HighNESS International School on Thermal Neutron Scattering Kernel Generation

BRIEF INTRODUCTION TO THE

THEORY OF NEUTRON SCATTERING

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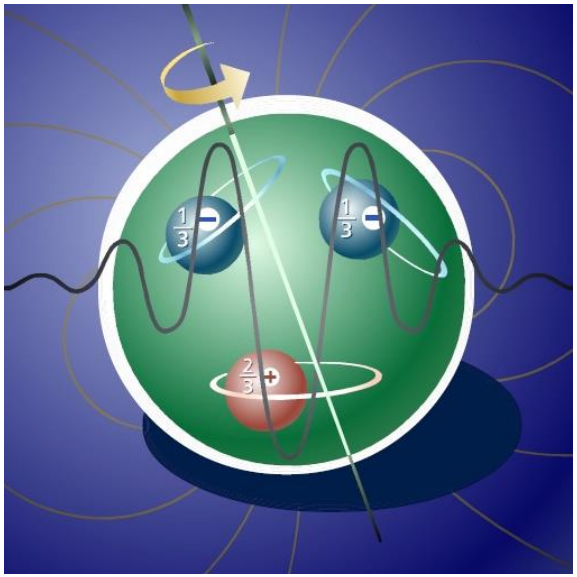
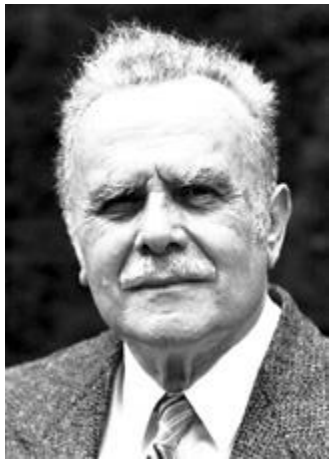
James Chadwick

The neutron



1932

- 1994, the Nobel Prize



Bertram N. Brockhouse

Clifford G. Shull


Transport
Communication
Health
Information
Food
Energy
New Knowledge
Industry
Education
Environment
Natural Resources
Materials design
Drug discovery
Biotechnology
Advanced Engineering
Biology
Material Science
Soft Condensed Matter
Structural Chemistry
Templating of nanostructures
Magneto electronics
Solid State Physics
Neutron Science
Fundamental Physics
Liquid and Glasses
Energy Resources
Particle physics Cosmology astrophysics
Earth Science
Unveiling ancient technologies
Hydrogen Economy
H_2

PROPERTIES OF NEUTRONS

STUDY DYNAMICS

Neutron energies are comparable to the time scales of molecular diffusion, vibrations and rotations.

STUDY STRUCTURE

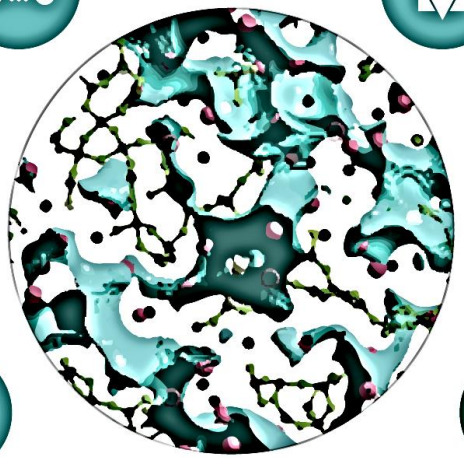
Neutron wavelengths are comparable to the spacings of atoms and molecules.

PENETRATION POWER

Neutrons can penetrate deep into matter (including many different metals) enabling the study of large samples - even within complex sample environments.

STUDY MAGNETISM

The neutron's magnetic moment can be used to study the microscopic magnetic properties of materials.



NON-DESTRUCTIVE

Neutrons are suitable for the characterisation of delicate and precious samples.

VERSATILE SAMPLE ENVIRONMENTS

Sophisticated sample environments enable studies under operating conditions, including extreme temperatures and pressures.

SENSITIVITY TO LIGHT ELEMENTS

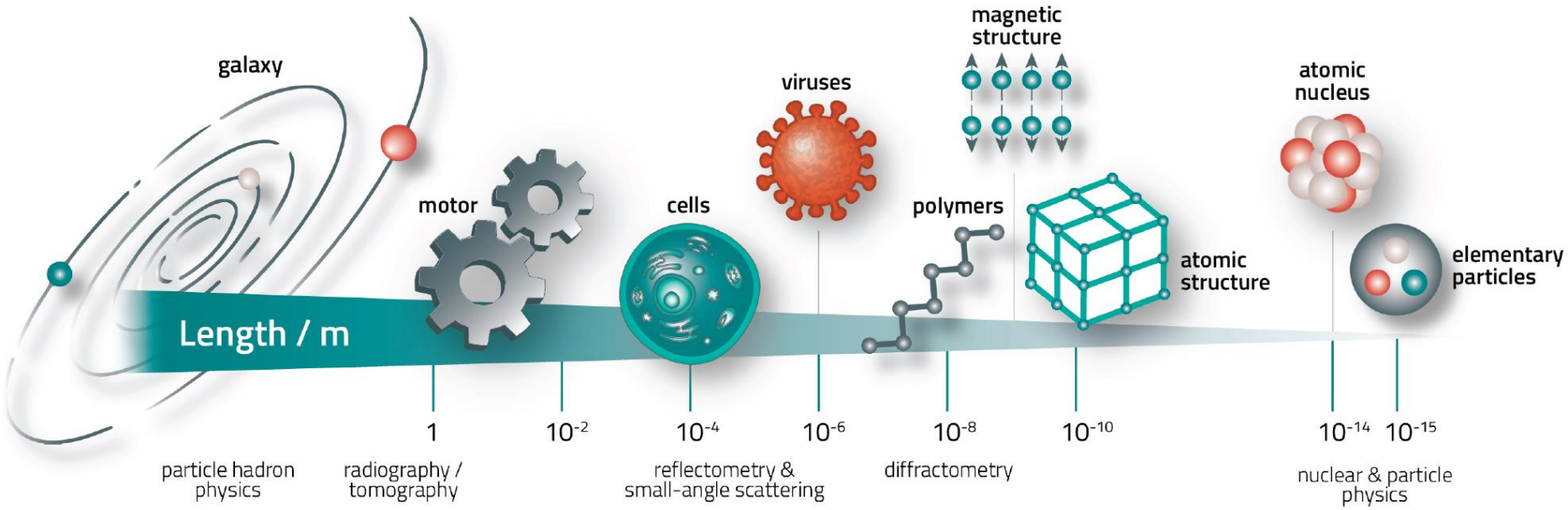
The neutron scattering power of nuclei varies in a quasi-random manner such that lighter atoms (e.g. H, Li) can be studied in the presence of heavier ones.

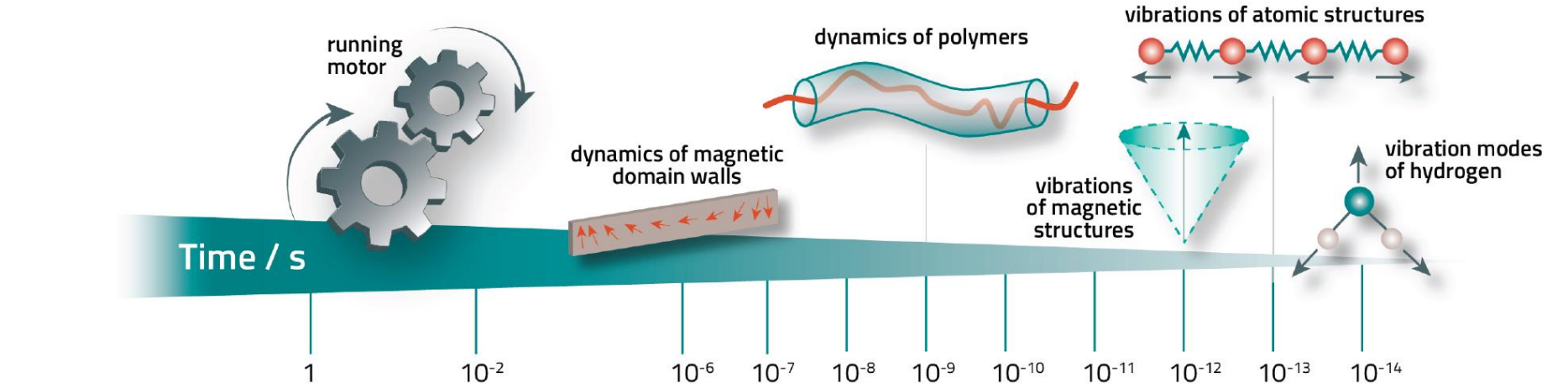
COMPLEMENTARITY

Neutron scattering is highly complementary to other techniques, such as X-ray scattering, electron microscopy, magnetic resonance and computational methods.

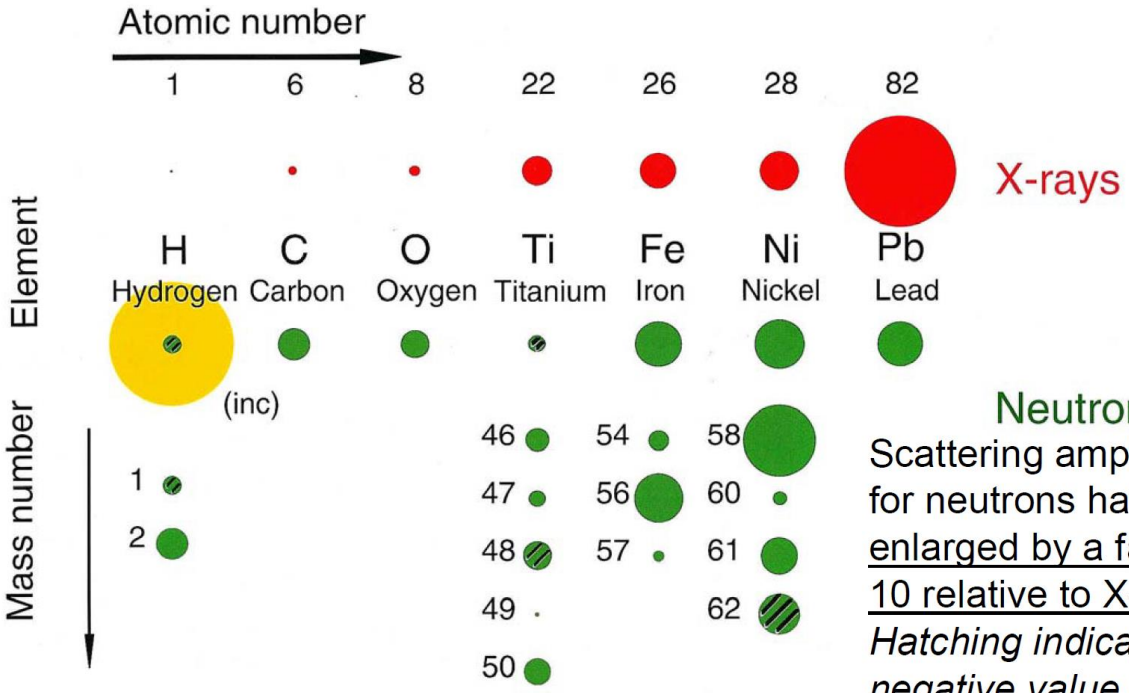
ISOTOPIC CONTRAST

Neutrons are sensitive to different isotopes of the same element, so isotopic substitution (e.g. H/D) can be used to highlight specific features.


galaxy
motor
cells
viruses
magnetic structure
polymers
atomic structure
atomic nucleus
elementary particles
Length / m
1
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-14}
10^{-15}
particle hadron physics
radiography / tomography
reflectometry & small-angle scattering
diffractometry
nuclear & particle physics


running motor
dynamics of magnetic domain walls
dynamics of polymers
vibrations of atomic structures
vibrations of magnetic structures
vibration modes of hydrogen
Time / s
1
10^{-2}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}

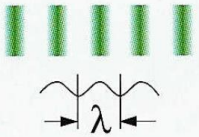
The Scattering Power for X-rays and Neutrons



Scattering amplitudes for neutrons are usually very small and vary in an irregular way between elements and isotopes. This yields important possibilities for contrast variation and eases theoretical interpretation (essentially no attenuation of the beam in the sample ⇒ “First Born approximation”)

The Neutron as a Particle and as a Wave

Particle



Wave

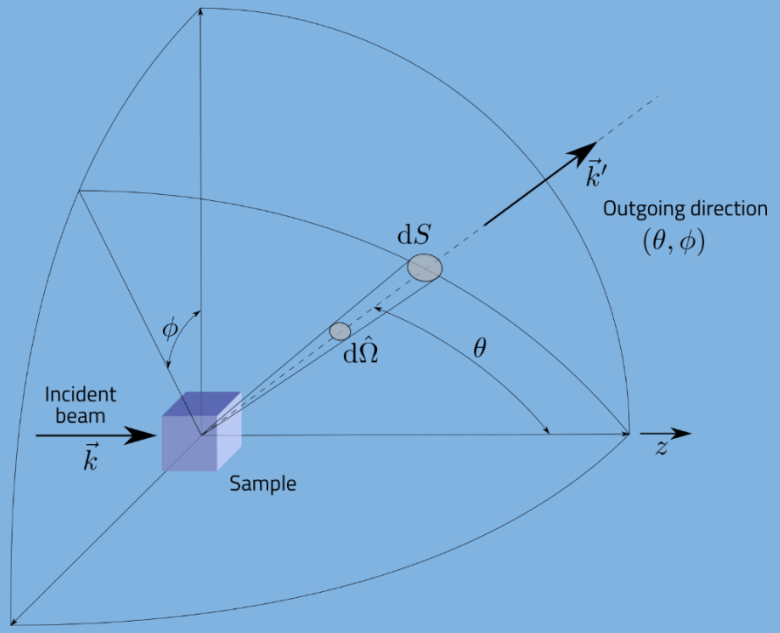
Charge	: 0		
Mass	$m = 1{,}67 \cdot 10^{-24}\,g$		
"Radius"	$r_0 = 6 \cdot 10^{-16}\,m$	**Wave length**	$\lambda = \frac{h}{m \cdot v}$
Spin	: 1/2	**Wave number**	$k = \frac{2\pi}{\lambda}$
Magn. Moment	$\mu = -1{,}9\,\mu_N$		
Momentum	$\vec{p} = m \cdot \vec{v}$	**Momentum**	$\vec{p} = \frac{h \cdot \vec{k}}{2\pi} = \hbar \cdot \vec{k}$
Energy	$E = \frac{m}{2} v^2$	**Energy**	$E = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 \cdot k^2}{2m}$
(v = velocity)		(h = Plank´s constant)	

STARTING DEFINITIONS

Suppose a monoenergetic incident beam of neutrons of energy *E*. The *incident flux* (Φ) is the number of neutrons that falls per unit time and unit area perpendicular to the beam.

Given the angles θ and φ, the *double differential cross section* is defined as the number of neutrons scattered per unit time at the solid angle $d\Omega$ in the direction (θ, φ) with final energies between E' and E'+d*E'*, per unit solid angle and energy.

$$\frac{d^2\sigma}{d\Omega\, dE'}$$



STARTING DEFINITIONS

The *differential cross section* is the number of neutrons scattered per unit of time and per unit solid angle in dΩ around the direction (θ, φ).

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \int \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'} \mathrm{d}E'$$

The *energy-transfer kernel* (or simply *transfer kernel*) is defined as the number of scattered neutrons, per unit of time and per unit of energy, with energies between E' and E'+d*E'*,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E'} = \int \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \, \mathrm{d}E'} \mathrm{d}\Omega$$

STARTING DEFINITIONS

The *total cross section* is defined as the total number of neutrons scattered per unit time in any direction and with any energy

$$\sigma_{\text{tot}} = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\,\mathrm{d}\Omega = \int \frac{\mathrm{d}\sigma}{\mathrm{d}E'}\,\mathrm{d}E'$$

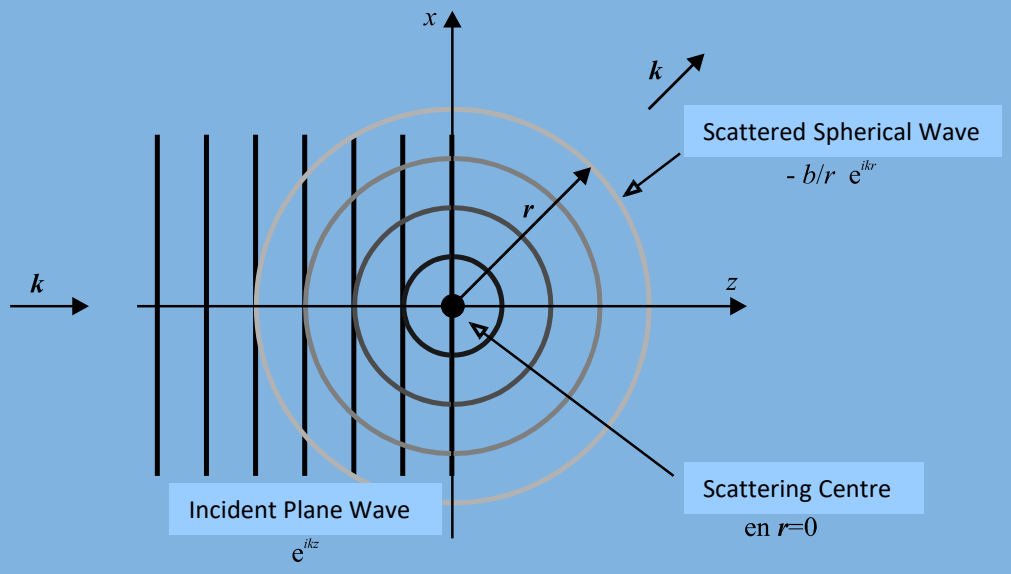
The basic problem of scattering theory is to obtain theoretical expressions for the cross sections, which are the quantities that are measured directly in scattering experiments.

SCATTERING BY A FIXED NUCLEI

We represent incident neutrons by a wave function $\psi_{inc} = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})$

And the wave function of the scattered neutrons is written as $\psi_{sc} = -\frac{b}{r}\exp(ikr)$

b is called the scattering length of the scattering nuclei.



The nuclear forces that cause the scattering process have a range of 10^{-14} to 10^{-15} m, which is much less than the wave-length of thermal neutrons, on the order of 10^{-10} m). In these circumstances, scat-tering comes entirely from s-waves, i.e. with a spheri-cally symmetrical angular distribution.

Appendix: Neutron Scattering Lengths and Cross Sections

(in *Neutron Scattering*, Academic Press Inc., 2013)

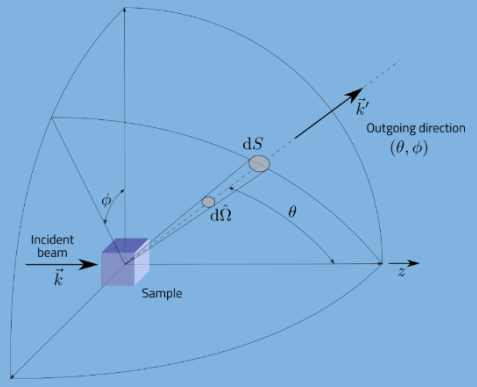
Element	Z	A	I(π)	c_a	$\bar{b}$	b^+	b^-	b_i	σ_c	σ_i	σ_s	σ_a
n	0	1	1/2(+)		-37.0(6)	0	-37.0(6)	16.0(3)	43.01(2)	0	43.01(2)	
H	1				-3.7390(11)				1.7568(10)	80.26(6)	82.02(6)	0.3326
1H		1	1/2(+)	99.9885	-3.7423(12)	10.817(5)	-47.420(14)	25.217(6)	1.7589(11)	79.91(4)	81.67(4)	0.3326
2H		2	1(+)	0.0115	6.674(6)	9.53(3)	0.975(60)	4.03(3)	5.597(10)	2.04(3)	7.64(3)	0.000519
3H		3	1/2(+)	12.32y	4.792(27)	4.18(15)	6.56(37)	-1.04(17)	2.89(3)	0.14(4)	3.03(5)	<6E-
He	2				3.26 (3)				1.34(2)	0	1.34(2)	0.00747
3He		3	1/2(+)	0.000134	5.74(7)-1.483(2)i	4.5(3)	9.3(5)	-2.1(3)+2.568(3)i	4.42(10)	1.38(16)	5.8(2)	5333.0(7
4He		4	0(+)	99.999866	3.26 (3)			0	1.34(2)	0	1.34(2)	
Li	3				-1.90(3)				0.454(10)	0.92(3)	1.37(3)	70.5
6Li		6	1(+)	7.59	2.00(11)-0.261(1)i	0.67(14)	4.67(17)	-1.89(10)+0.26(1)i	0.51(5)	0.46(5)	0.97(7)	940.0(4
7Li		7	3/2(-)	92.41	-2.22(2)	-4.15(6)	1.00(8)	-2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454
Be	4	9	3/2(-)	100	7.79(1)			0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076
B					5.30(4)-0.213(2)i				3.54(5)	1.70(12)	5.24(11)	767.0(8
10B	5	10	3(+)	19.9	-0.1(3)-1.066(3)i	-4.2(4)	5.2(4)	-4.7(3)+1.231(3)i	0.144(6)	3.0(4)	3.1(4)	3835.0(9
11B		11	3/2(-)	80.1	6.65(4)	5.6(3)	8.3(3)	-1.3(2)	5.56(7)	0.21(7)	5.77(10)	0.0055(
C					6.6484(13)				5.551(2)	0.001(4)	5.551(3)	0.00350
12C	6	12	0(+)	98.93	6.6535(14)			0	5.559(3)	0	5.559(3)	0.00353
13C		13	1/2(-)	1.07	6.19(9)	5.6(5)	6.2(5)	-0.25(3)	4.81(14)	0.034(11)	4.84(14)	0.00137
N					9.36(2)				11.01(5)	0.50(12)	11.51(11)	1.90
14N	7	14	1(+)	99.636	9.37(2)	10.7(2)	6.2(3)	2.1(3)	11.03(5)	0.50(12)	11.53(11)	1.91
15N		15	1/2(-)	0.364	6.44(3)	6.77(10)	6.21(10)	0.24(6)	5.21(5)	0.00005(10)	5.21(5)	0.000024
O					5.805(4)				4.232(6)	0.000(8)	4.232(6)	0.00019
16O	8	16	0(+)	99.757	5.805(5)			0	4.232(6)	0	4.232(6)	0.00010
17O		17	5/2(+)	0.038	5.66(5)	5.86(7)	5.41(17)	0.17(5)	4.20(22)	0.004(3)	4.20(22)	0.236(
18O		18	0(+)	0.205	5.84(7)			0	4.29(10)	0	4.29(10)	0.00016
F	9	19	1/2(+)	100	5.654(12)	5.632(10)	5.767(10)	-0.082(9)	4.017(14)	0.0008(2)	4.018(14)	0.0096
Ne					4.566(6)				2.620(7)	0.008(9)	2.628(6)	0.039
20Ne	10	20	0(+)	90.48	4.631(6)			0	2.695(7)	0	2.695(7)	0.036
21Ne		21	3/2(+)	0.27	6.66(19)			(+/-)0.6(1)	5.6(3)	0.05(2)	5.7(3)	0.67(
22Ne		22	0(+)	9.25	3.87(1)			0	1.88(1)	0	1.88(1)	0.046
Na	11	23	3/2(+)	100	3.63(2)	6.42(4)	-1.00(6)	3.59(3)	1.66(2)	1.62(3)	3.28(4)	0.530
Mg					5.375(4)				3.631(5)	0.08(6)	3.71(4)	0.063

If v is the speed of the neutrons (the same before and after scattering), the number of neutrons per second passing through the surface dS is

$$v\,dS\left|\psi_{sc}\right|^2 = v\,dS\frac{b^2}{r^2} = v b^2\,d\Omega$$

while the incident neutron flux is

$$\Phi = v\left|\psi_{inc}\right|^2 = v$$



From the definition of cross section it follows that

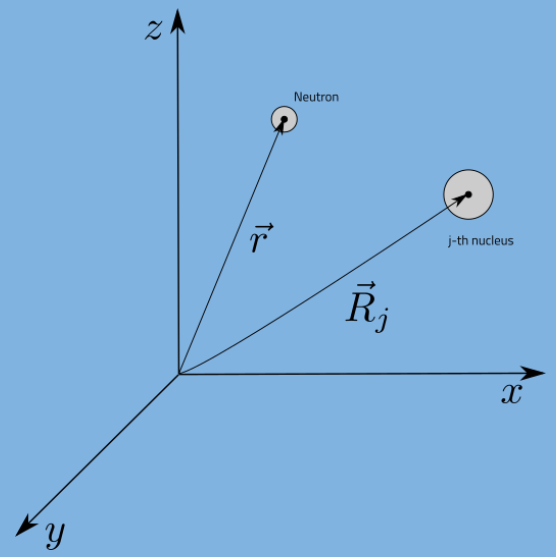
$$\frac{d\sigma}{d\Omega} = \frac{v b^2 d\Omega}{\Phi\, d\Omega} = b^2$$

that integrated over all angles allows to obtain for this case

$$\sigma_{tot} = 4\pi b^2$$

NUCLEAR SCATTERING

	Initial State		Final State	
Neutron:	$\boldsymbol{k}$	ψ_k	$\boldsymbol{k'}$	$\psi_{k'}$
Scatt.System:	λ	χ_λ	λ'	$\chi_{\lambda'}$



The differential cross section represents the sum of all processes in which the state of the scattering system changes from λ to λ', and the state of the neutron changes from k to k'

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\substack{\boldsymbol{k'}\\ \text{en } d\Omega}} W_{\boldsymbol{k},\lambda\to\boldsymbol{k'},\lambda'}$$

where $W_{\boldsymbol{k},\lambda\to\boldsymbol{k'},\lambda'}$ is the number of transitions per second from state {k, λ} to {k', λ'}, and Φ is the incident neutron flux.

NUCLEAR SCATTERING

Using Fermi´s Golden Rule:

$$\sum_{\substack{\mathbf{k}' \\ \text{en } d\Omega}} W_{\mathbf{k},\lambda\to\mathbf{k}',\lambda'} = \frac{2\pi}{\hbar}\rho_{\mathbf{k}'}\left|\left\langle \mathbf{k}'\,\lambda'\middle|V\middle|\mathbf{k}\lambda\right\rangle\right|^2$$

The matrix element is

$$\langle \boldsymbol{k}'\,\lambda'|V|\boldsymbol{k}\lambda\rangle = \int \psi^*_{\boldsymbol{k}'}\,\chi^*_{\lambda'}\,V\,\psi_{\boldsymbol{k}}\,\chi_{\lambda}\,\mathrm{d}\boldsymbol{R}\,\mathrm{d}\boldsymbol{r}$$

that is

$$\langle \boldsymbol{k}'\,\lambda'|V|\boldsymbol{k}\lambda\rangle = \frac{1}{Y}\int \exp(-i\boldsymbol{k}'\cdot\boldsymbol{r})\,\chi^*_{\lambda'}\,V\,\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\,\chi_{\lambda}\,\mathrm{d}\boldsymbol{R}\,\mathrm{d}\boldsymbol{r}$$

$$\Rightarrow \quad \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\mathrm{h}^2}\right)^2\left|\left\langle \mathbf{k}'\,\lambda'\middle|V\middle|\mathbf{k}\lambda\right\rangle\right|^2$$

$$\Downarrow$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\,\hbar}\right)^2\left|\langle \boldsymbol{k}'\,\lambda'|V|\boldsymbol{k}\lambda\rangle\right|^2\,\delta\left(E_{\lambda'} - E_{\lambda} + E - E'\right)$$

This is the *MASTER EQUATION* to describe scattering processes in the frame of the Born approximation.

The interaction potential between the slow neutron and the j-th nucleus has the form $V_j(\mathbf{r}-\mathbf{R}_j)$, so that for the complete scattering system the potential is

$$V(\boldsymbol{r}) = \sum_j V_j(\boldsymbol{r} - \boldsymbol{R}_j)$$

Using this expression in that of the matrix element yields

$$\langle \boldsymbol{k}'\,\lambda' | V | \boldsymbol{k}\lambda \rangle = \sum_j V_j(\boldsymbol{Q}) \langle \lambda' | \exp(i\boldsymbol{Q}\cdot\boldsymbol{R}_j) | \lambda \rangle$$

where $V_j(\boldsymbol{Q}) = \int V_j(\boldsymbol{x}_j) \exp(i\boldsymbol{Q}\cdot\boldsymbol{x}_j)\,\mathrm{d}\boldsymbol{x}_j$, $\langle \lambda' | \exp(i\boldsymbol{Q}\cdot\boldsymbol{R}_j | \lambda \rangle = \int \chi^*_{\lambda'} \exp(i\boldsymbol{Q}\cdot\boldsymbol{R}_j)\,\chi_\lambda\,\mathrm{d}\boldsymbol{R}$

$\hbar\mathbf{Q} = \hbar(\mathbf{k} - \mathbf{k'})$	*Momentum transfer*
$\hbar\omega = E - E'$	*Energy transfer*

Introducing the Fermi pseudo-potential

$$V_j(\boldsymbol{r}-\boldsymbol{R}_j)=\frac{2\pi\hbar^2}{m}b_j\,\delta(\boldsymbol{r}-\boldsymbol{R}_j)$$

where b_j is the scattering length of the j-th nucleus. Then

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda\to\lambda'}=\frac{k'}{k}\sum_{j,j'}b_{j'}^{*}\,b_j\langle\lambda'|\exp(-i\boldsymbol{Q}\cdot R_{j'})|\lambda\rangle\langle\lambda'|\exp(i\boldsymbol{Q}\cdot R_j)|\lambda\rangle$$
$$\times\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\left(i\frac{E_{\lambda'}-E_\lambda}{\hbar}t\right)\exp(-i\omega t)\,\mathrm{d}t$$

In a real case, we must add over all final states and average over the initial states corresponding to the thermodynamic state of the scattering system.

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}=\sum_{\lambda,\lambda'}p_\lambda\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\lambda\to\lambda'}=\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}b_{j'}\,b_j\int_{-\infty}^{\infty}\exp(-i\omega t)\,\mathrm{d}t\times$$
$$\times\left\langle\lambda\left|\exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}\right)\exp\left(iH_0t/\hbar\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j\right)\exp\left(-iH_0t/\hbar\right)\right|\lambda\right\rangle$$

In terms of Heisenberg´s time-dependent operators,

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_{j'}\,b_j \int_{-\infty}^{\infty} \left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right)\right\rangle \exp(-i\omega t)\,\mathrm{d}t$$

where the brakets represent a thermal-quantum average.
This is a more elaborated form of the *Master Equation* for describing neutron scattering by matter.
Finally, averaging over possible isotopic distributions in the system,

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} \overline{b_{j'}\,b_j} \int_{-\infty}^{\infty} \exp(-i\omega t)\;\chi_{jj'}(t)\,\mathrm{d}t$$

$$\chi_{jj'}(t) = \left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right)\right\rangle$$

Coherent and Incoherent Scattering

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

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

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

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

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

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

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

Incoherent Scattering
(scattering is uniform in all directions)

Note: N = number of atoms in scattering system

COHERENT AND INCOHERENT CROSS SECTIONS

Assuming there is no correlation between b_j corresponding to different nuclides, average values are obtained

$$\overline{b_{j'}\, b_j} = \begin{cases} \bar{b}^2 & j' \neq j \\ \overline{b^2} & j' = j \end{cases}$$

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\, \mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\bar{b}^2 \sum_{j,j'} \int_{-\infty}^{\infty} \exp(-i\omega t)\, \chi_{jj'}(t)\, \mathrm{d}t$$

$$+ \frac{k'}{k}\frac{1}{2\pi\hbar}\left(\overline{b^2} - \bar{b}^2\right) \sum_{j} \int_{-\infty}^{\infty} \exp(-i\omega t)\, \chi_{jj}(t)\, \mathrm{d}t$$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\, \mathrm{d}E'}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar} \sum_{j,j'} \int_{-\infty}^{\infty} \exp(-i\omega t)\, \chi_{jj'}(t)\, \mathrm{d}t$$

COHERENT X-section

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\, \mathrm{d}E'}\right)_{\mathrm{inc}} = \frac{\sigma_{\mathrm{inc}}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar} \sum_{j} \int_{-\infty}^{\infty} \exp(-i\omega t)\, \chi_{jj}(t)\, \mathrm{d}t$$

INCOHERENT X-section

If there are no spin correlations between nuclei in the molecules, the averages over the spatial and spin wavefunctions can be performed separately, giving rise to the *coherent* and *incoherent* contributions to the cross section of a general scattering system:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'} = \frac{1}{4\pi}\frac{k'}{k} N\left(\sigma_{\mathrm{coh}}\, S_{\mathrm{coh}}(\boldsymbol{Q},\omega) + \sigma_{\mathrm{inc}}\, S_{\mathrm{inc}}(\boldsymbol{Q},\omega)\right)$$

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- on the method of measurement, e.g. the choice of Ei,

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- on the method of measurement, e.g. the choice of Ei,
- on the strength of the interaction between neutrons and the sample (i.e. on the "scattering cross section"), and
- on the sample itself, through the scattering function S(**Q**,ω).

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According to the Incoherent and Coherent Scattering Laws:

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp(-i\omega t)\ \chi_{\mathrm{inc}}(\boldsymbol{Q},t)\,\mathrm{d}t$$

$$S_{\mathrm{coh}}(\boldsymbol{Q},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp(-i\omega t)\ \chi_{\mathrm{coh}}(\boldsymbol{Q},t)\,\mathrm{d}t$$

and their corresponding Intermediate Scattering Functions:

$$\chi_{\mathrm{coh}}(\boldsymbol{Q},t) = \frac{1}{N}\sum_{j,j'}\left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_{j}(t)\right)\right\rangle$$

$$\chi_{\mathrm{inc}}(\boldsymbol{Q},t) = \frac{1}{N}\sum_{j}\left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j}(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_{j}(t)\right)\right\rangle$$

These correlation functions, scattering laws and intermediate functions contain all the information about the structure and dynamics of the scattering system. Such information is therefore obtained directly in the measurement of a double differential cross section.

SOME ANALYTICAL PROPERTIES

We will review some analytic properties of the scattering functions. Due to the Hermiticity of the position operators the following equality holds:

$$S(\boldsymbol{Q},\omega) = S^{*}(\boldsymbol{Q},\omega)$$

that means that $S(\boldsymbol{Q},\omega)$ is real, which is evident because it is proportional to the observable scattering cross section.

Also,

$$S(-\boldsymbol{Q},-\omega) = \exp(-\beta\hbar\omega)\, S(\boldsymbol{Q},\omega)$$

known as *the principle of detailed balance*. This property expresses the microscopic reversibility of the scattering process, and it is very useful from a practical point of view as it permits to generate the complete scattering function from its calculation over only part of the $(\boldsymbol{Q},\omega)$ plane.

SOME ANALYTICAL PROPERTIES

A few general properties of the scattering functions:

Energy Moments

$$S_n(\mathbf{Q}) = \hbar \int_{-\infty}^{\infty} d\omega (\hbar\omega)^n S(\mathbf{Q},\omega) = \left(\frac{\hbar}{i}\right)^n \frac{\partial^n}{\partial t^n} \chi(\mathbf{Q},t) \Big|_{t=0}$$

Zero Moment:
Structure Factor

$$S_0(\mathbf{Q}) = \chi(\mathbf{Q},0) = \frac{1}{N} \left| \Sigma_l \exp\left(i\mathbf{Q}.\mathbf{R}_l\right) \right|^2$$

$$S_{0,inc}(\mathbf{Q}) = \chi_{inc}(\mathbf{Q},0) = 1$$

First Moment:
Mean Energy Transf.

$$S_1(\mathbf{Q}) = \frac{\hbar^2 Q^2}{2M}$$

1. Nuclei Free and at Rest

FREE NUCLEUS AT REST

Consider the simplest case of a scattering system composed of a single free atom of mass M and at rest in the laboratory system. Because it is at rest, the atom is in the eigen-state $|0\rangle$ of the momentum operator, whose eigenvalue is p=0.

Defining the operator ,

$$H_j(\boldsymbol{Q}) = \exp\left\{-i\boldsymbol{Q}\cdot\boldsymbol{R}_j\right\} H_0 \exp\left\{i\boldsymbol{Q}\cdot\boldsymbol{R}_j\right\} \quad ,$$

the intermediate scattering function is rewritten as ,

$$\chi_{\text{inc}}(\boldsymbol{Q},t) = \langle 0|\exp\left\{-iH_0(\boldsymbol{p}+\hbar\boldsymbol{Q})t/\hbar\right\} \exp\left\{iH_0(\boldsymbol{p})t/\hbar\right\}|0\rangle$$

where the Hamiltonian corresponds to that of a free particle, i.e.

$$H_0(\boldsymbol{p}) = \frac{p^2}{2M} \quad .$$

$$\chi_{\mathrm{inc}}(\boldsymbol{Q},t)=\exp\left\{i\frac{\hbar Q^2}{2M}t\right\} \quad ,$$

and its Fourier transform gives the scattering law

$$S_{\mathrm{inc}}(\boldsymbol{Q},\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{e}^{-\frac{it}{\hbar}\left(\hbar\omega-\frac{\hbar^2Q^2}{2M}\right)}\mathrm{d}t=\delta\left(\hbar\omega-\frac{\hbar^2Q^2}{2M}\right) \quad .$$

Then, the double differential cross section is

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{inc}}=\frac{\sigma_{\mathrm{inc}}}{4\pi}\frac{k'}{k}\delta\left(\hbar\omega-\frac{\hbar^2Q^2}{2M}\right)$$

And the energy-transfer kernel

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}E'}\right)_{\mathrm{inc}}=\frac{\sigma_{\mathrm{inc}}}{4\pi}\frac{k'}{k}\int_{\Omega}\delta\left(\hbar\omega-\frac{\hbar^2Q^2}{2M}\right)\mathrm{d}\Omega=\frac{\sigma_{\mathrm{inc}}}{2}\frac{k'}{k}\int_{-1}^{1}\delta\left(\hbar\omega-\frac{\hbar^2}{2M}(k^2+k'^2-2kk'\mu)\right)\mathrm{d}\mu$$

$$=\frac{\sigma_{\mathrm{inc}}A}{4E}\int_{\hbar\omega-\hbar^2/2M\,(k-k')^2}^{\hbar\omega-\hbar^2/2M\,(k+k')^2}\delta(z)\,\mathrm{d}z$$

where $A=M/m$ and μ represents the cosine of the scattering angle.

Finally, we obtainthe following result for the energy-transfer kernel

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}E'}\right)_{\mathrm{inc}} = \begin{cases} \dfrac{\sigma_{\mathrm{inc}} A}{4E} & \left(\dfrac{A-1}{A+1}\right)^2 E < E' < E \\ 0 & \text{en el resto} \end{cases}$$

The total cross section is the integral over all final energies of the transfer kernel

$$\sigma_{\mathrm{inc}}(E) = \sigma_{\mathrm{inc}}\left(\frac{A}{A+1}\right)^2 \quad ,$$

Which is the so called *free atom total cross section* (σ_{free}).

2. Nuclei in a Free Gas

NUCLEUS IN A FREE GAS

Let us consider the case where the scattering system is a gas of free particles. In this situation the atom of mass M is one of a set of such atoms, which are in thermodynamic equilibrium at a temperature T. Using the free particle Hamiltonian and performing the thermal average, the intermediate scattering function is obtained.

$$\chi_{\mathrm{inc}}(\boldsymbol{Q},t) = \exp\left\{\frac{\hbar Q^2}{2M}\left(it - \frac{k_{\mathrm{B}}T}{\hbar}t^2\right)\right\} \quad ,$$

whose Fourier transform leads to the double differential cross section

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{inc}} = N\frac{\sigma_{\mathrm{inc}}}{4\pi}\frac{k'}{k}\frac{1}{\sqrt{2\pi}\,\Lambda}\exp\left\{-\frac{\left(\hbar\omega - \hbar^2Q^2/2M\right)^2}{2\,\Lambda^2}\right\} \quad ,$$

where

$$\Lambda^2 = \frac{\hbar^2Q^2}{M}k_{\mathrm{B}}T \quad ,$$

Performing the integral over solid angles we get the energy-transfer kernel

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}E'}\right)_{\mathrm{gas}} = N\frac{\sigma_{\mathrm{inc}}A}{8E}\left\{\mathrm{erf}\left(\eta x'_{\mathrm{g}} - \rho x_{\mathrm{g}}\right) \pm \mathrm{erf}\left(\eta x'_{\mathrm{g}} + \rho x_{\mathrm{g}}\right) + \exp\left(x_{\mathrm{g}}^{\,2} - x'^{\,2}_{\mathrm{g}}\right)\left[\mathrm{erf}\left(\eta x_{\mathrm{g}} - \rho x'_{\mathrm{g}}\right) \mp \mathrm{erf}\left(\eta x_{\mathrm{g}} + \rho x'_{\mathrm{g}}\right)\right]\right\},$$

where $x_{\mathrm{g}}^{\,2} = E/k_{\mathrm{B}}T$, $x'^{\,2}_{\mathrm{g}} = E'/k_{\mathrm{B}}T$, $\eta = (A+1)/2\sqrt{A}$, $\rho = (A-1)/2\sqrt{A}$ and the upper sign corresponds to $E' \le E$ and the lower sign to $E' \ge E$.

The total cross section of a gas is obtained by integration over all final energies

$$\sigma_{\mathrm{inc}}(E) = N\sigma_{\mathrm{inc}}\left(\frac{A}{A+1}\right)^2\left\{\left(1+\frac{1}{2Ax_{\mathrm{g}}^{\,2}}\right)\mathrm{erf}(\sqrt{A}x_{\mathrm{g}}) + \frac{1}{\sqrt{\pi A}x_{\mathrm{g}}}\exp(-Ax_{\mathrm{g}}^{\,2})\right\}.$$

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where $x_{\mathrm{g}}^{\,2} = E/k_{\mathrm{B}}T$, $x'^{\,2}_{\mathrm{g}} = E'/k_{\mathrm{B}}T$, $\eta = (A+1)/2\sqrt{A}$, $\rho = (A-1)/2\sqrt{A}$ and the upper sign corresponds to $E' \le E$ and the lower sign to $E' \ge E$.

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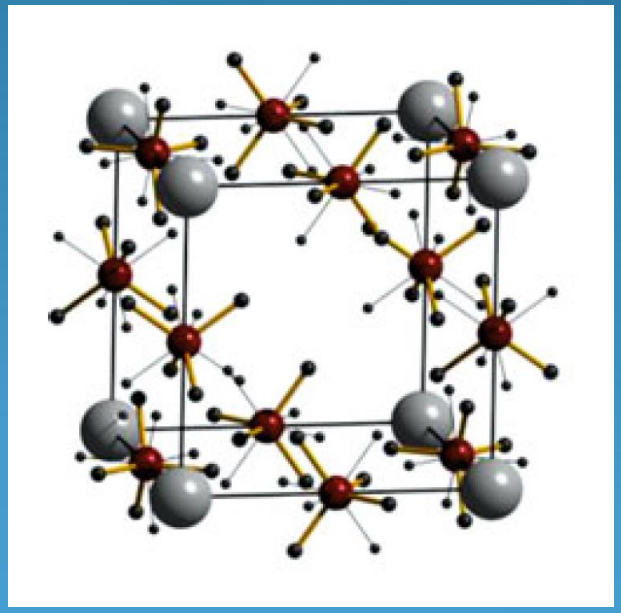
$$\sigma(E \gg \hbar\omega) \rightarrow \sigma_{inc}\left(\frac{A}{A+1}\right)^2\left[1+\frac{kT_{eff}}{2AE}\right]$$

Approach to the Free-atom X-Section

3. Scattering by Crystalline Solids



Let now be a Bravais crystal with only one atom per unit cell, where each site is determined by a vector $\boldsymbol{l}_j$. Allowing thermal movement of the j-nucleus, its instantaneous position will be

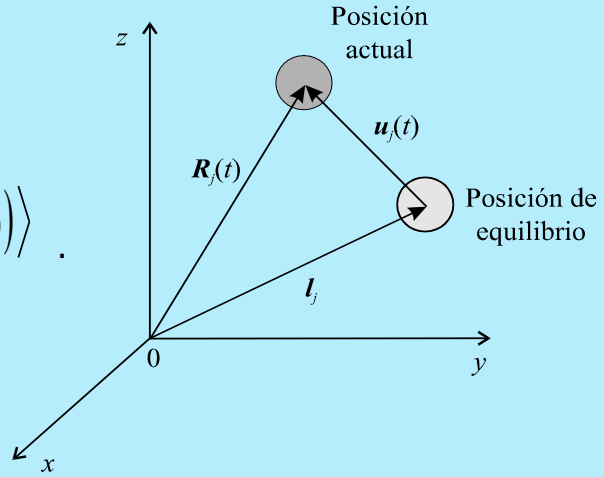
$$\boldsymbol{R}_j = \boldsymbol{l}_j + \boldsymbol{u}_j \quad ,$$

where $\boldsymbol{u}$ j is the displacement from the equilibrium position and $\boldsymbol{l}_j$ is constant.

For a Bravais crystal, the correlation between the positions of the nuclei j and j' depends only on $\boldsymbol{l}_j - \boldsymbol{l}_{j'}$. Thus, in the expression of the intermediate coherent scattering function, the sum over j is the same for each value of j', so that $j'=0$ can be assumed, resulting in

$$\chi_{\text{coh}}(\boldsymbol{Q},t) = \frac{1}{N}\sum_{j,j'}\left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_{j'}(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right)\right\rangle$$

$$= \sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{u}_0(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{u}_j(t)\right)\right\rangle \quad .$$



Making a similar reasoning for the intermediate incoherent scattering function, where each term in j is equal to the term $j = 0$, one obtains

$$\chi_{\text{inc}}(\boldsymbol{Q},t) = \frac{1}{N}\sum_j \left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{R}_j(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_j(t)\right)\right\rangle$$

$$= \left\langle \exp\left(-i\boldsymbol{Q}\cdot\boldsymbol{u}_0(0)\right)\exp\left(i\boldsymbol{Q}\cdot\boldsymbol{u}_0(t)\right)\right\rangle \quad .$$

In these expressions $\boldsymbol{u}_j(t)$ is the Heisenberg operator for $\boldsymbol{u}_j$.

Assuming that interatomic forces are linear with displacements, these can be expressed as sums of displacements due to normal modes of oscillation, i.e.

$$\boldsymbol{u}_j = \left(\frac{\hbar}{2MN}\right)^{1/2}\sum_s \frac{\boldsymbol{e}_s}{\sqrt{\omega_s}}\left\{a_s \exp(i\boldsymbol{q}\cdot\boldsymbol{l}_j) + a_s^{\dagger}\exp(-i\boldsymbol{q}\cdot\boldsymbol{l}_j)\right\} \quad ,$$

where $\boldsymbol{q}$ is the wave vector of the mode, p its polarization index (p=1, 2, 3) and s represents the pair of indices $\boldsymbol{q}$, p. The angular frequency and the mode polarization vector are ω_s and $\boldsymbol{e}_s$, respectively, and M is the mass of the nucleus, assumed equal for all sites. The annihilation and creation operators of the mode s, are a_s y $a_s^{\dagger}$. The sum is performed on the N values of $\boldsymbol{q}$ in the first Brillouin zone and on the three values of p.

With the expressions obtained for the intermediate scattering functions, the coherent cross section is rewritten as

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\int_{-\infty}^{\infty}\left\langle \exp U\,\exp V\right\rangle \exp(-i\omega t)\,\mathrm{d}t \quad ,$$

We proceed in a similar way with the incoherent cross section, obtaining the expressions for the coherent and incoherent differential cross sections :

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\left\langle U^2\right\rangle \sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\int_{-\infty}^{\infty}\exp\langle UV\rangle \exp(-i\omega t)\,\mathrm{d}t$$

and

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{inc}} = \frac{\sigma_{\mathrm{inc}}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\left\langle U^2\right\rangle \int_{-\infty}^{\infty}\exp\left\langle UV_0\right\rangle \exp(-i\omega t)\,\mathrm{d}t \quad ,$$

In the above expressions, an exponential factor is recognized, which is generally denoted as

$$\exp\{-2W\} = \exp\left\langle U^2\right\rangle = \exp\left\{-\left\langle\left\{\boldsymbol{Q}\cdot\boldsymbol{u}_0(0)\right\}^2\right\rangle\right\} \quad ,$$

known as *the Debye-Waller factor*.

$$2W = \frac{\hbar}{2MN} \sum_s \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s)^2}{\omega_s} \langle 2n_s + 1 \rangle \quad .$$

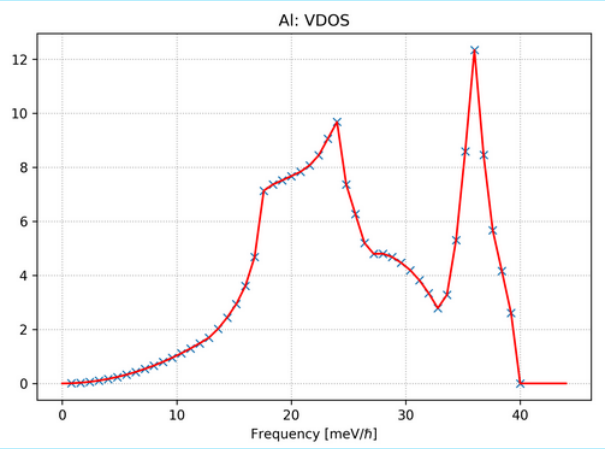
For *cubic crystals* the mean value of $(\boldsymbol{Q}.\boldsymbol{e}_s)^2$ is directly $Q^2/3$, then

$$2W = \frac{\hbar}{2MN} \frac{Q^2}{3} \sum_{\boldsymbol{q},p} \frac{\langle 2n(\omega_p(\boldsymbol{q})) + 1 \rangle}{\omega_p(\boldsymbol{q})} = \frac{\hbar}{2MN} \frac{Q^2}{3} \frac{V_c}{(2\pi)^3} \sum_p \int \frac{\langle 2n(\omega_p(\boldsymbol{q})) + 1 \rangle}{\omega_p(\boldsymbol{q})} \mathrm{d}\boldsymbol{q} \quad ,$$

where V_c is the volume of the crystal and the dependence with the wave vector and polarization modes has been made explicit. Even for non-cubic crystals these expressions are good approximations.

Since the number of degrees of freedom is of the order of 10^{23}, it is possible and convenient to express the sum over the oscillation modes as an integral over the frequencies, using the density of normal modes *Z(ω)*, or phonon density of states (DOS), defined so that *Z(ω)dω* is the fraction of the normal modes between ω y ω+dω. Then

$$\frac{V_c}{3N} \sum_p \int \frac{f(\omega_p(\boldsymbol{q}))}{(2\pi)^3} \mathrm{d}\boldsymbol{q} = \int Z(\omega)\, f(\omega)\, \mathrm{d}\omega \quad ,$$



where, by comparison, it follows that

$$Z(\omega) = \frac{V_c}{3N} \sum_p \int \frac{\delta\left(\omega - \omega_p(\boldsymbol{q})\right)}{(2\pi)^3} \mathrm{d}\boldsymbol{q} \quad .$$

So, we get the following expression for the Debye-Waller factor

$$2W = \frac{\hbar Q^2}{2M} \int_0^\infty \left\langle 2n(\omega) + 1 \right\rangle \frac{Z(\omega)}{\omega} \mathrm{d}\omega \quad ,$$

where the number $n(\omega)$, has the expression

$$\left\langle n(\omega) \right\rangle = \left[\exp\left(\beta\hbar\omega \right) - 1 \right]^{-1} \quad ,$$

which is the average boson occupation number.

In the case of the incoherent double differential cross section, for the factor $\exp\langle UV_0\rangle$ an analysis like that performed with the Debye-Waller factor can be made. Again, for cubic crystals and replacing the sum by an integral over the frequencies, one obtains

$$\langle UV_0\rangle = \frac{\hbar Q^2}{2M}\int_0^\infty \frac{Z(\omega)}{\omega}\left\{e^{-i\omega t}\langle n(\omega)+1\rangle + e^{i\omega t}\langle n(\omega)\rangle\right\} d\omega \quad .$$

Defining the function

$$\gamma(t) = \int_{-\infty}^{\infty} \frac{Z(\omega)}{\omega} n(\omega)\, e^{-i\omega t}\, d\omega \quad ,$$

And using symmetry properties of the occupation number, harmonic oscillators and density of states, we can write it as

$$\gamma(t) = \int_0^\infty \frac{Z(\omega)}{\omega}\left\{[n(\omega)+1]\, e^{i\omega t} + n(\omega)\, e^{-i\omega t}\right\} d\omega \quad ,$$

It clearly follows that *the intermediate incoherent scattering function* has the following expression

$$\chi_{\text{inc}}(\boldsymbol{Q},t) = \exp\left\{\frac{\hbar Q^2}{2M}\left[\gamma(t)-\gamma(0)\right]\right\} \quad ,$$

The Phonon Expansion

A crystal of N atoms has 3*N* normal modes, whose quantum numbers determine the initial state $|\lambda\rangle$ of the crystal. In a generic scattering process, the state of the crystal changes to $|\lambda'\rangle$, characterized by another set $n_1', n_2', \ldots, n_{3N}'$ of quantum numbers. Scattering processes can be classified according to changes in those quantum numbers.

Elastic processes: All quantum numbers remain unchanged, that is, $n_i' = n_i$ for all *i* from 1 to 3*N*.

One-phonon processes: All quantum numbers remain unchanged, except one corresponding to the oscillator α, which changes by one unit, i.e. $n_i' = n_i$ for all i $\neq\alpha$ and .

$n_\alpha' = n_\alpha \pm 1$

Two-phonon processes: All quantum numbers remain unchanged, except for two corresponding to the oscillators α and β, which change by one unit, i.e. for all i $\neq\alpha$ or β, and $n_\alpha' = n_\alpha \pm 1$, $n_\beta' = n_\beta \pm 1$

Similarly for processes of three, four and more phonons.

The development in phonons is obtained if the factor exp⟨*UV*⟩ in

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\langle U^2\rangle \sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\int_{-\infty}^{\infty}\exp\langle UV\rangle\exp(-i\omega t)\,\mathrm{d}t$$

is developed in Taylor series. (⟨*exp UV*$_0$⟩ in the incoherent expression), i.e.

$$\exp\langle UV\rangle = 1+\langle UV\rangle+\frac{1}{2!}\langle UV\rangle^2+\ldots+\frac{1}{p!}\langle UV\rangle^p+\ldots\,,$$

where the *pth* term produces the cross section for all *p* phonon processes. Thus, the first term gives the elastic cross section; the following ⟨*UV*⟩ term gives the cross section for all processes of a phonon in which α it is, in turn, each of the 1 to 3*N* and each n_α increases or decreases by one unit; the term (1/2!) ⟨*UV*⟩^{2} gives the cross section for all two-phonon processes in which the combination $\alpha\beta$, is, in turn, each of the 3N (3N-1)/2 combinations of two oscillators taken from 3*N* and, for each combination, n_β and n_α varies by one unit, and so on.

We will come back on this topic soon, to indicate more explicitly the way this expansion is performed.

Elastic coherent scattering

Replacing $\exp\langle UV\rangle$ by 1 in the double differential cross section, we obtain

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi} N \exp\left\langle U^2\right\rangle \sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\,\delta(\hbar\omega) \quad ,$$

situation that corresponds to elastic scattering. This expression can be easily integrated to obtain the differential cross section $\mathrm{d}\sigma/\mathrm{d}\Omega$, keeping the energy E of the incident neutron fixed:

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh\ el}} = \int_0^\infty \left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh\ el}} \mathrm{d}E' = \frac{\sigma_{\mathrm{coh}}}{4\pi} N \exp\left\langle U^2\right\rangle \sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j) \quad .$$

Finally it results

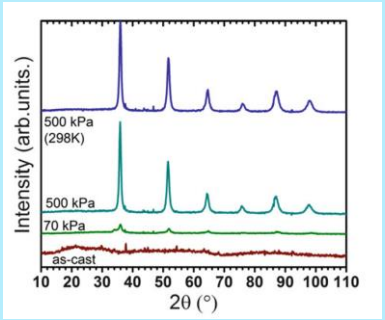
$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh\ el}} = \frac{\sigma_{\mathrm{coh}}}{4\pi} N \frac{(2\pi)^3}{v_0} \exp(-2W) \sum_{\boldsymbol{\tau}} \delta(\boldsymbol{Q}-\boldsymbol{\tau}) \quad ,$$

where the sum over the lattice was performed in the standard form, v_0 is the volume of the unit cell of the crystal and $\boldsymbol{\tau}$ is a vector of the reciprocal lattice. The latter equation indicates that scattering can only occur when the momentum transfer vector $\boldsymbol{Q}$ coincides with a vector of the reciprocal lattice $\boldsymbol{\tau}$, which is Bragg's Law.

For Bravais crystals with base, the following expression is obtained for the coherent elastic differential cross section

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\text{coh el}} = N\frac{(2\pi)^3}{v_0}\sum_{\boldsymbol{\tau}}\delta(\boldsymbol{Q}-\boldsymbol{\tau})\left|F_{\mathrm{N}}(\boldsymbol{Q})\right|^2 ,$$

Coherent Elastic Diff. Cross Section



where

$$F_{\mathrm{N}}(\boldsymbol{Q}) = \sum_{\boldsymbol{d}}\bar{b}_{\boldsymbol{d}}\exp(i\boldsymbol{Q}\cdot\boldsymbol{d})\exp(-W_{\boldsymbol{d}})$$

is known as the *nuclear structure factor of the unit cell*, the sum is performed over all the sites of the base (each characterized by the vector ***d*** that locates it with respect to the site of the network), the mean scattering length refers to that magnitude for each site of the base and $W_{\boldsymbol{d}}$ is given by

$$W_{\boldsymbol{d}} = \frac{\hbar Q^2}{4M_{\boldsymbol{d}}}\int_0^{\omega_{\mathrm{m}}}\coth\left(\tfrac{1}{2}\beta\hbar\omega\right)\frac{Z(\omega)}{\omega}\,\mathrm{d}\omega \quad ,$$

valid for a cubic crystal, where the sum over the normal modes has been replaced by the integral over the frequencies, and the occupation number has been used.

One Phonon Coherent scattering

Returning to scattering for a Bravais crystal, the coherent cross section of a phonon is obtained by replacing exp⟨UV⟩ by ⟨ UV⟩ in

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\langle U^2\rangle \sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\int_{-\infty}^{\infty} \langle UV\rangle \exp(-i\omega t)\,\mathrm{d}t$$

producing the cross section

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right)_{\mathrm{coh\,1\,ph}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{1}{4\pi M}\exp(-2W)\sum_j \exp(i\boldsymbol{Q}\cdot\boldsymbol{l}_j)\sum_s \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s)^2}{\omega_s}$$

$$\times\int_{-\infty}^{\infty}\Big[\exp\{-i(\boldsymbol{q}\cdot\boldsymbol{l}_j-\omega_s t)\}\langle n_s+1\rangle + \exp\{i(\boldsymbol{q}\cdot\boldsymbol{l}_j-\omega_s t)\}\langle n_s\rangle\Big]\exp(-i\omega t)\,\mathrm{d}t \quad .$$

Using the integral form of the Dirac delta and solving the sum over the lattice, each of the two terms in the above expression can be written as

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right)_{\mathrm{coh}\,\pm1\,\mathrm{ph}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k'}{k}\frac{(2\pi)^3}{v_0}\frac{\hbar}{2M}\exp(-2W)$$

$$\times\sum_s\sum_{\boldsymbol{\tau}}\frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s)^2}{\omega_s}\begin{Bmatrix}\langle n_s+1\rangle\\ \langle n_s\rangle\end{Bmatrix}\delta(\hbar\omega\mp\hbar\omega_s)\,\delta(\boldsymbol{Q}\mp\boldsymbol{q}-\boldsymbol{\tau}) \quad .$$

Due to those δ distributions that appear in the last expression, for the dispersion process to occur the two conditions must be met:

$\hbar\omega = \pm\hbar\omega_s$ and $\boldsymbol{Q} = \boldsymbol{\tau} \pm \boldsymbol{q}$

When the temperature tends to zero, $\langle n_s+1 \rangle$ tends to 1, and $\langle n_s \rangle$ tends to zero, so that the phonon absorption cross section tends to zero, a predictable result since at this limit all oscillators are in their ground state. For crystals with more than one atom per lattice site, the expression for the cross section generalizes as follows

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{coh}\,\pm 1\,\mathrm{ph}} = \frac{k'}{k}\frac{(2\pi)^3}{2v_0}\sum_s\sum_{\boldsymbol{\tau}}\frac{\hbar}{\omega_s}\left|\sum_d \frac{\bar{b}_d}{\sqrt{M_d}}\exp(-W_d)\exp(i\boldsymbol{Q}\cdot\boldsymbol{d})(\boldsymbol{Q}\cdot\boldsymbol{e}_{d,s})\right|^2 \times \left\{\begin{matrix}\langle n_s+1\rangle \\ \langle n_s\rangle\end{matrix}\right\}\delta(\hbar\omega \mp \hbar\omega_s)\,\delta(\boldsymbol{Q}\mp\boldsymbol{q}-\boldsymbol{\tau})$$

Phonon Dispersion Relation

Analyzing the situation corresponding to the sign (+), the first condition indicates that the energy of the neutron decreases by an amount equal to the energy of a phonon of the s-th normal mode; this process, in which a phonon is created, is known as *emission or creation of phonons*. The second condition can be considered as an expression of momentum conservation, since $\hbar\boldsymbol{Q}$ it is the change of the momentum of the neutron, while $\hbar(\boldsymbol{\tau}+\boldsymbol{q})$ it is the momentum delivered to the crystal. Similarly, the situation corresponding to the sign (-) can be analyzed, where in this process a phonon is annihilated and is known as a*bsorption* or *annihilation of phonons*.

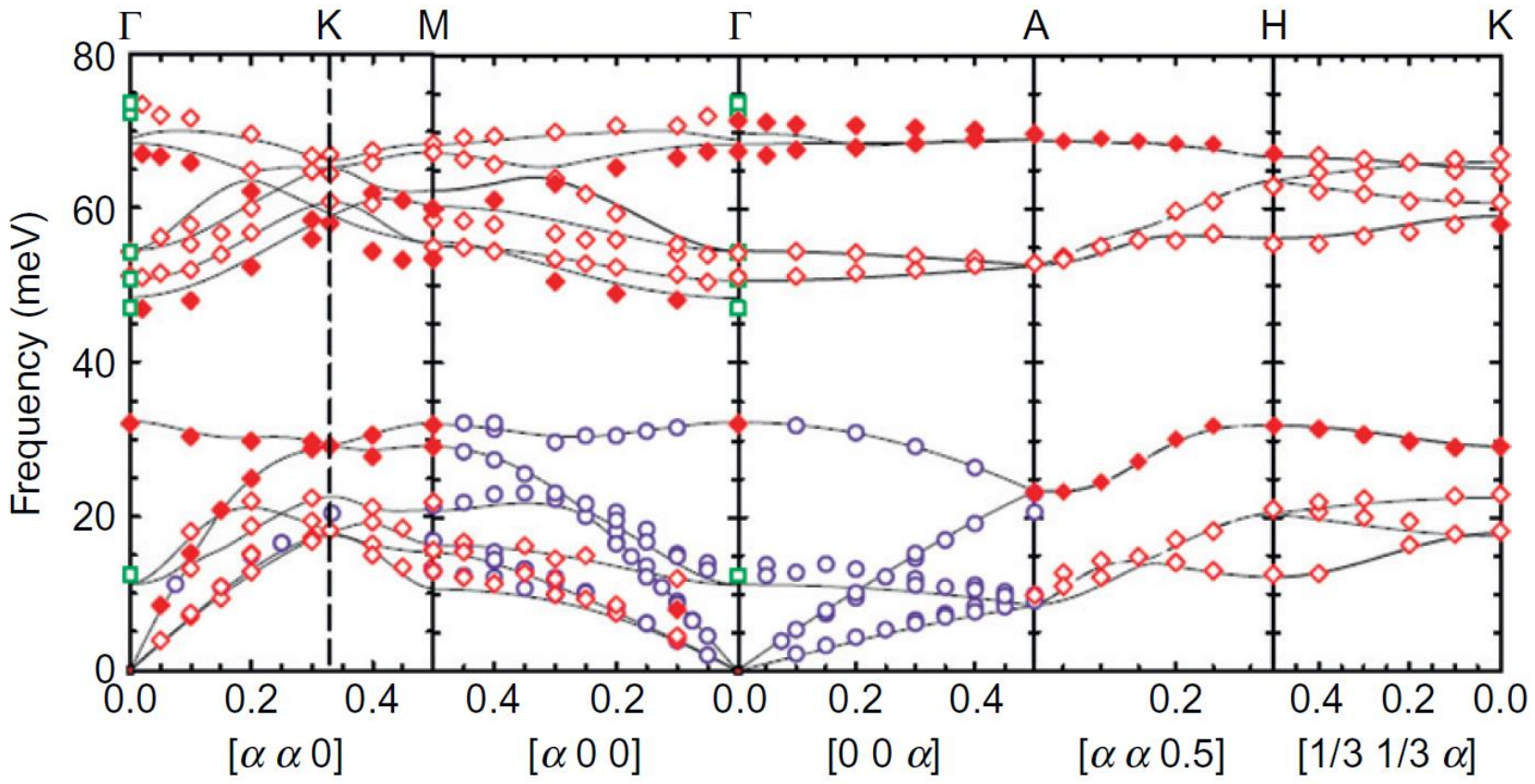


FIGURE 1.9 Phonon-dispersion relations for zinc oxide along the main symmetry directions. Diamonds and circles (red and blue) correspond to inelastic neutron-scattering data. Raman data at the Γ point ($Q=0$) are depicted by squares (green). *Ab initio* calculations are shown by the solid curves. *Reprinted with permission from Ref. [75].*

Multiphonon coherent scattering

The coherent cross section for p phonons is obtained by replacing exp ⟨UV⟩ by $\langle UV\rangle^p / p!$ and can be easily shown to contain two δ functions giving rise to the following equations

$$\hbar\omega = \sum_{n=1}^{p}(\pm\hbar\omega_{s_n})$$

and

$$\boldsymbol{Q} = \boldsymbol{\tau} \sum_{n=1}^{p}(\pm\boldsymbol{q}_n) \quad .$$

Both conditions must be met for this type of scattering to occur, where the neutron creates or annihilates a phonon in p different normal modes.

Unlike the coherent scattering case of one phonon, given a wave vector $\boldsymbol{k}$, it is always possible to find combinations of p normal modes such that their values of $\boldsymbol{q}$ and ω_s satisfy the scattering conditions for any value of k' . That is, the conservation of momentum and energy does not impose restrictions as severe as in the elastic case of one phonon. So multiphonon scattering tends to a function that depends smoothly on the angle of scattering and the incident energy.

The behaviour of that function becomes similar to the multiphonon incoherent scattering, which is why they are usually taken to be the same. This is the incoherent approximation to the multiphonon contribution to the scattering cross section.

Incoherent scattering

In the incoherent double differential cross section,

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\mathrm{inc}} = \frac{\sigma_{\mathrm{inc}}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\langle U^2\rangle\int_{-\infty}^{\infty}\exp\langle UV_0\rangle\exp(-i\omega t)\,\mathrm{d}t$$

$\exp\langle UV_0\rangle$ is developed in powers of $\langle UV_0\rangle$ in a totally analogous way to what was done for the coherent cross section. Thus it follows that the p-th term corresponds to a process of *p* phonons.

To calculate the elastic incoherent cross section, the $\exp\langle UV_0\rangle$ is replaced by 1 and proceeds in the same way that was done with the coherent contribution, to finally obtain

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{inc\ el}} = \frac{\sigma_{\mathrm{inc}}}{4\pi}N\exp(-2W)\,.$$

Incoherent Elastic Diff. X-S

The only dependence of this differential cross section with the direction of dispersion is on the Debye-Waller factor, which depends on ***Q***. At low temperatures scattering is isotropic, since the Debye-Waller factor is close to one.

The incoherent cross section of a phonon is obtained by replacing exp $\langle UV_0 \rangle$ by $\langle UV_0 \rangle$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\text{inc 1 ph}} = \frac{\sigma_{\text{inc}}}{4\pi}\frac{k'}{k}\frac{\hbar}{2M}\exp(-2W)\sum_s \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s)^2}{\omega_s}$$

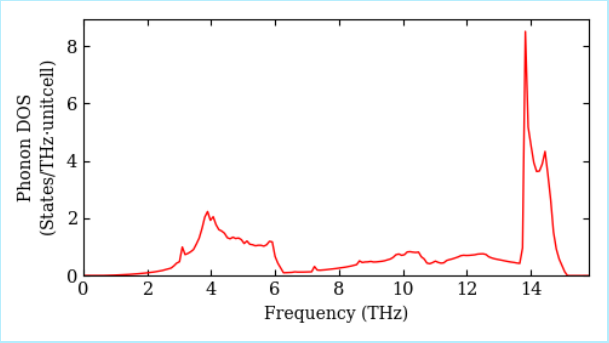
$$\times\left[\langle n_s+1\rangle\,\delta(\hbar\omega-\hbar\omega_s)+\langle n_s\rangle\,\delta(\hbar\omega+\hbar\omega_s)\right] .$$

The first term in the bracket corresponds to phonon creation and the second to annihilation.

This means that for fixed **k**, θ, and crystal orientation, there is incoherent scattering of a phonon for a continuous range of values of k', and for a given k' there is scattering of all normal modes whose ω_s satisfies the conservation of energy condition. Therefore, the cross section can be represented in terms of the phonon density of states $Z(\omega)$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\text{inc}\,\pm 1\,\text{ph}} = \frac{\sigma_{\text{inc}}}{4\pi}\frac{k'}{k}\frac{N}{4M}Q^2\exp(-2W)\frac{Z(\omega)}{\omega}\left[\coth\left(\tfrac{1}{2}\beta\hbar\omega\right)\pm 1\right] .$$

Phonon Density of States



The incoherent cross section of a phonon is obtained by replacing exp $\langle UV_0 \rangle$ by $\langle UV_0 \rangle$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\text{inc 1 ph}} = \frac{\sigma_{\text{inc}}}{4\pi}\frac{k'}{k}\frac{\hbar}{2M}\exp(-2W)\sum_s \frac{(\boldsymbol{Q}\cdot\boldsymbol{e}_s)^2}{\omega_s}$$

$$\times\left[\langle n_s+1\rangle\,\delta(\hbar\omega-\hbar\omega_s)+\langle n_s\rangle\,\delta(\hbar\omega+\hbar\omega_s)\right] .$$

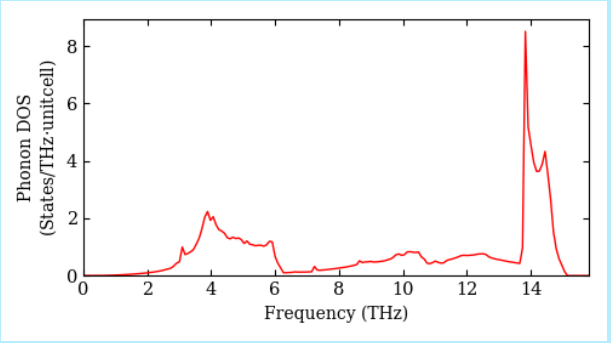
The first term in the bracket corresponds to phonon creation and the second to annihilation.

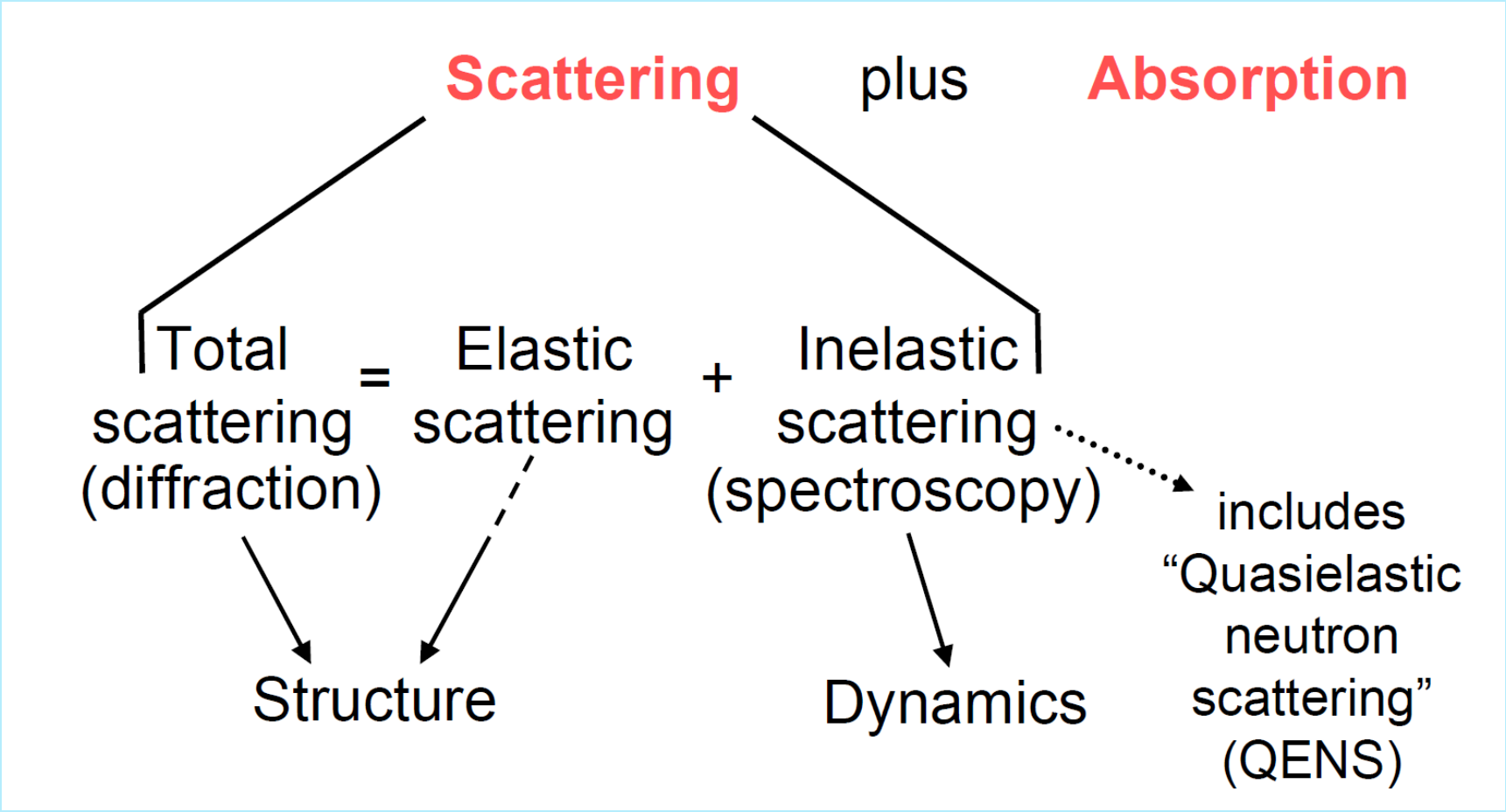
This means that for fixed **k**, θ, and crystal orientation, there is incoherent scattering of a phonon for a continuous range of values of k', and for a given k' there is scattering of all normal modes whose ω_s satisfies the conservation of energy condition. Therefore, the cross section can be represented in terms of the phonon density of states $Z(\omega)$

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{\text{inc}\,\pm 1\,\text{ph}} = \frac{\sigma_{\text{inc}}}{4\pi}\frac{k'}{k}\frac{N}{4M}Q^2\exp(-2W)\frac{Z(\omega)}{\omega}\left[\coth\left(\tfrac{1}{2}\beta\hbar\omega\right)\pm 1\right] .$$

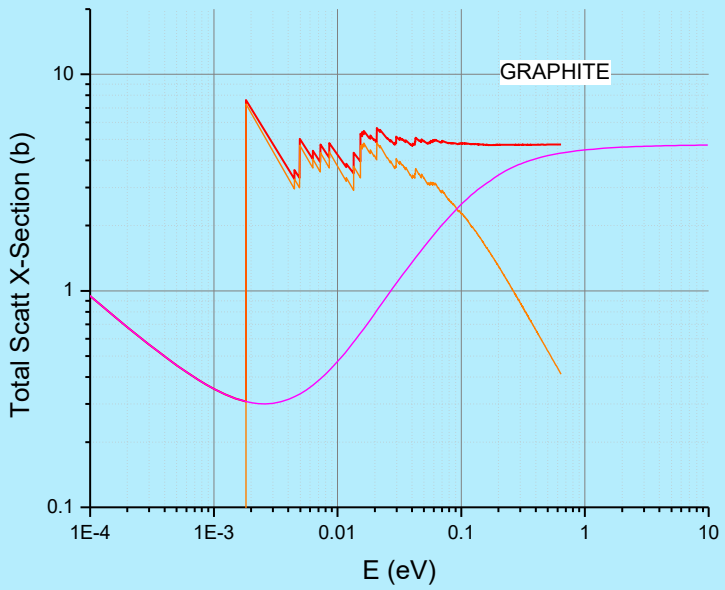
Phonon Density of States

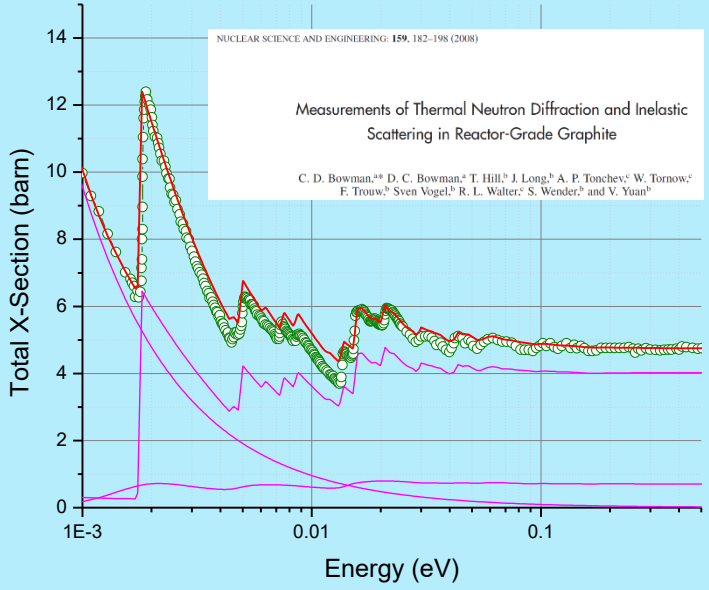
$$(\omega\to 0) \;\to\; \sim Q^2\,Z(\omega)/\omega^2 \;\Rightarrow\; Z(\omega\to 0)\sim\omega^2$$



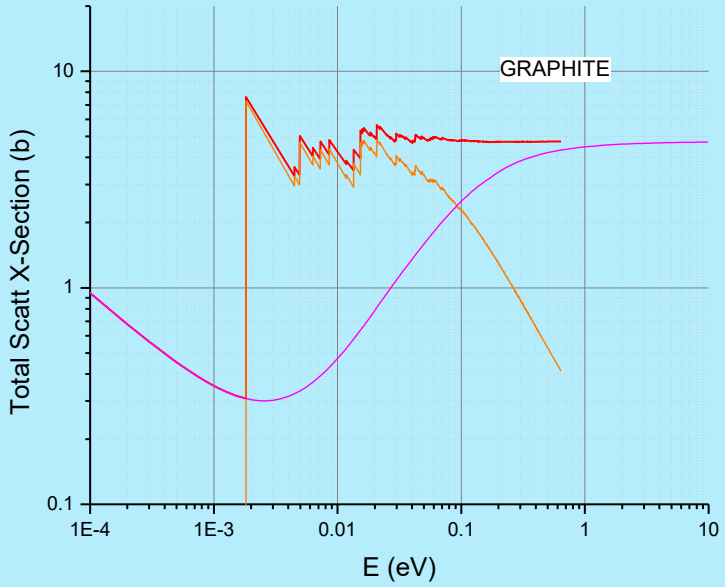

Scattering
plus
Absorption
Total scattering (diffraction)
=
Elastic scattering
+
Inelastic scattering (spectroscopy)
includes "Quasielastic neutron scattering" (QENS)
Structure
Dynamics

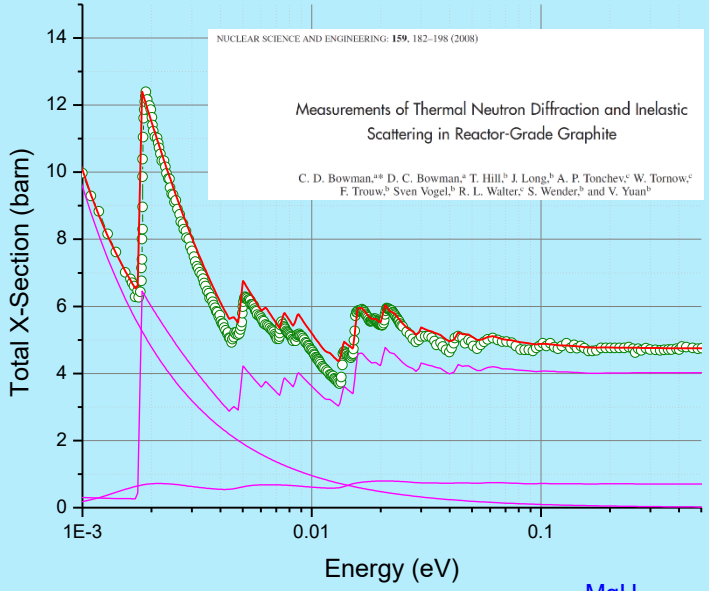
SCATTERING BY CRYSTALS

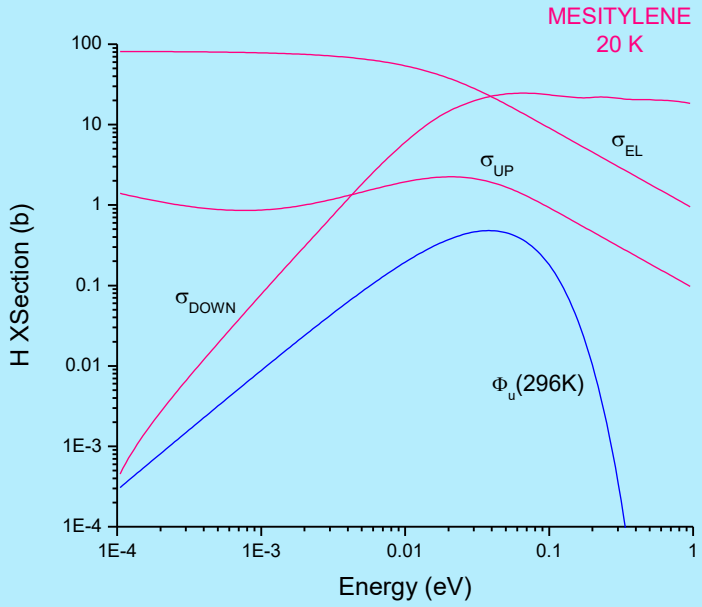


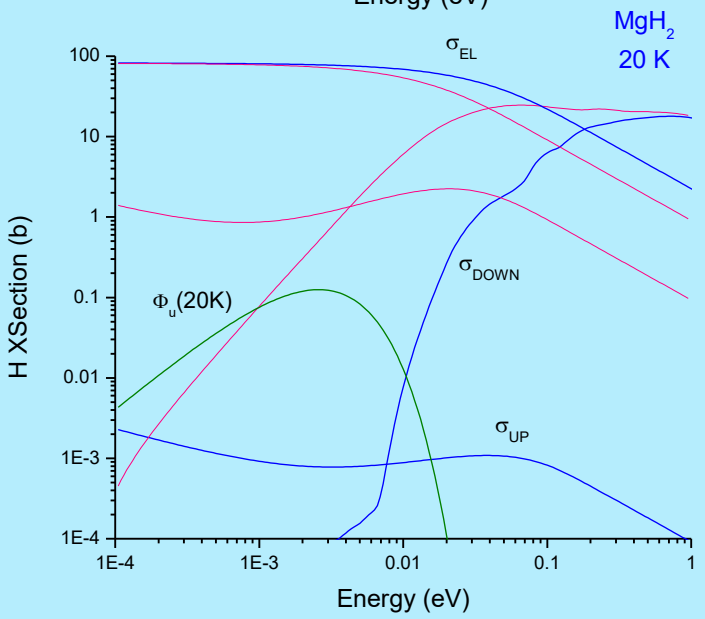


SCATTERING BY CRYSTALS









A GOOD COLD NEUTRON MODERATOR....

AND A GOOD COLD NEUTRON REFLECTOR

Sjölander´s Phonon Expansion

For the incoherent intermediate scattering function, in the isotropic (cubic) and harmonic (Gaussian) approximations to represent the motion of the crystal atoms, we obtain

$$\chi_{\text{inc}}(\boldsymbol{Q},t) = \exp\left\{\frac{\hbar Q^2}{2M}\left[\gamma(t)-\gamma(0)\right]\right\}$$

where

$$\gamma(t) = \int_{-\infty}^{\infty} \frac{Z(\omega)}{\omega}\, n(\omega)\, \mathrm{e}^{-i\omega t}\, \mathrm{d}\omega \quad ,$$

that, using symmetry properties of the occupation number *n(w)* and the phonon density of states *Z(ω)* can be written as

$$\gamma(t) = \int_{0}^{\infty} \frac{Z(\omega)}{\omega}\left\{[n(\omega)+1]\,\mathrm{e}^{i\omega t} + n(\omega)\,\mathrm{e}^{-i\omega t}\right\}\mathrm{d}\omega \quad ,$$

Because

$$2W = \frac{\hbar Q^2}{2M}\int_0^{\infty}\langle 2n(\omega)+1\rangle\frac{Z(\omega)}{\omega}\,\mathrm{d}\omega = \frac{\hbar \boldsymbol{Q}^2}{2M}\,\gamma(0) \;\rightarrow\; \chi_{inc}(\boldsymbol{Q},t) = e^{-2W}\exp\left[\frac{\hbar \boldsymbol{Q}^2}{2M}\,\gamma(t)\right]$$

Expanding the intermediate scattering function, we get

$$\chi(\boldsymbol{Q},t) = e^{-2W} \sum_{p=0}^{\infty} \frac{(2W)^p}{p!} \left[\frac{\gamma(t)}{\gamma(0)}\right]^p$$

where each term represents the interaction of the neutron with *p* phonons.

In the manner of Sjölander (1958), we can define the functions

$$G_p(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \left[\frac{\gamma(t)}{\gamma(0)}\right]^p dt$$

Which allow the scattering cross section to be written in the form

$$\frac{d^2\sigma}{d\omega\, dE'} = N \frac{\sigma_{inc}}{4\pi} \frac{\boldsymbol{k}'}{\boldsymbol{k}} e^{-2W} \sum_{p=0}^{\infty} (2W)^p \frac{G_p(\omega)}{\hbar p!}$$

This is the phonon expansion for the incoherent double differential cross section, within the cubic and the Gaussian approximations.

The integration limit in the definition of the $G_p(\omega)$ is formally extended to infinity, although the expression under the integral sign differs from zero only within a finite interval, determined by the condition $/\omega/ \leq p\omega_m$ for a given p, where ω_m is the maximum frequency of the normal modes (PDOS).

It is evident from the same definition that the $G_p(\omega)$ are normalized to unity. Also, and independently of the model for the solid

$$G_0(\omega) = \hbar\, \delta(\hbar\omega)$$

Using the convolution theorem for Fourier transforms, an important recurrence relationship is satisfied by the $G_p(\omega)$

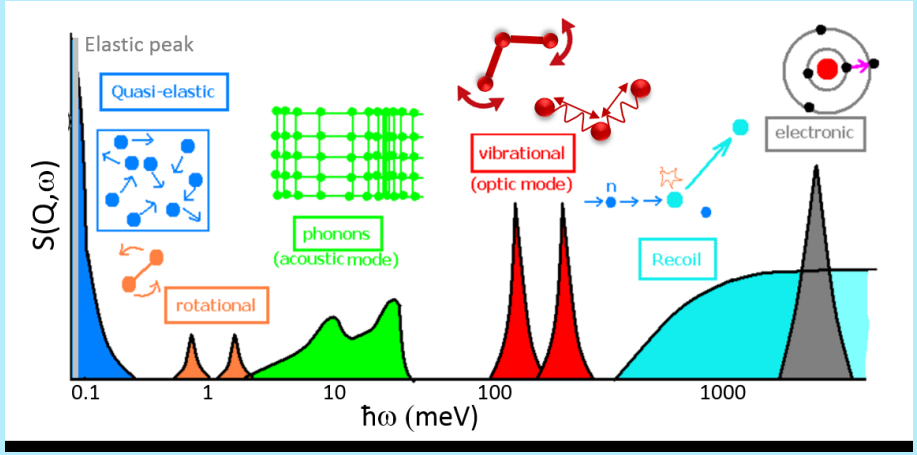
$$G_p(\omega) = \int_{-\infty}^{\infty} G_1(-\omega')\, G_{p-1}(\omega' + \omega)\, d\omega'$$

We have seen before that the zero-phonon term gives rise to the elastic component, which is completely different for the coherent and the incoherent cross sections. Therefore, these terms are treated exactly, whereas it is usual to approximate the coherent inelastic contribution by the incoherent inelastic contribution. This is the **incoherent approximation** for the inelastic cross section.

SCATTERING BY CONDENSED SYSTEMS

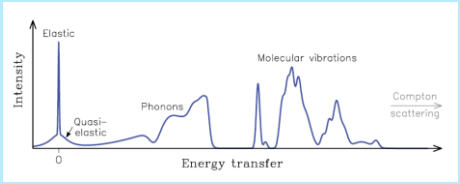
The neutron scattering techniques allow the study of dynamical phenomena of nuclear or magnetic origin in condensed matter.

The quasi-elastic region, which extends up to a few meV around the elastic peak (zero energy transfer point: $\hbar\omega = 0$ meV) is characteristic of phenomena and/or relaxations process-es in the system.



Over the whole energy range, from 0 to several hundreds meV, the signal can also corresponds to the exchange of quanta of energy between the neutron and the sample.

https://doi.org/10.1051/epjconf/201818805001



The case of Molecular Solids

An approximate density of states is used to represent the actual dynamics of the molecular solid:

$$Z(\omega) = a_s Z_s(\omega) + a_r Z_r(\omega) + a_v Z_v(\omega)$$; a_i are relative weights.

Under the assumption of no coupling between modes, the intermediate scattering function is

$$\chi(Q,t) = \chi_s(Q,t).\chi_r(Q,t).\chi_v(Q,t)$$

where each of the factors is further assumed to satisfy the Gaussian approximation

$$\chi_i(Q,t) = \exp\left\{\frac{\hbar Q^2}{2M} a_i [\ \gamma_i(t) - \gamma_i(0)\ ]\right\} \quad ; \qquad i = s, r, v$$

and the time-dependent mean-square displacement $\gamma(t)$ is given by

$$\gamma(t) = \int_0^\infty \frac{Z(\omega)}{\omega}\left[\{n(\omega)+1\}e^{i\omega t} + n(\omega)e^{-i\omega t}\right]d\omega = \sum_i a_i \gamma_i(t)$$

with $n(\omega)$ being the occupation number.

The complete scattering law is calculated as

$$S(Q,\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt\, \chi(Q,t)e^{-i\omega t} = S_s(Q,\omega) \otimes S_r(Q,\omega) \otimes S_v(Q,\omega)$$

Scattering Law

The thermal scattering cross section is defined as

$$\sigma(E \to E', \mu) = \frac{\sigma_b}{k_b T} \sqrt{\frac{E'}{E}}\, S_{n.sym}(\alpha, \beta)$$

where $S_{n.sym}(\alpha, \beta)$ is the non-symmetric form of the thermal scattering law, σ_b is the bound scattering cross section, and $k_b T$ is the temperature in eV.

Here, α is unitless momentum exchange and β is unitless energy exchange, as seen below:

$$\alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{A k_b T}$$

$$\beta = \frac{E' - E}{k_b T}$$

where initial and final neutron energies are E and E' respectively, A is the ratio of the scatterer mass to the neutron mass, and μ is the cosine of the scattering angle in the laboratory. Note that β is positive for neutron energy gain and negative for neutron energy loss.

Continuous, Solid-type Spectrum

For a solid-type spectrum, the scattering law is defined as

$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{i\beta t}\ \mathrm{e}^{\gamma(t)-\gamma(0)}\ dt$$

$$\gamma(t) = \alpha\int_{-\infty}^{\infty} P(\beta)\ \mathrm{e}^{-i\beta t}\ \mathrm{e}^{-\beta/2}\ d\beta$$

where

$$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)}$$

and the phonon distribution $\rho(\beta)$ is and even funcion and is normalized to the solid-type distribution weight ω_s,

$$\int_0^{\infty} \rho(\beta)\ d\beta = \omega_s.$$

The phonon distribution can be input without normalization - it will be normalized automatically by LEAPR.

Recall that while β is defined as unitless energy change $(E' - E)/k_bT$, the input phonon distribution must be provided energy exchange $E' - E$ in units of eV.

The Debye-Waller coefficient is defined as

$$\lambda_s = \int_{-\infty}^{\infty} P(\beta)\ \mathrm{e}^{-\beta/2}\ d\beta$$

which simplifies the scattering law $S_s(\alpha,\beta)$ to be

$$S_s(\alpha,\beta) = \frac{1}{2\pi}\mathbf{e}^{-\alpha\lambda_s}\int_{-\infty}^{\infty} \mathrm{e}^{i\beta t}\ \mathrm{e}^{\gamma(t)}\ dt$$

The exponential of $\gamma(t)$ is a complex and highly oscillatory.

$$\mathrm{e}^{\gamma(t)} = \exp\left[\alpha \int_{-\infty}^{\infty} P(\beta)\, \mathrm{e}^{-i\beta t}\, \mathrm{e}^{-\beta/2}\, d\beta\right]$$

To ease the burden of calculating the scattering law, LEAPR uses the phonon expanion method, which involves expanding the $\gamma(t)$ exponential as a Taylor series,

$$\mathrm{e}^{\gamma(t)} = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\alpha \int_{-\infty}^{\infty} P(\beta)\, \mathrm{e}^{-i\beta t}\, \mathrm{e}^{-\beta/2}\, d\beta\right]^n$$

which, when used in the solid-type scattering law definition, results in

$$\begin{aligned} S_s(\alpha,\beta) = {} & \mathbf{e}^{-\alpha\lambda_s} \sum_{n=0}^{\infty} \frac{1}{n!}\alpha^n \\ & \times \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{i\beta t} \left[\int_{-\infty}^{\infty} P(\beta)\, \mathrm{e}^{-i\beta t}\, \mathrm{e}^{-\beta/2}\, d\beta\right]^n dt \end{aligned}$$

(note that the order of summation and integral have been swapped). Now, the second line of the above equation is redefined as $\lambda_s^n \mathcal{T}_n(\beta)$. This allows for the solid-type scattering law to be redefined as

$$S_s(\alpha,\beta) = \mathrm{e}^{-\alpha\lambda_s} \sum_{n=0}^{\infty} \frac{1}{n!}\left[\alpha\lambda_s\right]^n \mathcal{T}_n(\beta)$$

where

$$\mathcal{T}_0(\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{i\beta t}\, dt = \delta(\beta)$$

and

$$\begin{aligned}\mathcal{T}_1(\beta) &= \frac{1}{\lambda_s}\int_{-\infty}^{\infty} P(\beta')\, \mathrm{e}^{-\beta'/2} \left[\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{i(\beta-\beta')t}\, dt\right] d\beta' \\ &= \frac{1}{\lambda_s} P(\beta')\, \mathrm{e}^{-\beta/2}.\end{aligned}$$

In general subsequent $\mathcal{T}_n(\beta)$ terms can be obtained by convolving the first term with the previous one,

$$\mathcal{T}_n(\beta) = \int_{-\infty}^{\infty} \mathcal{T}_1(\beta')\, \mathcal{T}_{n-1}(\beta-\beta')\, d\beta'.$$

These $\mathcal{T}_n(\beta)$ follow the relationship

$$\mathcal{T}_n(\beta) = \mathrm{e}^{-\beta}\, \mathcal{T}_n(-\beta)$$

and are normalized to unity,

$$\int_{-\infty}^{\infty} \mathcal{T}_n(\beta)\, d\beta = 1.$$

Formulation in dimensionless variables: α,β

(q,ω) preferred in neutron scattering community, (α,β) preferred in nuclear industry (incl. MCNP, ENDF, …)

α: dimensionless q^2

β: dimensionless ΔE

$$\beta = \frac{E_f - E}{kT} = -\frac{\hbar\omega}{kT}$$

$$\begin{aligned}\alpha &= \frac{\hbar^2}{2m_n kT} q^2 \\ &= \frac{E + E_f - 2\mu\sqrt{EE_f}}{kT} \qquad \mu = \cos\theta_{\mathrm{scat}} \\ &= \frac{2E}{kT} + \beta - 2\mu\sqrt{\frac{E}{kT}\left(\frac{E}{kT} + \beta\right)}\end{aligned}$$

Scattering lengths taken outside definition of S:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E_f \mathrm{d}\Omega} = \sqrt{\frac{E_f}{E}} \frac{\sigma_b}{4\pi} \frac{S(\alpha,\beta)}{k_b T}$$

$\sigma_b = 4\pi b^2$

Total cross section, with explicit kinematic limits:

μ=-1, complete backwards scattering

$$\sigma(E) = \frac{\sigma_b kT}{4E} \int_{-E/kT}^{\infty} \int_{\alpha_-(E,\beta)}^{\alpha_+(E,\beta)} S(\alpha,\beta) d\alpha d\beta$$

constant affects σ(E), but not (α,β)-sampling

neutron lose all its energy

μ=+1, complete forward scattering

$$\alpha_\pm(E,\beta) = \frac{2E}{kT} + \beta \pm 2\sqrt{\frac{E}{kT}\left(\frac{E}{kT} + \beta\right)}$$

kinematically accessible region is a parabola in the (α,β)-plane

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