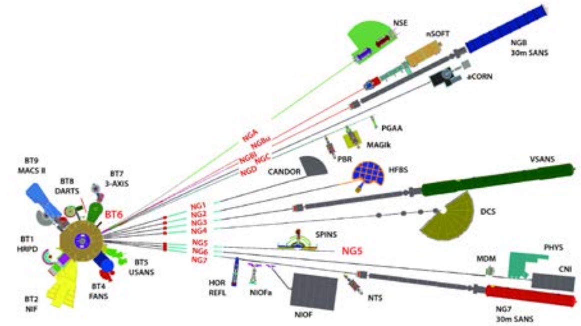
2019 NCNR Summer School on Methods and Applications of Neutron Spectroscopy



Basic Elements of Neutron Inelastic Scattering

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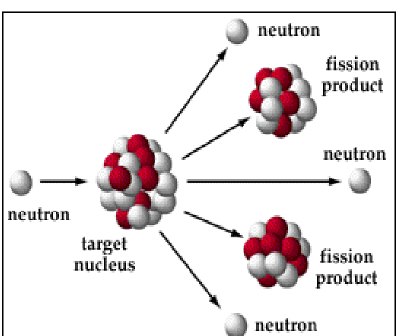
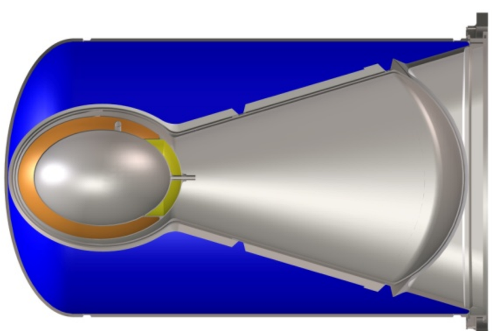
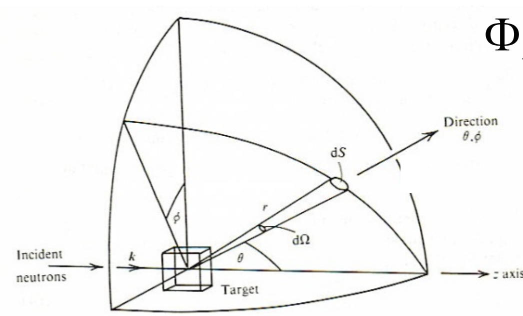
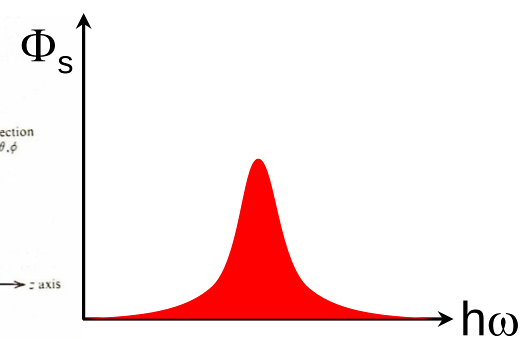
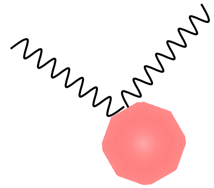




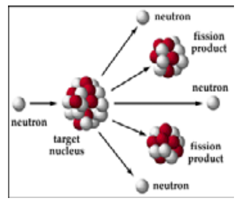




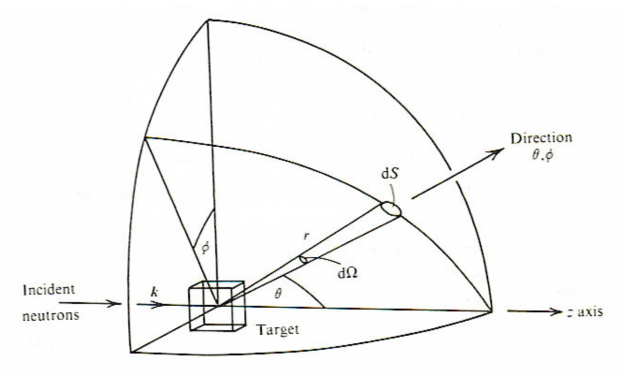
Outline



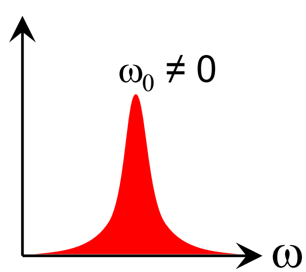
1. Introduction
   - Motivation
   - Scattering Probes

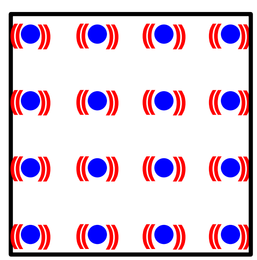


2. The Neutron
   - Production and Moderation
   - Wave/Particle Duality



3. Basic Elements of Neutron Scattering
   - The Scattering Length b
   - Scattering Cross Sections
   - Pair Correlation Functions
   - Coherent and Incoherent Scattering
   - Neutron Scattering Methods

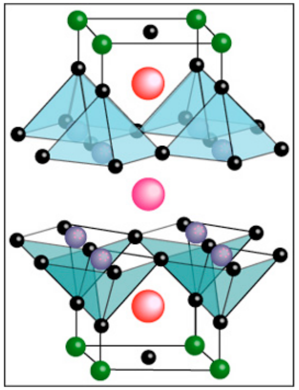




4. Summary of Scattering Cross Sections
   - Elastic (Bragg versus Diffuse)
   - Quasielastic (Diffusion)
   - Inelastic (Phonons)

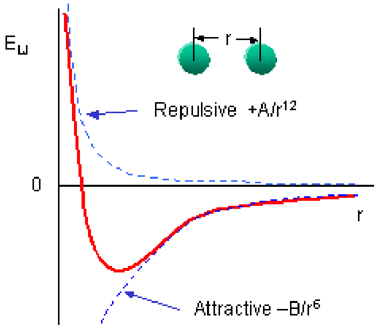
Motivation

Structure and Dynamics



$Bi_2Sr_2CaCu_2O_{8+\delta}$

The most important property of any material is its underlying atomic / molecular structure (structure dictates function).

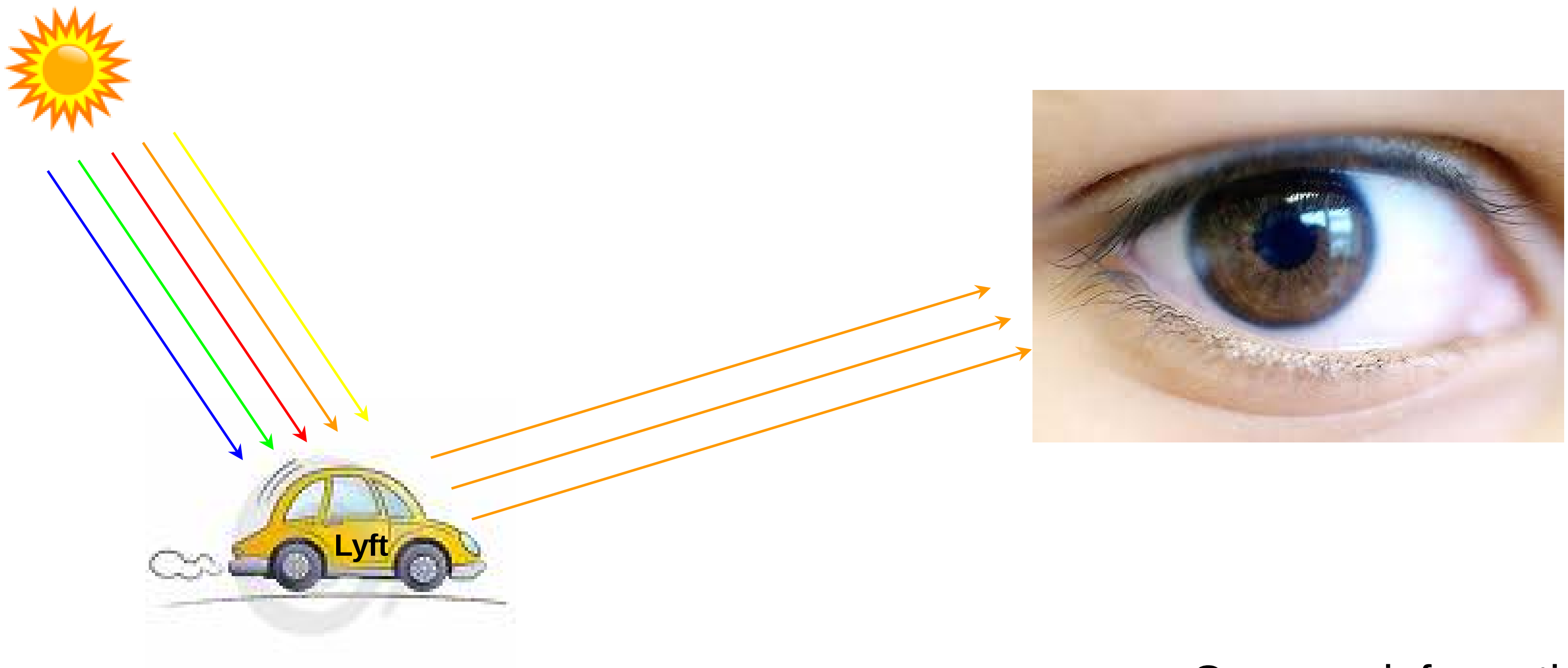


The motions of the atoms (dynamics) are extremely important because they provide information about the interatomic potentials.

An ideal method of characterization would provide detailed information about both structure and dynamics.

Motivation

Why Should We Scatter?



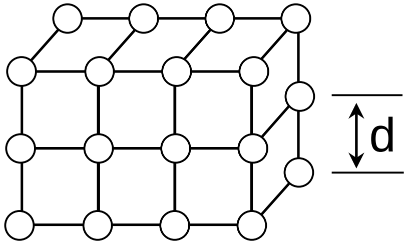
- We see something when light scatters from it. → Conveys information: location, speed, shape
- Light is composed of electromagnetic waves. → $\lambda \sim 4000$ Å – 7000 Å
- However, the details of what we can see are ultimately limited by the wavelength.

Motivation

The tracks of a compact disk act as a diffraction grating, producing a separation of the colors of white light when it scatters from the surface.

From this one can determine the nominal distance between tracks on a CD, which is 1.6×10^{-6} meters = 16,000 Angstroms.

To characterize materials we must determine the underlying structure. We do this by using the material as a diffraction grating.



Problem: Distances between atoms in materials are of order Angstroms → light is inadequate. Moreover, most materials are opaque to light.

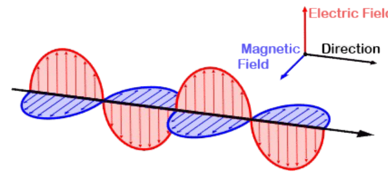
$$\boxed{\lambda_{Light} \gg d \sim 4\ \text{Å}}$$

Scattering Probes

To measure atomic structure requires a probe with a λ ~ length scale of interest.

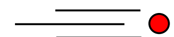
Some candidates …

X rays



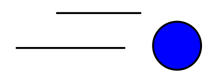
EM - wave

Electrons



Charged particle

Neutrons



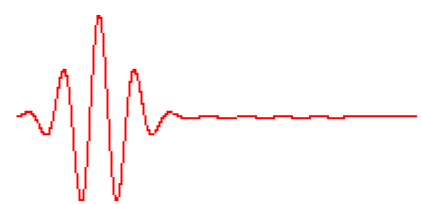
Neutral particle

1929 Nobel Laureate
in Physics

From Louis de Broglie:

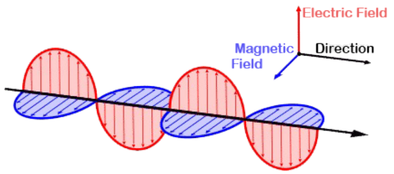
$$\lambda = h/p = h/mv$$

Particles have wave properties too.



Scattering Probes

X rays: Pros and Cons



If we wish only to determine relative atomic positions, then we should choose x rays almost every time.

1. Relatively cheap

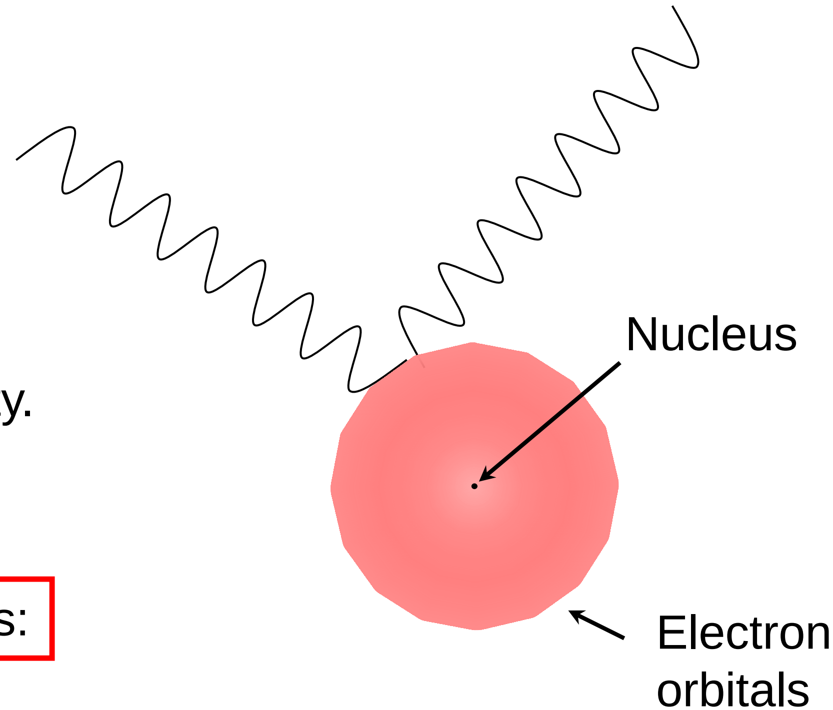
2. Sources are ubiquitous → easy access

3. High flux → can study small samples

4. Extremely good resolution

However …

Scattering Probes

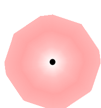


X rays are electromagnetic radiation.
Thus they scatter from the charge density.

Consequences:

Low-Z elements are hard to see.

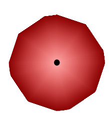
Hydrogen



(Z = 1)

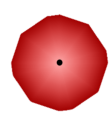
Elements with similar atomic numbers have very little contrast.

Cobalt



??

Nickel

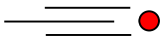


(Z = 27) (Z = 28)

X rays are strongly attenuated when passing through furnaces, cryostats, and samples too.

Scattering Probes

Electrons: Pros and Cons



Electrons are charged particles → they see both the atomic electrons and nuclear protons at the same time.

1. Relatively cheap

2. Sources are not uncommon → easy access

3. Fluxes are extremely high → can study tiny crystals

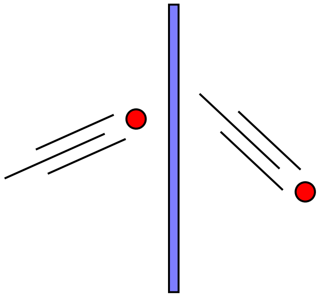
4. Very small wavelengths → more information

However …

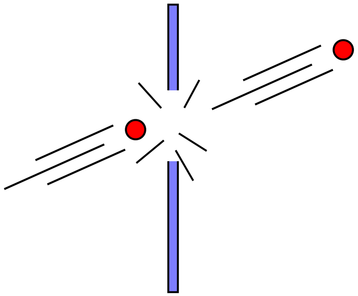
Scattering Probes

Electrons have some deficiencies too ...

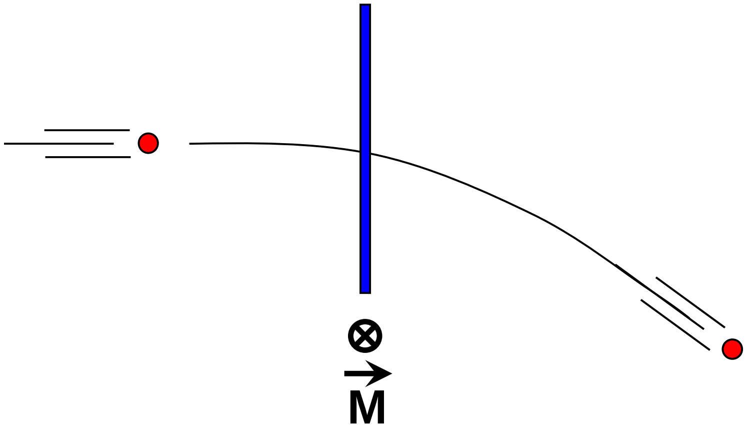
Requires very thin samples.



Radiation damage is a concern.

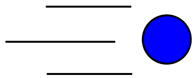


Magnetic structures are hard to determine because electrons are deflected by the internal magnetic fields.



Scattering Probes

Neutrons: Pros and Cons



Zero charge → not strongly attenuated by furnaces, etc.

Magnetic dipole moment → can study magnetic structures

Nuclear interaction → can see low-Z elements easily like H → good for the study of biomolecules and polymers.

Nuclear interaction is simple → scattering is easy to model

Low energies → Non-destructive probe

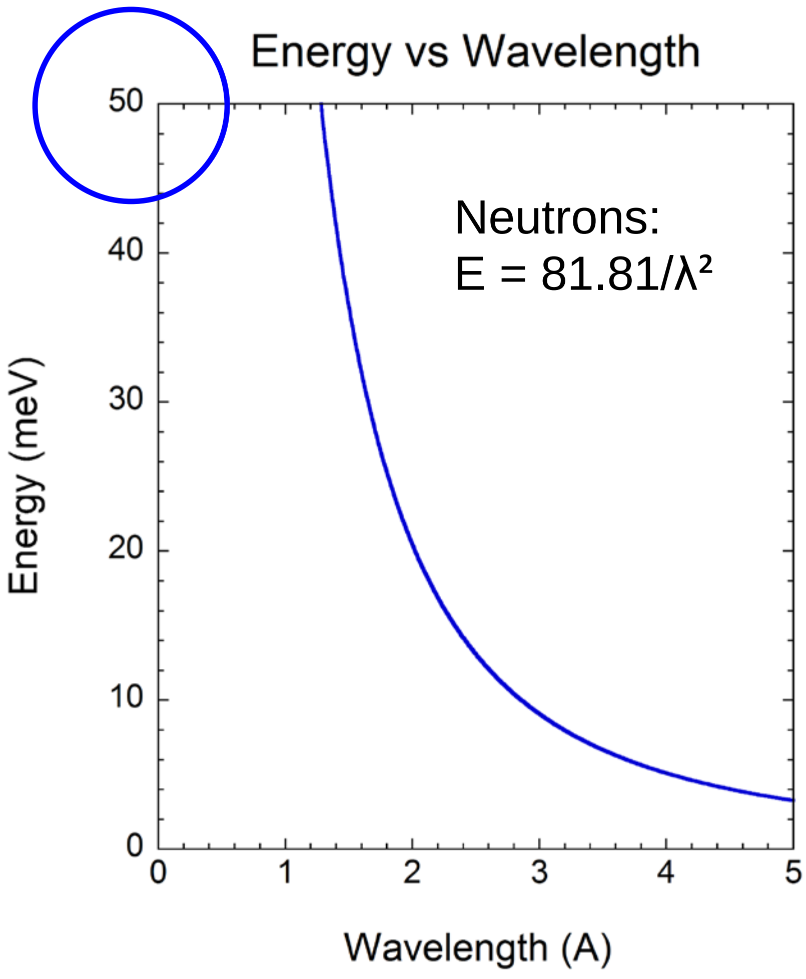
Neutrons expensive to produce → access not as easy

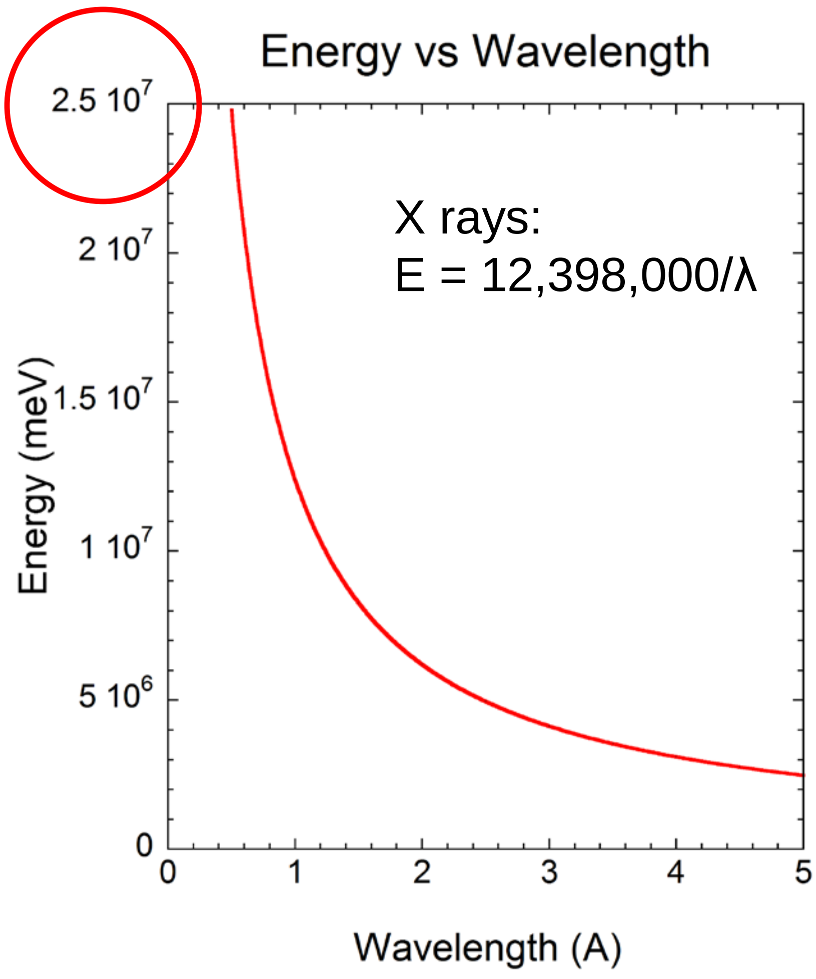
Interact weakly with matter → often require large samples

Available fluxes are low compared to other methods

Scattering Probes

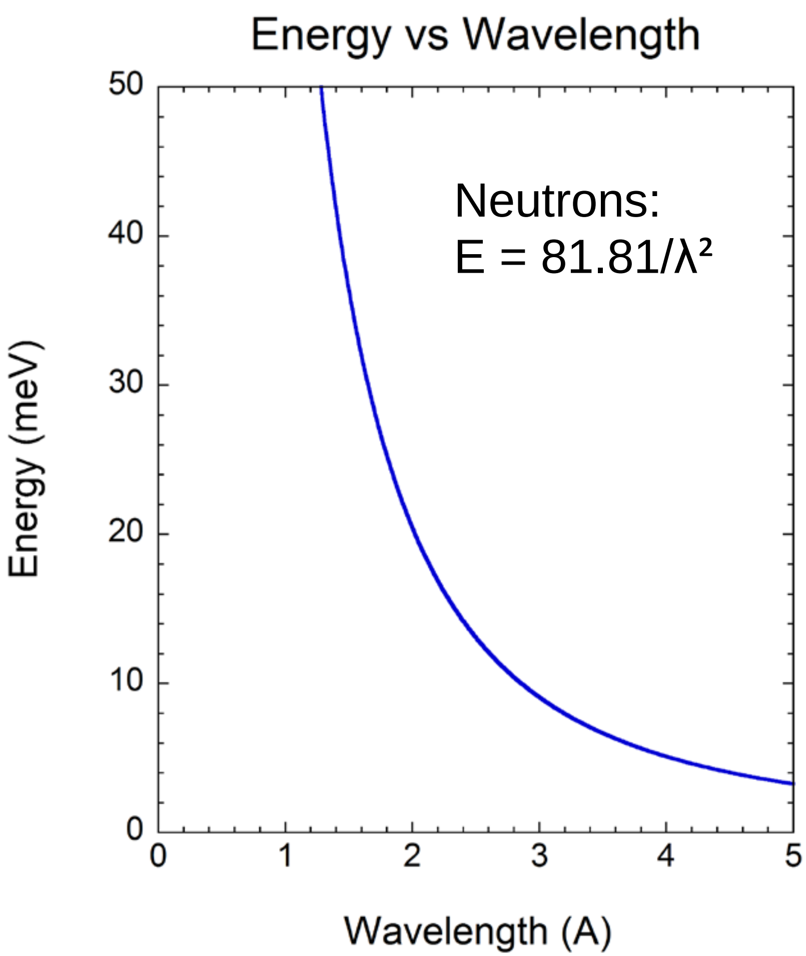
To characterize atomic dynamics requires a probe with $h\omega$ ~ energy scale of interest.

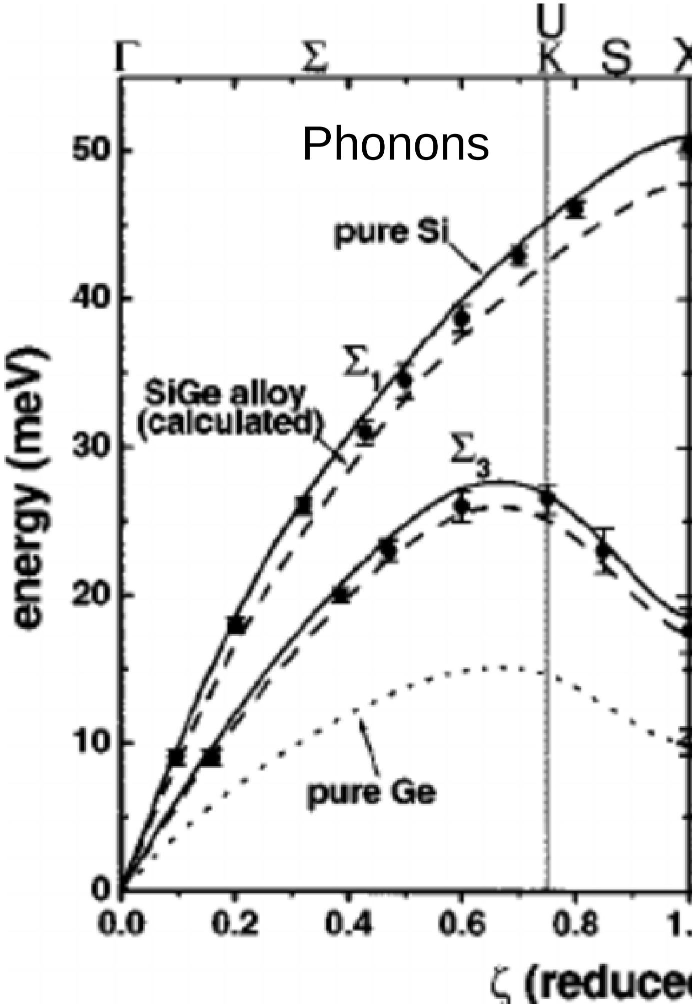




Scattering Probes

To characterize atomic dynamics requires a probe with hω ~ energy scale of interest.





Scattering Probes

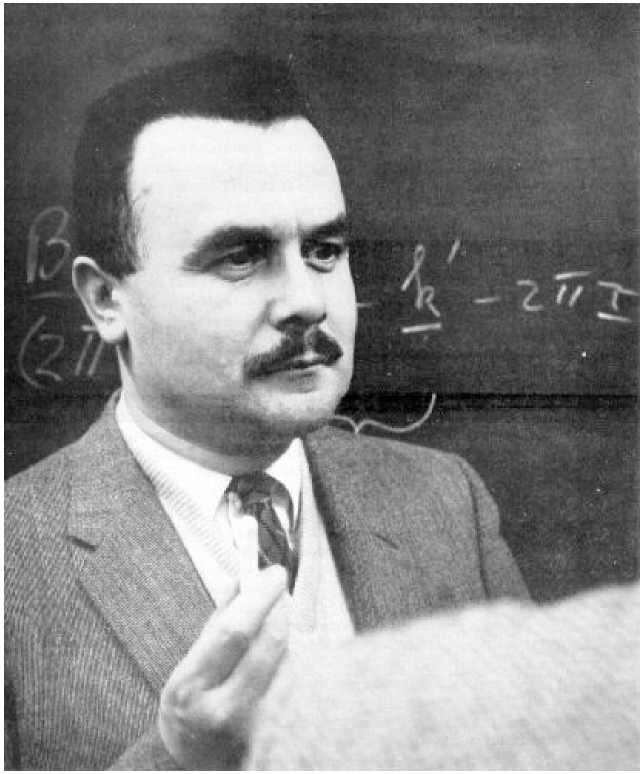
Neutron: A Lucky Coincidence

$$E = p^2/2m = h^2k^2/2m = 81.81/\lambda^2$$

The mass of the neutron is such that one can <u>simultaneously</u> study structure and dynamics.

Thus neutron scattering methods can directly measure the <u>geometry</u> of dynamic processes.

The Neutron



"If the neutron did not exist, it would need to be invented."

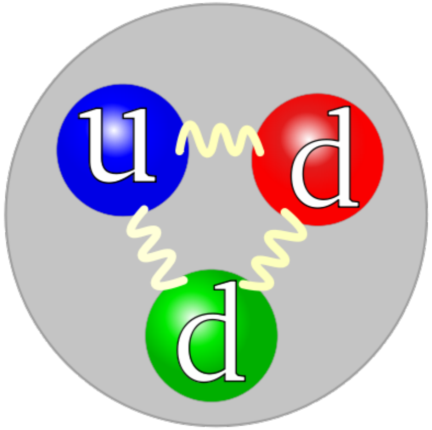
Bertram Brockhouse
1994 Nobel Laureate in Physics

The Neutron

"… for the discovery of the neutron."

Sir James Chadwick
1935 Nobel Laureate in Physics

The Neutron



$m_n = 1.675 \times 10^{-27}$ kg
$Q = 0$
$S = ½ \hbar$
$\mu_n = -1.913\ \mu_N$

Interactions:

Strong, Electro-weak, Gravity

$\lambda = 1$ Å
$v = 4000$ m/s
$E = 82$ meV

de Broglie Relation:
$\lambda = h/p = h/m_n v$

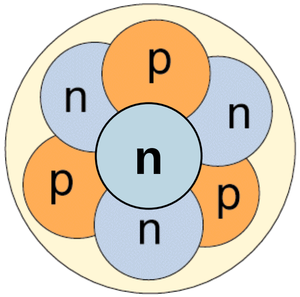
$\lambda = 9$ Å
$v = 440$ m/s
$E = 1$ meV

Production

Free neutrons decay via the weak force.
Lifetime ~ 888 seconds (15 minutes).

$$n \rightarrow p + e^{-} + \nu_e$$

A useful source of neutrons requires a nuclear process by which bound neutrons can be freed from the nuclei of atoms and that is easily sustainable.

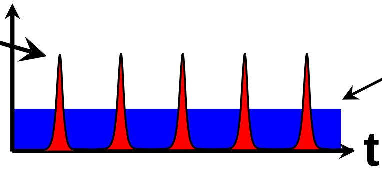


There are two such processes, spallation and fission …

Fission

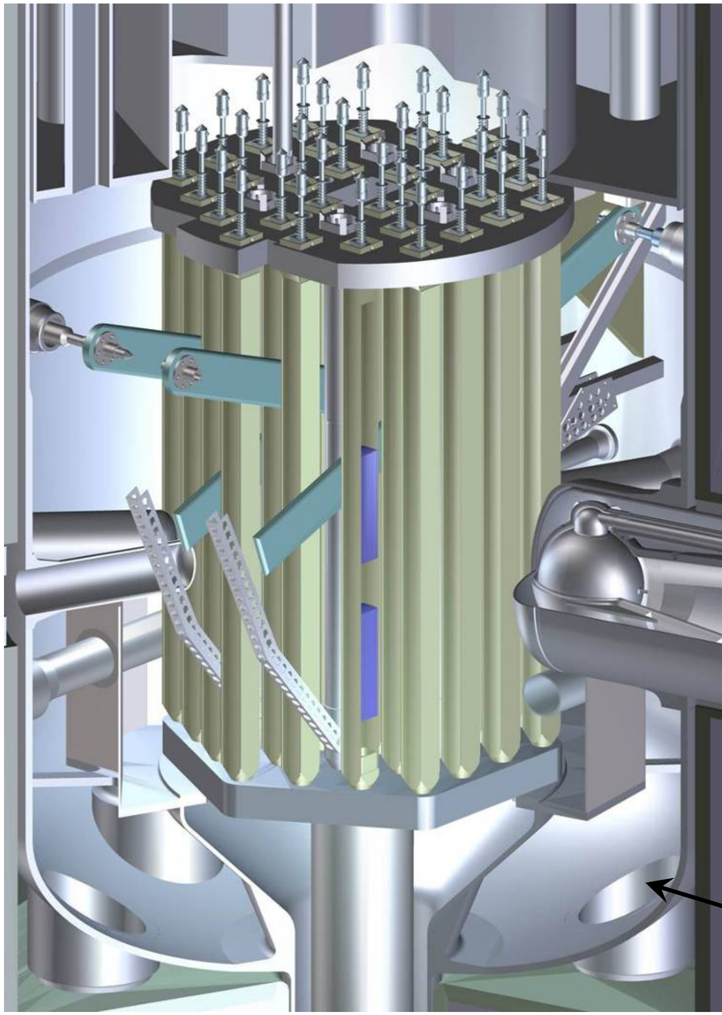
Spallation

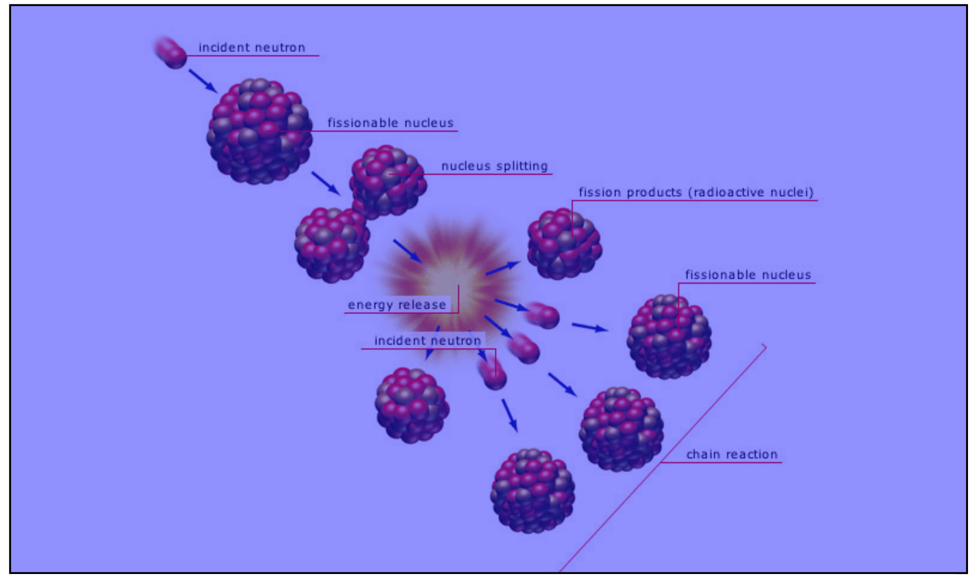
Fission



Nuclear fission is used in power and research reactors.

$$^{235}_{92}U_{143} + n \rightarrow \left[^{236}_{92}U_{144}\right]^* \rightarrow X + Y + 2.44n$$





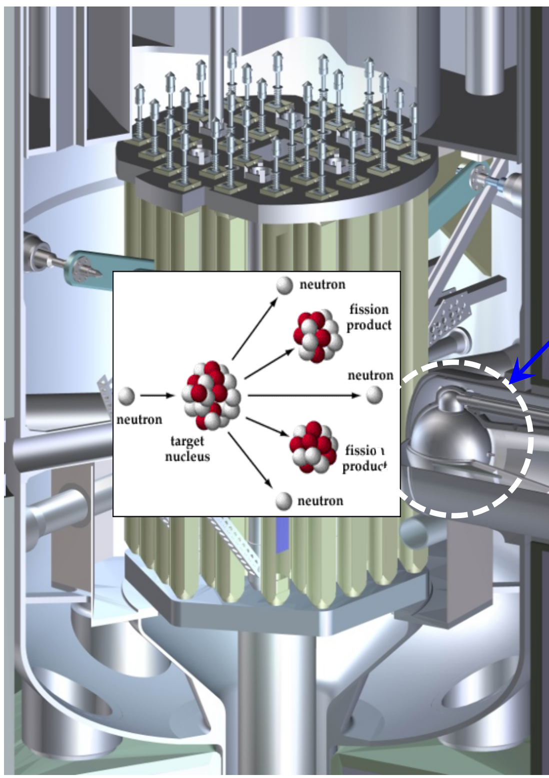
A liquid medium (D_2O, or heavy water) is used to moderate the fast fission neutrons to room temperature (2 MeV → 50 meV).

The fission process and moderator are confined by a large containment vessel.

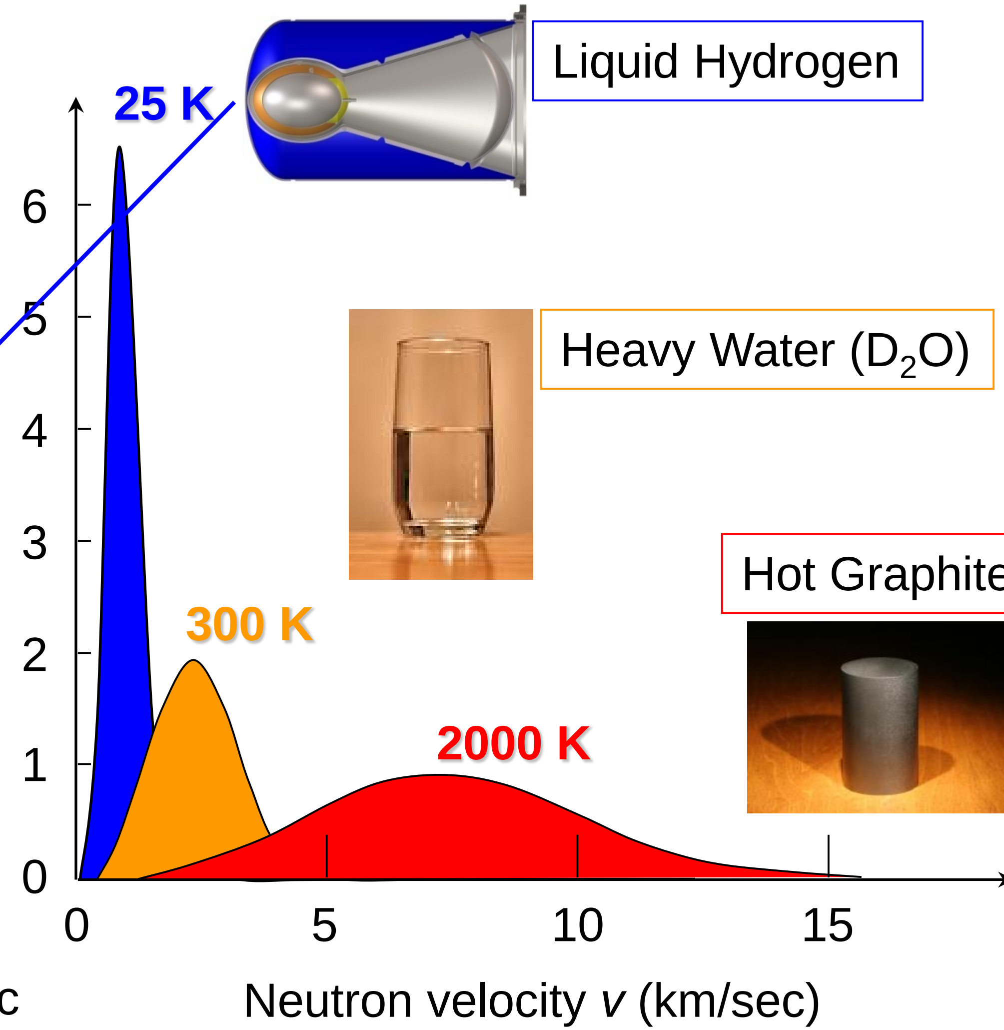
Moderation

Maxwellian Distribution

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



Liquid Hydrogen



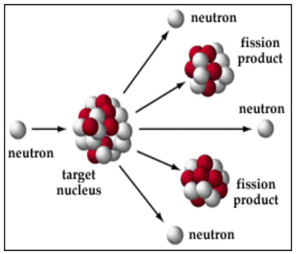
Heavy Water (D_2O)

Hot Graphite

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

Moderation

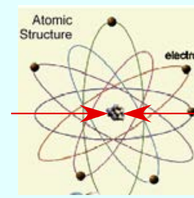
de Broglie Relation $\lambda = h/m_n v$

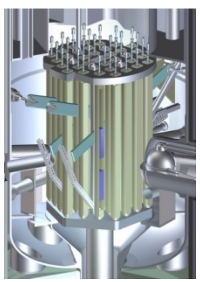


Fast Neutron,

V ~ 20,000,000 m/sec

~ 0.00002 nm

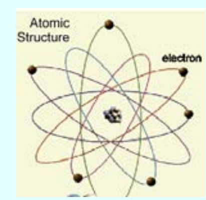


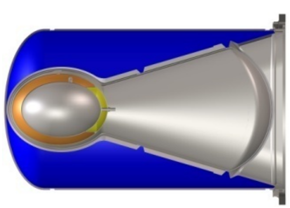


Thermal Neutron,

V ~ 2,000 m/sec

~ 0.2 nm





Cold Neutron,

V ~ 200 m/sec

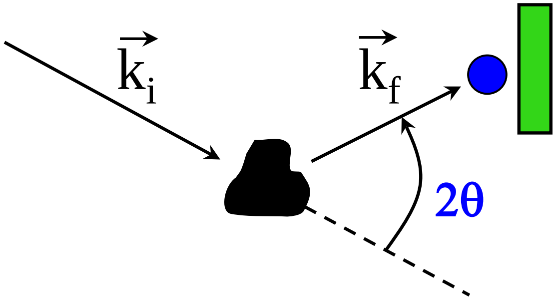
~ 2 nm

Scattering Basics

Neutron scattering experiments measure the flux Φ_s of neutrons scattered by a sample into a detector as a function of the change in neutron wave vector ($\vec{Q}$) and energy ($\hbar\omega$).

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

<u>Momentum</u>	<u>Energy</u>
$\hbar k = \hbar(2\pi/\lambda)$	$\hbar\omega_n = \hbar^2 k_n{}^2/2m$
$\hbar\vec{Q} = \hbar\vec{k}_i - \hbar\vec{k}_f$	$\hbar\omega = \hbar\omega_i - \hbar\omega_f$



The expressions for the scattered neutron flux Φ_s involve the positions and motions of atomic nuclei or unpaired electron spins.

$\Phi_s \Rightarrow$ Contains information about <u>structure</u> and <u>dynamics</u>!

Scattering Basics

These "cross sections" are what we measure experimentally.

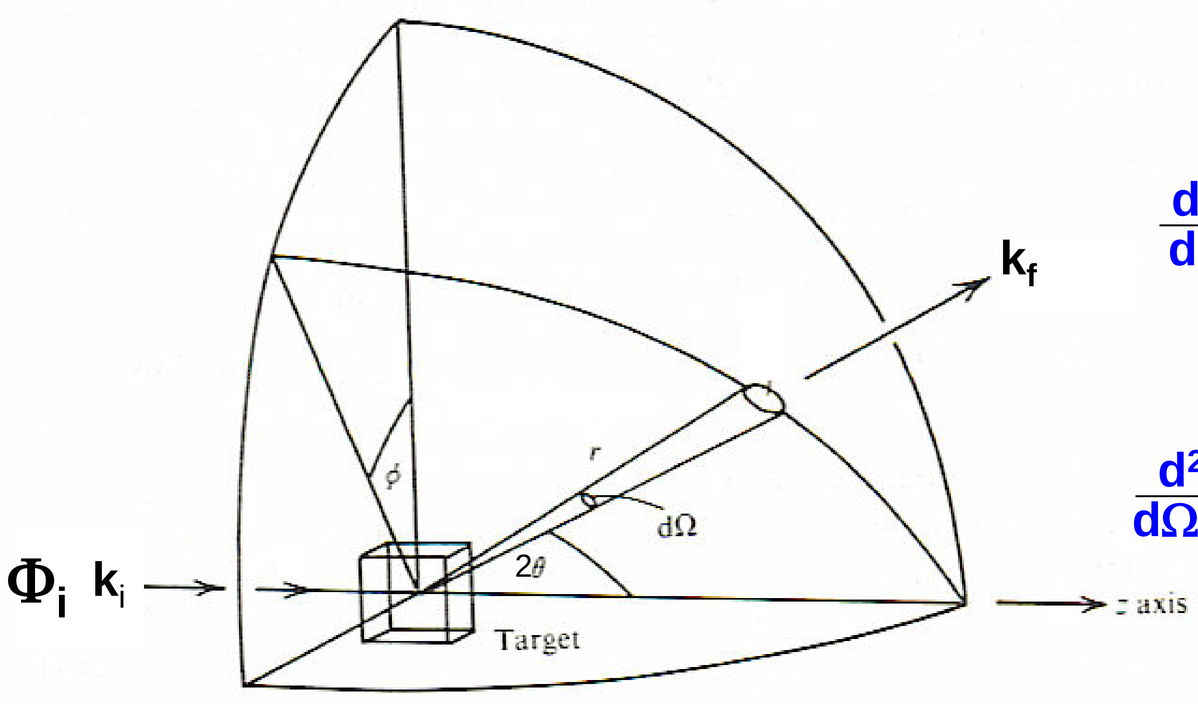
Consider an incident neutron beam with flux Φ_i (~10^6 to 10^9 n/sec/cm^2) and wave vector $\mathbf{k}_i$ on a non-absorbing sample.

We define three cross sections:

σ = Total cross section

$\frac{d\sigma}{d\Omega}$ = Differential cross section

$\frac{d^2\sigma}{d\Omega dE_f}$ = Partial differential cross section



Cross Sections

What are the physical meanings of these three cross sections?

σ Total # of neutrons scattered per second / Φ_i.
(Typically of order 1 barn = 10^{-24} cm^2.)

$\dfrac{d\sigma}{d\Omega}$ Total # of neutrons scattered per second into $d\Omega$ / $d\Omega\ \Phi_i$.
(Diffraction → structure.

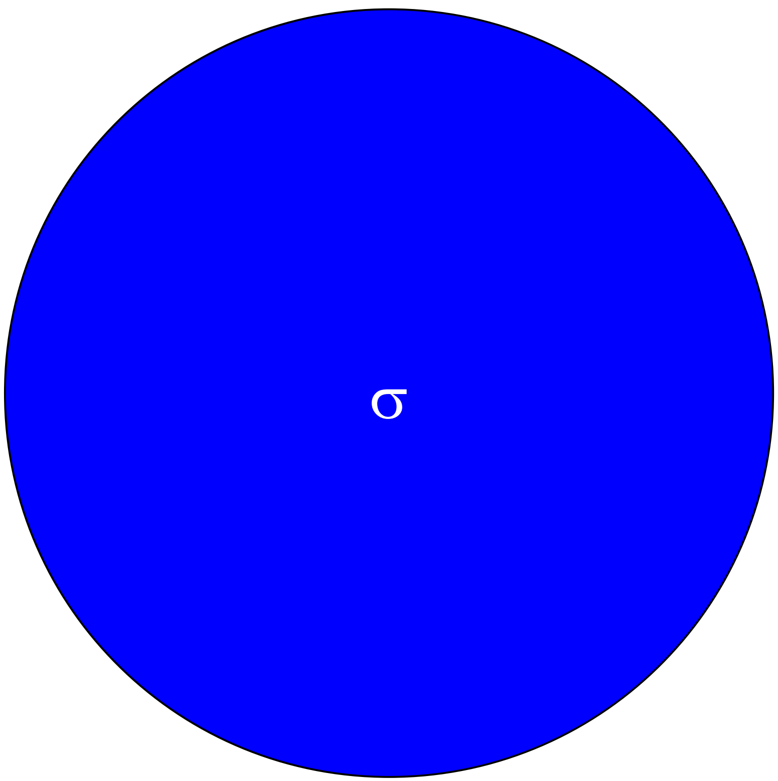
$\dfrac{d^2\sigma}{d\Omega dE_f}$ Total # of neutrons scattered per second into $d\Omega$ with a final energy between E_f and dE_f / $d\Omega\ dE_f\ \Phi_i$.
(Inelastic scattering → dynamics.

Cross Sections

What are the relative sizes of the cross sections?

Clearly: $$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int \frac{d^2\sigma}{d\Omega dE_f} d\Omega dE_f$$

Thus: $$\sigma >> \frac{d\sigma}{d\Omega} >> \frac{d^2\sigma}{d\Omega dE_f}$$



$$\frac{d^2\sigma}{d\Omega dE_f}$$

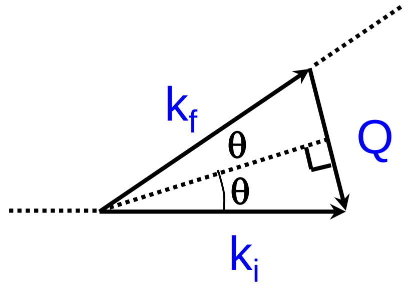
Typically, $$\frac{d\sigma}{d\Omega} \sim \underline{\underline{10^6}} \times \frac{d^2\sigma}{d\Omega dE_f}$$

Elastic vs Inelastic

Note that <u>both</u> of these cases are described by …

$$\frac{d^2\sigma}{d\Omega dE_f}$$

Elastic (k_i=k_f) $\neq \dfrac{d\sigma}{d\Omega}$



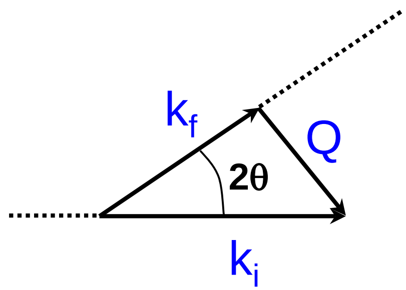
$\sin\theta = (Q/2)/k$

$Q = 2k\sin\theta = 4\pi\sin\theta/\lambda$

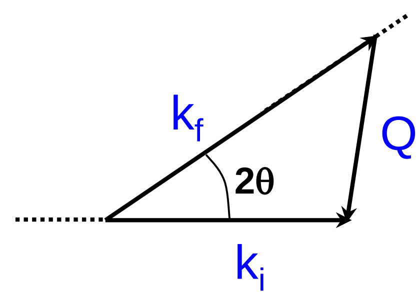
<u>Elastic Scattering:</u>

- Change in neutron energy = 0
- Probes changes in momentum only

Inelastic ($k_i \neq k_f$)



Energy loss ($h\omega$>0)



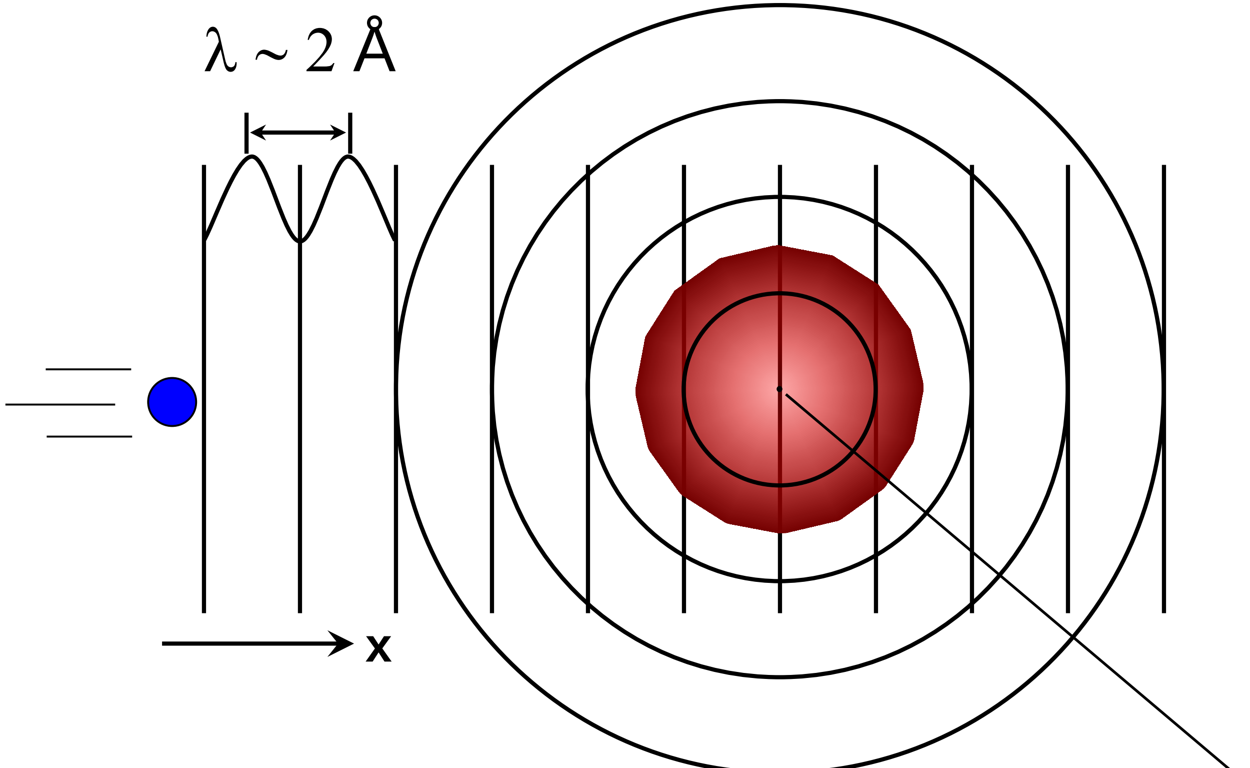
Energy gain ($h\omega$<0)

<u>Inelastic Scattering:</u>

- Change in neutron energy ≠ 0
- Probes changes in <u>both</u> momentum and energy

Nuclear Scattering

Consider the simplest case:
A fixed, isolated nucleus.



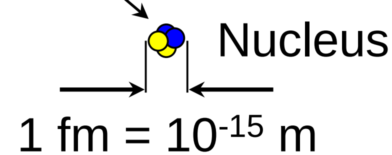
The scattered (final) neutron Ψ_f is a <u>spherical</u> wave:

$$\boxed{\Psi_f(\mathbf{r}) \sim (-b/r)e^{i\mathbf{kr}-\omega t}}$$

QUESTIONS:

1. The scattering is <u>elastic</u> ($k_i = k_f = k$). Why?

2. The scattering is <u>isotropic</u>. Why?



The incident neutron Ψ_i is a <u>plane</u> wave:

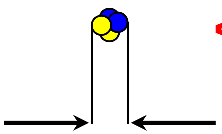
$$\boxed{\Psi_i(\mathbf{r}) \sim e^{i\mathbf{kx}-\omega t}} \quad (k = 2\pi/\lambda)$$

Nuclear Scattering

ANSWERS:

1. The scattering is elastic because the nucleus is fixed, so no energy can be transferred to it from the neutron (ignoring any excitations of the nucleus itself).

2. A basic result of diffraction theory states: if waves of any kind scatter from an object of a size $\ll \lambda$, then the scattered waves are spherically symmetric. (This is also known as s-wave scattering.)



$\ll \lambda$

$\sim 10^{-15}$ m $\ll 10^{-10}$ m

$$V(r) = \left(\frac{2\pi h^2}{m_n}\right) \sum_{j=1}^{N} b_j \, \delta(r - r_j)$$

Details of V(r) are unimportant!
V(r) can be parametrized by a scalar b that depends only the nucleus and isotope!

Fermi Pseudopotential

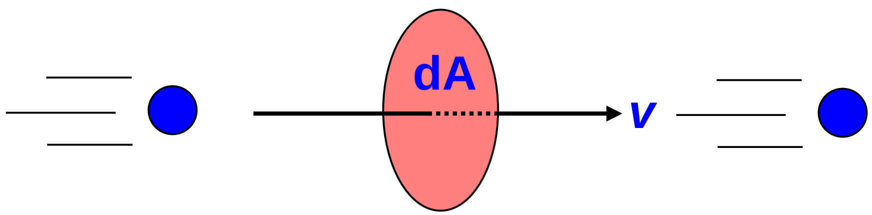
Nuclear Scattering

Calculate σ for a single, fixed nucleus:

Def.

$\sigma \cdot \Phi_i$ = Total number of neutrons scattered per second by the nucleus.

v = Velocity of neutrons (elastic → same before and after scattering).



$v\, dA\, |\Psi_f|^2$ = Total number of neutrons scattered per second through **dA**.

$$\int v\, dA\, |\Psi_f|^2 = \int v (r^2 d\Omega)(b/r)^2 = \int v\, b^2 d\Omega = v\, 4\pi b^2 = \sigma \cdot \Phi_i$$

Since $\Phi_i = v\, |\Psi_i|^2 = v$ → $\boxed{\sigma = 4\pi b^2}$

Try calculating $\dfrac{d\sigma}{d\Omega}$

Nuclear Scattering

The Neutron Scattering Length - b

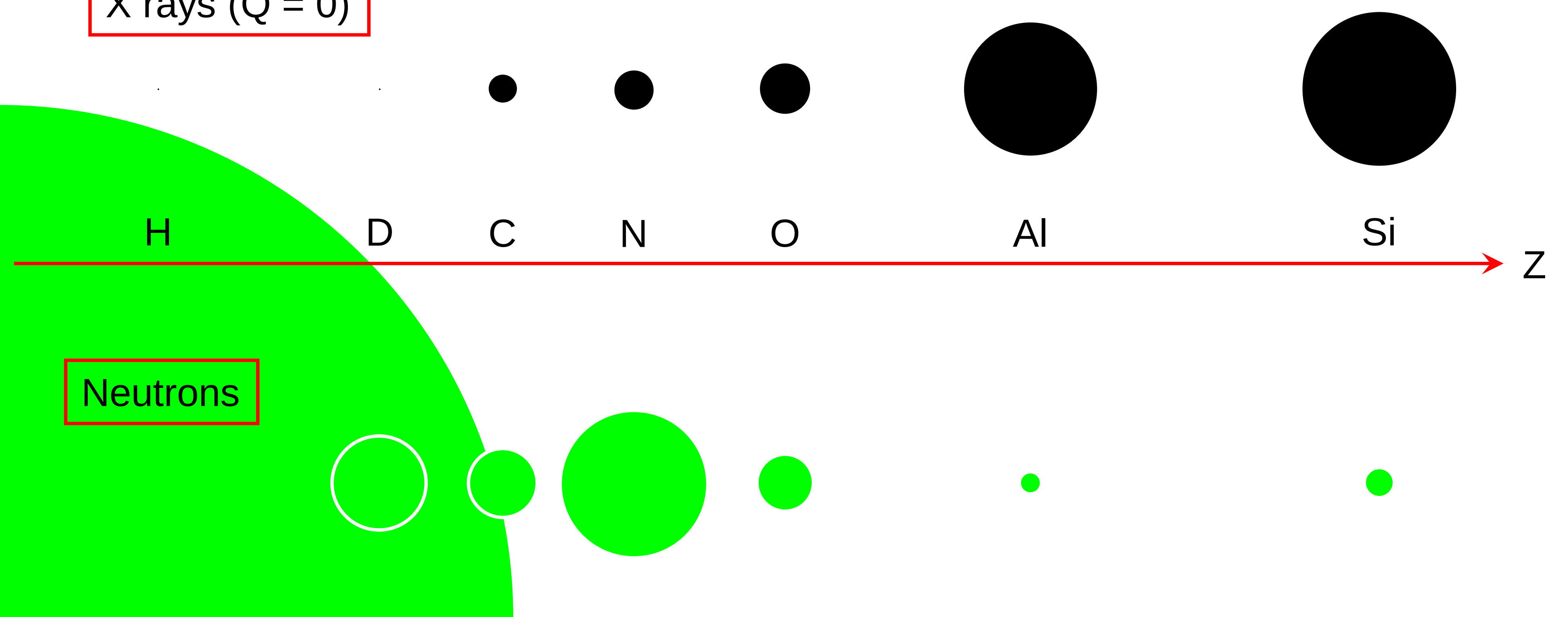
Units of length: $b \sim 10^{-12}$ cm.

Analogous to f(Q), the x-ray form factor.

Varies randomly with Z and isotope
→ Neutrons "see" atoms x rays can't.

Total Scattering Cross Section: $\sigma = 4\pi b^2$

X rays (Q = 0)



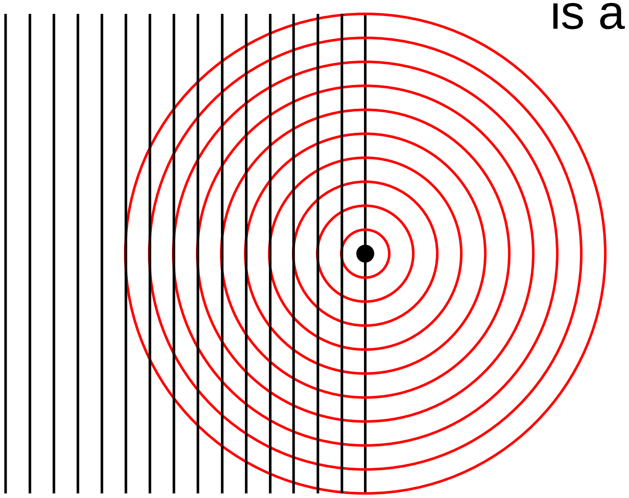
Nuclear Scattering

What if many atoms are present?

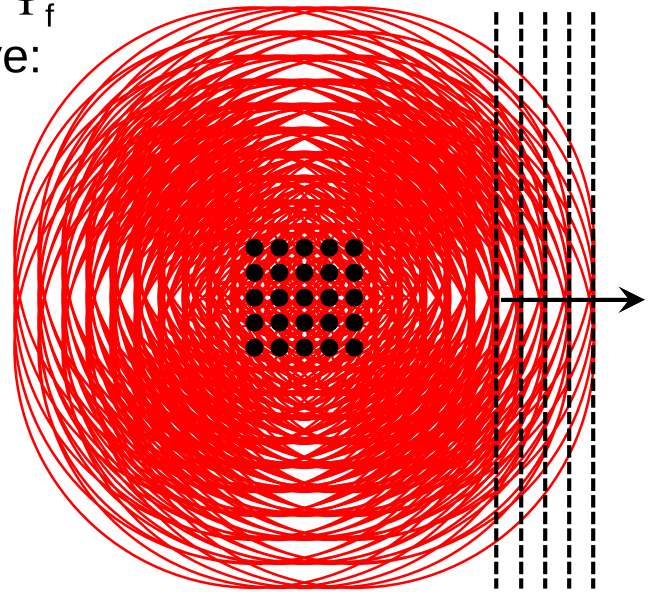
Scattering from one nucleus

Scattering from many nuclei

Scattered neutron Ψ_f is a <u>spherical</u> wave:



The incident neutron Ψ_i is a <u>plane</u> wave:



Constructive interference

Get strong scattering in some directions, but not in others. Angular dependence yields information about how the nuclei are arranged or <u>correlated</u>.

Magnetic Scattering

Magnetic vs Nuclear Scattering

<u>Nuclear Potential</u>

$$V_N(\mathbf{r}) = \frac{2\pi h^2}{m_n} b\delta(\mathbf{r})$$

Scalar interaction →
Isotropic scattering

Very short range

Depends on nucleus, isotope, and nuclear spin

<u>Magnetic Potential</u>

$$V_M(\mathbf{r}) = -\boldsymbol{\mu}_n \bullet \mathbf{B}(\mathbf{r})$$

Vector interaction →
Anisotropic scattering

Longer range

Depends on neutron spin orientation.

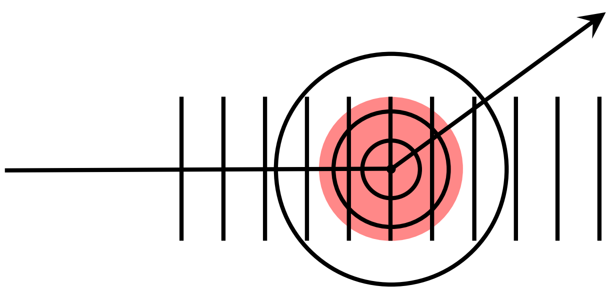
Polarized neutrons can measure the different components of M.

Magnetic Scattering

Magnetic Form Factor

Nuclear Potential

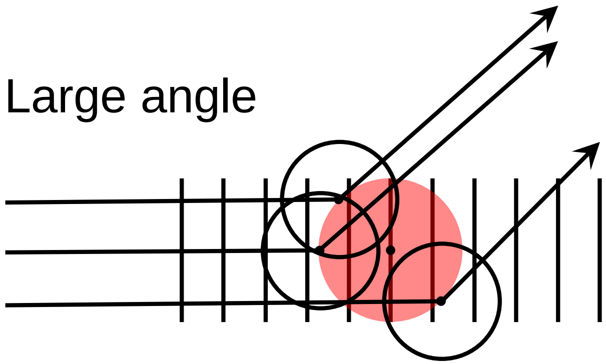
$$V_N(\mathbf{r}) = \frac{2\pi h^2}{m_n} b\delta(\mathbf{r})$$

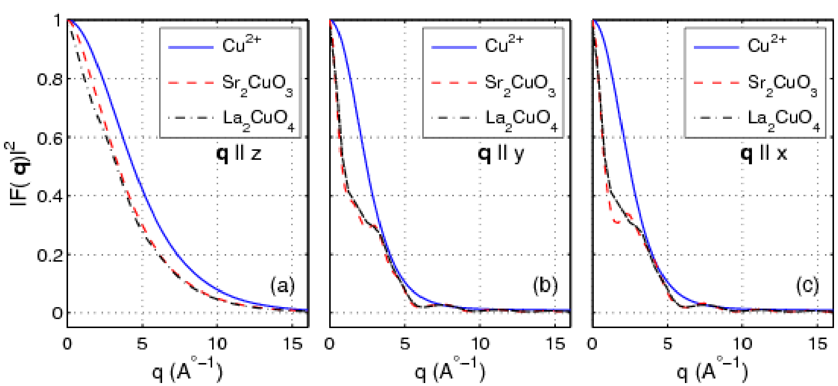


Magnetic Potential

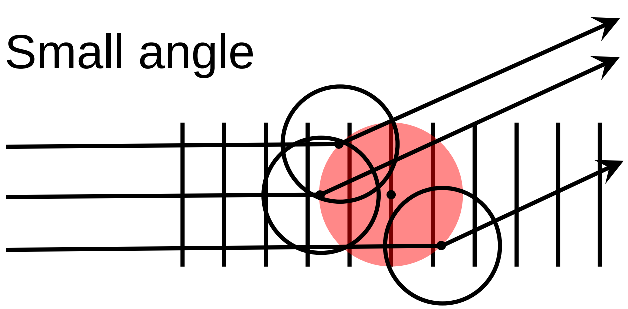
$$V_M(\mathbf{r}) = -\boldsymbol{\mu}_n \bullet \mathbf{B}(\mathbf{r})$$

Large angle





Small angle



Magnetic Scattering

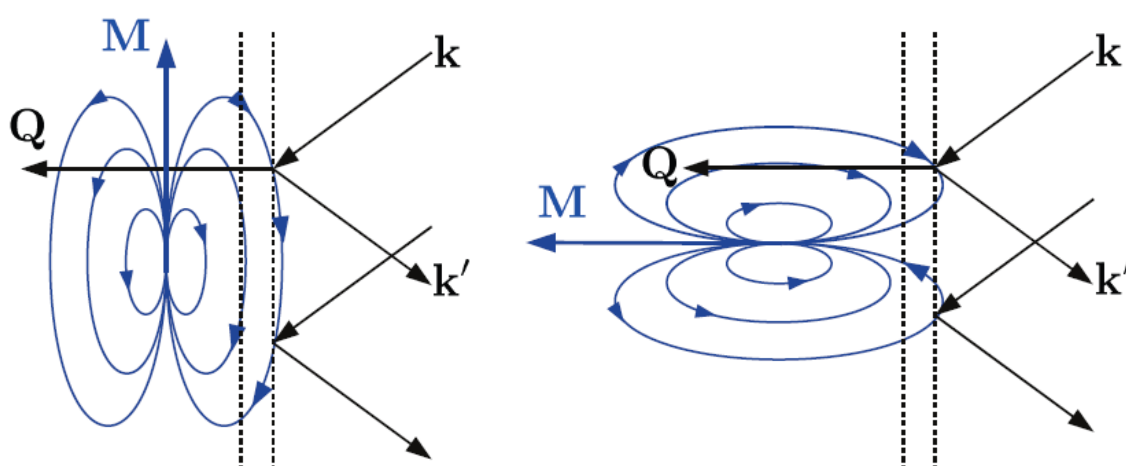
Neutrons Scatter from M Perpendicular to Q

Magnetic scattering depends on Fourier transform of interaction potential $V_M(\mathbf{r})$:

James Clerk Maxwell
(1831 – 1879)

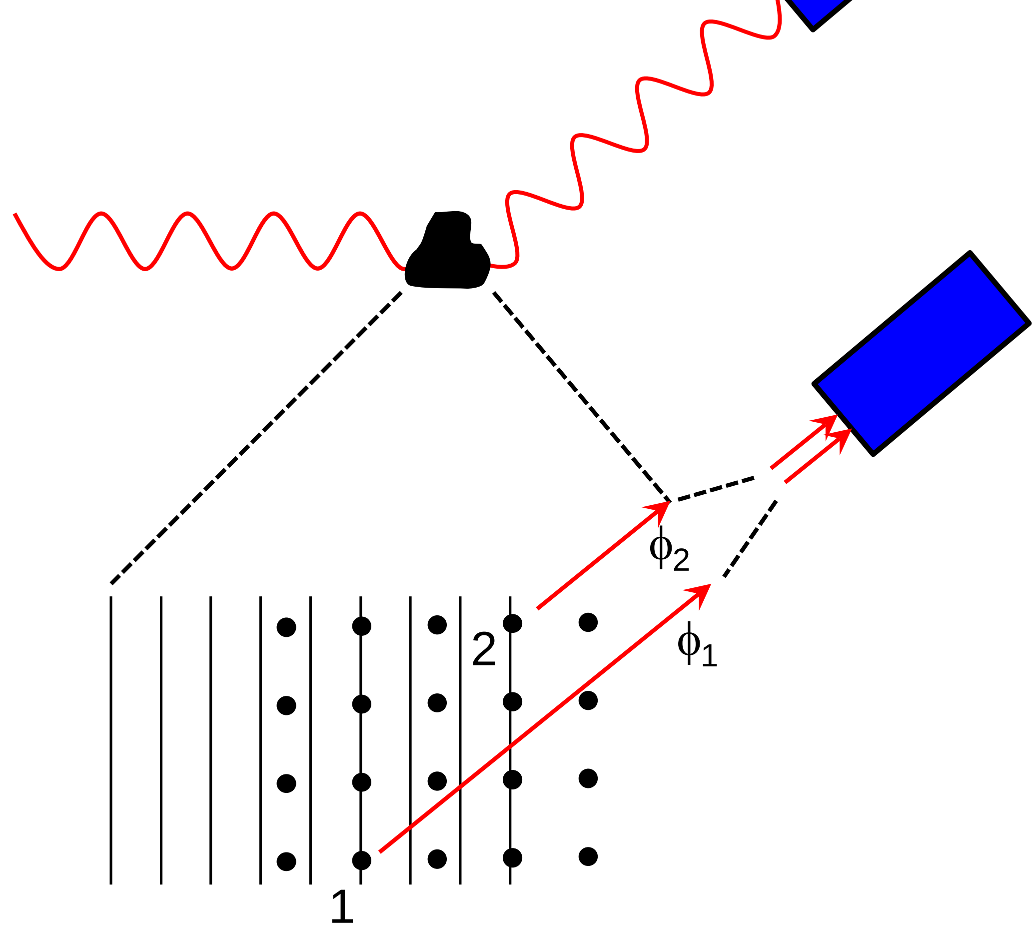
$$V_M(\mathbf{Q}) = -\mu_n \bullet \mathbf{B}(\mathbf{Q})$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}) = 0 \xrightarrow{\text{F.T.}} i\mathbf{Q} \cdot \mathbf{B}(\mathbf{Q}) = 0$$



Correlation Functions

Two-particle or pair correlations



(1) Born Approximation:
Assumes neutrons scatter only once (single scattering event).

(2) Superposition:
Amplitudes of scattered neutrons ϕ_n add linearly.

$$\Phi_s = \phi_1 + \phi_2 + \ldots$$

$$\text{Intensity} = |\Phi|^2 = |\phi_1 + \phi_2 + \ldots|^2 = |\phi_1|^2 + |\phi_2|^2 + \ldots + \underbrace{\phi_1{}^*\phi_2{}^* + \phi_2{}^*\phi_1}_{} + \ldots$$

Depends on relative positions of 1 and 2 → pair correlations!

After Andrew Boothroyd
PSI Summer School 2007

Correlation Functions

From Van Hove (1954) …

The measured quantity Φ_s depends only on time-dependent correlations between the positions of *pairs* of atoms.

This is true because *neutrons interact only weakly with matter*. Thus only the lowest order term in the perturbation expansion contributes.

Differential Cross-Section

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} b_i b_j \, e^{-i(\mathbf{k}_i-\mathbf{k}_j)\cdot(\mathbf{r}_i-\mathbf{r}_j)}$$

Depends only on:
where the atoms are
and
what the atoms are.

Correlation Functions

From Squires (1996):
Introduction to the theory of thermal neutron scattering

Partial Differential Cross-Section

$$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{k_0\rightarrow k_1} = \frac{1}{N}\frac{k_f}{k_i}\left(\frac{m}{2\pi\hbar^2}\right)^2 \sum p_i p_f \sum | < \mathbf{k}_f | V | \mathbf{k}_i > |^2 \delta(E+E_i-E_f)$$

$$\left(\frac{d^2\sigma}{d\Omega dE}\right)_{k_0\rightarrow k_1} = N\frac{k_f}{k_i} b^2 S(\mathbf{Q},\omega)$$

Neutron Structure Factor

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int G(\mathbf{r},t) e^{i(\mathbf{Q}\cdot r - \omega t)} d\mathbf{r}dt$$

Fourier Transform

Pair Correlation Function

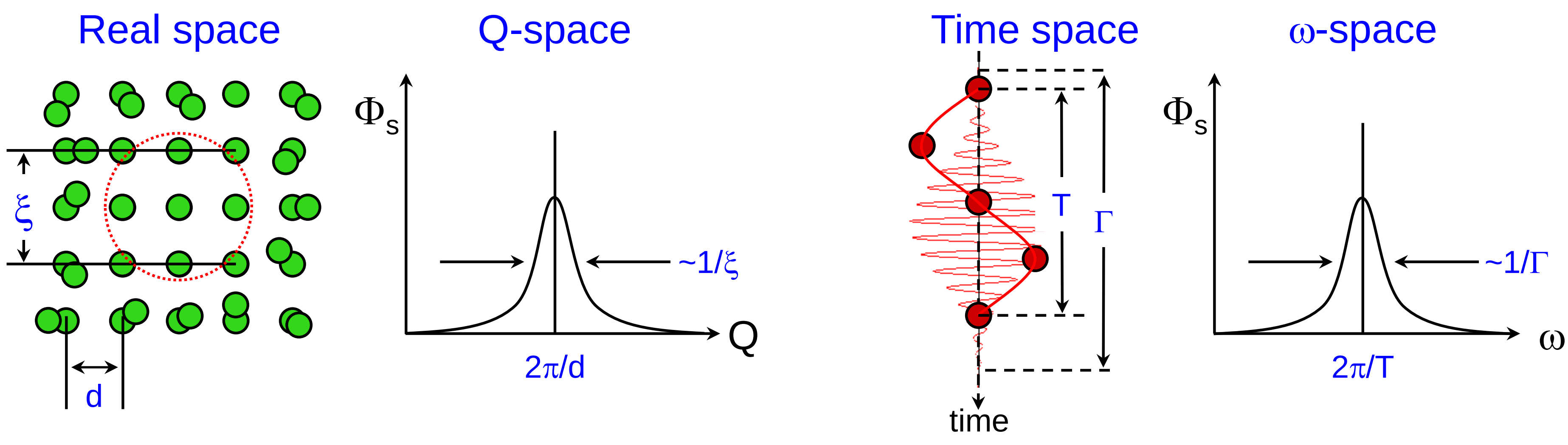
$$G(\mathbf{r},t) = (\frac{1}{2\pi})^3 \frac{1}{N}\int \sum_{jj'} e^{i\mathbf{Q}\cdot\mathbf{r}} < e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)} e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)} > d\mathbf{Q}$$

Correlation Functions

KEY IDEA – Neutron interactions are <u>weak</u> → Scattering only probes <u>two-particle</u> correlations in space and time, but does so simultaneously!

The scattered neutron flux $\Phi_s(\vec{Q},\hbar\omega)$ is proportional to the space ($\vec{r}$) and time (t) Fourier transform of the <u>probability</u> $G(\vec{r},t)$ of finding an atom at ($\vec{r}$,t) given that there is another atom at r = 0 at time t = 0.

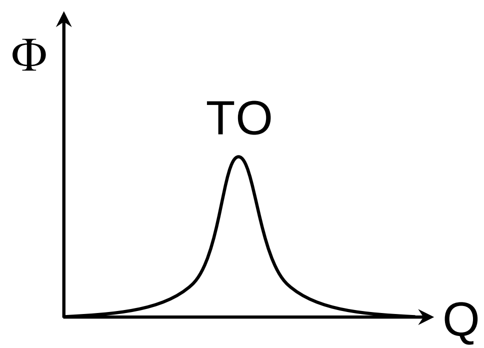
$$\Phi_s \propto \frac{\partial^2 \sigma}{\partial\Omega\partial\omega} \propto \iint e^{i(\vec{Q}\cdot\vec{r}-\omega t)} G(\vec{r},t)\, d^3\vec{r}\, dt$$



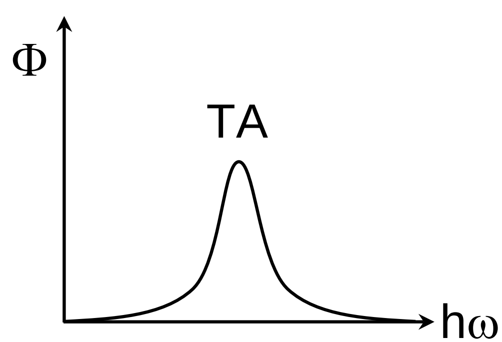
Correlation Functions

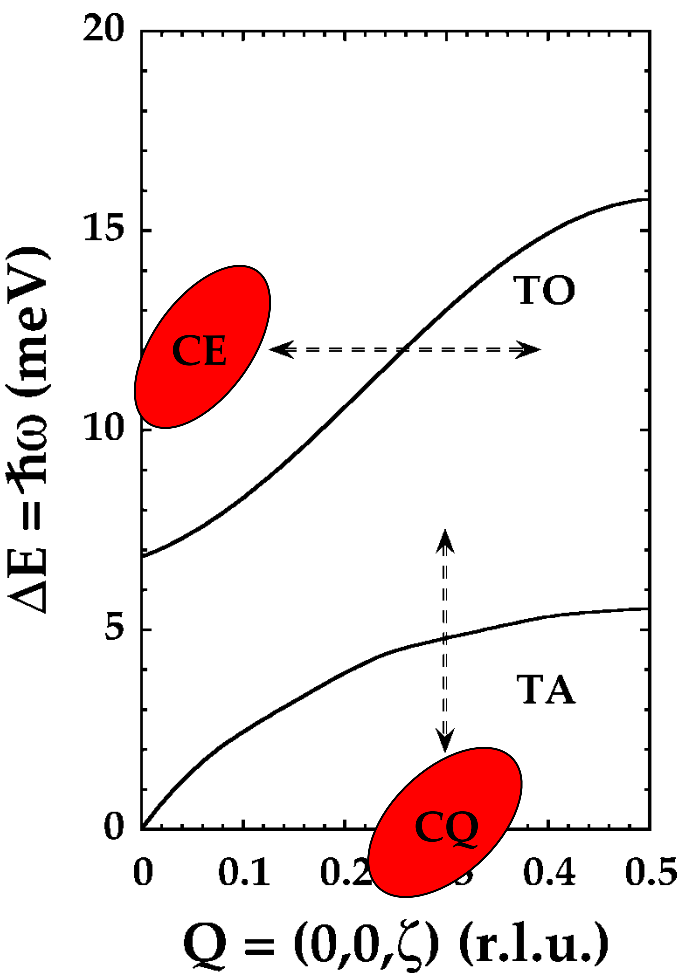
There are two main ways of measuring the neutron scattering cross section $S(Q,\omega)$.

Constant-E scans: vary Q at fixed $h\omega$.



Constant-Q scans: vary $h\omega$ at fixed Q.





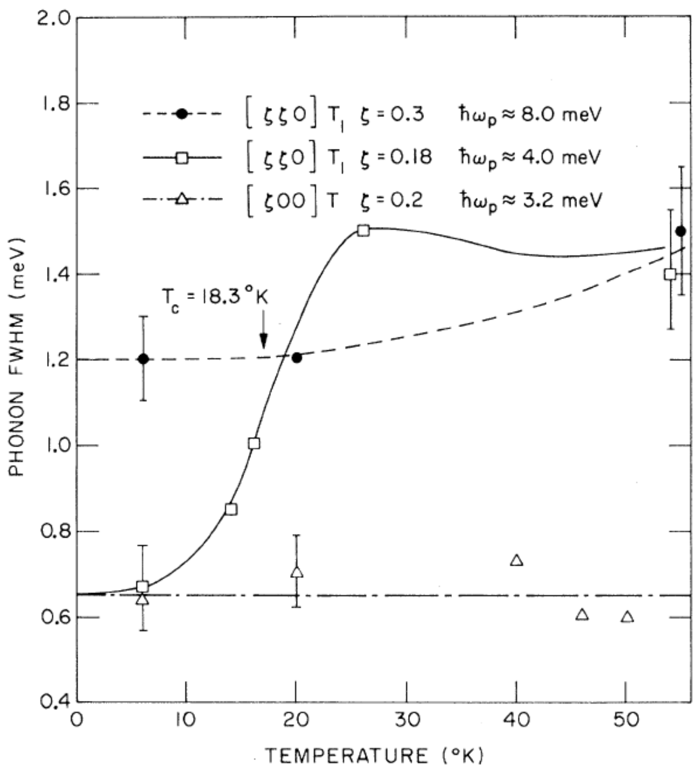
Classic Example

BCS Superconductivity

VOLUME 30, NUMBER 6 PHYSICAL REVIEW LETTERS 5 FEBRUARY 1973

Influence of the Superconducting Energy Gap on Phonon Linewidths in Nb_3Sn†

J. D. Axe and G. Shirane
Brookhaven National Laboratory, Upton, New York 11973
(Received 7 December 1972)

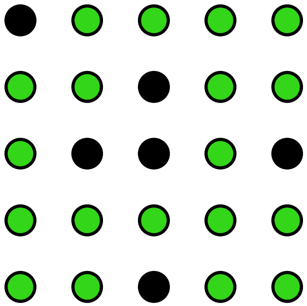


Coherent vs Incoherent

What happens when two different nuclei are randomly distributed throughout the crystal?

This situation could arise for two reasons.
1. Isotopic incoherence
2. Nuclear spin incoherence

Both reasons can occur because the scattering interaction is <u>nuclear</u>.



Recall that $\left(\frac{d^2\sigma}{d\Omega dE}\right)_{k_0 \to k_1} = N \frac{k_f}{k_i} b^2 S(\mathbf{Q}, \omega)$

Then the above equation must be generalized:

$$\frac{d^2\sigma}{d\Omega dE_f} = \sum_{i,j} \overline{b_i b_j}\, S_{ij}(Q,\omega)$$

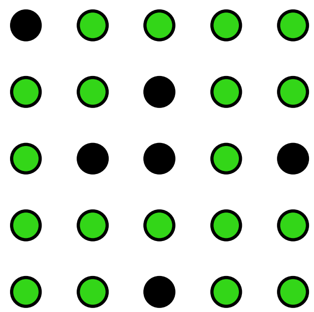
$$\overline{b_i b_j} = (\overline{b})^2, \text{ for } i=j$$

$$\overline{b_i b_j} = \overline{b^2}, \text{ for } i \neq j$$

$\overline{}$ = average

Coherent vs Incoherent

What happens when two different nuclei are randomly distributed throughout the crystal?



Our partial differential cross section can then be recast into the form:

$$\boxed{\frac{d^2\sigma}{d\Omega dE_f} = \sigma_c S_c(Q,\omega) + \sigma_i S_i(Q,\omega)}$$, where

$\sigma_c = 4\pi(\overline{b})^2$ c = coherent

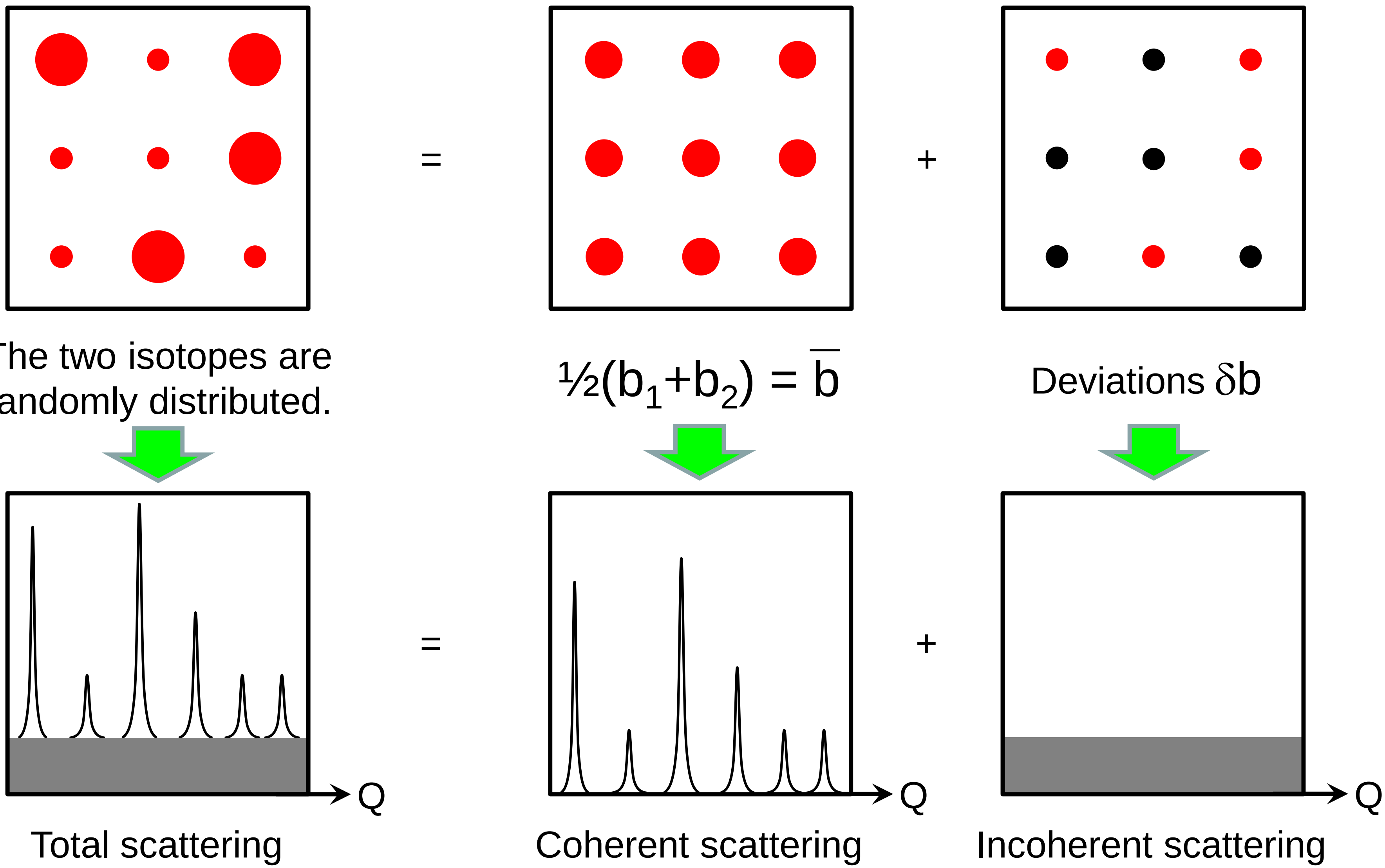
$\sigma_i = 4\pi\{\overline{b^2} - (\overline{b})^2\}$ i = incoherent

Coherent vs Incoherent

Consider a system composed of two different scattering lengths, b_1 and b_2.

$b_1 =$ ●

$b_2 =$ ⬤



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PSI Summer School 2007

Coherent vs Incoherent

What do these expressions mean physically?

Coherent Scattering

Measures the Fourier transform of the *pair* correlation function $G(r,t)$ → interference effects.

This cross section reflects collective phenomena such as:

Phonons

Spin Waves

Incoherent Scattering

Measures the Fourier transform of the *self* correlation function $G_s(r,t)$ → no interference effects.

This cross section reflects single-particle scattering:

Atomic Diffusion

Vibrational Density of States

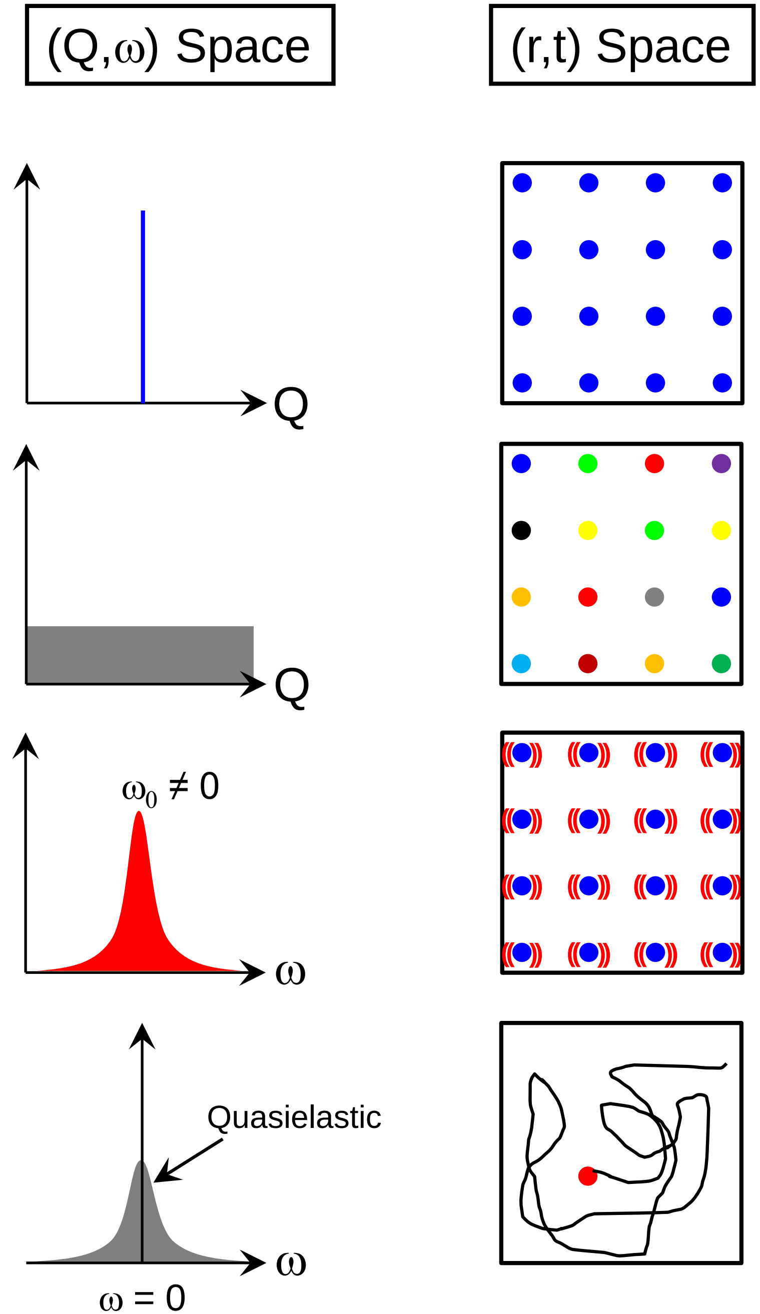
Brief Summary

$$\left.\frac{d\sigma}{d\Omega}\right|_{coh} = \frac{\sigma_{coh}}{4\pi} S(Q)$$

$$\left.\frac{d\sigma}{d\Omega}\right|_{inc} = \frac{\sigma_{inc}}{4\pi}$$

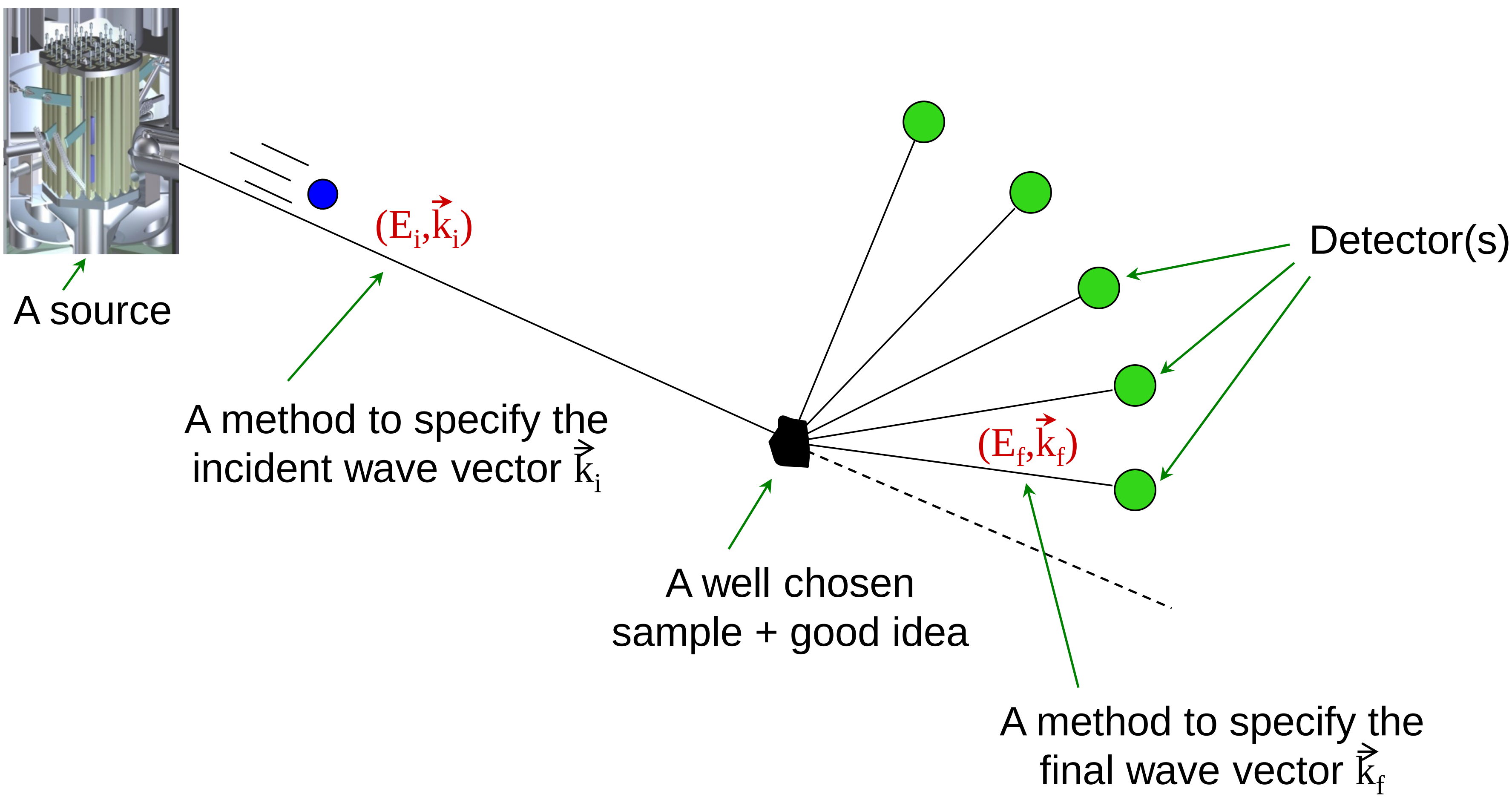
$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right|_{coh} = \frac{k_f}{k_i}\frac{\sigma_{coh}}{4\pi} S_{coh}(Q,\omega)$$

$$\left.\frac{d^2\sigma}{d\Omega dE_f}\right|_{inc} = \frac{k_f}{k_i}\frac{\sigma_{inc}}{4\pi} S_{inc}(Q,\omega)$$



Basics of Scattering

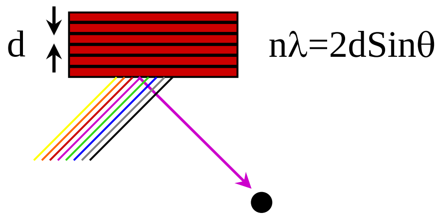
Elements of all scattering experiments



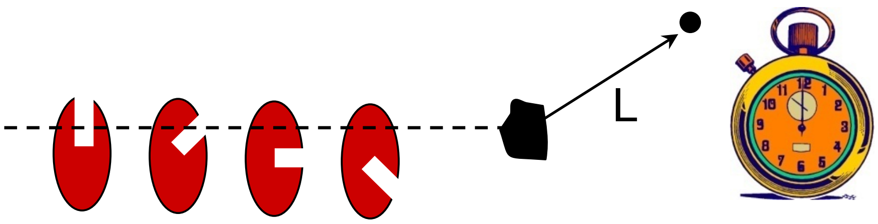
Basics of Scattering

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

1. Bragg Diffraction

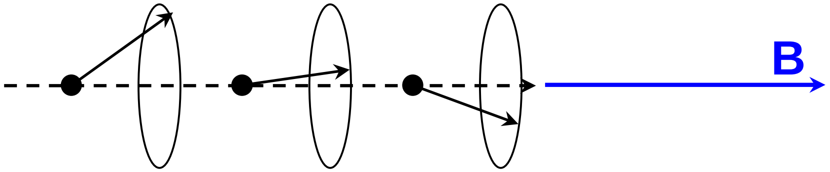


2. Time-of-Flight (TOF)



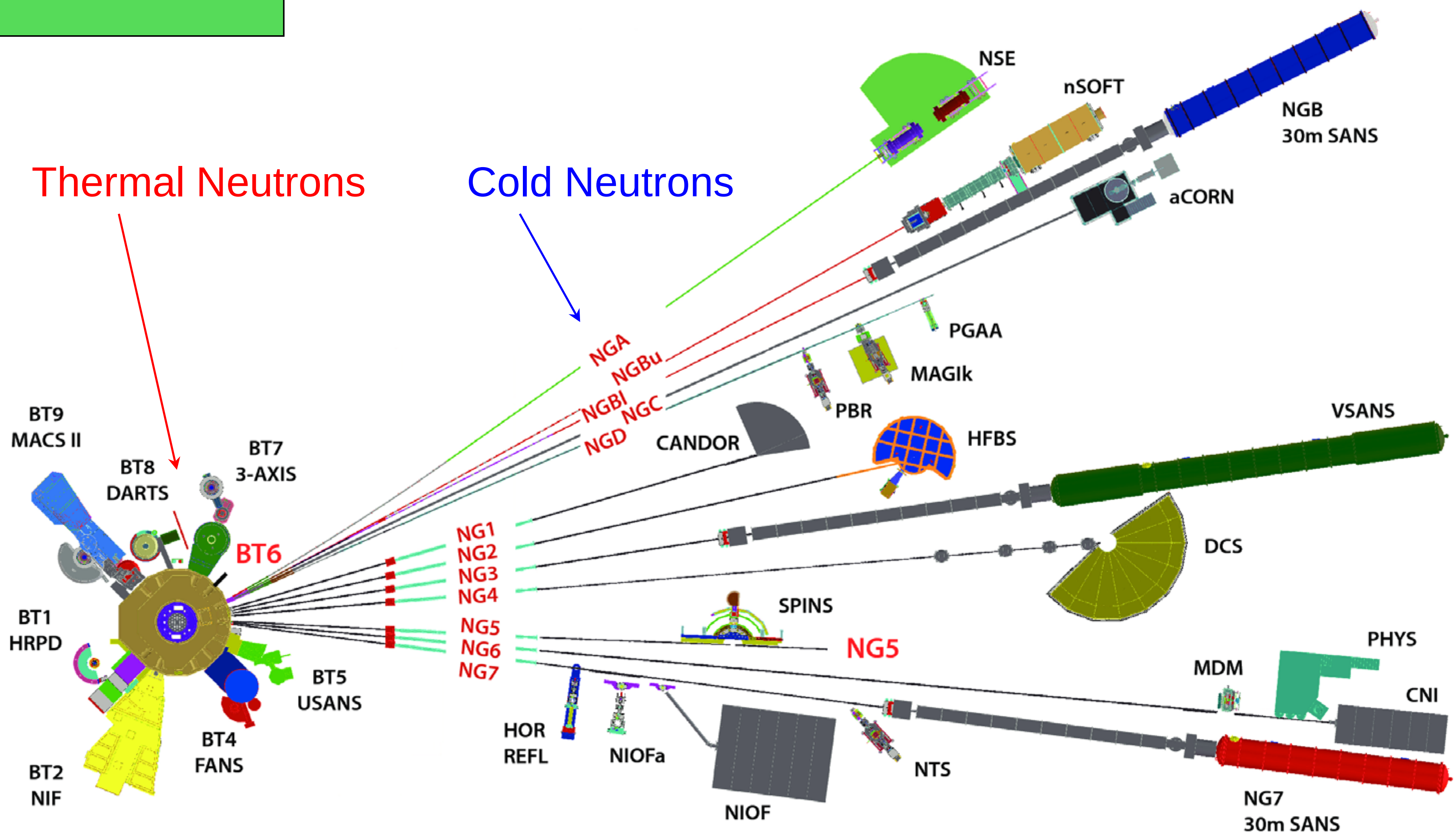
$v = L/t$

3. Larmor Precession



Neutron Instruments

You will see many of these on the tour …



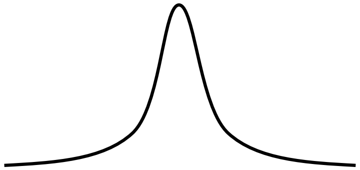
Neutron Instruments

Why so many different kinds?

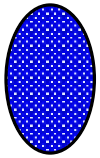
Because neutron scattering is an intensity-limited technique. Thus detector coverage and resolution MUST be tailored to the science.

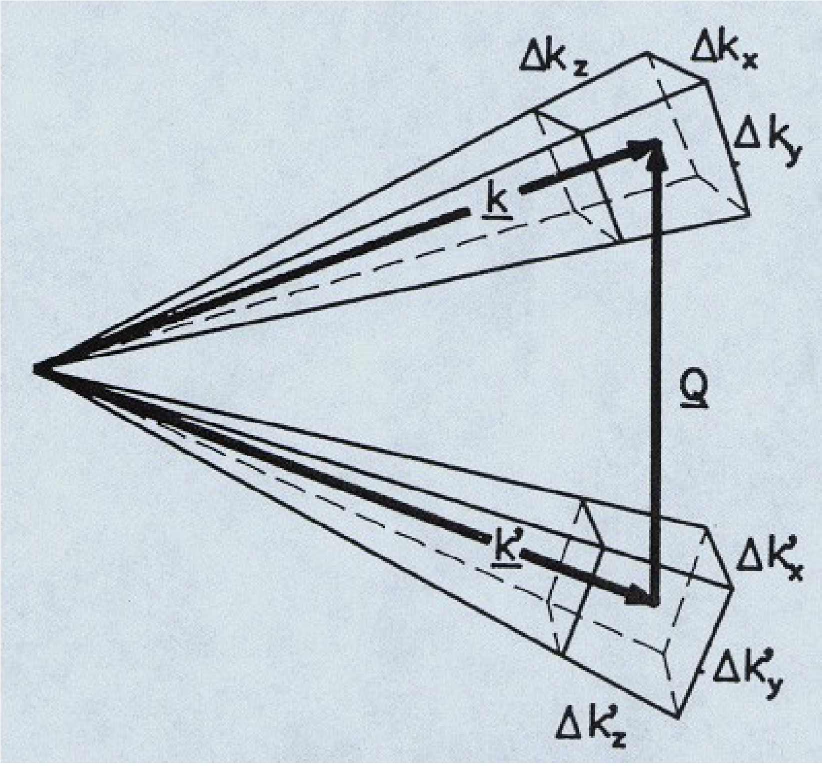
Uncertainties in the neutron wavelength and direction imply **Q** and $\hbar\omega$ can only be defined with a finite precision.

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



$\propto$





Courtesy of R. Pynn

Quick Review

Please try to remember these things …

1. Neutrons scattering probes two-particle correlations in both space and time (simultaneously!).

2. The neutron scattering length, b, varies randomly with Z → allows access to atoms that are usually unseen by x-rays.

3. Coherent Scattering

Measures the Fourier transform of the pair correlation function $G(r,t)$ → interference effects.

This cross section reflects collective phenomena.

4. Incoherent Scattering

Measures the Fourier transform of the self correlation function $G_s(r,t)$ → no interference effects.

This cross section reflects single-particle scattering.

More Examples

OK, after all of this, just exactly what can neutron scattering do for you?

More Examples

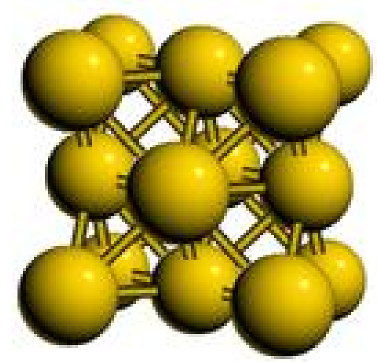
Phonons

After Bruce Gaulin
NXS 2016

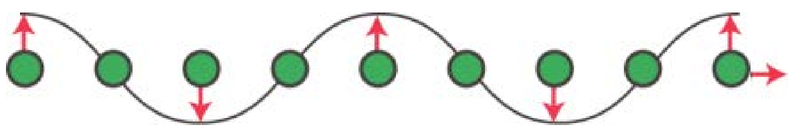
- Normal modes in periodic crystal → wavevector

$$\mathbf{u}(l,t)=\frac{1}{\sqrt{NM}}\sum_{j\mathbf{q}}\boldsymbol{\varepsilon}_j(\mathbf{q})\exp(i\mathbf{q}\cdot\mathbf{l})\hat{B}(\mathbf{q}j,t)$$

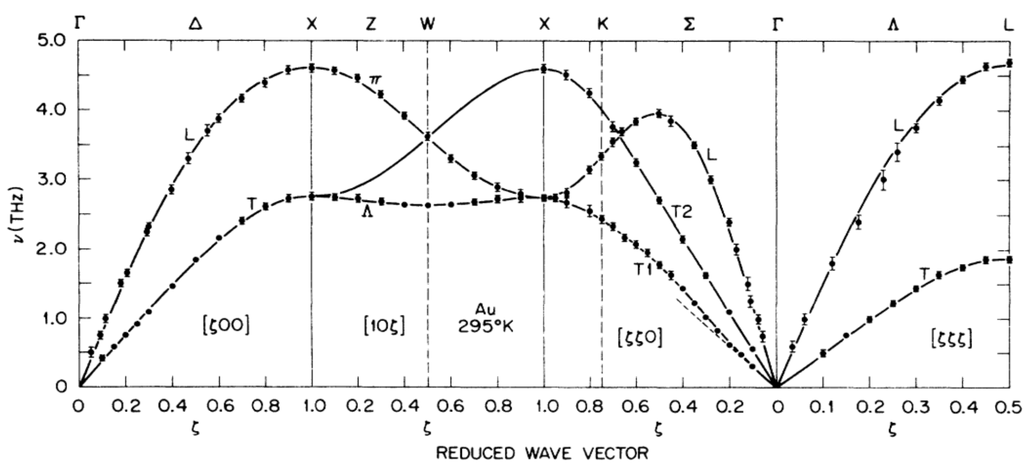
- Energy of phonon depends on **q** and polarization



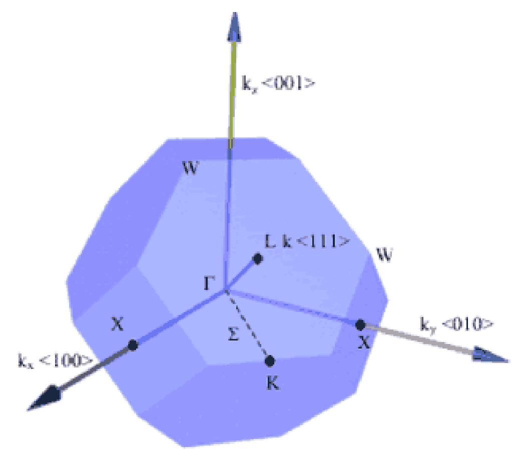
FCC structure



Longitudinal mode
Transverse mode



Lynn, *et al.*, *Phys. Rev. B* **8**, 3493 (1973).

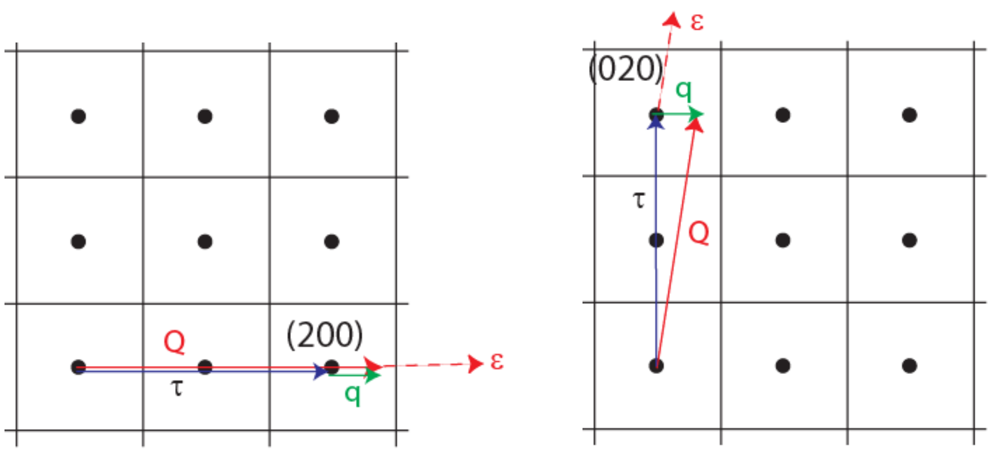


FCC Brillouin zone

One-Phonon Scattering Cross Section

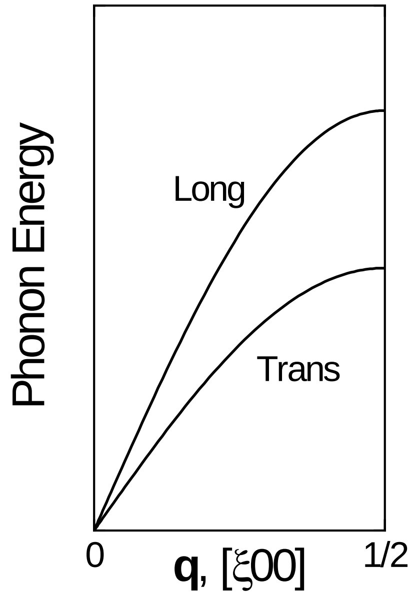
Structure (polarization) factor

$$S_{1+}(\mathbf{Q},\omega)=\frac{1}{2NM}e^{-Q^2\langle u^2\rangle}\sum_{j\mathbf{q}}\frac{\left|\mathbf{Q}\cdot\boldsymbol{\varepsilon}_j(\mathbf{q})\right|^2}{\omega_j(\mathbf{q})}\left(1+n(\omega)\right)\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})\delta\left(\omega-\omega_j(\mathbf{q})\right)$$



Longitudinal scan, **q** || ε

Transverse scan, **q** ⊥ ε

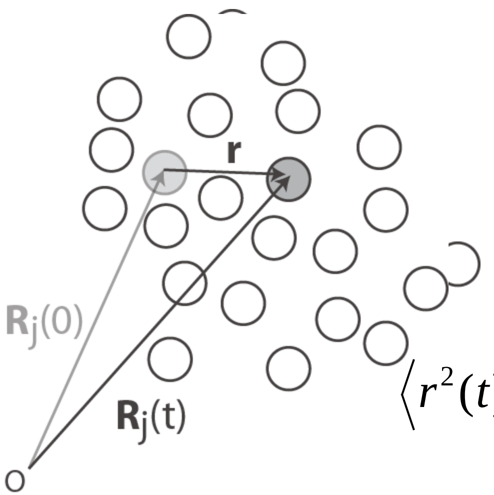


After Bruce Gaulin
NXS 2016

More Examples

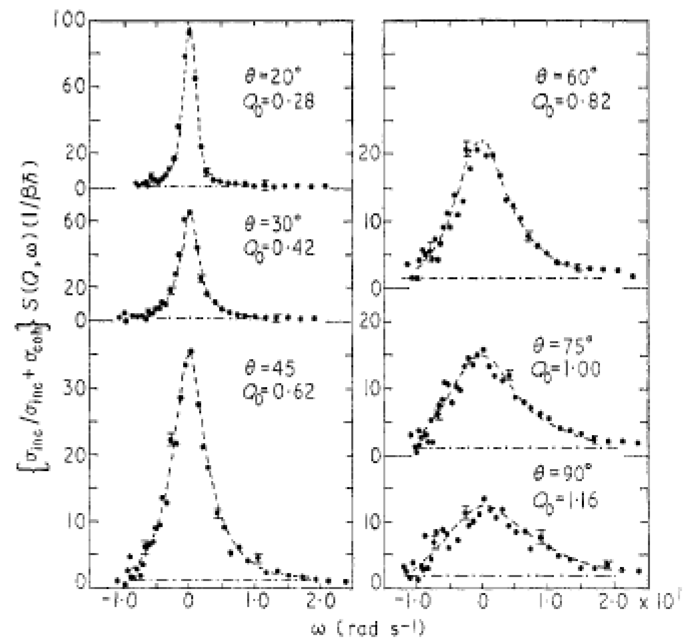
Diffusion Scattering Cross Section

For times that are long compared to the collision time, atom diffuses



$$\langle r^2(t)\rangle \approx 6Dt$$

Liquid Na



Cocking, *J. Phys. C* **2**, 2047 (1969)..

Auto-correlation function

$$G_s(r,t) = \left\{6\pi\langle r^2(t)\rangle\right\}^{-3/2} \exp\left(-\frac{r^2}{6\langle r^2(t)\rangle}\right)$$

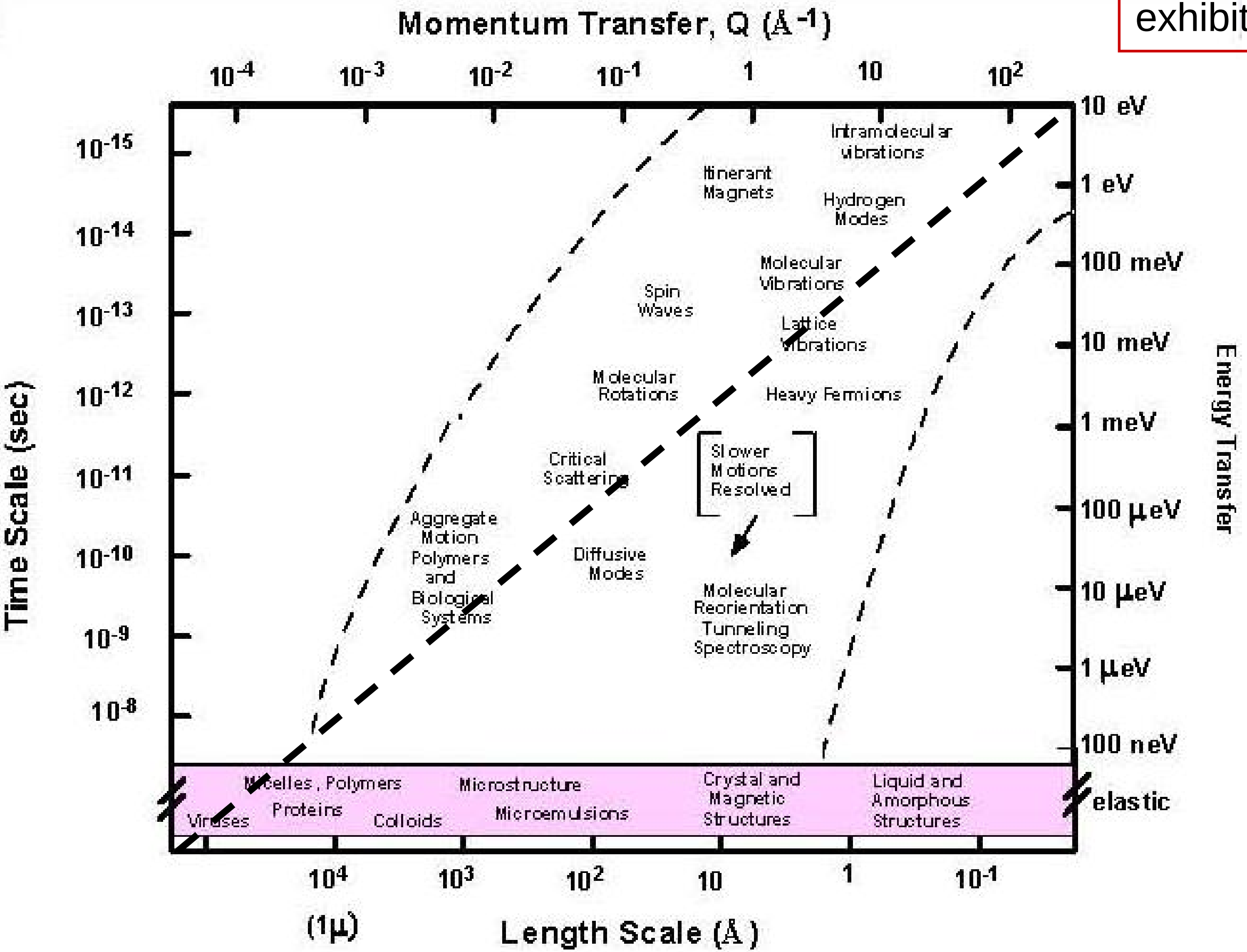
$$S(Q,\omega) = \frac{1}{\pi\hbar}\exp\left(\frac{\hbar\omega}{2k_BT}\right)\frac{DQ^2}{\omega^2+(DQ^2)^2}$$

After Bruce Gaulin
NXS 2016

Length and Time Scales

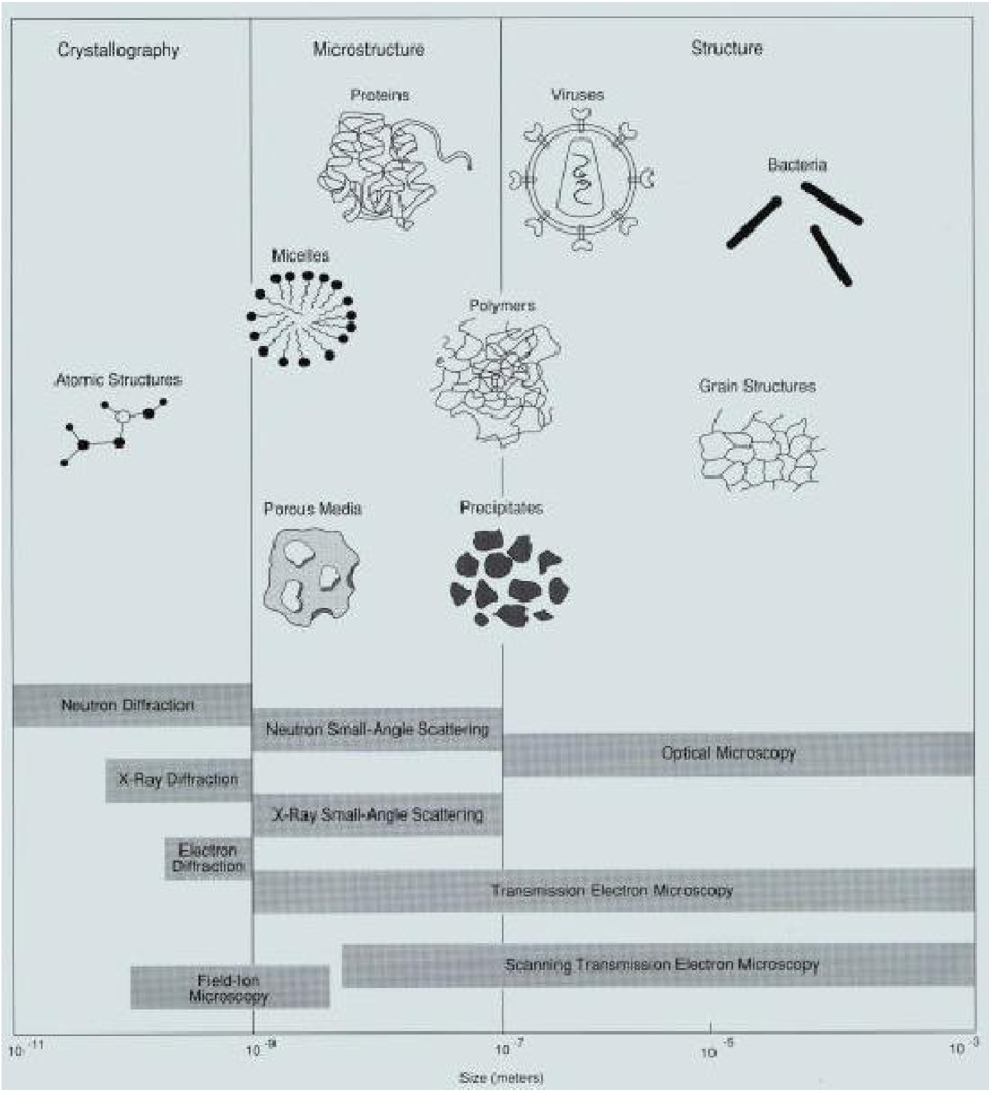
Do you see a pattern here?

Larger “objects” tend to exhibit slower motions.

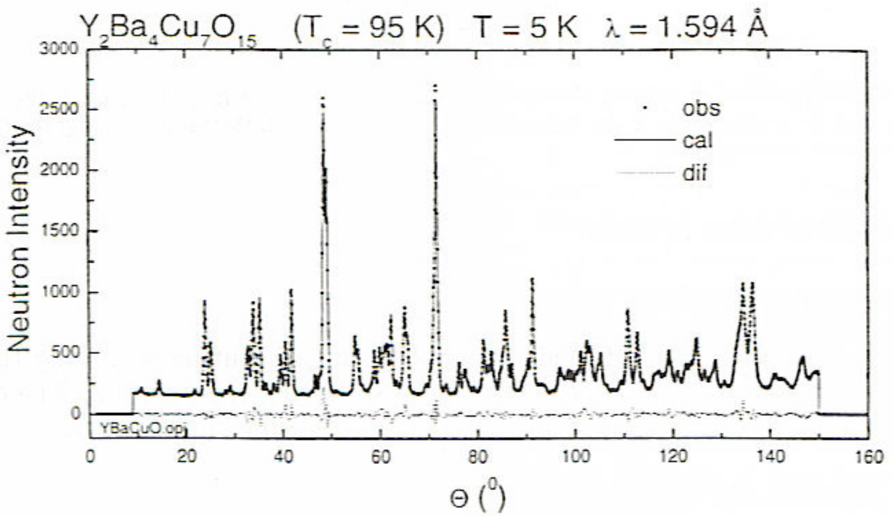


Elastic Scattering

Neutrons can probe length scales ranging from ~0.1 Å to ~1000 Å



Pynn, *Neutron Scattering: A Primer* (1989)



Mitchell et. al, *Vibrational Spectroscopy with Neutrons* (2005)

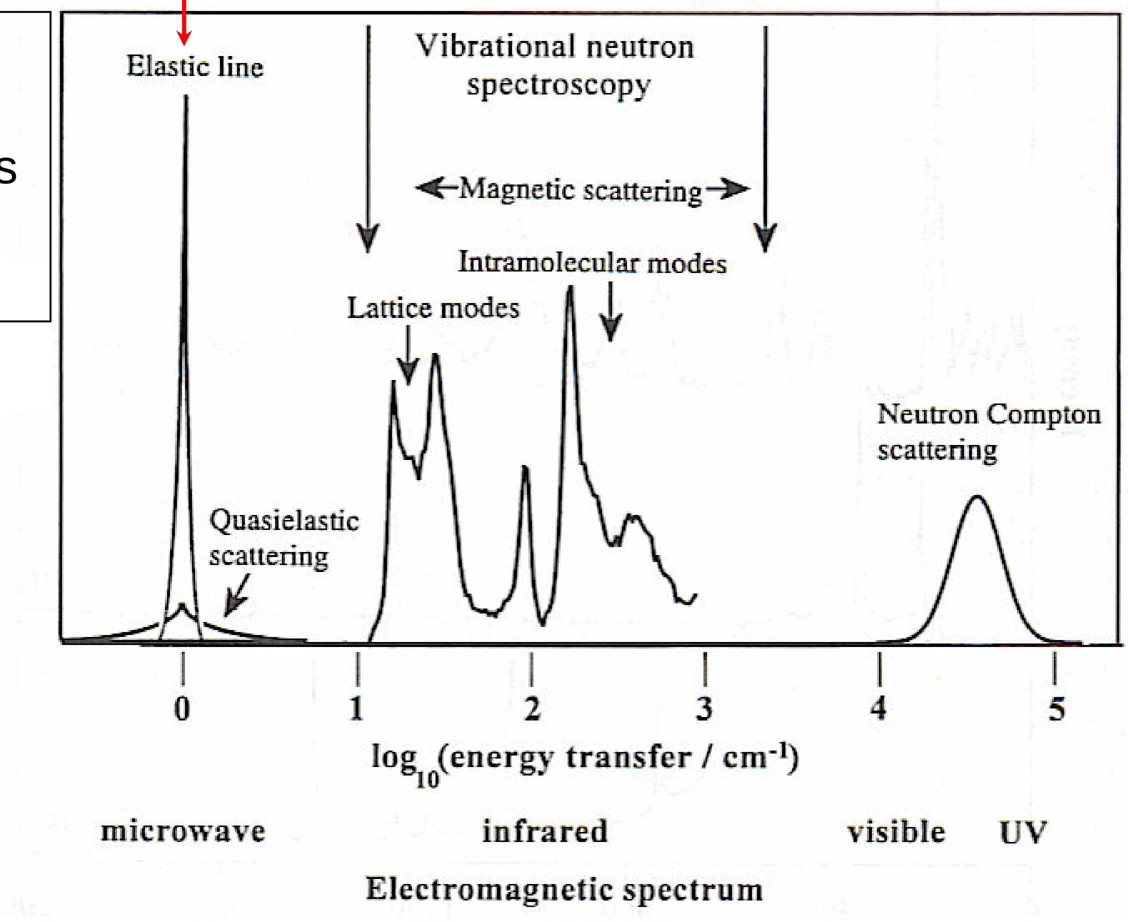
Neutrons needed to determine structure of 123 high-T_c cuprates because x rays weren’t sufficiently sensitive to the oxygen atoms.

Inelastic Scattering

Neutrons can probe time scales ranging from ~10^{-14} s to ~10^{-8}s.

$\hbar\omega = 0$

Probes the vibrational, magnetic, and lattice excitations (dynamics) of materials by measuring changes in the neutron momentum and energy simultaneously.



Mitchell et. al, *Vibrational Spectroscopy with Neutrons* (2005)

Elastic Scattering

Pop Quiz

Can one measure elastic scattering from a liquid?

If Yes, explain why?
If No, explain why not?

Hint: What is the correlation of one atom in a liquid with another after a time t?

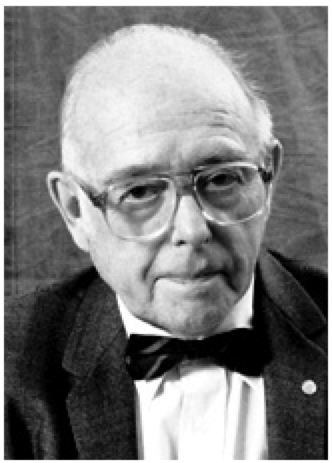
Nobel Prize in Physics 1994

The Fathers of Neutron Scattering

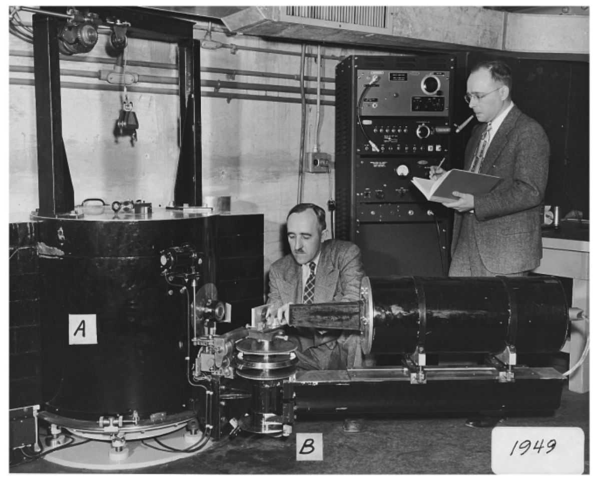
"For pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

"For the development of the neutron diffraction technique"

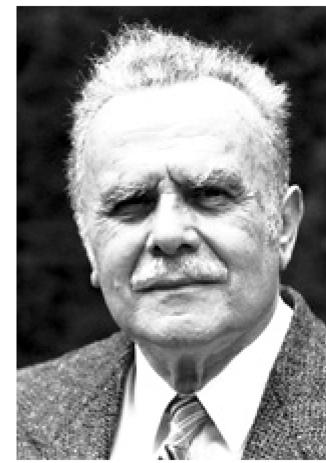
"For the development of neutron spectroscopy"



Clifford G Shull
MIT, USA
(1915 – 2001)



Ernest O Wollan
ORNL, USA
(1910 – 1984)



Bertram N Brockhouse
McMaster University, Canada
(1918 – 2003)

Showed us where the atoms are …

Did first neutron diffraction expts …

Showed us how the atoms move …

Useful References

- http://www.mrl.ucsb.edu/~pynn/primer.pdf
- "Introduction to the Theory of Thermal Neutron Scattering"
  - G. L. Squires, Cambridge University Press
- "Theory of Neutron Scattering from Condensed Matter"
  - S. W. Lovesey, Oxford University Press
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  - G. E. Bacon, Clarendon Press, Oxford
- "Structure and Dynamics"
  - M. T. Dove, Oxford University Press
- "Elementary Scattering Theory"
  - D. S. Sivia, Oxford University Press