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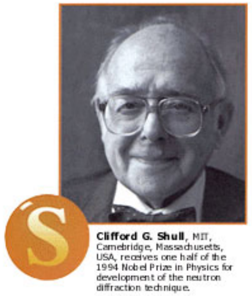
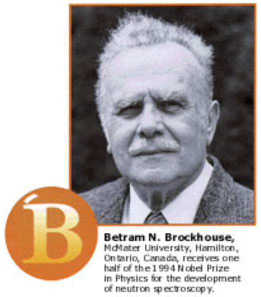
Basics of Neutron Scattering

Luis Carlos Pardo Soto



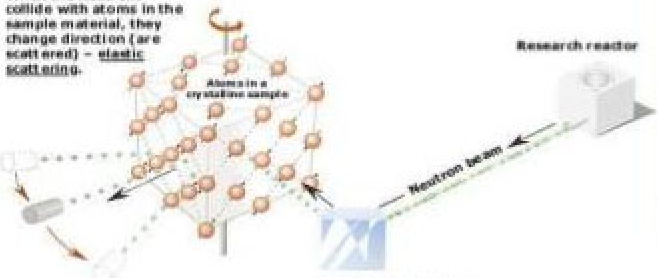
Clifford G. Shull, MIT, Camebridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

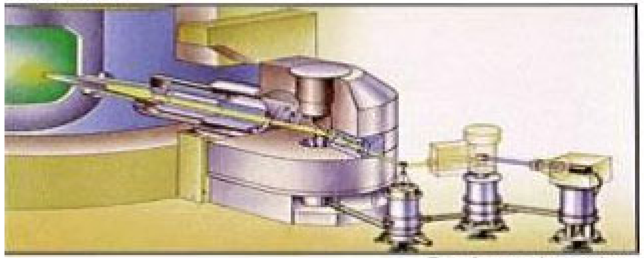


Betram N. Brockhouse, McMater University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

The 1994 Nobel Prize in Physics – Shull & Brockhouse.

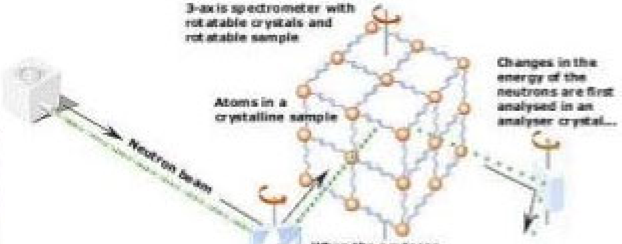
Neutrons show where the atoms.......





3-axis spectrometer

...and what the atoms do.



THE NEUTRON

WAVE

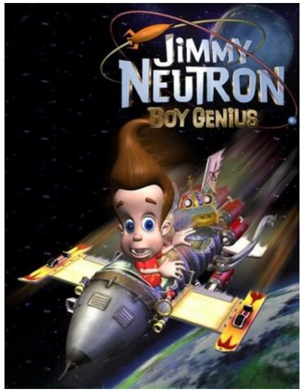
They can interfere

$$\lambda = h / mv$$

diffraction

POSITION

PARTICLE



Energy is related to velocity ➔ to λ

$$E = 1/2mv^2 = h^2 / 2m\lambda^2$$

Energy exchanged with sample

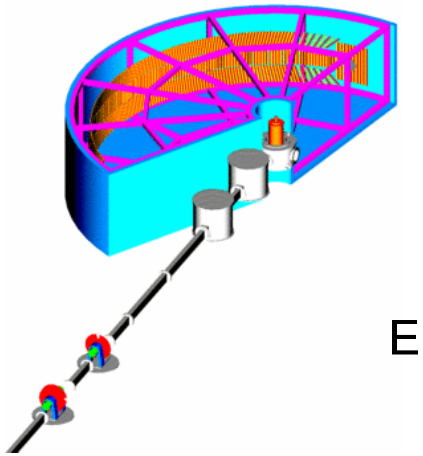
DYNAMICS

$m_n = 1.675 \cdot 10^{-27}$ kg

…wave-Particle duality was never so nicely exploited

The neutron

STRUCTURE
Position = detectors



DYNAMICS
Energy = Time of flight
"1/2mv^2"   v=x/t

TEMPERATURE

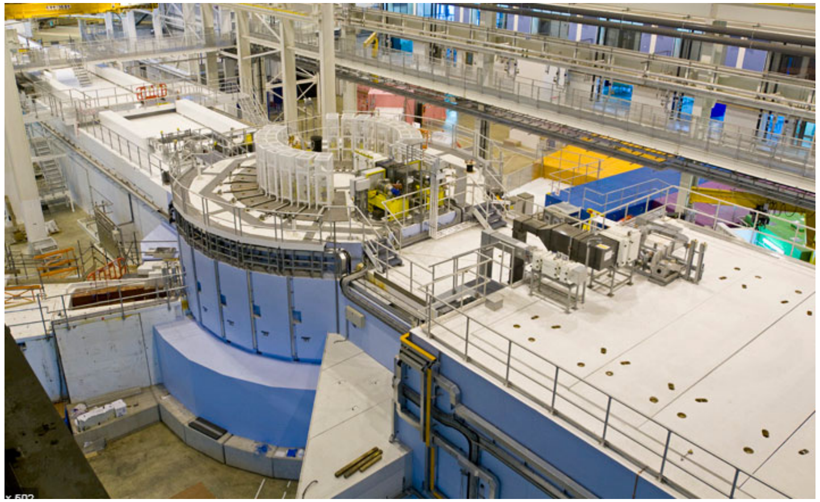
	cold	**thermal**	**hot**
Temperature	*T=25K*	*T=300K*	*T=2000K*
Energy	*E=2meV*	*E=25meV*	*E=170meV*
Velocity	*v=500m/s*	*v=2200m/s*	*v=m/s*
Wavelength λ	*λ=3.5Å*	*λ=1.8Å*	*λ=0.5Å*

FAST MOTIONS (energy range) →

← **SLOW MOTIONS (resolution)**

NEUTRON PRODUCTION

Spallation



ISIS (UK)

ess (Lund)

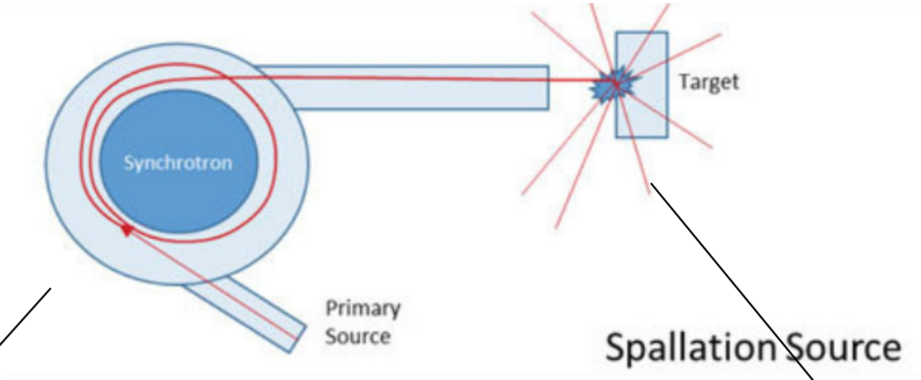
Fission

ILL (france)

FRMII(germany)

Spallation

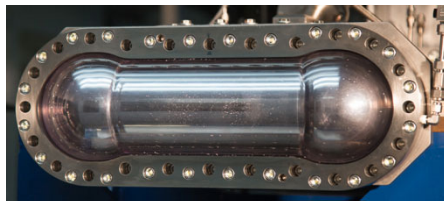
pulsed source



1GeV protons accelerated
by LINAC or Synchrotron

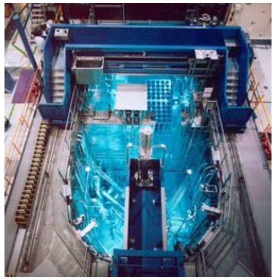
shoot against a

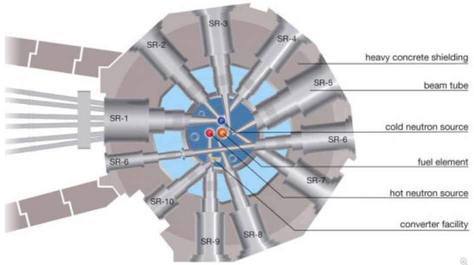
Heavy metal (Hg) target



Fission

continuous source



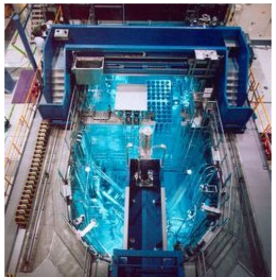


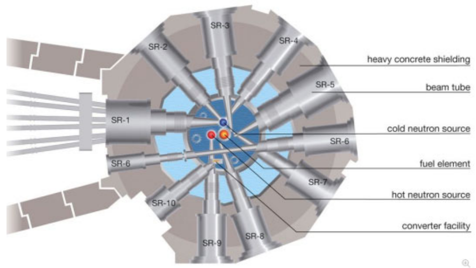
How do we take out the neutrons from the reactor
They are unstopable (more or less)

like a stone that bounces in a lake...

Fission

continuous source

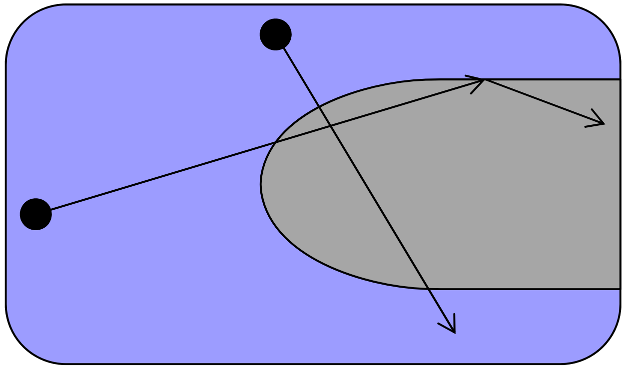




How do we take out the neutrons from the reactor
They are unstopable (more or less)

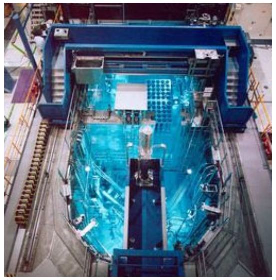
neutron crosses

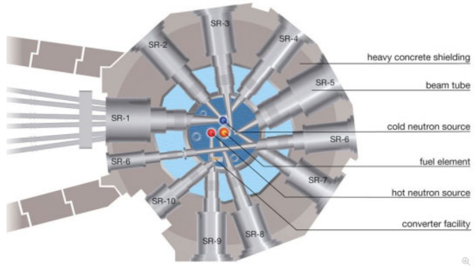
neutron bounces



Fission

continuous source





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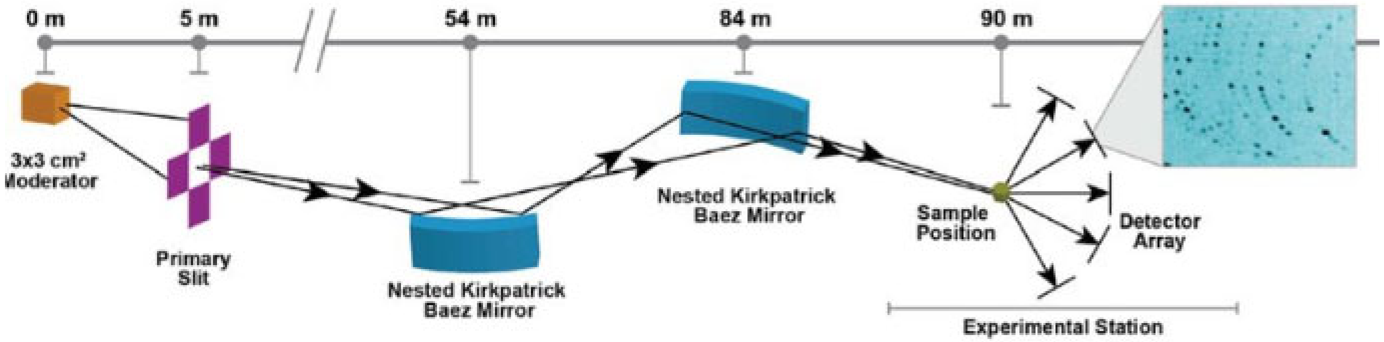
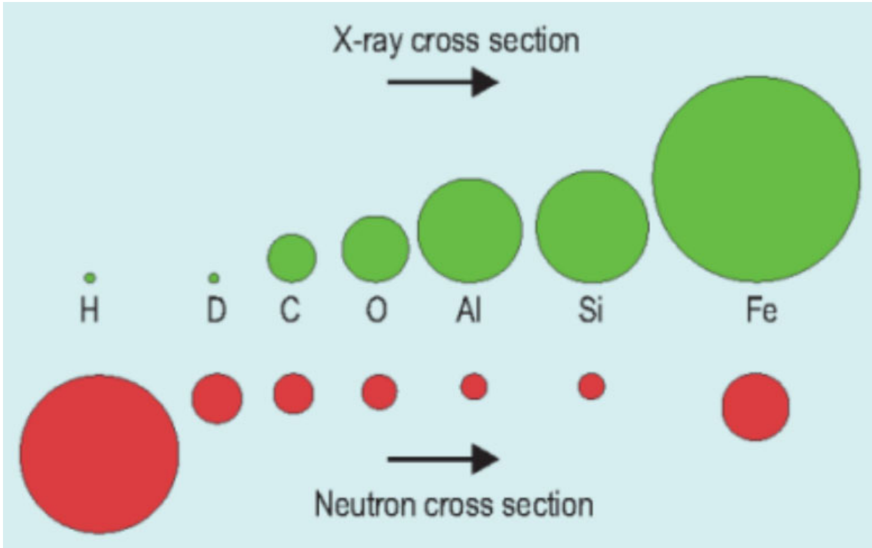


This makes neutron “optics” quite funny...

Nice thing about neutrons



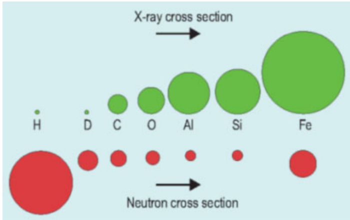
they are complementary (or necessary) to X-Rays:

You CANNOT see hydrogen with X-rays, but you see metals very nicelly

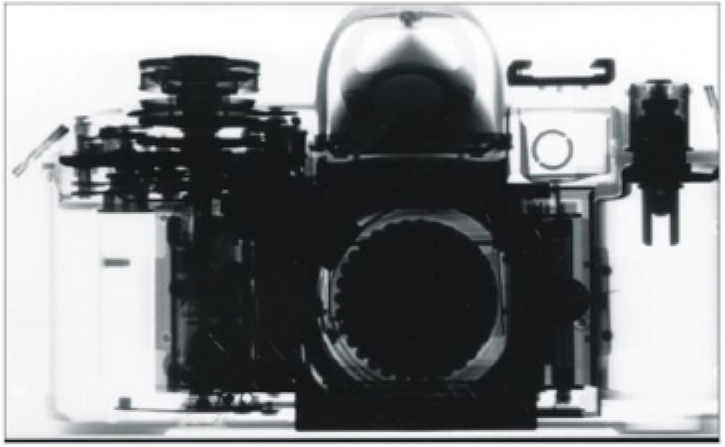
You CANNOT see metals with neutrons, but you see hydrogen very nicelly

(this means that you can have "heavy ancilliary" equipment)

Nice thing about neutrons

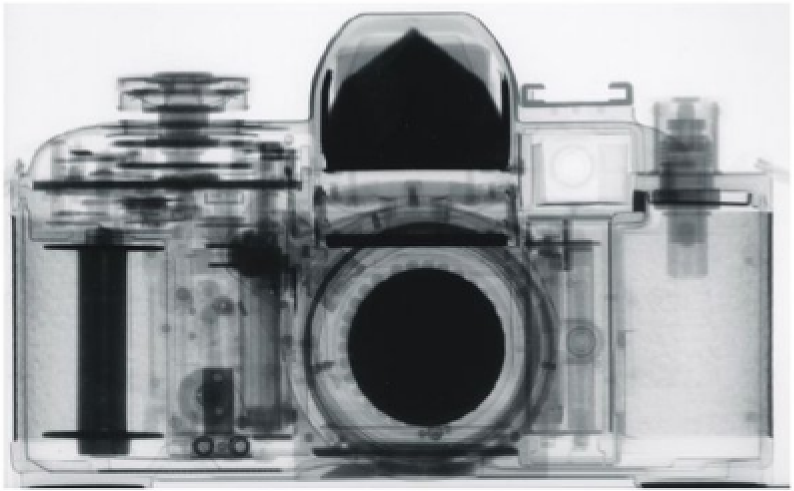


Comparison of X-ray and Neutron Radiographs



X-ray

you see metal



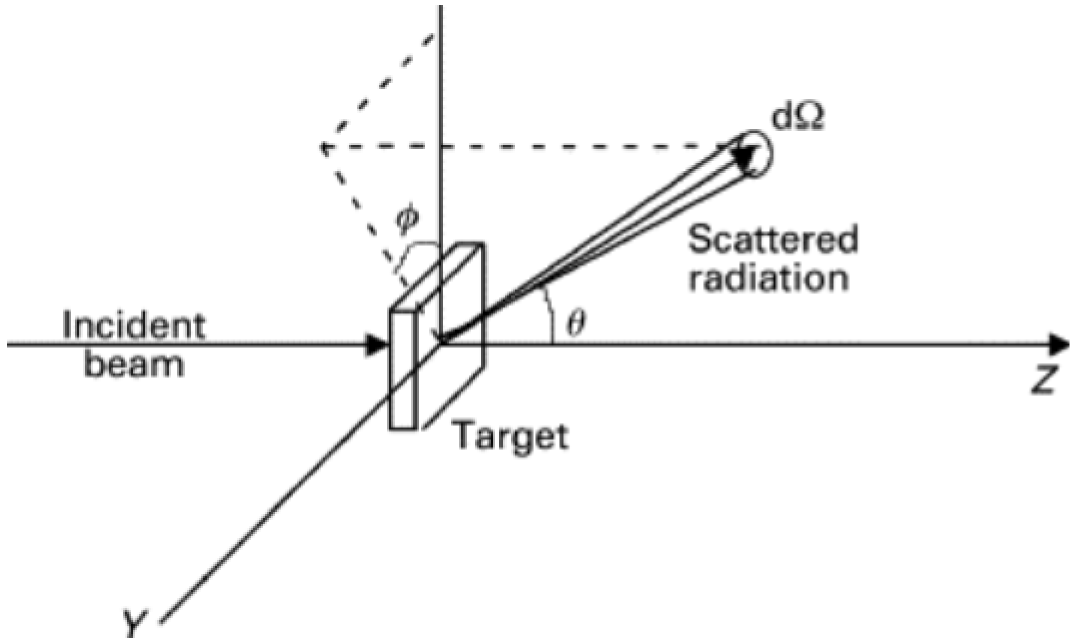
Neutrons

you see plastic

https://www.youtube.com/watch?v=VESMU7JfVHU

SCATTERING CROSS SECTION

What do we measure?



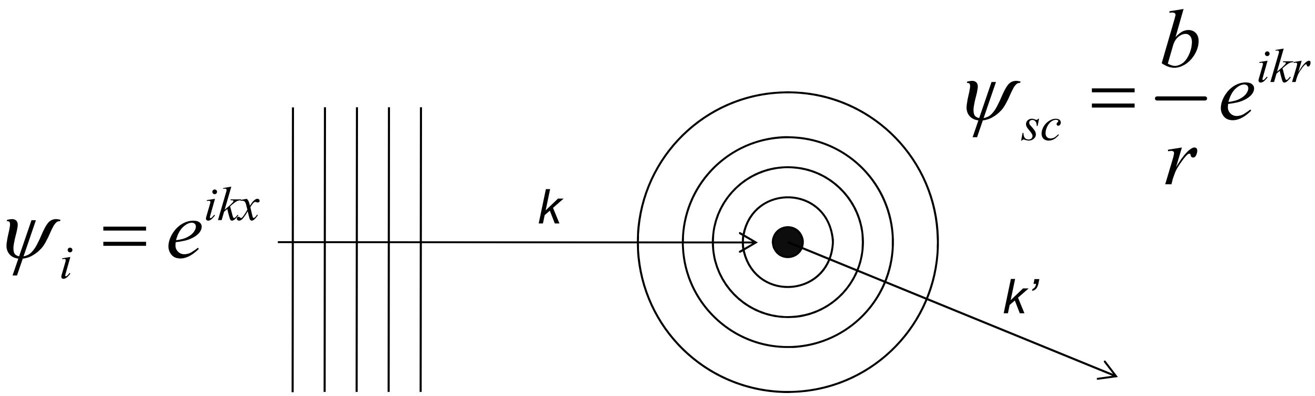
<u>*Partial differential cross section:*</u>
number of neutrons/photons scattered per second into a small solid angle dΩ in the direction θ and φ with final energy between E' and E'+dE

$$\frac{\partial^2 \sigma}{\partial \Omega \partial E}$$

<u>*you can integrate (marginalize) the energy*</u>
number of neutrons/photons scattered per second into a small solid angle dΩ in the direction θ and φ

$$\frac{\partial^2 \sigma}{\partial \Omega}$$

Scattering by a single nucleous:



TOTAL scattering cross section

$$\sigma_{tot} = \iint \frac{\partial \sigma}{\partial \Omega \partial E} 4\pi b^2 d\Omega dE = 4\pi b^2$$

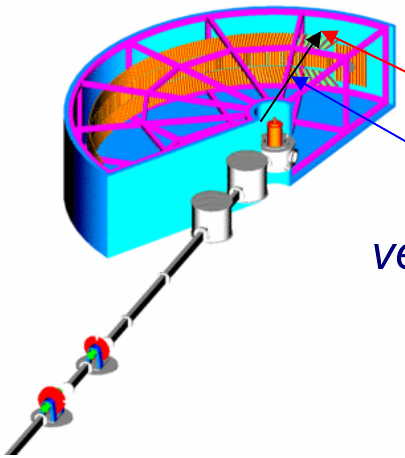
... which is related to the interaction potential between neutron and nucleus

$$V(r) = \frac{2\pi\hbar^2}{m} b \cdot \delta(r)$$

What do we measure?

Where do neutrons go?

What energy do they have?

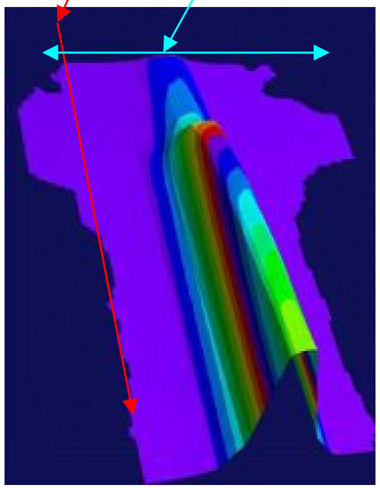


detector

velocity

$$\frac{\partial^2 \sigma}{\partial \Omega \partial E}$$

Double differential scattering cross-section



E related to energy transfer DYNAMICS

Ω related to momentum transfer (q) STRUCTURE

How is it related to the sample physics?

Neutron change of direction *(and energy)* → *Neutron change of energy*

$$\vec{Q} = \vec{k} - \vec{k}_0$$

$$\hbar\omega = E - E_0 = \frac{\hbar^2}{2m}(k^2 - k_0^2)$$

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} = \frac{k}{k_0} \frac{1}{N \cdot 2\pi} \int_{-\infty}^{\infty} \sum_i \sum_j \left\langle b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot b_j e^{-i\vec{Q}\vec{R}_j(0)} \right\rangle e^{-i\omega t} dt$$

Scattering cross section depends on spin and isotope

Particle position at times 0 and t emits a spherical wave
(CLASSICAL APPROXIMATION!)

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$$\hbar\omega = E - E_0 = \frac{\hbar^2}{2m}(k^2 - k_0^2)$$

… and some factors

$$\frac{\partial^2 \sigma}{\partial\Omega\partial\omega} = \frac{k}{k_0}\frac{1}{N \cdot 2\pi}\int_{-\infty}^{\infty}\sum_i \sum_j \left\langle b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot b_j e^{-i\vec{Q}\vec{R}_j(0)} \right\rangle e^{-i\omega t} dt$$

Sumation over all i,j

Fourier transform

i=j and i≠j !!!!!

- i=j measurement **of a single particle** trajectory
- i≠j measurement **of diferent particles** trajectory

COHERENT AND INCOHERENT SCATTERING

Coherent and incoherent scattering

GOAL: *separate "one particle" from "different particles"*

$b_{i:}$ depends on isotope and spin state (scheisse!)

$$\sum_i \sum_j b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot b_j e^{-i\vec{Q}\vec{R}_j(0)}$$

DISTINCT *SELF*

$$\sum_{i\neq j} b_i b_j e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} + \sum_{i=j} b_i b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

GOAL: *separate "one particle" from "different particles"*

b_i: depends on isotope and spin state

$$\sum_i \sum_j b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot b_j e^{-i\vec{Q}\vec{R}_j(0)}$$

DISTINCT — *SELF*

$$\sum_{i\neq j} b_i b_j \left\langle e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} \right\rangle + \sum_{i=j} b_i b_i \left\langle e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)} \right\rangle$$

$\bar{b}\;\bar{b}$

$$\sum_{i\neq j} \bar{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)} + \sum_{i=j} \overline{b^2} e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$$+ \sum_{i=j} \bar{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)} - \sum_{i=j} \bar{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$$\sum_{i,j} \bar{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} + \sum_{i=j} \left(\overline{b^2} - \bar{b}^2\right) \cdot e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$$\sum_{i,j} b_{coh}^2 \left\langle e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} \right\rangle + \sum_{i=j} b_{inc}^2 \cdot \left\langle e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)} \right\rangle$$

COHERENT — *INCOHERENT*

Coherent and incoherent scattering

***GOAL**: separate "one particle" from "different particles"*

b_i: depends on isotope and spin state (scheisse!)

$$\sum_i \sum_j b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot b_j e^{-i\vec{Q}\vec{R}_j(0)}$$

DISTINCT | SELF

$$\sum_{i\neq j} b_i b_j e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} + \sum_{i=j} b_i b_i e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$\overline{b}\ \overline{b}$

$$\sum_{i\neq j} \overline{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} + \sum_{i=j} \overline{b^2} e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$$+ \sum_{i=j} \overline{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)} - \sum_{i=j} \overline{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$$\sum_{i,j} \overline{b}^2 e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} + \sum_{i=j} \left(\overline{b^2} - \overline{b}^2\right) \cdot e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)}$$

$$\sum_{i,j} b_{coh}^2 \left\langle e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_j(0)} \right\rangle + \left\langle \sum_{i=j} b_{inc}^2 \cdot e^{i\vec{Q}\vec{R}_i(t)} \cdot e^{-i\vec{Q}\vec{R}_i(0)} \right\rangle$$

COHERENT | *INCOHERENT*

COHERENT

(warning!!! it does include the self part!!!!!)

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right)_{coh} = \frac{k}{k_0}\frac{b_{coh}^2}{N\cdot 2\pi}\int_{-\infty}^{\infty}\sum_{i,j}\left\langle e^{i\vec{Q}\vec{R}_i(t)}\cdot e^{-i\vec{Q}\vec{R}_j(0)}\right\rangle e^{-i\omega t}dt$$

$b_{coh}^2 = \overline{b}^2$ and $\sigma_{coh} = 4\pi\overline{b}^2$

INCOHERENT

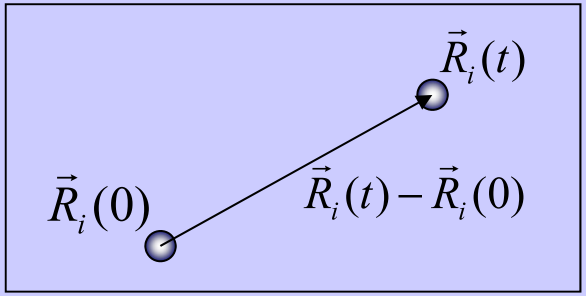
$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right)_{inc} = \frac{k}{k_0}\frac{b_{inc}^2}{N\cdot 2\pi}\int_{-\infty}^{\infty}\sum_{i}\left\langle e^{i\vec{Q}\vec{R}_i(t)}\cdot e^{-i\vec{Q}\vec{R}_i(0)}\right\rangle e^{-i\omega t}dt$$

$b_{inc}^2 = \overline{b^2} - \overline{b}^2$ and $\sigma_{inc} = \overline{b^2} - \overline{b}^2$

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \left[\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right]_{coherent} + \left[\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right]_{incoherent}$$

INCOHERENT SCATTERING

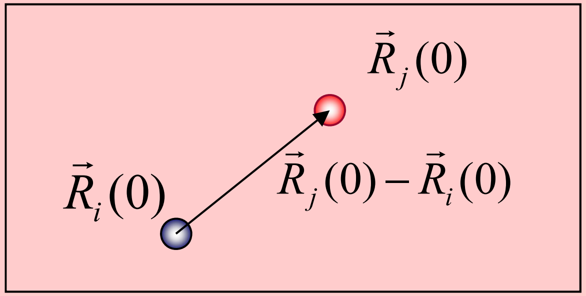
- i = j $\quad b_{inc}^2 e^{i\vec{Q}\left[\vec{R}_i(t)-\vec{R}_i(0)\right]}$



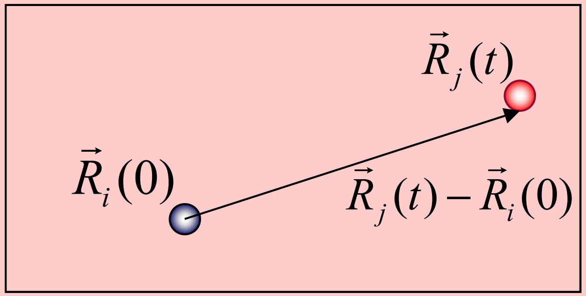
COHERENT SCATTERING

- ∀ i, j $\quad b_{coh}^2 \cdot e^{i\vec{Q}\left[\vec{R}_j(t)-\vec{R}_i(0)\right]}$

t=0



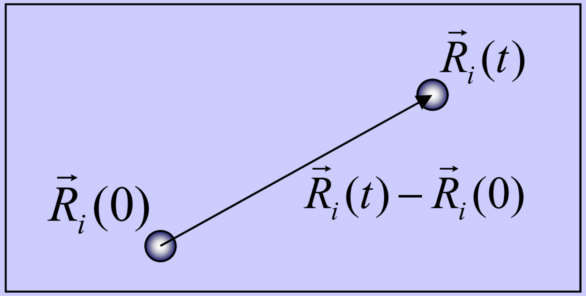
t



INCOHERENT SCATTERING

- i = j $\quad b_i^2 e^{i\vec{Q}\left[\vec{R}_i(t)-\vec{R}_i(0)\right]}$

$$\left[\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right]_{incoherent} = \frac{1}{N}\frac{k}{k_0}\sum_{\alpha=1}^{n} b_\alpha^{incoh}\cdot S_{inc}^{\alpha}(\vec{Q},\omega)$$



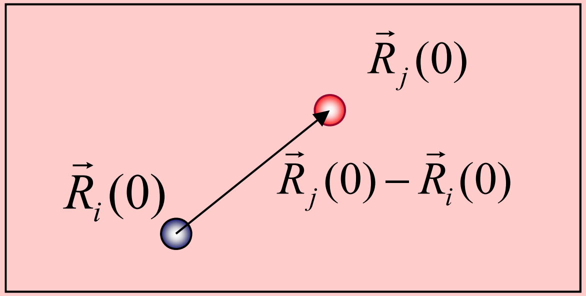
a single particle

COHERENT SCATTERING

- ∀ i, j $\quad b_i b_j \cdot e^{i\vec{Q}\left[\vec{R}_j(t)-\vec{R}_i(0)\right]}$

$$\left[\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right]_{coherent} = \frac{1}{N}\frac{k}{k_0}\sum_{\alpha=1}^{n}\sum_{\beta=1}^{n} b_\alpha^{coh} b_\beta^{coh}\sqrt{N_\alpha N_\beta}\cdot S^{\alpha\beta}(\vec{Q},\omega)$$

t=0



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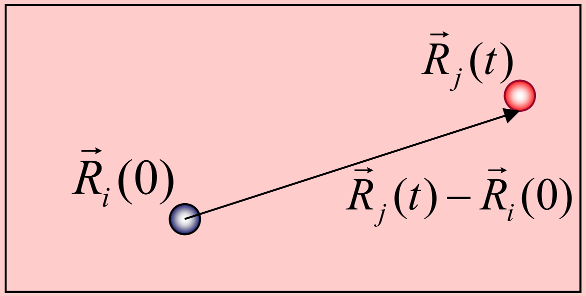


a lot of them

INCOHERENT SCATTERING ⟺ i = j

a single particle
“self” contribution

COHERENT SCATTERING ⟺ ∀ i, j

including i=j!!!
distinct + self

In the scattering cross-section:
Is the “self” part of coherent scattering the same as the “self”?

NO: *one goes with σ_{coh} and the other with σ_{inc} !!!*

WHY IS THAT IMPORTANT?

INCOHERENT SCATTERING ⟺ **movement of a single particle**

COHERENT SCATTERING ⟺ **diffraction & collective movements**

BIOLOGY!=hydrogen!!

INCOHERENT SCATTERING

movement of a single particle

σ_{inc} (H)=80.26 barn σ_{inc} (D)=2.05 barn

COHERENT SCATTERING

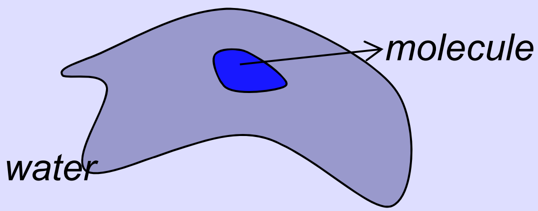
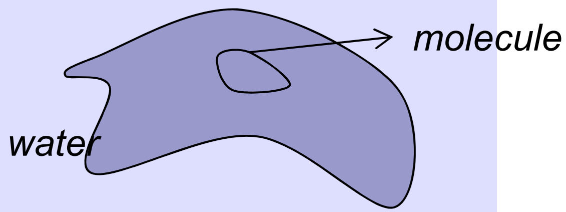
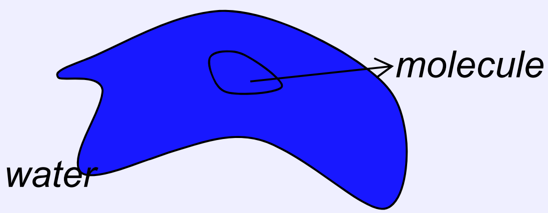
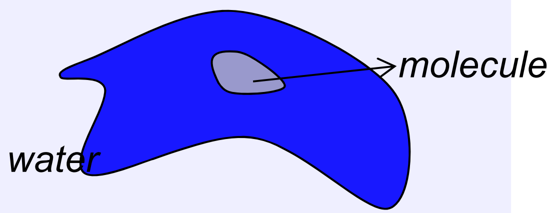
diffraction & collective movements

σ_{coh} (H)=1.7568 barn σ_{coh} (D)=5.592 barn

Contrast (diffraction)

Let’s mix water with a byological molecule...

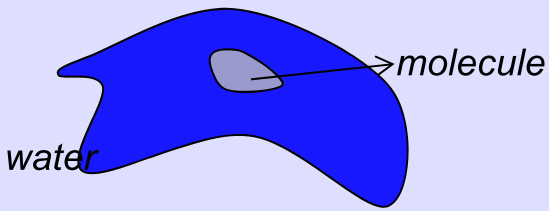
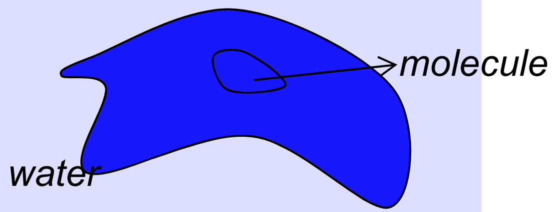
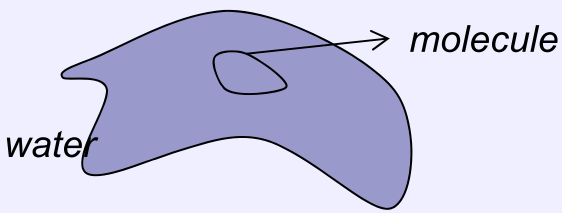
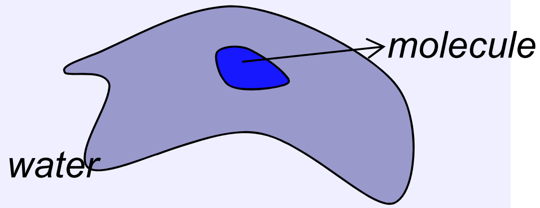
σ_{coh} (H)=1.7568 barn σ_{coh} (D)=5.592 barn

	deuterated	not-deuterated
Molecule Water Not deuterated		
Molecule Water deuterated		

Contrast (movements)

Let's mix water with a byological molecule...

σ_{inc} (H)=80.26 barn σ_{inc} (D)=2.05 barn

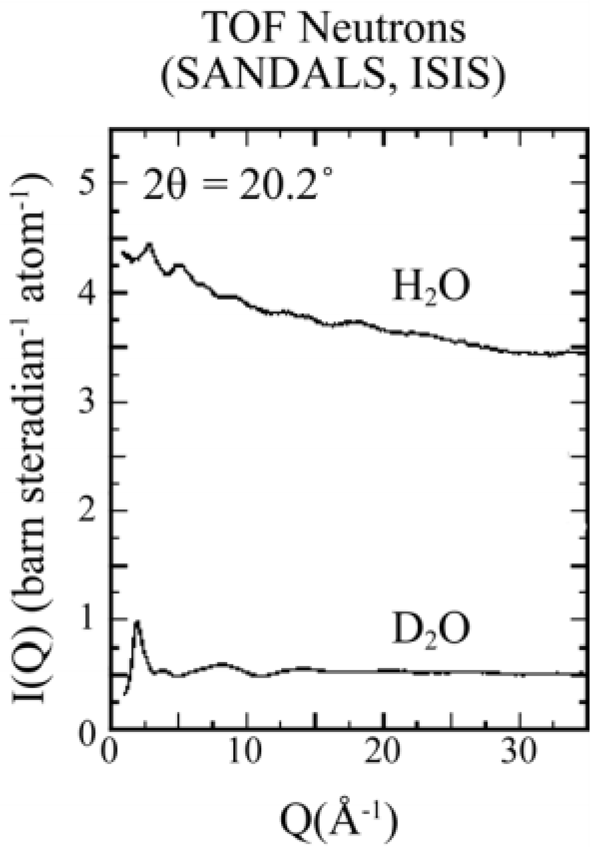
	deuterated	**not-deuterated**
Molecule Water Not deuterated		
Molecule Water deuterated		

Contrast (diffraction)

With other substances... for example in water. let's play...

σ_{coh} (H)=1.7568 barn σ_{coh} (D)=5.592 barn σ_{coh} (O)=4.232 barn

σ_{inc} (H)=80.26 barn σ_{inc} (D)=2.05 barn σ_{inc} (O)=0.0008 barn



$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \left[\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right]_{coherent} + \left[\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right]_{incoherent}$$

DOI: 10.1021/acs.chemrev.5b00663