1st Lecture

Scattering Principle & Static Scattering

Norman J. WAGNER

NSF NSE Workshop October 28th, 2021

University of Delaware

Acknowledgement to Dr. Yun Liu, NCNR NIST

THURSDAY, OCTOBER 28th, 2021

08:30 AM – 09:00 AM	MEET & GREET– Conference Room (Salon E & F)		
09:00 AM – 09:10 AM	OPENING REMARKS – Robert Dimeo, NCNR Director		
09:10 AM – 10:40 AM	1st LECTURE – Static Scattering – Norman Wagner		
10:40 AM – 11:00 AM	TEA BREAK		
11:00 AM – 12:30 PM	2nd LECTURE – Dynamic Scattering – Antonio Faraone		
12:30 PM – 01:30 PM	LUNCH BREAK		
01:30 PM – 03:00 PM	3rd LECTURE – NSE– Michihiro Nagao		
03:00 PM – 03:20 PM	TEA BREAK		
03:20 PM – 05:30 PM	INTEREST GROUPS		
	Polymer Antonio Faraone	Protein Michihiro Nagao	Membrane Elizabeth Kelley
06:15 PM – 07:45 PM	BANQUET – Group Picture		
07:45 PM – 08:25 PM	AFTER DINNER TALK – Edward Lyman		

FRIDAY, OCTOBER 29th, 2021	
08:15 AM – 08:30 AM	MEET & GREET– Conference Room (Salon E & F)
08:30 AM – 09:10 AM	COMPLEMENTARY METHODS – Madhusudan Tyagi
09:10 AM – 09:50 AM	PROPOSAL WRITING – Paul Butler
09:50 AM – 10:10 AM	TEA BREAK
10:10 AM – 11:25 AM	PRESENTATION SOUNDBITES
11:25 AM – 11:30 PM	CLOSING REMARKS – Dan Neumann, CHRNS Director
11:30 AM – 12:15 PM	LUNCH
12:20 PM – 01:00 PM	TRAVEL to NIST
01:30 PM – 03:00 PM	NCNR GUIDE HALL TOUR
03:30 PM – 04:30 PM	RETURN to HOTEL

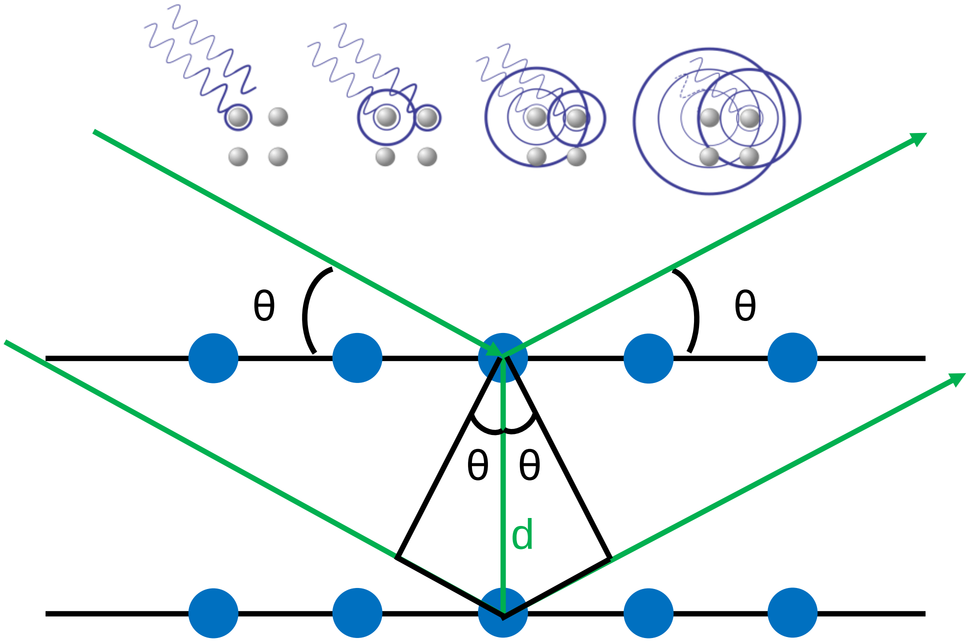
Learning Goal

- ✓ Learn basic concepts of scattering.
- ✓ Understand the relationship between reciprocal space and real space.
- ✓ Learn the properties of neutrons and understand why neutrons are a good probe to be used to study soft matter.
- ✓ Understand the principle of small-angle neutron scattering.

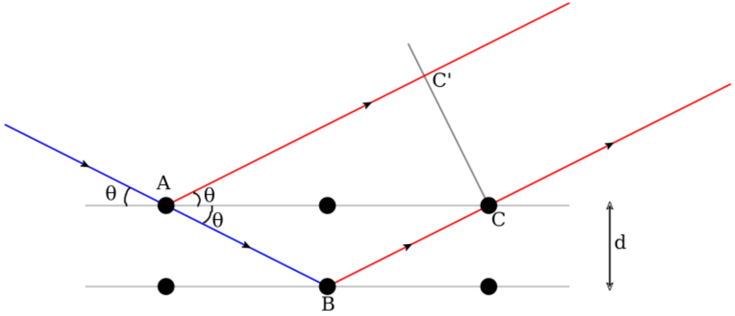
Outline

- Scattering Event
- Properties of Neutron
- Coherent and Incoherent Scattering
- Scattering Form Factors
- Principle of Small-angle Neutron Scattering

Bragg Diffraction 1913, Nobel Prize 1915



Bragg Diffraction

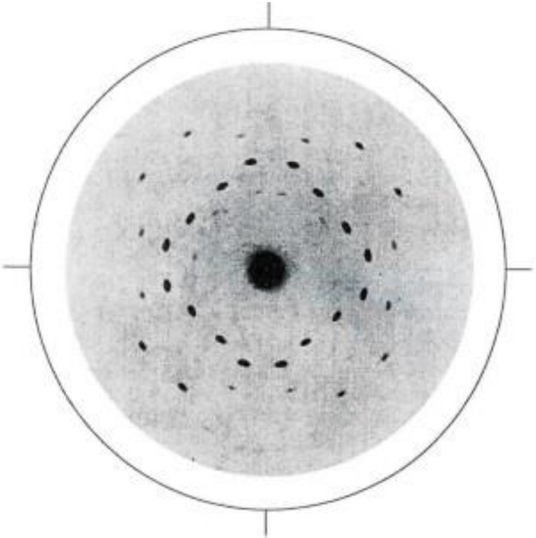


Bragg's law of diffraction:

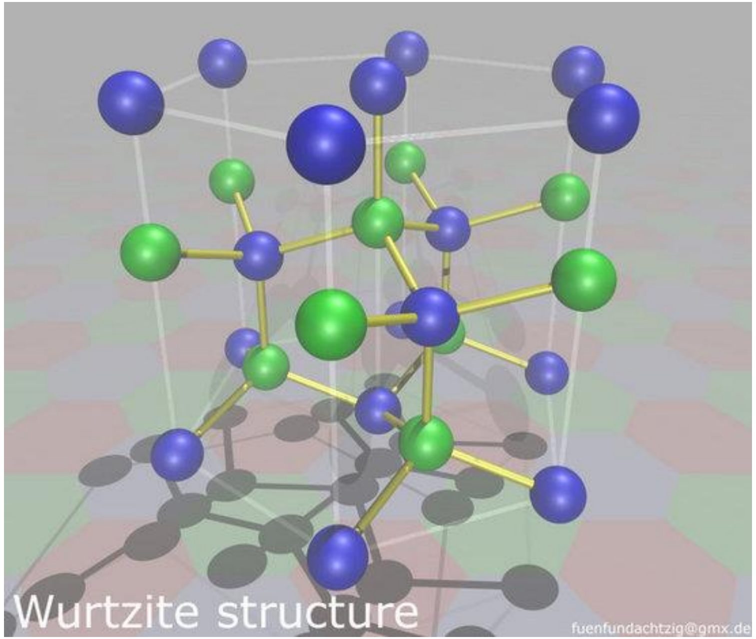
$$2d sin\,\theta = n\lambda$$

https://en.wikipedia.org/wiki/Bragg's_law

Max von Laue 1912



Friedrich, W., Knipping, P. & Laue, M. In *Sitzungsberichte der Math. Phys. Klasse (Kgl.) Bayerische Akademie der Wissenschaften* 303–322 (1912).



HCP structure of wurtzite. (Creator: Alexander Mann Date: 01/14/2006

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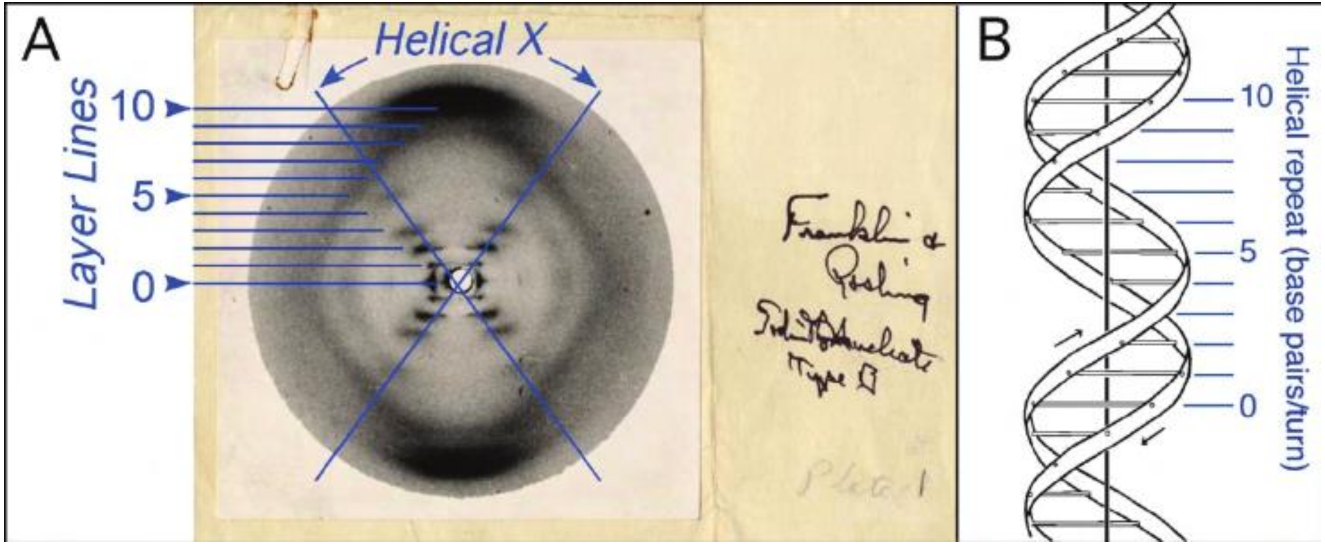
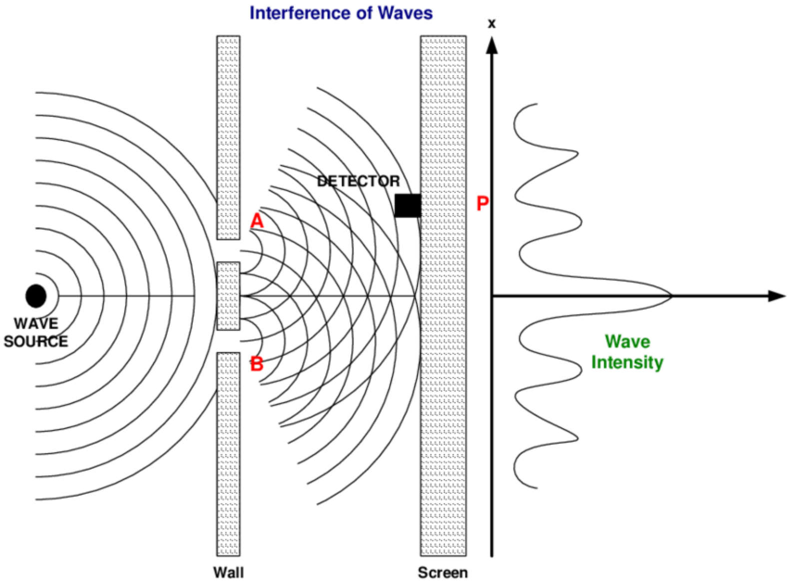
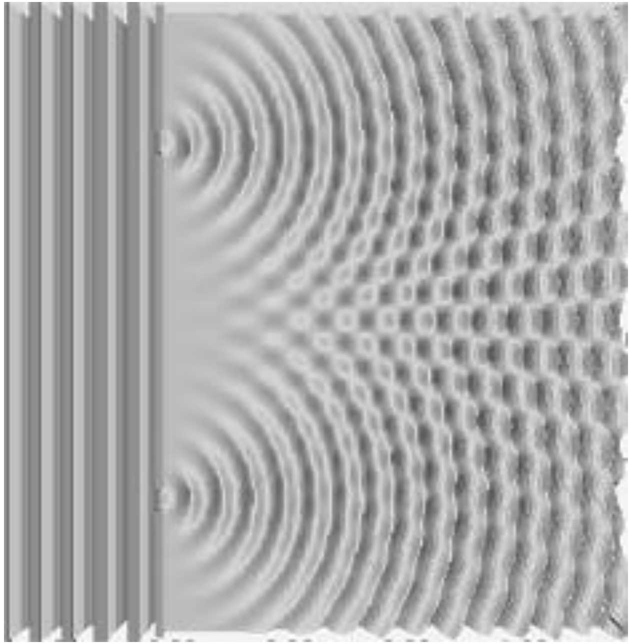
Rosalind Franklin & Raymond Gosling, 1952



Wave properties of the Neutron: Young's experiment 1801

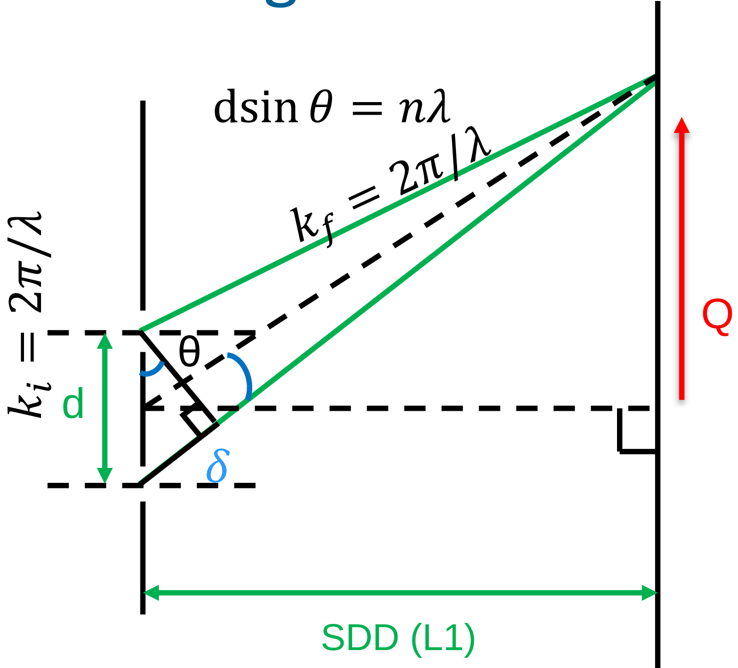


Elhoushi, Mostafa. (2011). Modeling a Quantum Computer.



https://gifimage.net/wp-content/uploads/2017/10/double-slit-experiment-gif-6.gif

Young's Double Slit Experiment (1801)



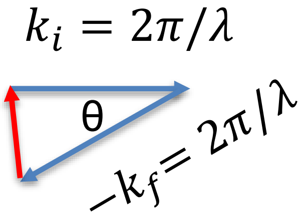
Double Slit Experiment

Intensity of scattering is:

$I(Q) = \psi(Q)\,\psi(Q)^* = |\psi(Q)|^2$

Vector Diagram defining Q:

$Q = \frac{4\pi}{\lambda}\sin\theta/2$



Extra distance traveled by second wave

$\delta = d * sin\theta$

Phase difference at detector:

$\delta = d * sin\theta = \mathrm{m} * \lambda; \quad m = 0, \pm 1, \pm 2, \pm 3, \ldots$

$I(Q) = \psi(Q)\,\psi(Q)^* = |\psi(Q)|^2 = |\psi_0|^2\,(1 + \cos(Qd))$

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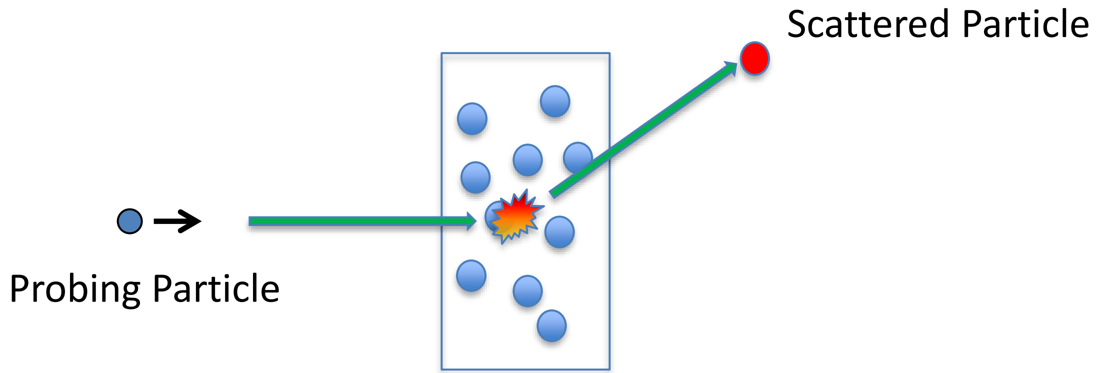
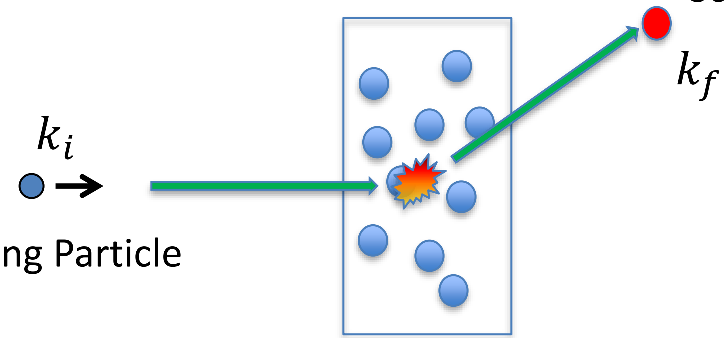
Scattering Geometry



Probing Particles:

low energy photon (light scattering such as SLS, DLS)
high energy photon (X-ray scattering)
neutron (neutron scattering)

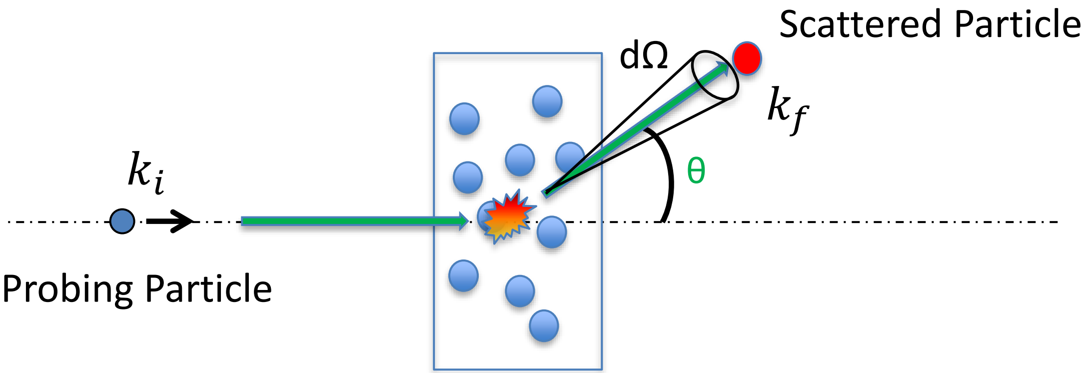
Scattering Geometry



Properties Probing Particles: energy E_i, and momentum $\overrightarrow{p_i} = \hbar\overrightarrow{k_i}$, where k_i is the wave vector of particles. And $k_i = \frac{2\pi}{\lambda_i}$. (λ is the wavelength of the particle.)

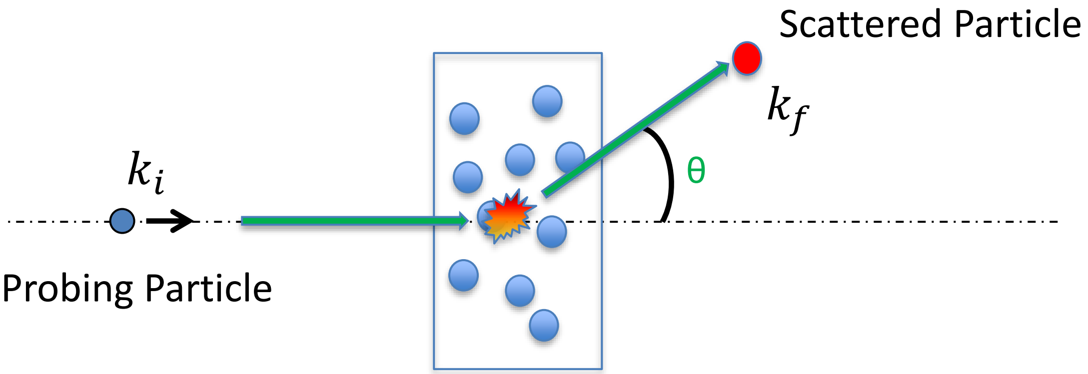
Properties Scattered Particles: energy E_f, and momentum $\overrightarrow{p_f} = \hbar\overrightarrow{k_f}$. And $k_f = \frac{2\pi}{\lambda_f}$.

Scattering Geometry

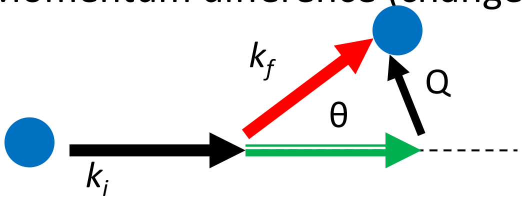


What we measure is the number of scattered particles at certain angles (θ) with a certain energy, (E_f).
In other words, it is essentially to measure the probability that a particle is scattered at a solid angle with a certain energy (E_f).
This probability is called the scattering intensity function, $I(\theta, E_i, E_f)$ which is proportional to the Differential Scattering Cross Section (dσ/dΩ).

Scattering Geometry



1. Momentum difference (change of wave vector)



2. Energy difference

$$\Delta \mathrm{E} = E_f - E_i = \hbar\omega$$

The scattering intensity, $I(\theta, E_i, E_f)$, can be rewritten as $I(Q, \Delta E), or\ I(Q, \omega)$.

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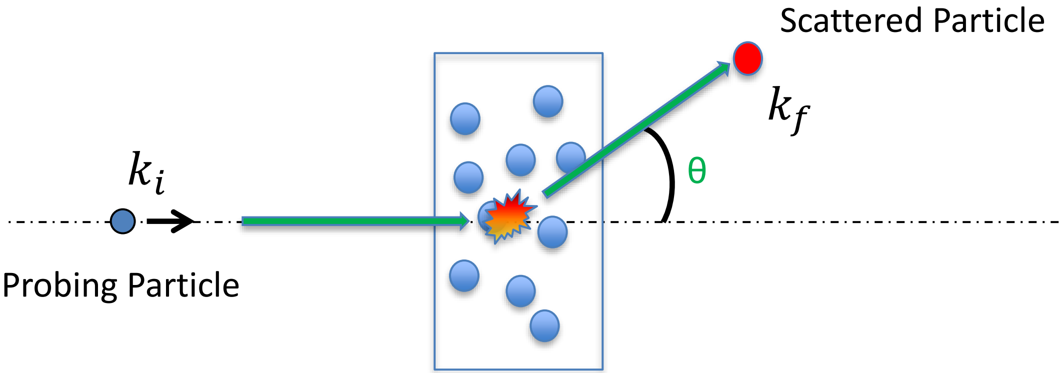
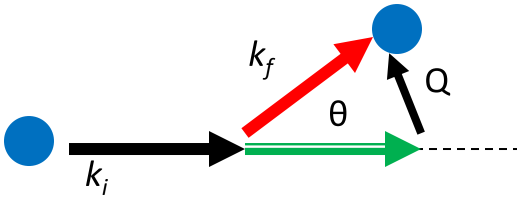
Scattering Geometry





Static scattering intensity function

The static scattering intensity is $I(Q) = \int I(Q,\omega)d\omega$.

If $k_i = k_f = k$, $Q = 2ksin\left(\frac{\theta}{2}\right) = \frac{4\pi}{\lambda}sin\left(\frac{\theta}{2}\right)$.

In many cases, the static scattering function is essentially the elastic scattering function, i.e., $\Delta\mathrm{E} = 0$. Therefore, $I(Q) \approx I(Q,\omega = 0)\Delta\omega$.

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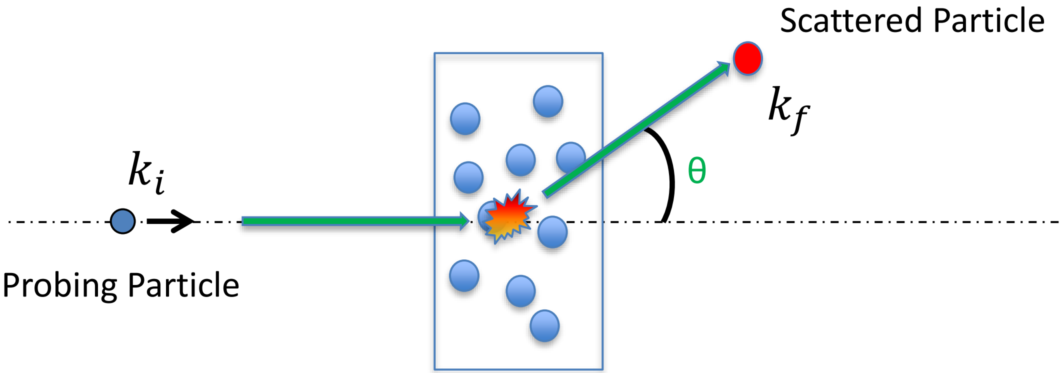
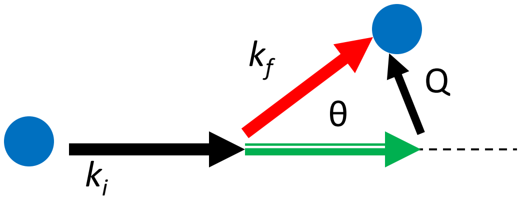
Scattering Geometry



Static scattering intensity function



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If $k_i = k_f = k$, $Q = 2ksin\left(\frac{\theta}{2}\right) = \frac{4\pi}{\lambda}sin\left(\frac{\theta}{2}\right)$.

In many cases, the static scattering function is essentially the elastic scattering function, i.e., $\Delta E = 0$. Therefore, $I(Q) \approx I(Q, \omega = 0)\Delta\omega$.

But they are different functions! Elastic scattering is NOT static scattering!

Properties of Probes

	X-ray	Neutron	Light
Weight	No	Yes	No
Wavelength (λ)	0.1 – 10 Å	0.1 - 10 Å	4000 - 7000 Å
Interaction	With Electrons	With Nucleus & Magnetic Moment	Polarizability Tensor
Charge	N/A	N/A	N/A
Spin	No	Yes	No
Magnetic Moment	No	Yes	No

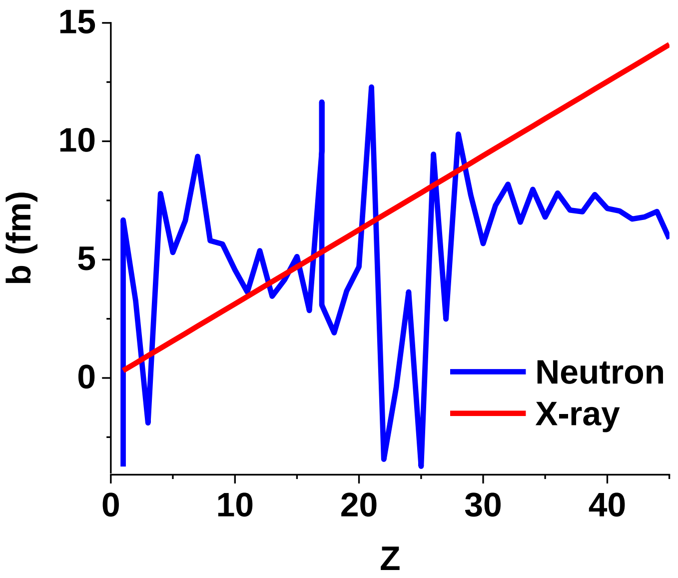
Nuclear Interaction

Neutrons are scattered by the nuclei.

Fermi pseudo-potential:

$$V(\underline{r}) = \frac{2\pi\hbar^2}{m_n} b_i \delta(\underline{r} - \underline{r_i})$$

b_i is the scattering length



Scattering power varies “non-systemically” from isotope to isotope.

The scattering also depends on nuclear spin state of the atom.

Isotopes & nuclear spin: the example of hydrogen

Proton with nuclear spin of ½ versus , isotope deuterium with nuclear spin of 1

Hydrogen:

$$b^{+} = 1.085x10^{-14}\ m$$
$$b^{-} = -4.750x10^{-14}\ m$$

$$\langle b\rangle = \frac{3}{4}\,b^{+} + \frac{1}{4}\,b^{-} = -0.374x10^{-14}\ m$$

$$\langle b^2\rangle = \frac{3}{4}(b^{+})^2 + \frac{1}{4}(b^{-})^2 = 6.524x10^{-14}\ m$$

$$\Delta b = \sqrt{\langle b^2\rangle - \langle b\rangle^2} = 2.527x10^{-14}\ m$$

Deuterium:

$$b^{+} = 0.953x10^{-14}\ m$$
$$b^{-} = 0.098x10^{-14}\ m$$

$$\langle b\rangle = \frac{2}{3}\,b^{+} + \frac{1}{3}\,b^{-} = 0.668x10^{-14}\ m$$

$$\Delta b = \sqrt{\langle b^2\rangle - \langle b\rangle^2} = 0.403x10^{-14}\ m$$

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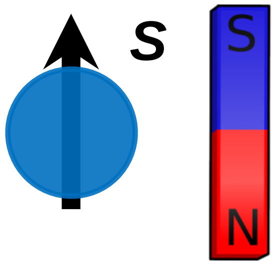
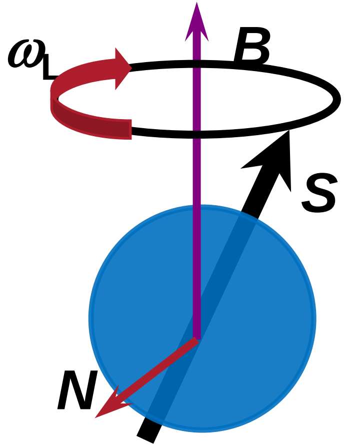
Nuclear Spin





Neutron Properties

- ✓ Mass, m_n = 1.675×10^{-27} kg
- ✓ Spin, S = 1/2 [in units of $h/(2\pi)$]
- ✓ Gyromagnetic ratio $\gamma = g_n \mu_n / [h/(2\pi)]$ = 1.832×10^{8} s^{-1}T^{-1} (29.164 MHz T^{-1})

In a Magnetic Field

- ✓ The neutron experiences a torque from a magnetic field B perpendicular to its spin direction. $N = S \times B$
- ✓ Precession with the Larmor frequency: $\omega_L = \gamma B$

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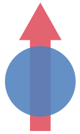
Spin-flip/Non-spin-flip Scattering

Sample scattering events sometimes involve with spin-flip scattering

Coherent scattering: Non-Spin-Flip Scattering

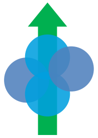
Isotope incoherent scattering: Non-Spin-Flip Scattering

Spin incoherent scattering: Spin-Flip Scattering -- 2/3 Spin-Flip probability



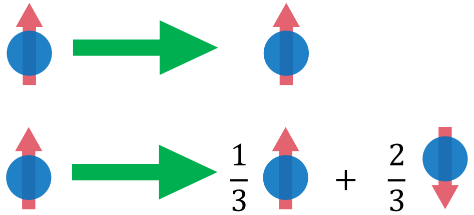
Neutron spin $\frac{1}{2}$

Quantization in an axis



Nuclear spin Sn

Random orientation



Spin-incoherent

Non-spin flip in the quantization axis

Spin flip in other axes

Spin-flip/Non-spin-flip Scattering

Sample scattering events sometimes involve with spin-flip scattering

Coherent scattering: Non-Spin-Flip Scattering

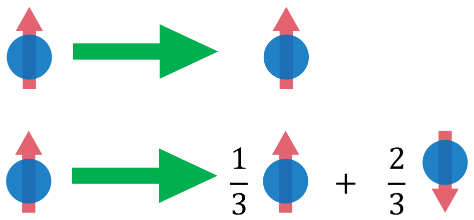
Isotope incoherent scattering: Non-Spin-Flip Scattering

Spin incoherent scattering: Spin-Flip Scattering -- 2/3 Spin-Flip probability

$$I_{NSF} = I_{coh} + I_{i-inc} + \frac{1}{3} I_{s-inc}$$

$$I_{SF} = \frac{2}{3} I_{s-inc}$$

$$I_{total} = I_{coh} + I_{i-inc} + I_{s-inc} = I_{NSF} + I_{SF}$$

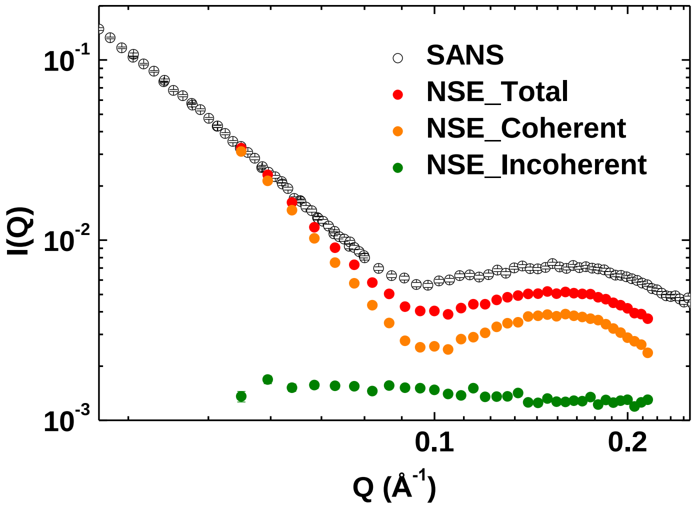


Separation of coherent + isotope-incoherent from spin-incoherent scattering

$$I_{coh} + I_{i-inc} = I_{NSF} - \frac{1}{2} I_{SF}$$

$$I_{s-inc} = \frac{3}{2} I_{SF}$$

Separation of Coherent/Incoherent Scattering

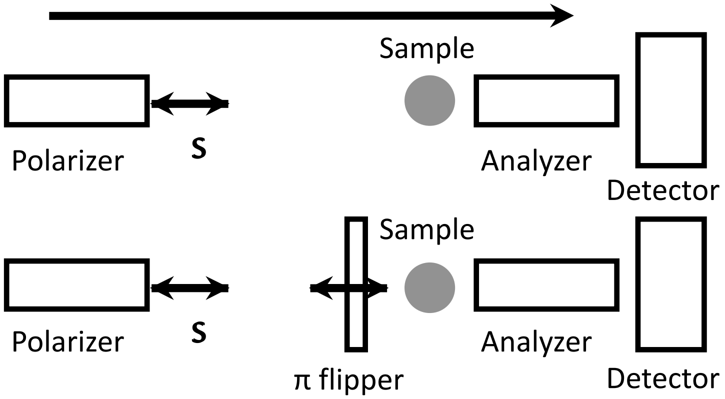


d54-DMPC in D_2O

Separation of coherent + isotope-incoherent from spin-incoherent scattering

$$I_{coh} + I_{i-inc} = I_{NSF} - \frac{1}{2} I_{SF} \qquad I_{s-inc} = \frac{3}{2} I_{SF}$$

How do We Measure NSF and SF in Practice



I_{NSF}

$$I_{NSF} = I_{coh} + I_{i-inc} + \frac{1}{3} I_{s-inc}$$

I_{SF}

$$I_{SF} = \frac{2}{3} I_{s-inc}$$

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Differential Scattering Cross Section

In a neutron scattering text book, you will find

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{n,m} b_n b_m \langle \exp[-i\vec{Q}\cdot(\vec{r}_m - \vec{r}_n)]\rangle$$

Here we consider average scattering lengths $\sum_{n,m} b_n b_m = \sum_{n,m}\left[\overline{b_n b_m} + \left(b_n b_m - \overline{b_n b_m}\right)\right]$

As the sample contains a large number of independent, distinct subsamples, we take an ensemble

$$\overline{b_n} = \langle b_n\rangle = \langle b\rangle$$

$$\overline{b_n b_m} = \langle b\rangle^2$$

For $n \neq m$, $\langle b_n b_m - \overline{b_n b_m}\rangle = \langle b_n\rangle\langle b_m\rangle - \overline{b_n b_m} = 0$

For $n = m$, $\langle b_n b_n - \overline{b_n b_n}\rangle = \langle b_n b_n\rangle - \langle b_n\rangle\langle b_n\rangle = \langle b^2\rangle - \langle b\rangle^2$

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar} \times \left[\langle b\rangle^2 \sum_{n,m}\langle \exp[-i\vec{Q}\cdot(\vec{r}_m - \vec{r}_n)]\rangle + (\langle b^2\rangle - \langle b\rangle^2)\sum_{n}\langle \exp[-i\vec{Q}\cdot(\vec{r}_n - \vec{r}_n)]\rangle\right]$$

Coherent scattering $I_{coh}(\vec{q},t)$

Incoherent scattering $I_{inc}(\vec{q},t)$

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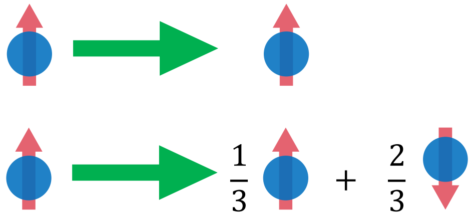
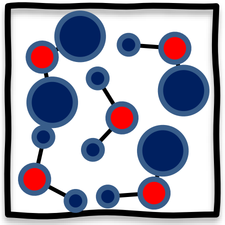
Coherent/Incoherent Summary

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{n,m} b_n b_m \langle \exp[-i\vec{Q}\cdot(\vec{r}_m - \vec{r}_n)]\rangle$$

$$= \frac{k_f}{k_i}\frac{1}{2\pi\hbar} \times \left[\langle b\rangle^2 \sum_{n,m}\langle \exp[-i\vec{Q}\cdot(\vec{r}_m - \vec{r}_n)]\rangle + (\langle b^2\rangle - \langle b\rangle^2)\sum_{n}\langle \exp[-i\vec{Q}\cdot(\vec{r}_m - \vec{r}_n)]\rangle\right]$$

Coherent scattering   Incoherent scattering





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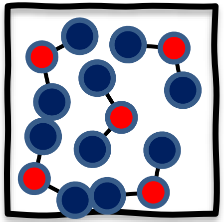

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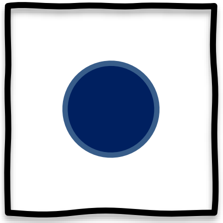

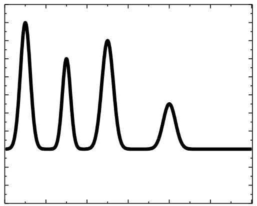

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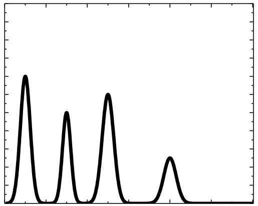

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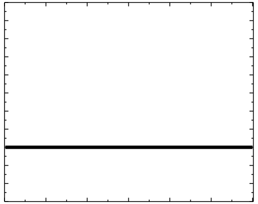

$\sigma = 4\pi\langle b^2\rangle$

Total

$\sigma_{coh} = 4\pi\langle b\rangle^2$

All correlation
Coherent

$\sigma_{inc} = 4\pi(\langle b^2\rangle - \langle b\rangle^2)$

Self correlation
Incoherent

Total

Coherent

Incoherent

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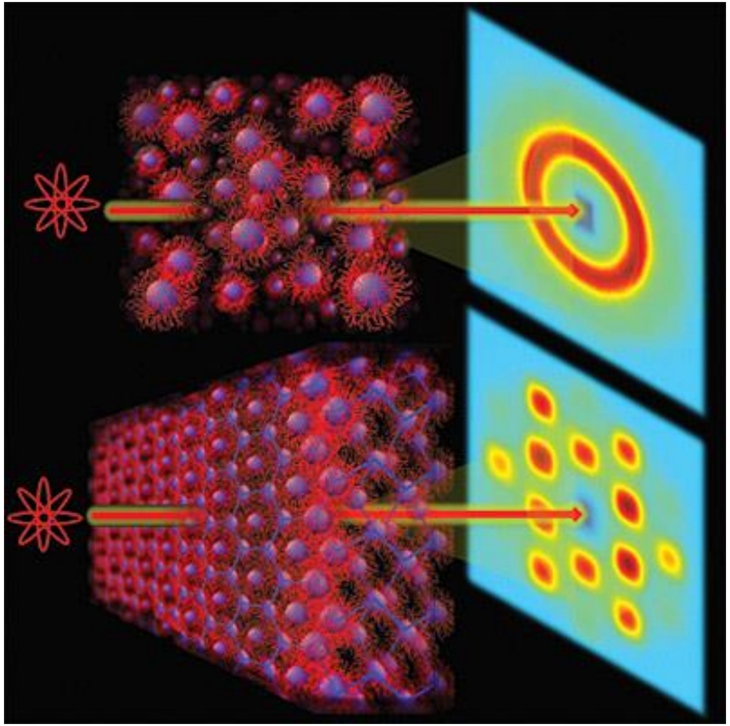
Scattering and Correlation Functions



$$S(Q) = FT\{\langle -i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)\rangle\} = FT_S\{g(r)\}$$

Fourier Transform of the Space Correlation Function

Remember Bragg's law

$$q = \frac{2\pi}{r}$$

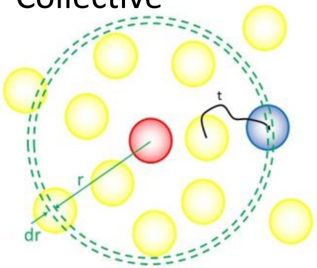
Adapted from: Lopez-Barron, C.R., L. Porcar, A.P.R. Eberle, and N.J. Wagner, "Dynamics of Melting and Recrystallization in a Polymeric Micellar Crystal Subjected to Large Amplitude Oscillatory Shear Flow," Physical Review Letters **108**, 258301 (2012).

Scattering Functions

$S_N(Q) = S_{inc}(Q) + S_{coh}(Q)$

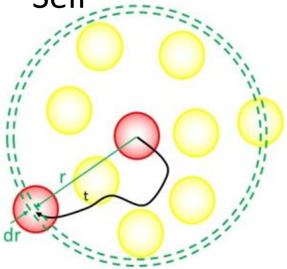
$S_{coh}(Q)$ is the time Fourier transform of the ***PAIR*** correlation function

$$S_{coh}(Q) = \frac{1}{N} FT\left\{\sum_{i,j} \langle b_i \rangle \langle b_j \rangle \langle \exp[-i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)] \rangle \right\}$$



$S_{inc}(Q)$ is the space Fourier transform of the ***SELF*** correlation function

$$S_{inc}(Q) = \frac{1}{N} FT\left\{\sum_{i} [\langle b_i^2 \rangle - \langle b_i \rangle^2] \langle \exp[-i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)] \rangle \right\}$$



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Scattering Functions

$S_N(Q) = S_{inc}(Q) + S_{coh}(Q)$

$S_{coh}(Q)$ is the time Fourier transform of the ***PAIR*** correlation function

$$S_{coh}(Q) = \frac{1}{N} FT \left\{ \sum_{i,j} \langle b_i \rangle \langle b_j \rangle \langle \exp[-i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)] \rangle \right\}$$

Coherent Scattering Cross Section

$$\sigma_i^{coh} = 4\pi \langle b_i \rangle^2$$

$S_{inc}(Q)$ is the space Fourier transform of the ***SELF*** correlation function

$$S_{inc}(Q) = \frac{1}{N} FT \left\{ \sum_{i} [\langle b_i^2 \rangle - \langle b_i \rangle^2] \langle \exp[-i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)] \rangle \right\}$$

Incoherent Scattering Cross Section

$$\sigma_i^{incoh} = 4\pi [\langle b_i^2 \rangle - \langle b_i \rangle^2]$$

Scattering Functions

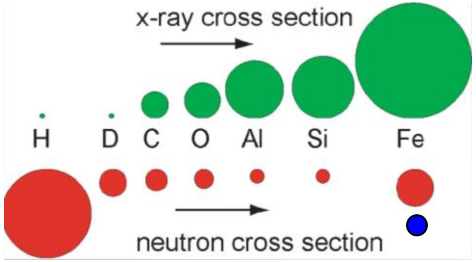
$S_N(Q) = S_{inc}(Q) + S_{coh}(Q)$

$S_{coh}(Q)$ is the time Fourier transform of the ***PAIR*** correlation function

$$S_{coh}(Q) = \frac{1}{N} FT \left\{ \sum_{i,j} \langle b_i \rangle \langle b_j \rangle \langle \exp[-i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)] \rangle \right\}$$

$S_{inc}(Q)$ is the space Fourier transform of the ***SELF*** correlation function

$$S_{inc}(Q) = \frac{1}{N} FT \left\{ \sum_{i} [\langle b_i^2 \rangle - \langle b_i \rangle^2] \langle \exp[-i\vec{Q} \cdot (\vec{r}_m - \vec{r}_n)] \rangle \right\}$$



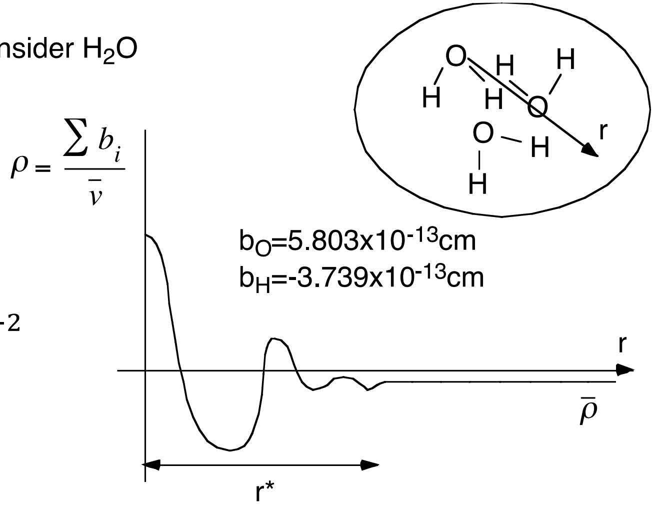
Hydrogen has a high scattering cross section

Scattering Length Density

When Length scales are large the details of atomic properties cannot be appreciated, a continuous medium approach is more appropriate.

$$\rho(r) = \frac{1}{v}\sum_{i\in v} b_i \delta(r - r_i) \quad \text{or} \quad \rho = \frac{\sum b_i}{v}$$

consider H_2O



r*~10Å

q≤0.1Å^{-1}

$$\rho_{SLD,H_2O} = \left(\frac{6\times 10^{23}}{mol}\right)\left(\frac{1.0g/cm^3}{18g/mol}\right)(2\times b_H + b_O) = -0.56\times 10^{10}cm^{-2}$$

$$\rho_{SLD,D_2O} = \left(\frac{6\times 10^{23}}{mol}\right)\left(\frac{1.1g/cm^3}{20g/mol}\right)(2\times b_D + b_O) = 6.32\times 10^{10}cm^{-2}$$

What matter is the contrast!! $\Delta\rho = \rho_1 - \rho_2$

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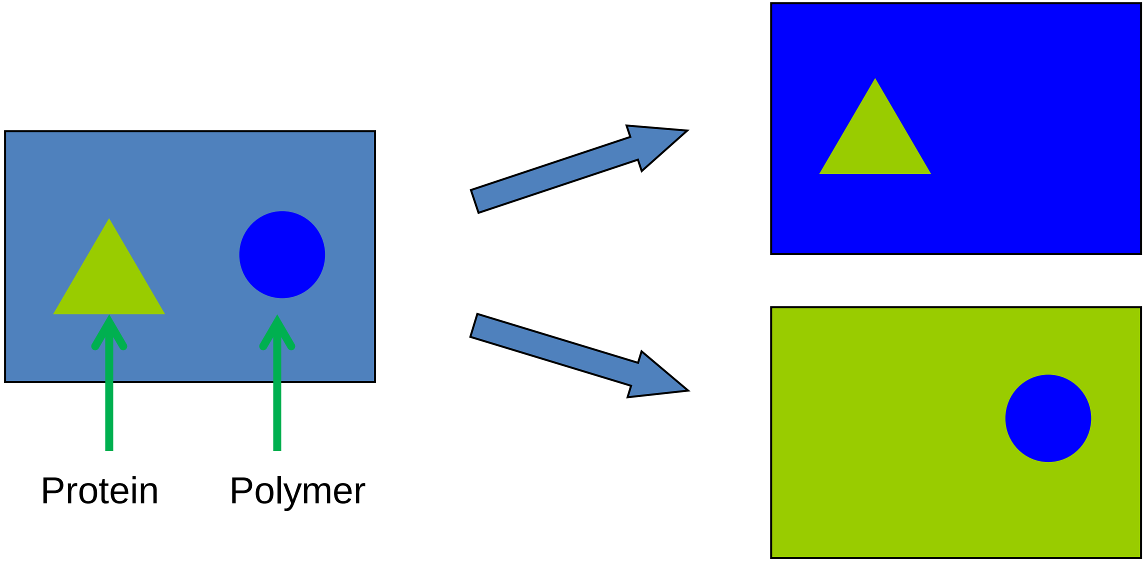
Scattering Contrast



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Neutron scattering lengths and cross sections

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

NOTE: The above are only thermal neutron cross sections. I do not have any energy dependent cross sections. For energy dependent cross sections please go to the National Nuclear Data Center at Brookhaven National Lab.

Select the element, and you will get a list of scattering lengths and cross sections. All of this data was taken from the Special Feature section of neutron scattering lengths and cross sections of the elements and their isotopes in *Neutron News*, Vol. 3, No. 3, 1992, pp. 29-37.

The scattering lengths and cross sections only go through element number 96 Cm (Curium)

A long table with the complete list of elements and isotopes is also available.

https://www.ncnr.nist.gov/resources/n-lengths/

Back to the top-level Center for Neutron Research page.

These data were entered by hand from the above cited paper. As such some errors may exist. Report errors or make inquiries to Alan Munter, *<alan.munter@nist.gov>*

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All of this data was taken from the Special Feature section of neutron scattering lengths and cross sections of the elements and their isotopes in *Neutron News*, Vol. 3, No. 3, 1992, pp. 29-37.

The contents of the columns are as follows:

Column	Unit	Quantity
1	---	Isotope
2	---	Natural abundance (For radioisotopes the half-life is given instead)
3	fm	bound coherent scattering length
4	fm	bound incoherent scattering length
5	barn	bound coherent scattering cross section
6	barn	bound incoherent scattering cross section
7	barn	total bound scattering cross section
8	barn	absorption cross section for 2200 m/s neutrons

Note: 1fm=1E-15 m, 1barn=1E-24 cm^2, scattering lengths and cross sections in parenthesis are uncertainties.

Neutron scattering lengths and cross sections							
Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
H	---	-3.7390	---	1.7568	80.26	82.02	0.3326
1H	99.985	-3.7406	25.274	1.7583	80.27	82.03	0.3326
2H	0.015	6.671	4.04	5.592	2.05	7.64	0.000519
3H	(12.32 a)	4.792	-1.04	2.89	0.14	3.03	0

Back up to the periodic table.

Last Modified 23, November 1999

These data were entered by hand from the above cited paper. As such some errors may exist. Report errors or make inquiries to Alan Munter, *<alan.munter@nist.gov>*

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Material

Co

Neutron Activation

For rabbit system [Calculate]

Thermal flux	Cd ratio	Thermal/fast ratio
1e8	0	0
Mass	**Exposure**	**Decay**
	10	1 y

Absorption and Scattering

[Calculate]

Density	Thickness
	1
Source neutrons	**Source X-rays**
1 Ang	Cu Ka

Neutron activation and scattering calculator

This calculator uses neutron cross sections to compute activation on the sample given the mass in the sample and the time in the beam, or to perform scattering calculations for the neutrons which are not absorbed by the sample.

1. Enter the sample formula in the material panel.

2. To perform activation calculations, fill in the thermal flux, the mass, the time on and off the beam, then press the calculate button in the neutron activation panel.

3. To perform scattering calculations, fill in the wavelength of the neutron and/or xrays, the thickness and the density (if not given in the formula), then press the calculate button in the absorption and scattering panel.

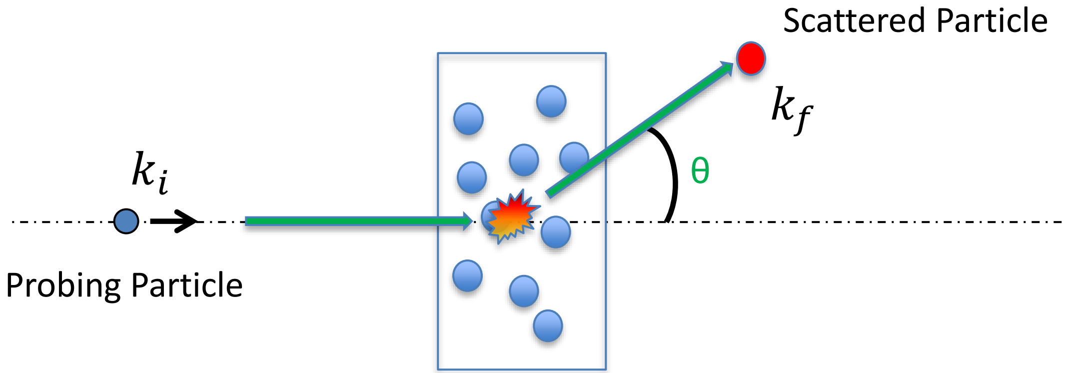
Chemical formula

Questions?
Neutron activation: NCNR Health Physics <hp@nist.gov>
Scattering calculations: Paul Kienzle <paul.kienzle@nist.gov>

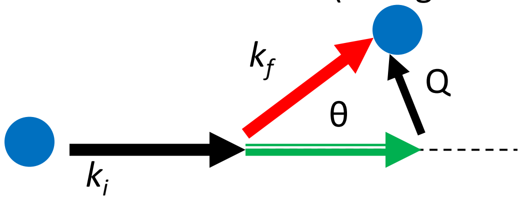
Last modified 05-November-2020 by website owner: NCNR (attn: Paul Kienzle)

https://www.ncnr.nist.gov/resources/activation/

Small-angle Scattering



1. Momentum difference (change of wave vector)



2. Energy difference

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

The scattering intensity, $I(\theta, E_i, E_f)$, can be rewritten as $I(Q, \Delta E), or\ I(Q, \omega)$.

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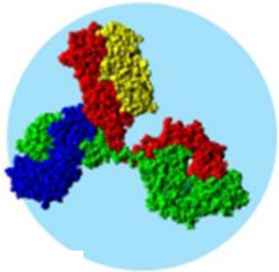
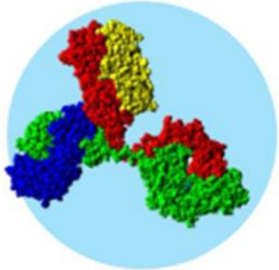
Static Scattering Intensity Function

What is the relation between I(Q) and the structure of investigated material?



$$I(Q) = \left| \sum_m b_m e^{-i\overrightarrow{r_m}\cdot\vec{Q}} \right|^2 = |F(Q)|^2$$

$$F(Q) = \sum_m b_m e^{-i\overrightarrow{r_m}\cdot\vec{Q}} = \int \rho(r) e^{-i\vec{r}\cdot\vec{Q}} d\vec{r}$$



Fourier transformation of the image

$F(Q)$ (Q: reciprocal space)

Static scattering function is related with the amplitude of the FT of the structure.

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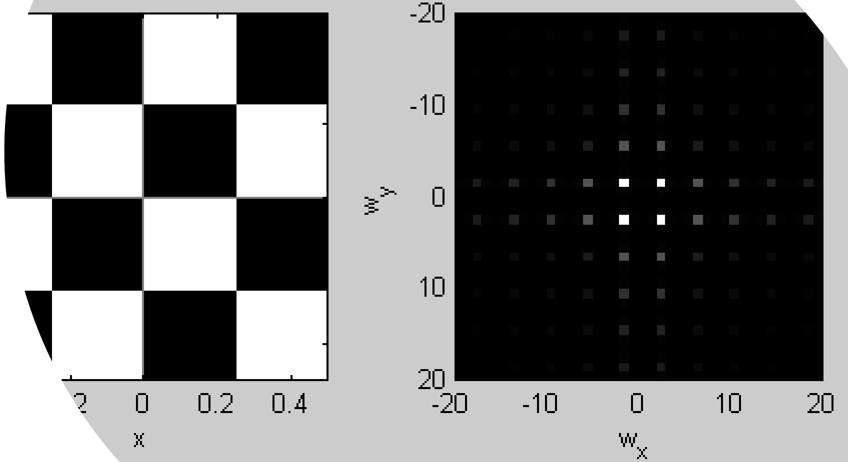
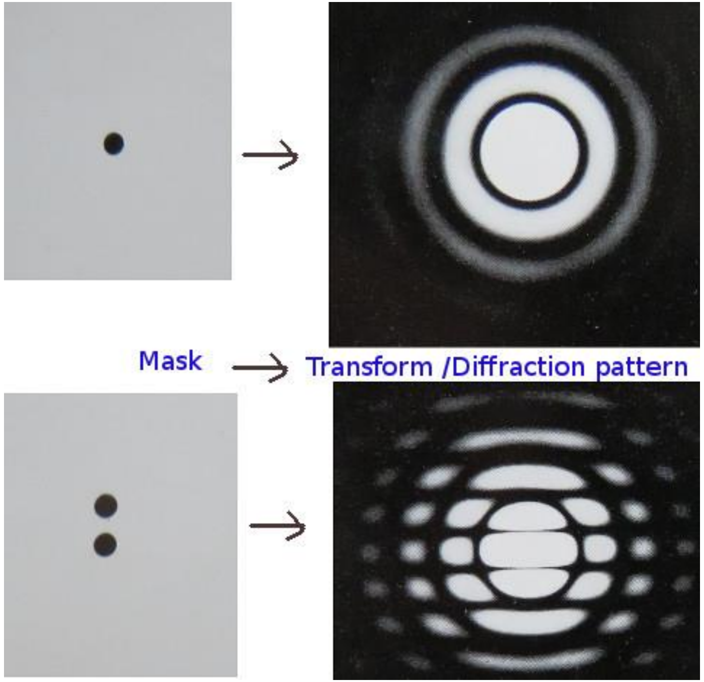


2-D Fourier transforms-symmetry

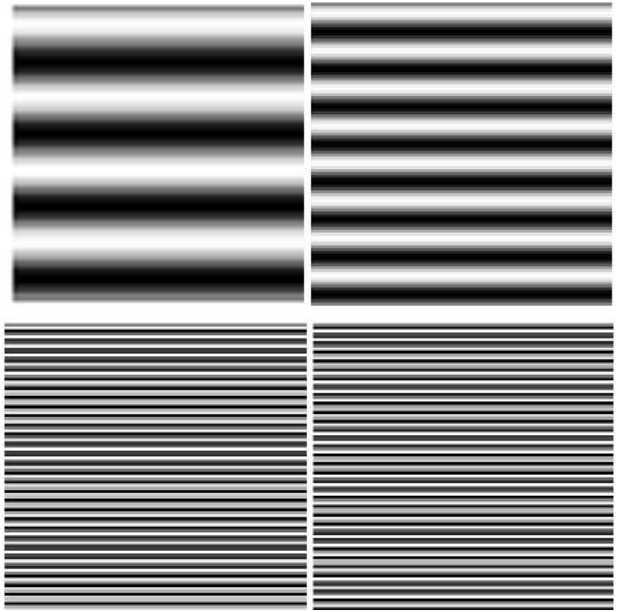
Remember Bragg's law

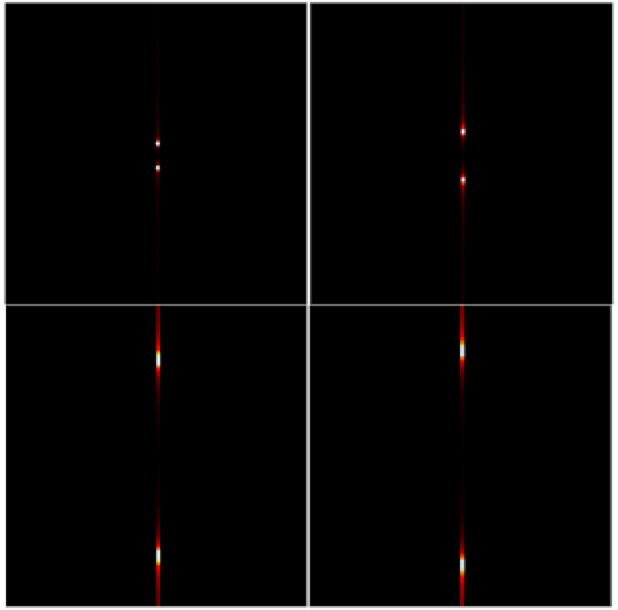
$$q = \frac{2\pi}{r}$$

FFT of an aperature

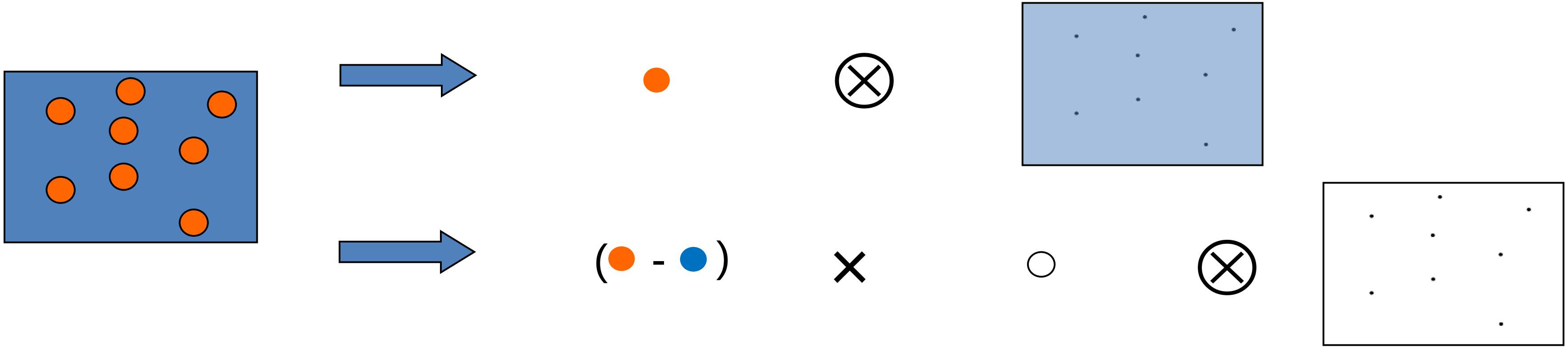


Mental gymnastics

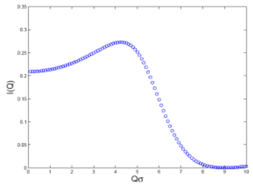


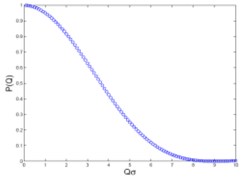


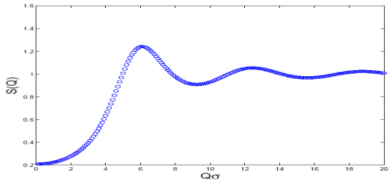
Static Scattering Intensity Function



$$I(Q) = A \times P(Q) \times S(Q)$$

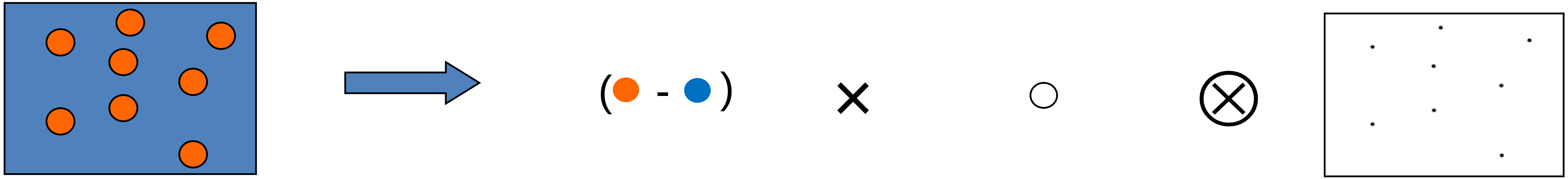




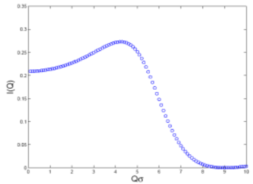


Static Scattering function | Prefactor | Normalized form factor | Inter-particle structure factor

Static Scattering Intensity Function



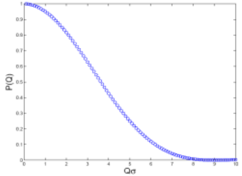
$I(Q) = A \times P(Q) \times S(Q)$



Static Scattering function

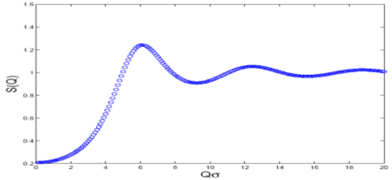
Prefactor

→ Molecular mass
Aggregate mass



Normalized form factor

→ Particle size
Particle shape
Aggregate size



Inter-particle structure factor

→ Particle-Particle interaction
Phase transition
Fractal structure

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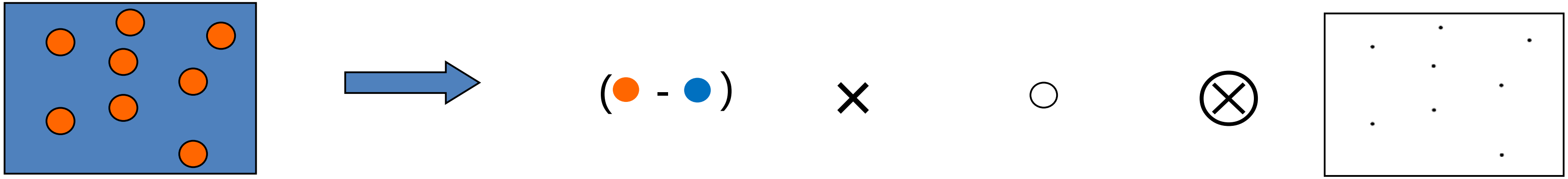
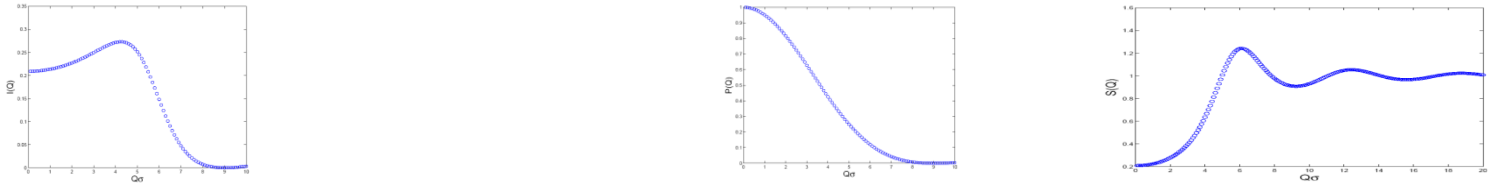
Static Scattering Intensity Function



$I(Q) = A \times P(Q) \times S(Q)$



Dilute sample: S(Q) ≈ 1. Low Q (Q ≈0 for SLS): P(Q ≈0)=1.

Case 1: small Q (Q ≈ 0) and dilute sample, I(Q ≈0) = A.

Case 2: dilute sample, I(Q)= A P(Q).

Case 3: small Q (Q ≈ 0) and concentrated sample, I(Q≈0)=A S(Q ≈0).

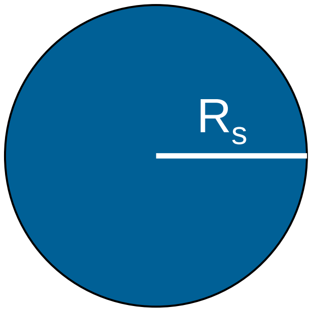
Case 4: concentrated sample, I(Q)=A P(Q) S(Q).

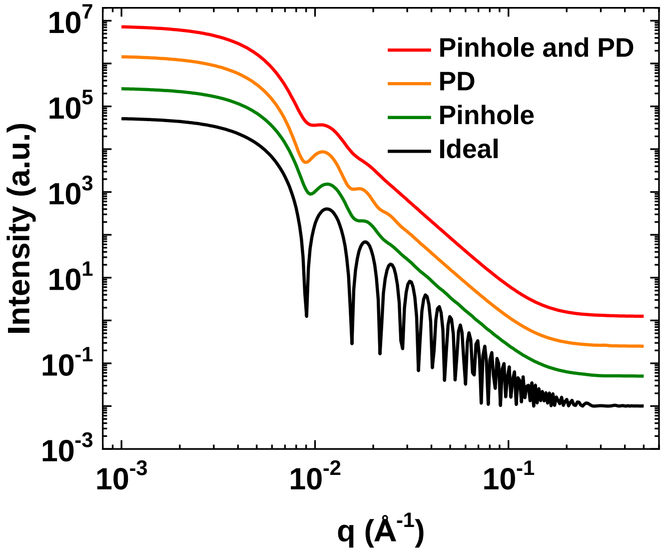
P(q) for Membrane, Polymer and Protein

P(q) for Membrane, Polymer and Protein

Sphere

$$I(Q) = A \times \left[3v_S \times (\rho_S - \rho_{sol}) \times \frac{\sin(QR_s) - QR_s \cos QR_s}{(QR_s)^3} \right]^2 + bkg$$





R_s = 50 nm

https://www.sasview.org/docs/user/models/sphere.html

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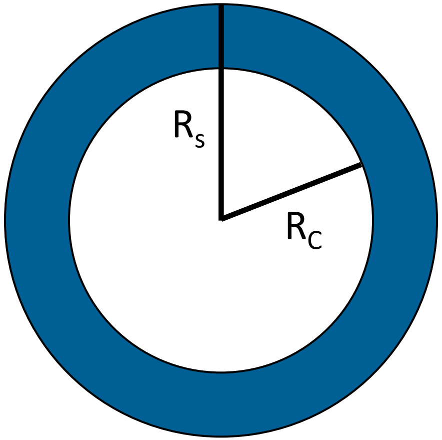
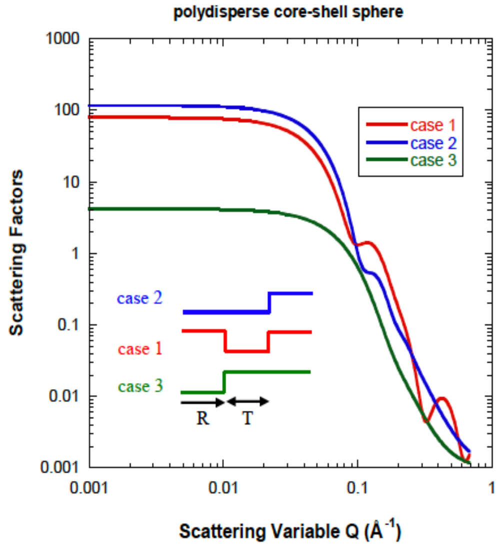
P(q) for Membrane, Polymer and Protein

Core-Shell Sphere



SansToolBox, p. 278



$$I(Q) = A \times \left[\frac{3}{v_s} \times v_c(\rho_c - \rho_{shell}) \times \frac{\sin(QR_c) - QR_c \cos QR_c}{(QR_c)^3} \right.$$

$$\left. + v_s \times (\rho_{shell} - \rho_{sol}) \times \frac{\sin(QR_{CsSph}) - QR_s \cos QR_{CsSph}}{(QR_{CsSph})^3} \right]^2 + bkg$$

https://www.sasview.org/docs/user/models/core_shell_sphere.html

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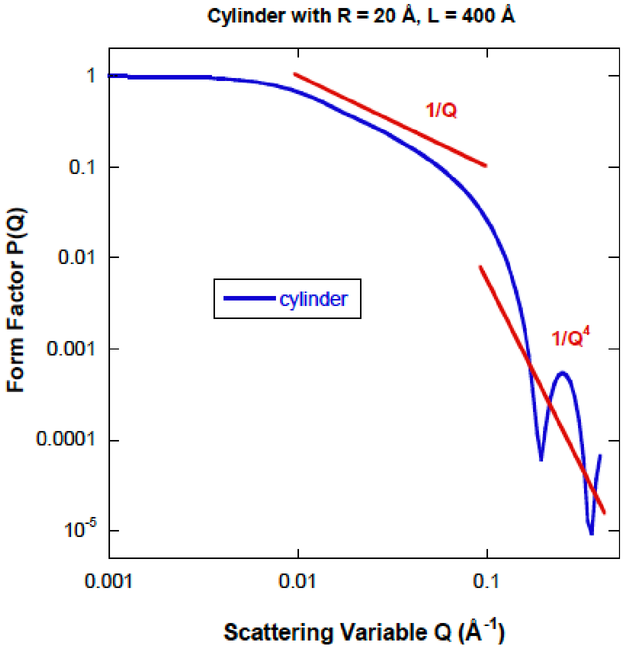
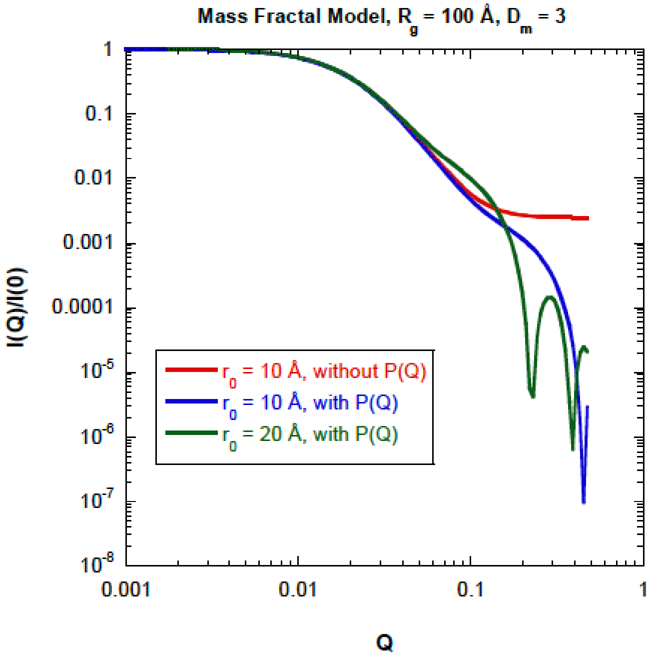
Cylinder



SANS ToolBox p. 282

Fractal

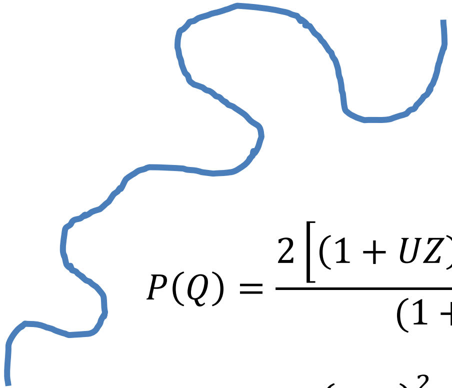


SANS ToolBox p. 339

P(q) for Membrane, Polymer and Protein

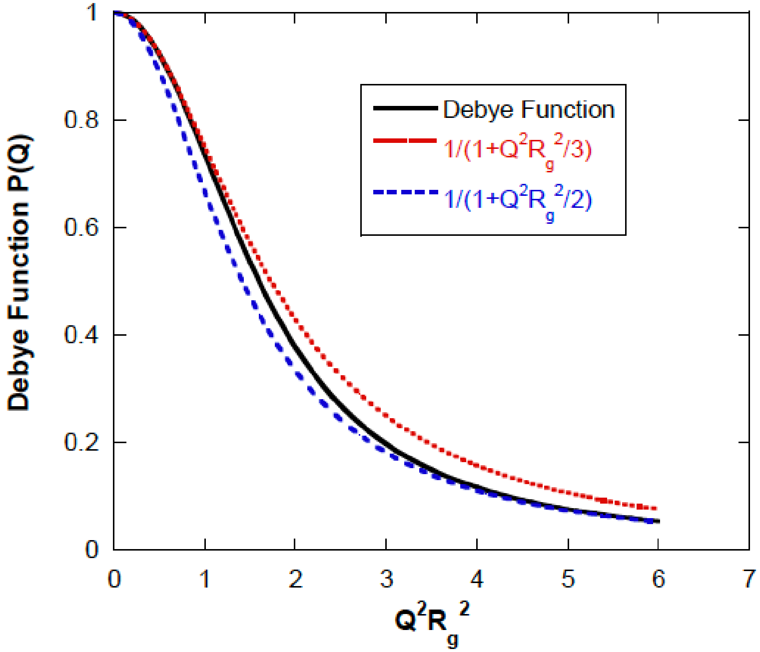
Gaussian coil

$$I(Q) = A \times \phi_{poly} \times v_{poly} \times (\rho_{poly} - \rho_{sol}) \times P(Q) + bkg$$



$$P(Q) = \frac{2\left[(1+UZ)^{-1/U} + Z - 1\right]}{(1+U)Z^2}$$

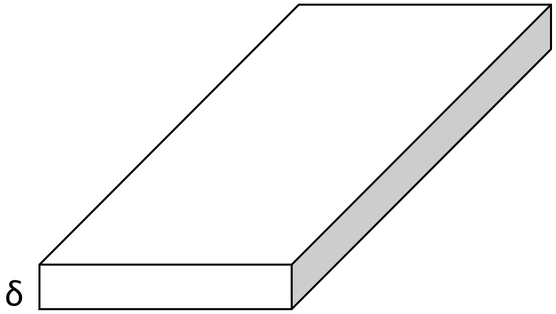
$$Z = \frac{(qR_g)^2}{1+2U} \quad U = \frac{M_w}{M_n} - 1$$



https://www.sasview.org/docs/user/models/poly_gauss_coil.html

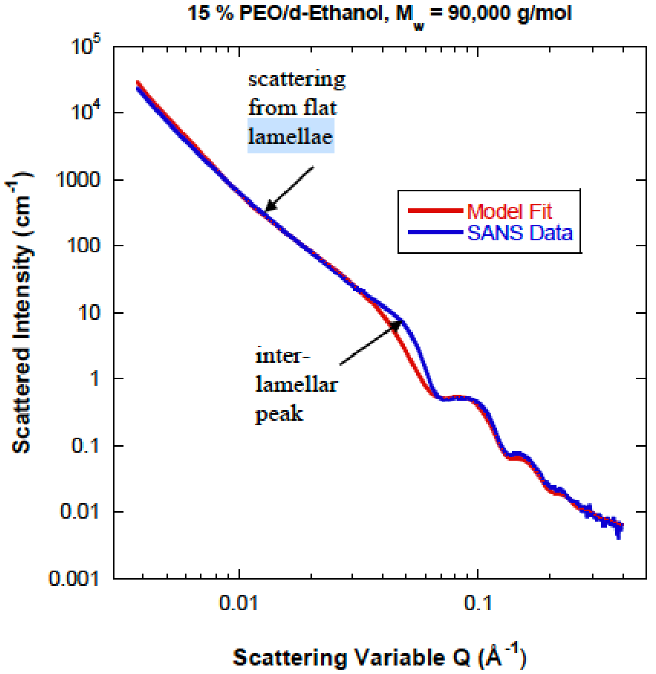
P(q) for Membrane, Polymer and Protein

Lamellae



$$I(Q) = A \times \frac{8\pi \times (\rho_L - \rho_{Sol})^2 \times \sin^2(^{Q\delta}/_2)}{Q^4\delta} + bkg$$

https://www.sasview.org/docs/user/models/lamellar.html



Guinier Plot

$$R_G^2 = \sum_i b_i (r_i - \bar{r})^2$$

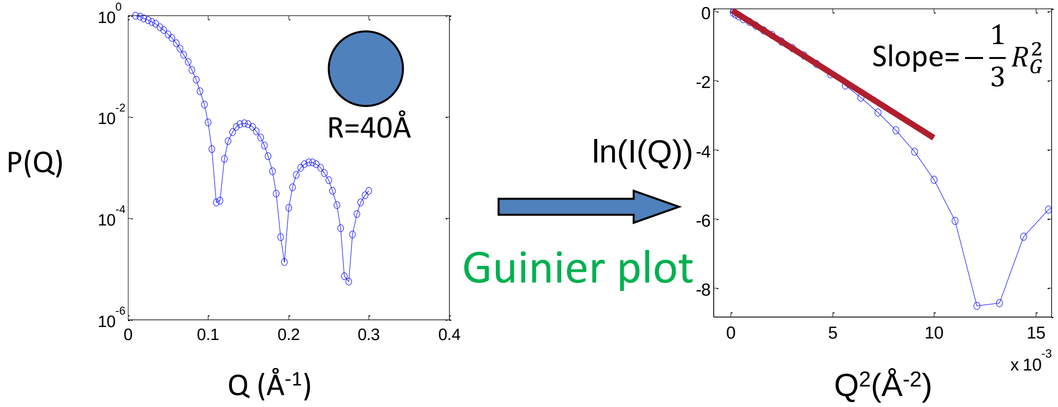
(Weighted by the scattering length)

Radius of gyration R_G: a measure of size of an object

When $QR_G << 1$, where R_G is the largest length scale in a measured object,

$$P(Q) = \exp(-\frac{1}{3} R_G^2 Q^2) \quad \text{or} \quad \ln(P(Q) = 1 - \frac{1}{3} R_G^2 Q^2$$

The equation is independent of shape, size and contrast.



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Interparticle Structure Factor S(q)

I(Q) = A × P(Q) × S(Q)

S(Q): Inter-particle structure factor

$$S(Q) = \frac{1}{N}\sum_{j,k} e^{-i\vec{Q}\cdot\vec{r}_j} e^{i\vec{Q}\cdot\vec{r}_k}$$

$$= 1 + \frac{1}{N}\sum_{j\neq k} e^{-i\vec{Q}\cdot\vec{r}_j} e^{i\vec{Q}\cdot\vec{r}_k}$$

$$= 1 + n\int (g(r) - 1)\, e^{i\vec{Q}\cdot\vec{r}} d\vec{r}^3$$

n: number density

g(r): pair distribution function

S.-H. Chen *Ann. Rev. Phy. Chem.* 1986, **37,** 351

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Interparticle Structure Factor S(q)

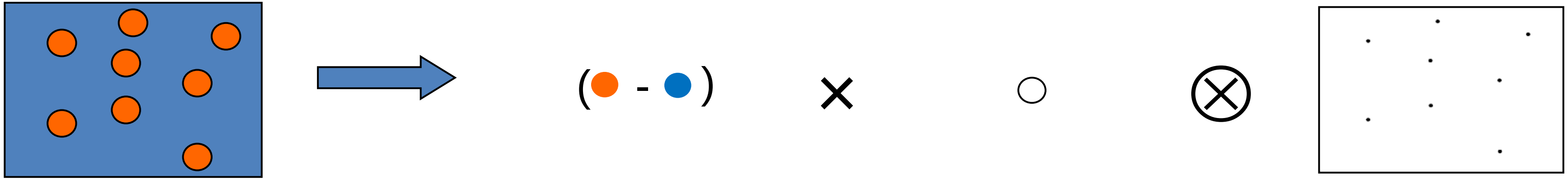
I(Q) = A × P(Q) × S(Q)

S(Q): Inter-particle structure factor

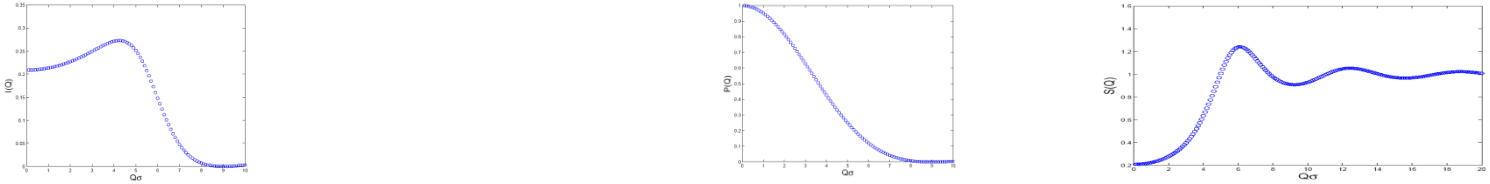
$$S(Q) = 1 + n \int (g(r) - 1)\, e^{i\vec{Q}\cdot\vec{r}} d\vec{r}^3$$

n: number density

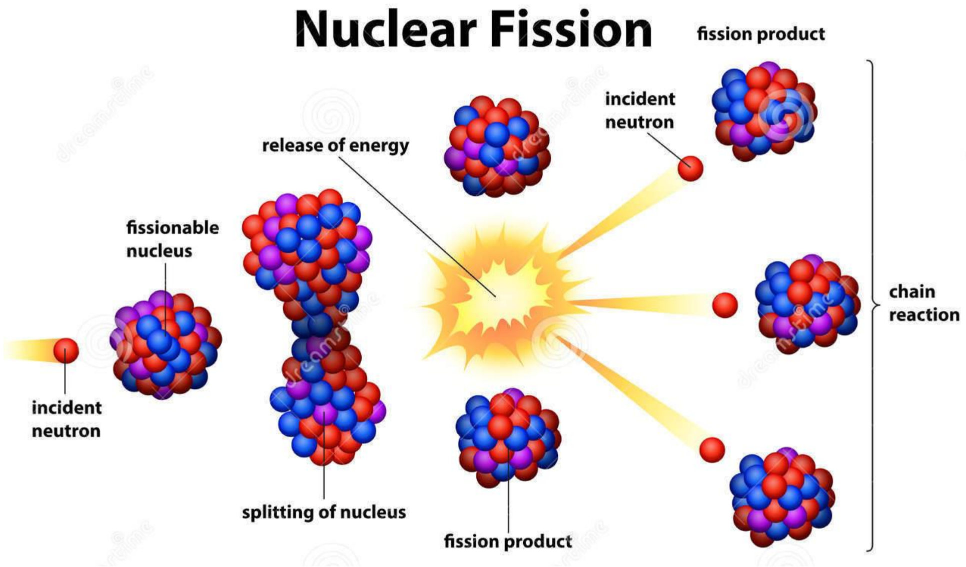
g(r): pair distribution function

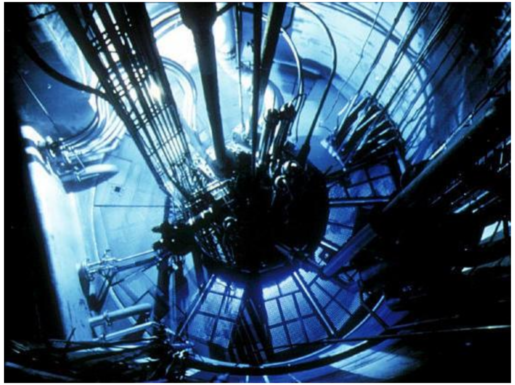


I(Q) = A × P(Q) × S(Q)



How do we obtain neutrons?





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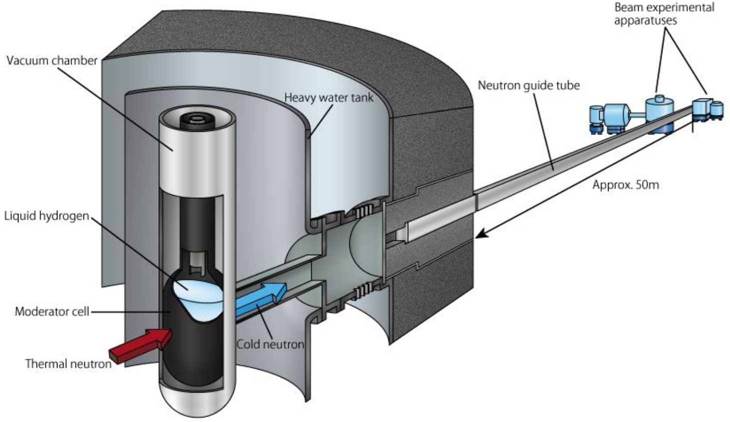
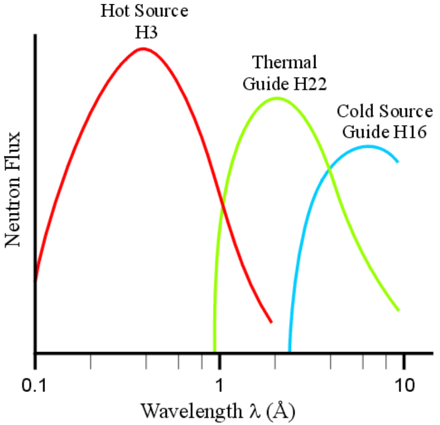
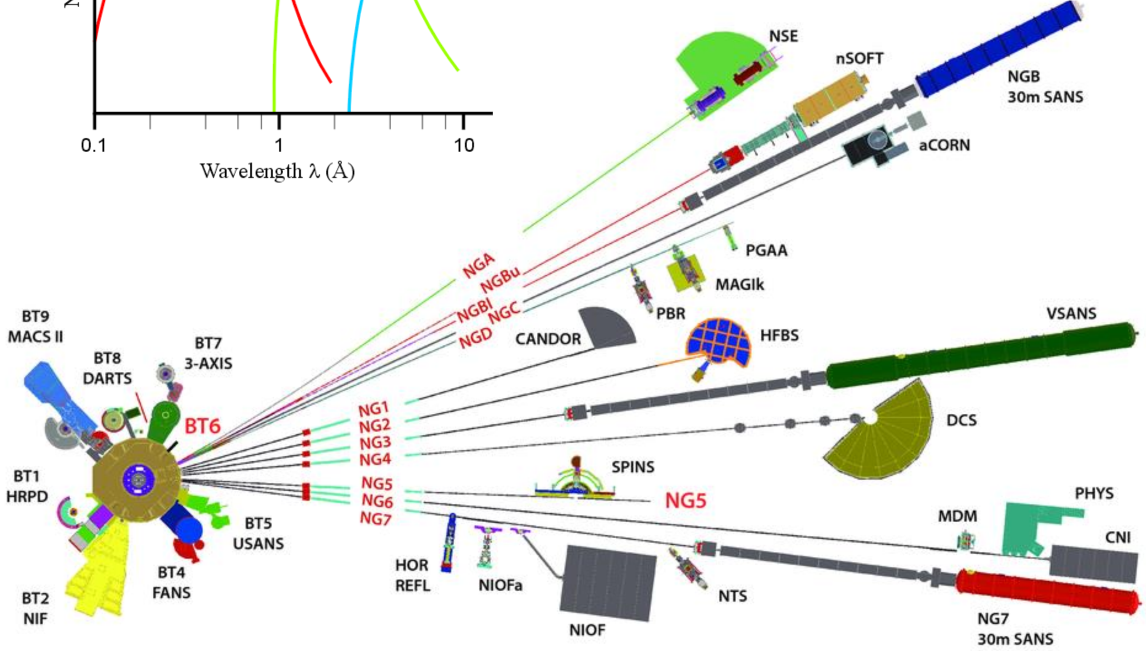
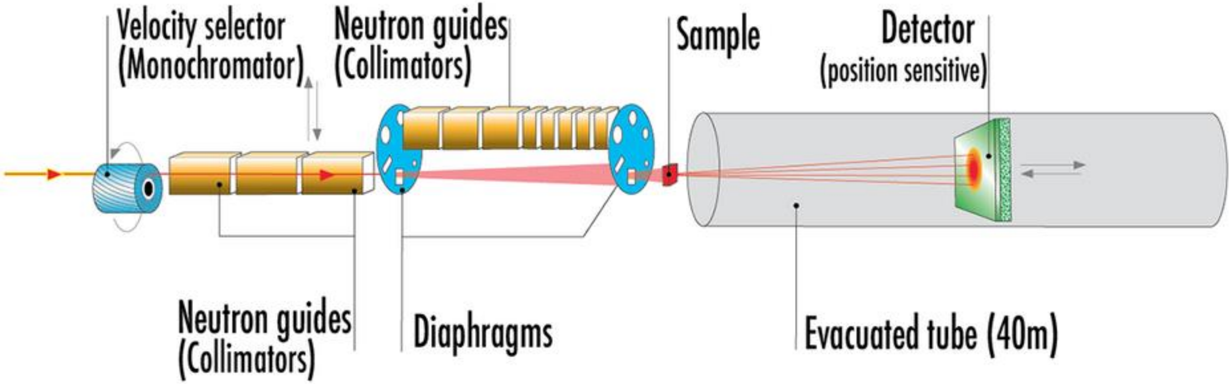
Obtaining Cold Neutrons

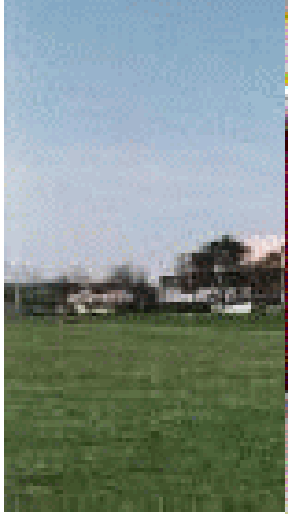


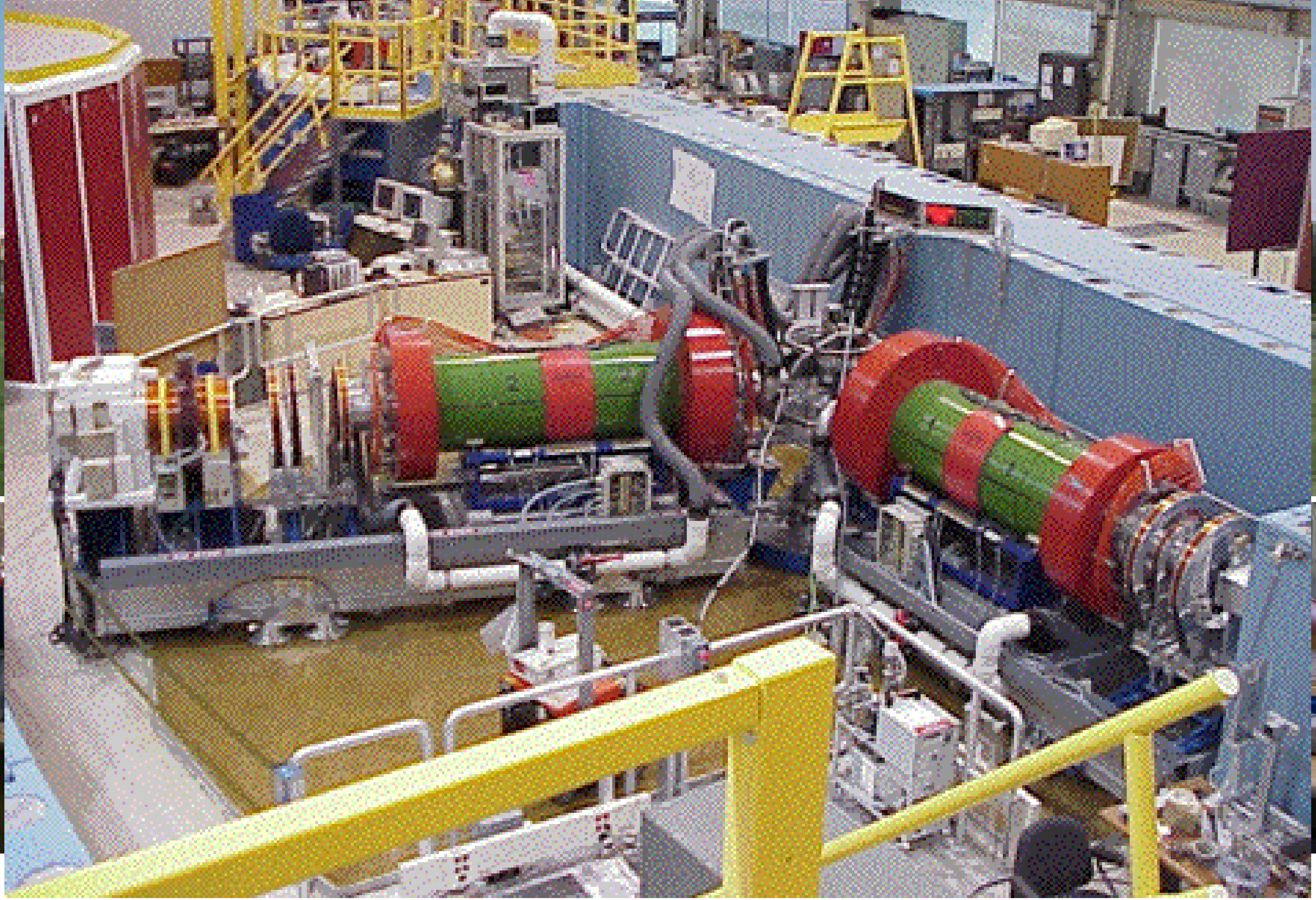




SANS Instrumentation








In class example problem:

Neutrons are produced in a nuclear reactor with an energy of many ev. They are then passed through a cold source (such as liquid hydrogen or deuterium) and thermalized at 20 K for use in neutron diffraction experiments. These are called "Cold Neutrons":

Questions:

- What is the distribution of velocities for these thermal neutrons.
- What is the most probably velocity
- What is the average velocity
- What is the standard deviation of the velocity?
- What is the corresponding wavelength and energy (in *ev*) of the most probable velocity?
- Thought question, why do we use thermal neutrons and not those produced in the reactor?

Data:

1 ev = 1.6×10^{-19} J

Mass neutron: 1.674927×10^{-27} kg

Speed of light in vacuum: 2.997925×10^{8} m/s

$K = 1.38 \times 10^{-23}$ J/K

$h = 6.26069 \times 10^{-34}$ Js

$$E = \frac{1}{2}mv^2 = \frac{h^2}{2m\lambda^2}$$

Solution:

Cold neutrons are thermalized at 20K with the Maxwell-Boltzmann distribution:

$$p(v) = 4\pi(m/2\pi kT)^{3/2} e^{-mv^2/2kT}$$

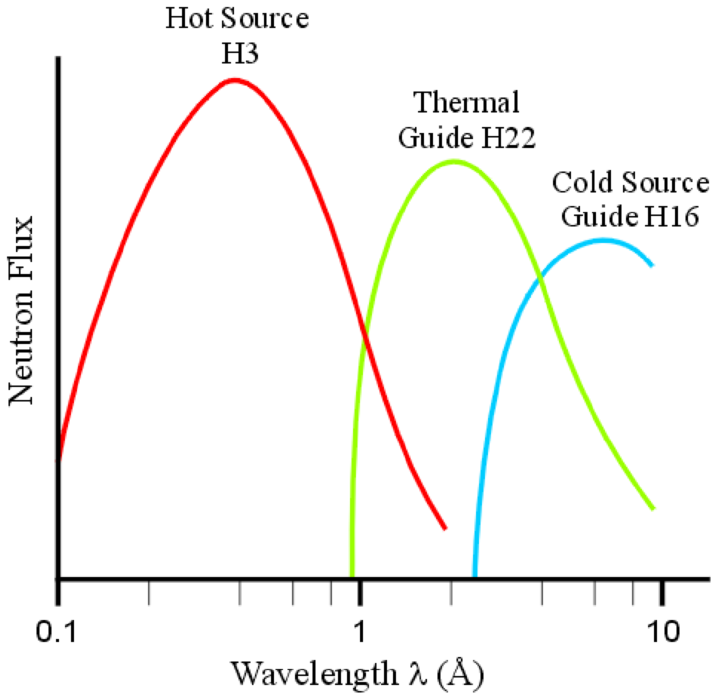
$$v_{max} = \sqrt{\frac{2kT}{m}} = 574\frac{m}{s}$$

$$\langle v \rangle^2 = \frac{8kT}{\pi m}, v = 648\frac{m}{s}$$

$$\langle v^2 \rangle = \frac{3kT}{m}, \sqrt{\langle v^2 \rangle} = 703m/s$$

$$\sqrt{\langle v^2 \rangle - \langle v \rangle^2} = 273$$

Energy: 3.5e-22J, 2.2mev, λ=6.1Å



We use these cold neutrons for diffraction as their wavelength is comparable to atomic spacings and their energies are low enough that they do not damage materials.