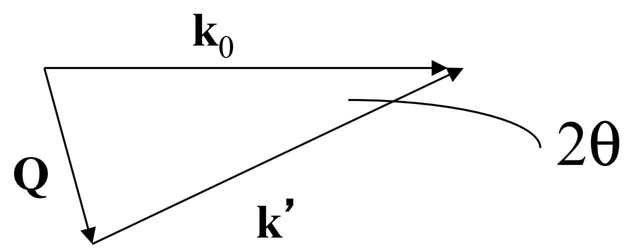


Summarizing:

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered through angle } 2\theta \text{ per second into d}\Omega}{\text{number of incident neutrons per square cm per second}}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = \sum_{i,j} b_i^{coh} b_j^{coh} e^{i(\vec{k}_0 - \vec{k}').(\vec{R}_i - \vec{R}_j)} = \sum_{i,j} b_i^{coh} b_j^{coh} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)}$$

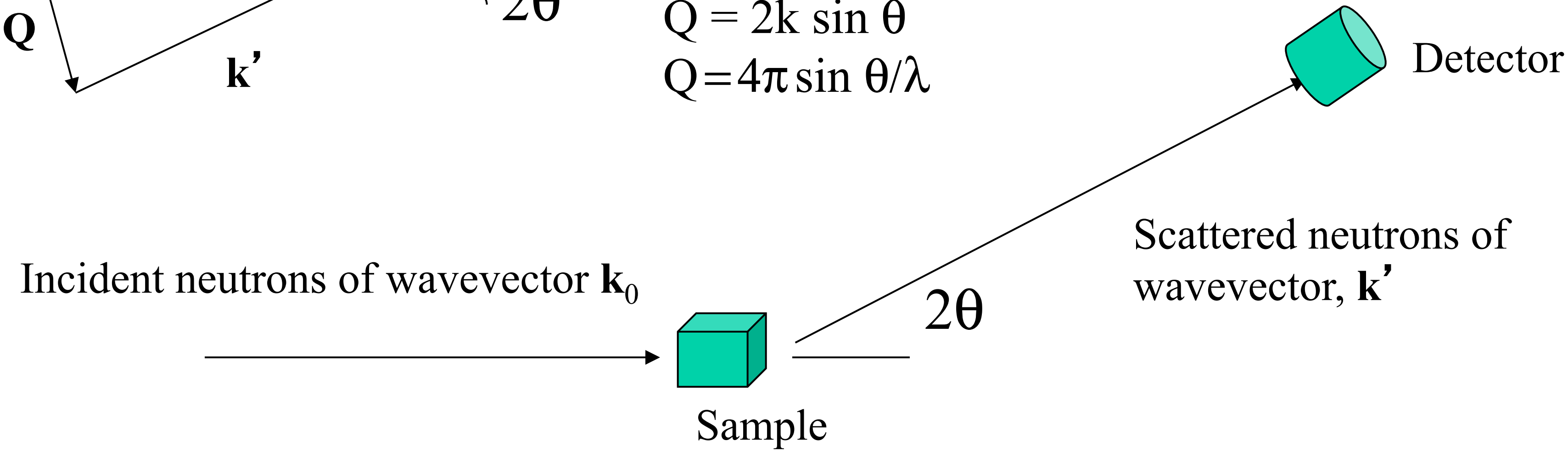
where the wavevector transfer $\vec{Q}$ is defined by $\vec{Q} = \vec{k}' - \vec{k}_0$



For elastic scattering $k_0 = k' = k$:

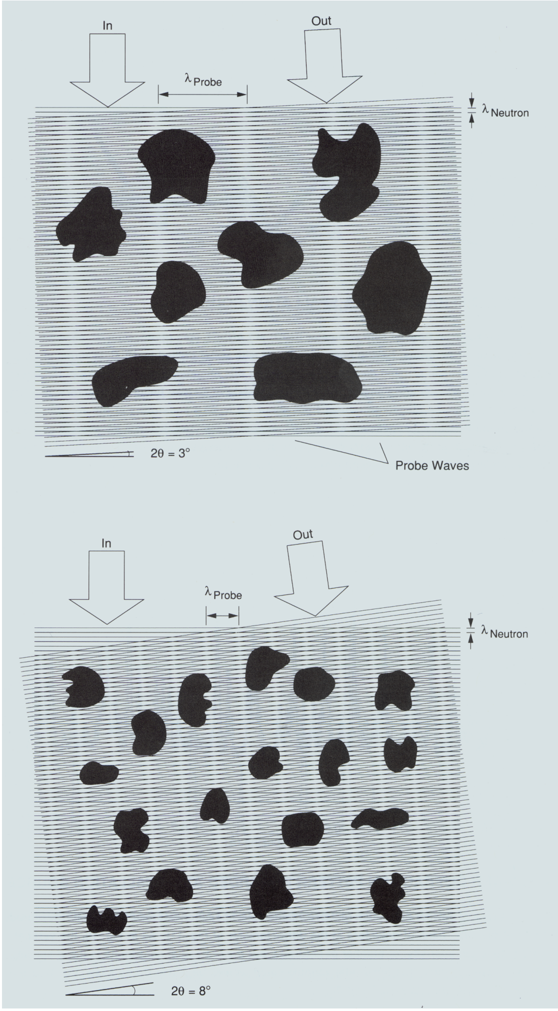
$Q = 2k \sin\theta$

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



Neutron Diffraction

- Neutron diffraction is used to measure the differential cross section, dσ/dω
  - Crystalline solids
    - Unit cell size; crystal symmetry; atomic arrangement and thermal motions (ellipsoids)
  - Liquids and amorphous materials
  - Large scale structures



- Depending on the scattering angle, structure on different length scales, d, is measured:

$$2\pi / Q = d = \lambda / 2\sin(\theta)$$

- For crystalline solids & liquids, use wide angle diffraction. For large structures, e.g. polymers, colloids, micelles, etc. use small-angle neutron scattering

The Kinematical Approximation

- Note that the approximation we have just seen ignores
  - Depletion of the incident beam by scattering or absorption
  - Multiple scattering

  i.e. energy is not conserved

- This so-called "kinematic approximation" is OK for weak scattering, very small crystals or "bad" crystals

- It is usually used for interpreting diffraction experiments, though "extinction corrections" are often needed with single crystals
  - If it's not adequate, use dynamical theory

- In addition, we have so-far ignored thermal motion of atoms

Bragg Scattering from Crystals

Working through the math (see, for example, Squires' book), we find:

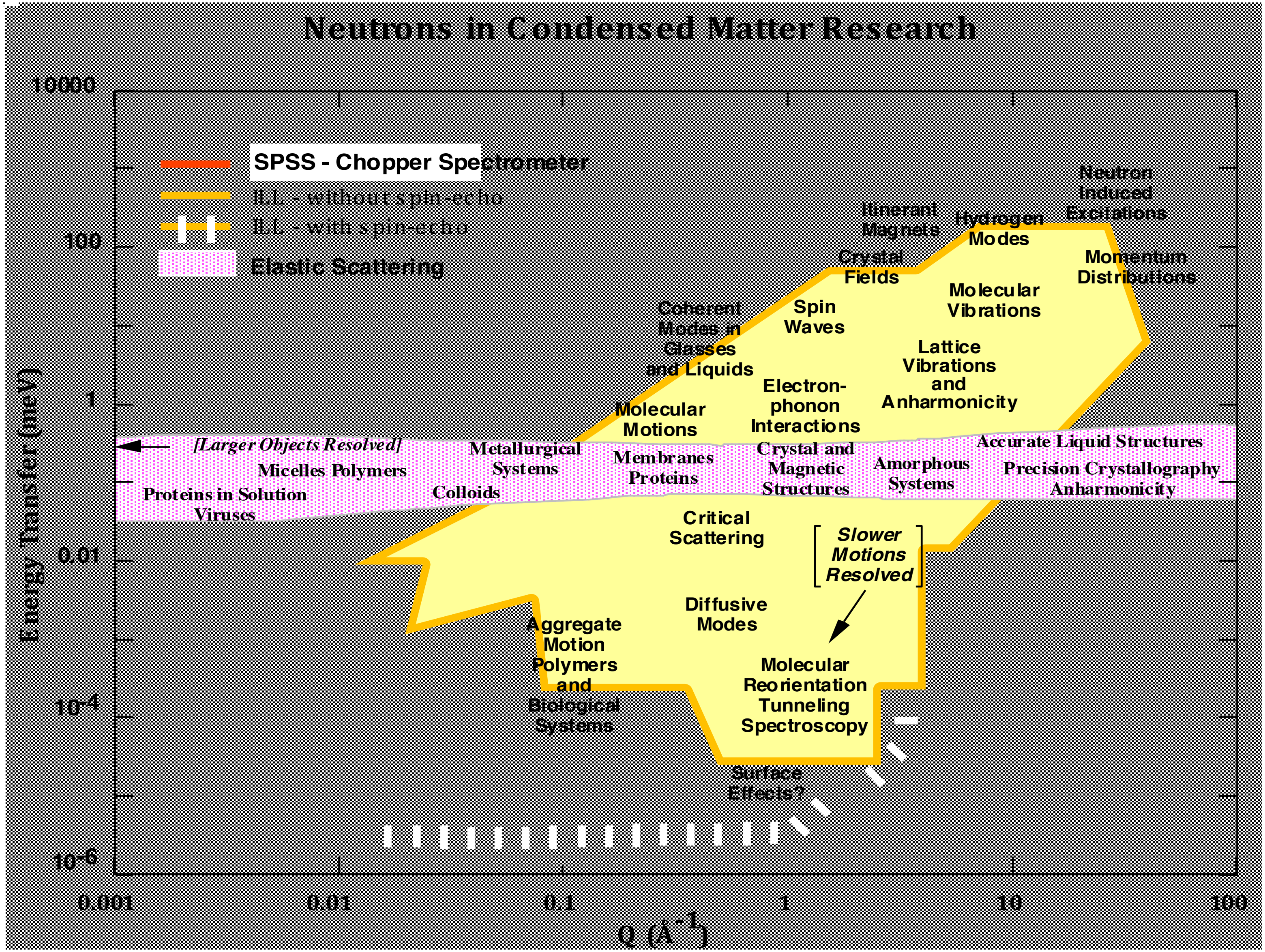
$$\left(\frac{d\sigma}{d\Omega}\right)_{Bragg} = N\frac{(2\pi)^3}{V_0}\sum_{hkl}\delta(\vec{Q}-\vec{G}_{hkl})\left|F_{hkl}(\vec{Q})\right|^2$$

where the unit-cell structure factor is given by

$$F_{hkl}(\vec{Q}) = \sum_d \overline{b}_d e^{i\vec{Q}.\vec{d}} e^{-W_d}$$

and W_d is the Debye-Waller factor that accounts for thermal motions of atoms

- Using either single crystals or powders, neutron diffraction can be used to measure F^2 (which is proportional to the intensity of a Bragg peak) for various values of (hkl).
- Direct Fourier inversion of diffraction data to yield crystal structures is not possible because we only measure the magnitude of F, and not its phase => models must be fit to the data
- Neutron powder diffraction has been particularly successful at determining structures of new materials, e.g. high T_c materials



Neutron scattering experiments measure the number of neutrons scattered at different values of the wavevector and energy transfered to the neutron, denoted Q and E. The phenomena probed depend on the values of Q and E accessed.

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