17th Oxford School on Neutron Scattering

5 to 15 September, 2022

Introductory Theory

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Books on Neutron Scattering

- General (with introductory theory)

Willis, B.T.M. and Carlile, C.G.
Experimental Neutron Scattering,
O.U.P., 2009, £37
General introduction to neutron scattering; v. good on experimental methods

Furrer, A., Mesot, J., Strässle, T.
Neutron Scattering in Condensed Matter Physics
World Scientific, 2009, £27
Basic principles of neutron scattering with applications in a range of different materials and phenomena

Carpenter, J.M. and Loong, C.-K.
Elements of Slow-Neutron Scattering
C.U.P., 2015, £42
Basic principles of neutron scattering and its application. More detailed than Furrer *et al*.

Boothroyd, A. T.
Principles of Neutron Scattering from Condensed Matter
O.U.P., 2020, £50
No introduction required.

Oxford Series on Neutron Scattering in Condensed Matter
O.U.P., 1988–2008
15 books on different individual fields of application of neutron scattering

- Theory

Lovesey, S.W. [formerly Marshall, W. and Lovesey, S.W.]
Theory of Neutron Scattering from Condensed Matter
O.U.P., 1984, 2 volumes, ~£78 each
Definitive formal treatment, but not for the faint-hearted!

Squires, G.L.
Introduction to the Theory of Thermal Neutron Scattering
C.U.P., 1978 (reprinted 2012), ~£35;
More elementary than Lovesey, excellent for basic theory

Sivia, D.S.
Elementary Scattering Theory for X-ray and Neutron Users
O.U.P., 2011, £22
Basic principles of neutron scattering from a wave perspective

- Online: www.neutronsources.org

Community web site with wide range of neutron resources

Neutrons as Particles and Waves

Matter Wave:

- Oscillations $\rightarrow$ wave
  Envelope $\rightarrow$ particle

- Increase ξ to define λ better:

  Decrease ξ to define position better,
  but lose information on λ.

  Cannot define both ξ and λ to arbitrary precision
  (Heisenberg's Uncertainty Principle)

- Kinematics — Einstein, de Broglie

  1) Energy: $E = hf$
  $= \hbar\omega$

  h = Planck's constant
  f = frequency
  $\hbar = h/2\pi$, $\omega = 2\pi f$

  2) Momentum: $p = h/\lambda$
  $\mathbf{p} = \hbar\mathbf{k}$

  $\mathbf{k}$ = wavevector
  $|\mathbf{k}| = k = 2\pi/\lambda$

Elastic Scattering from Bound Nuclei

Single nucleus

Weak disturbance of a plane wave

Result: plane wave + spherical wave

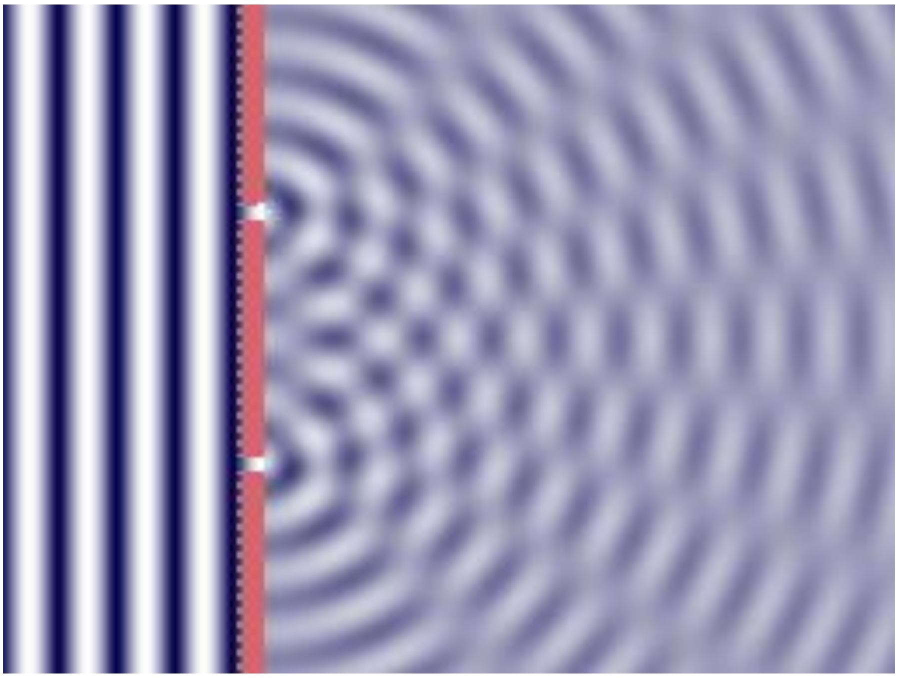
Model for neutrons interacting with a nucleus:

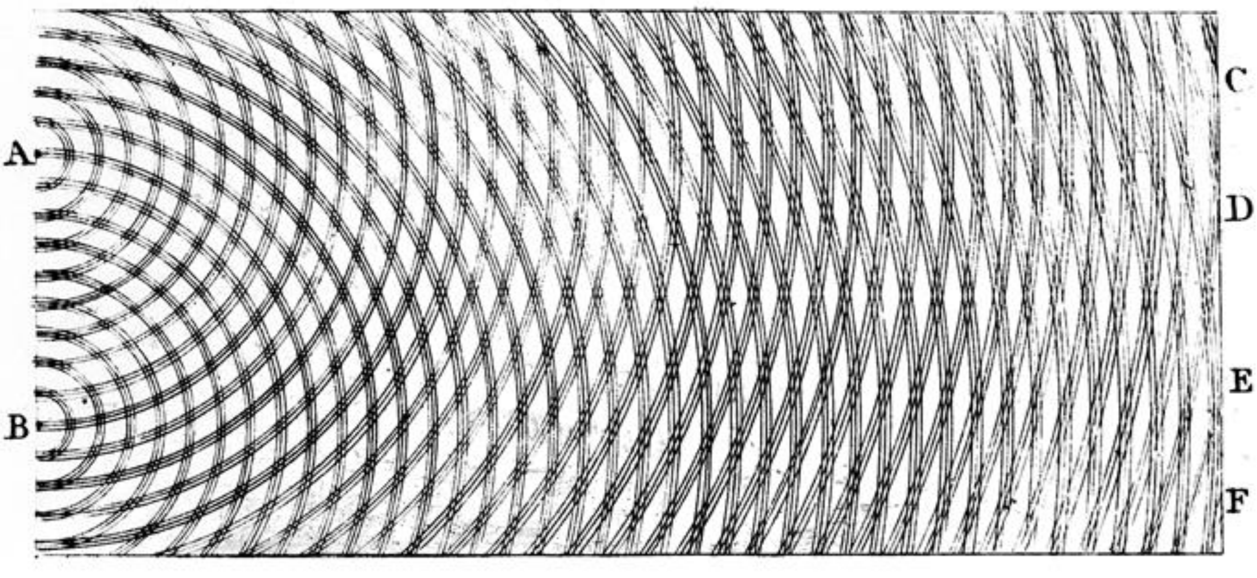
- Assumption – small fraction are scattered
- Justification – nuclear potential is short range
  most neutrons 'miss' nucleus

Born Approximation

[• Formal theory uses a *pseudopotential:* $V(\mathbf{r}) = (2\pi\hbar^2 b/m_n)\,\delta(\mathbf{r} - \mathbf{R})$]

Wave interference from 2 slits:

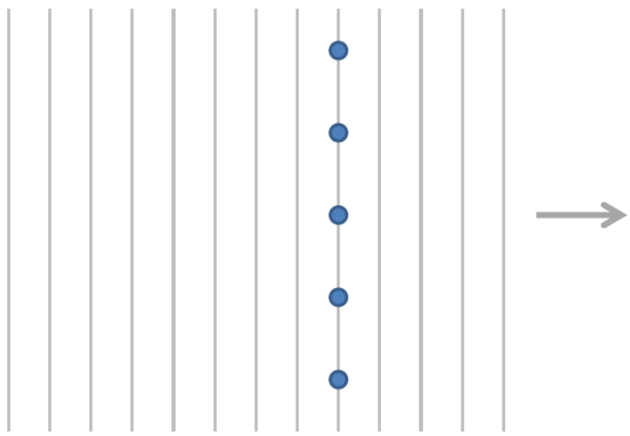


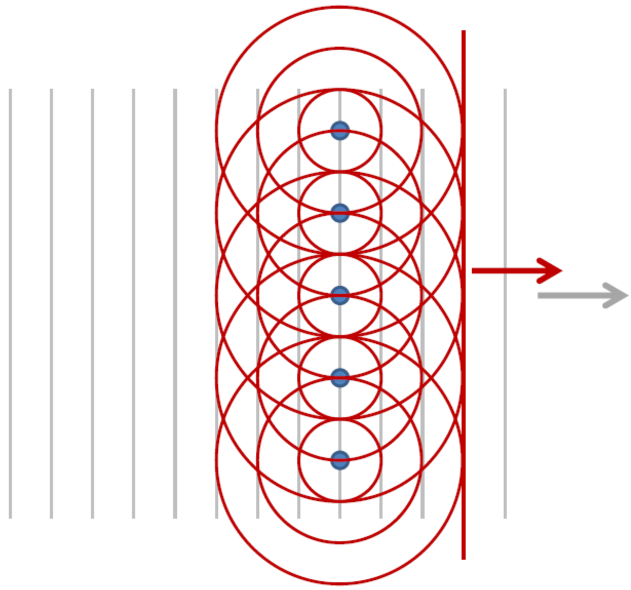


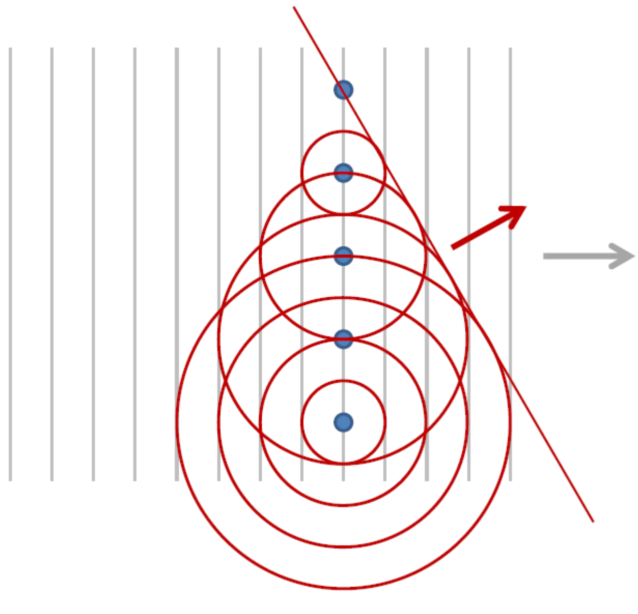
Thomas Young's sketch to explain the interference pattern from two-slits, which he presented to the Royal Society in 1803.

Scattering from a line of nuclei

a) Normal incidence







What is the diffraction angle ?

For constructive interference
the path difference = λ

$$\sin\theta = \lambda/d$$

Suppose path difference = 2λ:

$$\sin\theta = 2\lambda/d$$

In general:

$$\sin\theta = n\lambda/d$$

b) Incident angle = diffracted angle

diffraction condition:

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

Notes

- At large distances, diffracted waves are plane waves
- N nuclei:

  amplitude of diffracted wave ~N

  elsewhere, amplitude ~1

Elastic Scattering from a Crystal

a) Normal Incidence

In general, AA' ≠ AB, so diffraction from 2nd column of atoms not usually in phase with diffraction from first.

Only achieve constructive interference when a and d are in special ratios.

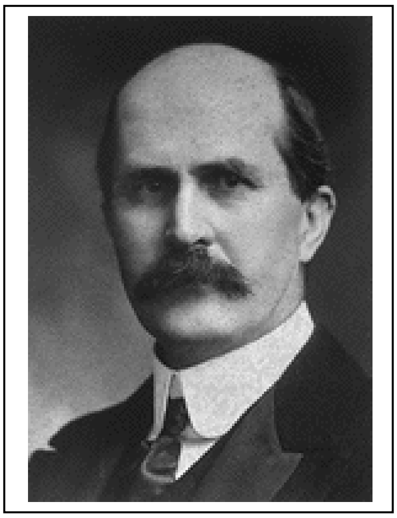
b) Angle of incidence = angle of reflection

This time, AA' = BB', so always achieve constructive interference from successive columns of atoms.

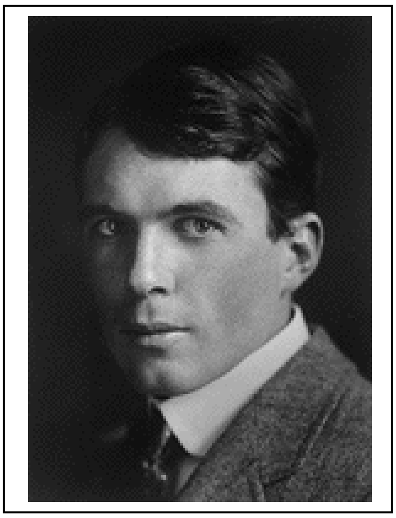
Hence, diffraction from a crystal occurs when

$$n\lambda = 2d \sin \theta \qquad \text{(Bragg's Law)}$$

The Braggs — founders of crystallography



W.H. Bragg
(1862–1942)



W.L. Bragg
(1890–1971)

- Developed X-ray diffraction techniques for solving crystal structures (1913)

- Bragg's law:

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

Proceedings of the Cambridge Philosophical Society **17**, 43 (1913)

- Measure diffraction peaks $\rightarrow$ d-spacings
  $\rightarrow$ crystal structure

- Braggs shared Nobel Prize in Physics (1915)

Debye-Waller factor

In reality, nuclei are not stationary:

Instantaneous positions

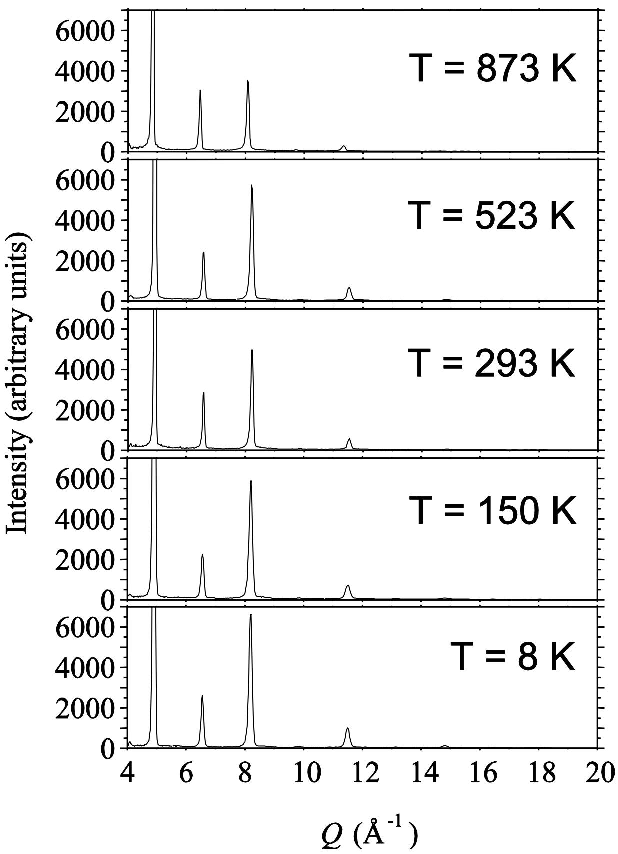
Time-average

- causes decrease in intensity of diffracted beam because waves are not so well in phase.
- Effect worsens as k ($=2\pi/\lambda$) and θ increase

- Bragg's Law the same, but $d \rightarrow \langle d \rangle$.
- smearing increases with temperature :

$$I = I_0 \exp\{-\langle(\mathbf{Q.u})^2\rangle\} = I_0 \exp(-2W)$$

Debye-Waller Factor



Single crystal diffraction data from $Nd_{0.5}Pb_{0.5}MnO_3$ taken on the SXD diffractometer, courtesy of Dr Dave Keen (ISIS).

Particle Waves (again)

2 assumptions of quantum mechanics :

1. A particle is represented mathematically by a complex wavefunction, $\psi(\mathbf{r})$.
2. Probability of finding the particle in a (infinitesimal) volume $\mathrm{d}V$ is $|\,\psi(\mathbf{r})\,|^2\,\mathrm{d}V$.

Examples

(i) Infinite plane wave :

$$\psi = \exp\{\,\mathrm{i}kz\,\} \qquad (=\cos kz + \mathrm{i}\sin kz\,)$$

$$\begin{aligned} |\,\psi|^2 &= \psi\,\psi^* \\ &= \exp\{\,\mathrm{i}kz\,\}\exp\{\,-\mathrm{i}kz\,\} \\ &= 1 \end{aligned}$$

→ 1 particle per unit volume everywhere

(ii) Spherical wave :

$$\psi = -\frac{b\exp\{\,\mathrm{i}kr\,\}}{r}$$

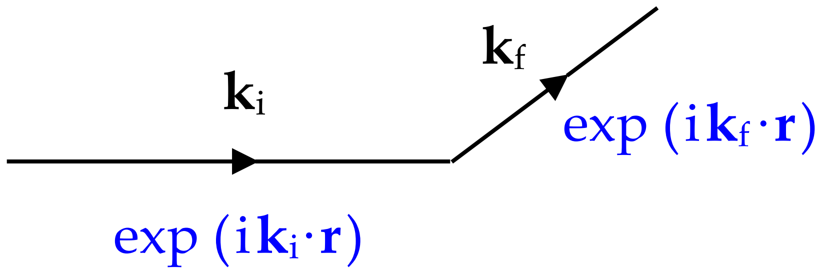
$$|\,\psi|^2 = b^2/r^2$$

→ density of particles falls off as $1/r^2$

Flux of particles

$$\begin{aligned} I &= \text{number incident normally on unit area per sec.} \\ &= \text{particle density} \times \text{velocity} \\ &= |\,\psi|^2\,v \\ &= |\,\psi|^2\,\hbar k/m \end{aligned}$$

Scattering as a Fourier transform



Fermi's Golden Rule and Born approximation:

Scattering probability ~ $|M|^2$

where

$$M = \int \exp(-i\mathbf{k}_f \cdot \mathbf{r})\, V(\mathbf{r})\, \exp(i\mathbf{k}_i \cdot \mathbf{r})\, d^3\mathbf{r}$$

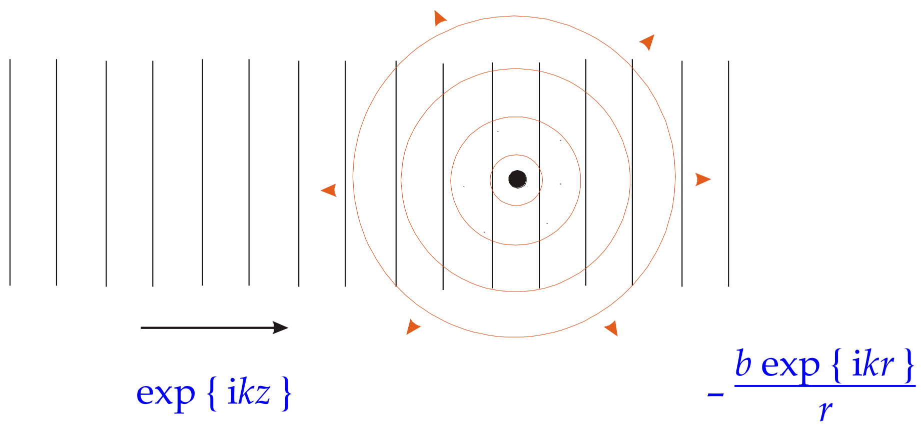
$$= \int V(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathrm{r})\, d^3\mathbf{r} \qquad (\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f)$$

$$= V(\mathbf{Q})$$ --- Fourier transform of $V(\mathbf{r})$

Neutron scattering is determined by the Fourier transform of the interaction potential (exception is reflectometry).

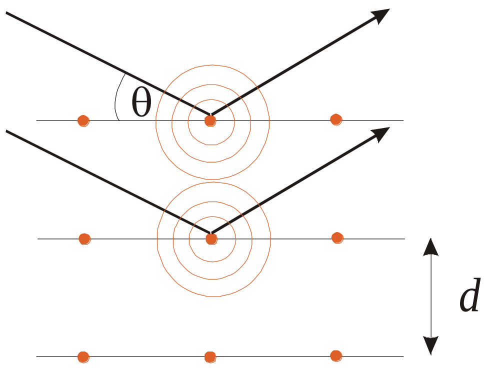
Summary of Lecture 1

- Nucleus provides a weak perturbation to the incident neutrons, scattered neutrons are described by spherical waves:



- Diffraction: interference pattern of neutron waves scattered from sample

- Diffraction from crystals:



$$\boxed{n\lambda \;=\; 2d \sin\theta}$$

Bragg's Law

d = spacing between planes
θ = half the scattering angle

- Thermal motion of atoms does not affect use of Bragg's Law, but does reduce peak intensities from their values for a perfectly rigid structure.

- Neutron scattering depends on Fourier transform of interaction potential

Cross-Sections

Total cross-section

Total cross-section σ is defined by,

$$\sigma = \frac{\text{total no. particles scattered in all directions per sec.}}{\text{incident flux } (I_0)}$$

(i) Classical case — scattering from a solid sphere, radius a

No. particles scattered per sec. $= \quad I_0 \quad \times \quad \pi a^2$

$$\rightarrow \quad \sigma = \pi a^2$$

(ii) Quantum case — scattering from an isolated stationary nucleus

Incident wave, $\quad \psi_0 = \exp\{ikz\}$

Incident flux, $\quad I_0 = |\psi_0|^2 v = v$

Scattered wave, $\quad \psi_{sc} = -\dfrac{b \exp\{ikr\}}{r}$

Scattered flux, at distance r $\quad I^{sc} = |\psi_{sc}|^2 v = b^2 v / r^2$

Total no. particles scattered per sec. $= \quad I^{sc} \quad \times \quad$ total area

$= b^2 v / r^2 \times 4\pi r^2$

$= 4\pi b^2 v$

$$\rightarrow \quad \sigma = 4\pi b^2$$

Notes:

- σ is the *effective area* of the target as viewed by the incident neutrons
- if the target is a nucleus, then b is the nuclear scattering length; b is the effective range of the nuclear potential
- units of b : Fermi (f) 1 Fermi = 10^{-15} m
  " " σ : barn (b) 1 barn = 10^{-28} m^2

Differential cross-section

Differential cross-section, $\dfrac{d\sigma}{d\Omega}$ is defined by,

$$\frac{d\sigma}{d\Omega} = \frac{\text{No. particles scattered into solid angle } d\Omega \text{ per sec.}}{I_0 \times d\Omega}$$

Solid angle subtended by detector at sample is $\Delta\Omega = A/L^2$

From definition of $\dfrac{d\sigma}{d\Omega}$, no. particles detected per sec. = $I_0 \, \Delta\Omega \dfrac{d\sigma}{d\Omega}$

but also, " " " " " = $|\psi^{sc}|^2 v \times A$

$$\rightarrow \quad \frac{d\sigma}{d\Omega} = \frac{|\psi^{sc}|^2}{|\psi_0|^2} L^2$$

Example : isolated nucleus

At detector scattered wave is $\psi^{sc} = -\dfrac{b \exp\{ikL\}}{L}$

$$\rightarrow \quad \frac{d\sigma}{d\Omega} = b^2 = \frac{\sigma}{4\pi}$$

Note:

- units of $\dfrac{d\sigma}{d\Omega}$: barns (steradian)$^{-1}$ (b sr^{-1})

Scattering cross-section for an assembly of stationary nuclei

Recall :
$$\frac{d\sigma}{d\Omega} = \frac{|\psi^{sc}|^2}{|\psi_0|^2} L^2$$

At detector,
$$\psi_o^{sc} = -\frac{b_o \exp\{ikL\}}{L}$$
$$\psi_n^{sc} = -\frac{b_n \exp\{ik(L+\Delta L_n)\}}{(L+\Delta L_n)}$$

What is ΔL_n ?

$$\Delta L_n = An + nB$$
$$= \frac{\mathbf{k}_i \cdot \mathbf{r}_n}{k} - \frac{\mathbf{k}_f \cdot \mathbf{r}_n}{k}$$
$$\rightarrow \quad k\Delta L_n = (\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}_n,$$
$$= \mathbf{Q} \cdot \mathbf{r}_n,$$

Total scattered wave,
$$\psi^{sc} = \sum_n \psi_n^{sc} = -\frac{\exp\{ikL\}}{L} \sum_n b_n \exp\{i\mathbf{Q} \cdot \mathbf{r}_n\}$$

Cross-section :
$$\frac{d\sigma}{d\Omega} = \left|\sum_n b_n \exp\{i\mathbf{Q} \cdot \mathbf{r}_n\}\right|^2$$

Bragg diffraction from a rigid crystal

Crystal is a periodic array of atoms.

Lattice is a periodic array of points representing the periodicity of the crystal. The lattice points are displaced from the origin by lattice vectors

$$\mathbf{l} \;=\; n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}, \qquad (n_1, n_2, n_3 \;\; \textbf{integers})$$

Basis (or motif) is the collection of atoms associated with each lattice point.

Unit cell is a lding block from which the crystal is constructed.

Usually it is a parallelepiped with edges **a**, **b**, **c**:

Cross-section :

$$\frac{d\sigma}{d\Omega} \;=\; \Big|\sum_{n} b_n \exp\{\, i\mathbf{Q}\,.\,\mathbf{r}_n \}\Big|^2$$

Position of nucleus $\mathbf{r}_n$:

$$\mathbf{r}_n \;=\; \mathbf{l} \;+\; \mathbf{d}$$

$$\rightarrow \qquad \frac{d\sigma}{d\Omega} \;=\; \Big|\sum_{\mathbf{l}} \exp\{\, i\mathbf{Q}\,.\,\mathbf{l}\,\} \sum_{\mathbf{d}} b_{\mathbf{d}} \exp\{ i\mathbf{Q}\,.\,\mathbf{d}\,\}\Big|^2$$

Coherent (Bragg) scattering occurs when all terms in **l** sum are equal, i.e.

$$\exp\{\, i\mathbf{Q}\,.\,\mathbf{l}\,\} \;=\; 1 \qquad \textbf{for all } \mathbf{l}$$

Which values of **Q** satisfy this equation? Answer:

$$\mathbf{Q} \;=\; h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \qquad (h, k, l \;\; \textbf{integers})$$

where,

$$\mathbf{a}^* \;=\; (2\pi/v_0)\, \mathbf{b} \times \mathbf{c}, \qquad \mathbf{b}^* \;=\; (2\pi/v_0)\, \mathbf{c} \times \mathbf{a}, \qquad \mathbf{c}^* \;=\; (2\pi/v_0)\, \mathbf{a} \times \mathbf{b}$$

and $\quad v_0 \;=\; \mathbf{a}\,.\,\mathbf{b} \times \mathbf{c} \;=\; \mathbf{b}\,.\,\mathbf{c} \times \mathbf{a} \;=\; \mathbf{c}\,.\,\mathbf{a} \times \mathbf{b}\,.$

Note also that $\mathbf{a}\,.\,\mathbf{a}^* = \mathbf{b}\,.\,\mathbf{b}^* = \mathbf{c}\,.\,\mathbf{c}^* = 2\pi$, **and** $\mathbf{a}\,.\,\mathbf{b}^* = \mathbf{a}\,.\,\mathbf{c}^* = \ldots = 0$

Proof:

Now consider summation over position vector **d**.

Write **d** in terms of fractional coordinates ($x_\mathbf{d}$, $y_\mathbf{d}$, $z_\mathbf{d}$) of nucleus

$$\mathbf{d} = x_\mathbf{d}\mathbf{a} + y_\mathbf{d}\mathbf{b} + z_\mathbf{d}\mathbf{c}$$

When **Q** satisfies the condition $\mathbf{Q} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$, then

$$\frac{d\sigma}{d\Omega} = N^2 \left| \sum_\mathbf{d} b_\mathbf{d} \exp\{ i\,(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \cdot (x_\mathbf{d}\mathbf{a} + y_\mathbf{d}\mathbf{b} + z_\mathbf{d}\mathbf{c}) \} \right|^2$$

$$= N^2 \,|\, F_{hkl} \,|^2 \qquad (N \text{ is the no. unit cells in the crystal})$$

where,

$$F_{hkl} = \sum_\mathbf{d} b_\mathbf{d} \exp\{ 2\pi i\,(hx_\mathbf{d} + ky_\mathbf{d} + lz_\mathbf{d}) \}$$

F_{hkl} is known as the **structure factor** for the reflection hkl.

Reciprocal Lattice

Paul Peter Ewald
(1888–1985)
The inventor of the
reciprocal lattice

Max von Laue
(1879–1960)
Nobel Prize (1914)

Strong elastic scattering occurs when

$$\mathbf{Q} = \mathbf{G}_{hkl} \qquad \text{(Laue condition)}$$

where, $\mathbf{G}_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$

The set of all vectors $\{\mathbf{G}_{hkl}\}$ is called the Reciprocal Lattice.

2 properties:

(i) $\mathbf{G}_{hkl}$ is normal to the plane (hkl).

(ii) $|\mathbf{G}_{hkl}| = 2\pi/d_{hkl}$

Bragg ≡ Laue:

$$|\mathbf{Q}| = |\mathbf{G}_{hkl}| \qquad \text{Laue Condition}$$

$$\rightarrow \quad \frac{4\pi}{\lambda}\sin\theta = 2\pi/d_{hkl}$$

$$\rightarrow \quad \lambda = 2d\sin\theta \qquad \text{Bragg's Law}$$

Summary of Lecture 2

- σ = total scattering cross-section
  – probability that the neutron is scattered

- $\dfrac{d\sigma}{d\Omega}$ = differential scattering cross-section
  – probability that the neutron is scattered into a specified direction

- For elastic scattering from a rigid structure

$$\frac{d\sigma}{d\Omega} = \left| \sum_n b_n \exp\{ i\mathbf{Q}\cdot\mathbf{r}_n \} \right|^2$$

- For a rigid crystal, Bragg scattering occurs when

$$\mathbf{Q} = \mathbf{G}_{hkl} \qquad \text{(Laue condition)}$$

where,

$$\mathbf{G}_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \qquad \text{(reciprocal lattice vectors)}$$

The cross-section for Bragg scattering is given by

$$\frac{d\sigma}{d\Omega} = N^2 \, | \, F_{hkl} |^2$$

where,

$$F_{hkl} = \sum_{\mathbf{d}} b_{\mathbf{d}} \exp\{ 2\pi i \, (hx_{\mathbf{d}} + ky_{\mathbf{d}} + lz_{\mathbf{d}}) \} \qquad \text{(structure factor)}$$

- Corollary: for a non-rigid crystal:

$$F_{hkl} = \sum_{\mathbf{d}} \exp(-W_{\mathbf{d}}) \; b_{\mathbf{d}} \exp\{ 2\pi i \, (hx_{\mathbf{d}} + ky_{\mathbf{d}} + lz_{\mathbf{d}}) \}$$

Coherent and Incoherent (nuclear) Scattering

$$\frac{d\sigma}{d\Omega} = |\sum_n b_n \exp\{i\mathbf{Q}\cdot\mathbf{r}_n\}|^2$$

Recall: b_n characterizes the range of the neutron–nucleus interaction.

b_n depends upon :

(i) which element;

(ii) which isotope;

(iii) relative spins of neutron and nucleus.

In principle, we can calculate $\frac{d\sigma}{d\Omega}$ exactly if we know the isotope and spin state of every nucleus. Not feasible in practice.

Simplifying assumption

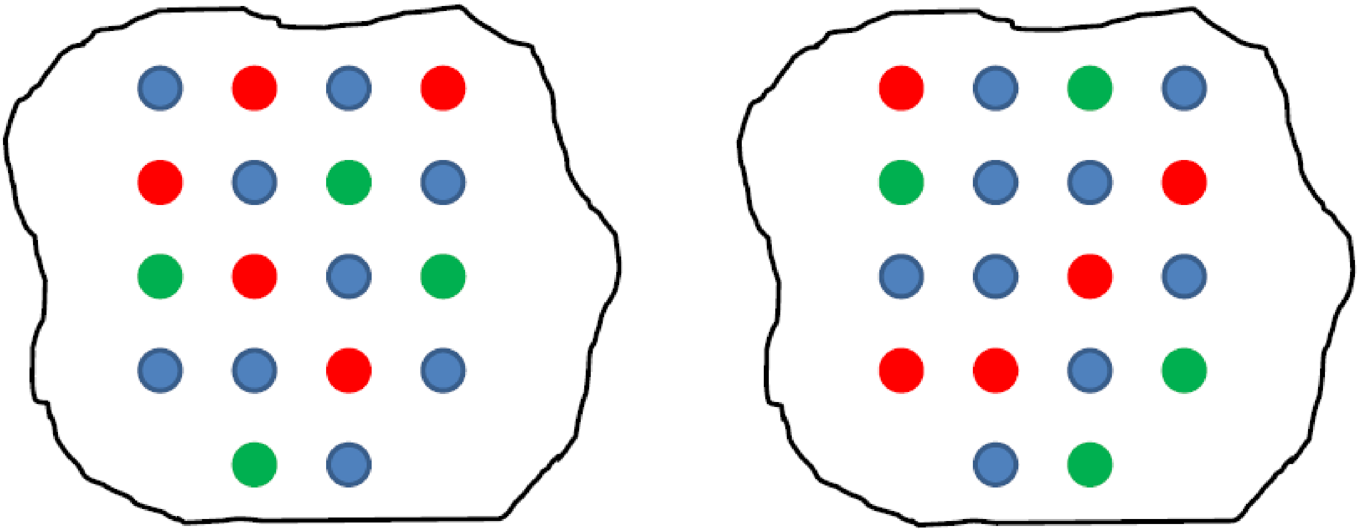
Assume that distribution of isotopes and spin states is random and uncorrelated between the sites.

$\rightarrow$ $\frac{d\sigma}{d\Omega}$ for one particular sample is the same as the average over many samples with same nuclear positions

$$\rightarrow \qquad \frac{d\sigma}{d\Omega} \approx \overline{\frac{d\sigma}{d\Omega}} \qquad \text{ensemble average}$$

In order to proceed we need $\overline{b}$ and $\overline{b^2}$

Ensemble averaging



Suppose sample contains only 1 type of atom, which has 3 different isotopes:

isotope r	natural abundance c_r	scattering length b_r
●	50 %	b_B
●	25 %	b_R
●	25 %	b_G

$$\bar{b} = 0.5\, b_B + 0.25\, b_R + 0.25\, b_G$$

$$\overline{b^2} = 0.5\, b_B^2 + 0.25\, b_R^2 + 0.25\, b_G^2$$

In general (see Section E of tutorial problems),

$$\bar{b} = \sum_r c_r b_r = \sum_r c_r (w_r^+ b_r^+ + w_r^- b_r^-)$$

$$\overline{b^2} = \sum_r c_r b_r^2 = \sum_r c_r [w_r^+ (b_r^+)^2 + w_r^- (b_r^-)^2]$$

Note that, $$\frac{d\sigma}{d\Omega} = \left|\sum_n b_n \exp\{i\mathbf{Q}\cdot\mathbf{r}_n\}\right|^2$$

$$= \sum_n\sum_m b_n b_m \exp\{i\mathbf{Q}\cdot(\mathbf{r}_n - \mathbf{r}_m)\}$$

Ensemble averaging $\rightarrow$ replace $b_n b_m$ by $\overline{b_n b_m}$

Sites uncorrelated $\rightarrow$ $\overline{b_n b_m} = \bar{b}_n \bar{b}_m$ if $n \neq m$

$= \overline{b_n^2}$ if $n = m$

Therefore,

$$\overline{\frac{d\sigma}{d\Omega}} = \sum_{n\neq m}\sum \bar{b}_n \bar{b}_m \exp\{i\mathbf{Q}\cdot(\mathbf{r}_n - \mathbf{r}_m)\} + \sum_{n=m} \overline{b_n^2}$$

$$= \sum_n\sum_m \bar{b}_n \bar{b}_m \exp\{i\mathbf{Q}\cdot(\mathbf{r}_n - \mathbf{r}_m)\} + \sum_{n=m} (\overline{b_n^2} - \bar{b}_n^2)$$

coherent scattering incoherent scattering

coherent scattering — correlations between the same, and different nuclei — interference, structure (also collective dynamics)

incoherent scattering — no information on structure — 'flat background' (also dynamics of single particles)

Values of $\bar{b}$ and $\overline{b^2}$ are tabulated (e.g. *Neutron News* vol. 3 No. 3 (1992) 29–37; http://www.ncnr.nist.gov/resources/n-lengths/; A. T. Boothroyd, *Principles of Neutron Scattering from Condensed Matter*, Appendix A).

Often written as $\sigma_{coh} = 4\pi\bar{b}^2$

and $\sigma_{inc} = 4\pi\,(\overline{b^2} - \bar{b}^2)$

Examples

	σ_{coh} (barns)	σ_{inc} (barns)
hydrogen	1.8	80.2
carbon	5.6	0
vanadium	0	5

Examples of coherent and incoherent scattering

(i) Bragg diffraction from a powdered crystal

(i) Elastic scattering from a liquid or glass

Magnetic Scattering

- Neutron is uncharged, but possesses a magnetic dipole moment $\boldsymbol{\mu}_n$ ($\sim 0.001\mu_B$) which can interact with magnetic fields from <u>unpaired</u> electrons via :

  (i) the intrinsic spin dipole moment of the electron,
  (ii) magnetic fields produced by orbital motion of electrons.

- Strength of magnetic interaction: $\sigma_{mag} \sim r_0^2 \sim 0.1$ barn
  " " nuclear " $\sigma_{coh} \sim b^2 \sim 1$ barn

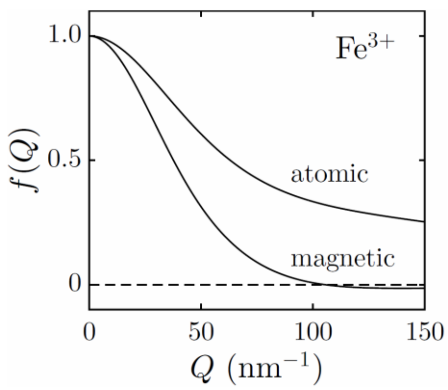
  so similar magnitude (r_0 = classical electron radius = 2.82 fm)

- Theory similar to nuclear scattering except scatter from magnetic moments in sample, and this occurs via a vector interaction

$$\begin{aligned} V_M(\mathbf{r}) &= -\boldsymbol{\mu}_n . \mathbf{B}(\mathbf{r}) \\ V_M(\mathbf{Q}) &= -\boldsymbol{\mu}_n . \mathbf{B}_\perp(\mathbf{Q}) \\ &= -\mu_0 \boldsymbol{\mu}_n . \mathbf{M}_\perp(\mathbf{Q}) \end{aligned}$$

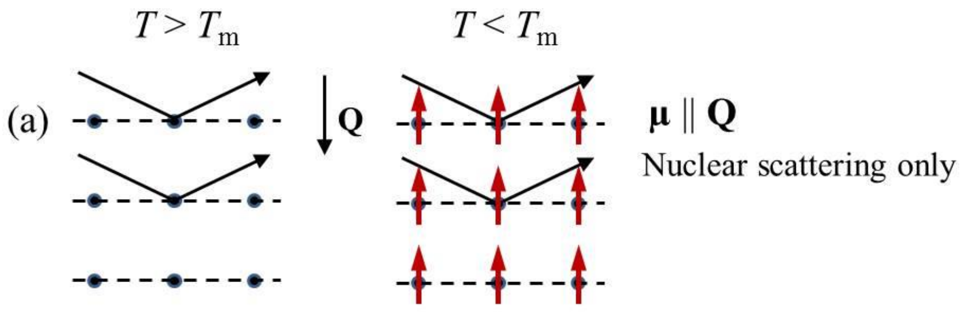
- Neutron probes component of the magnetization perpendicular to **Q**.

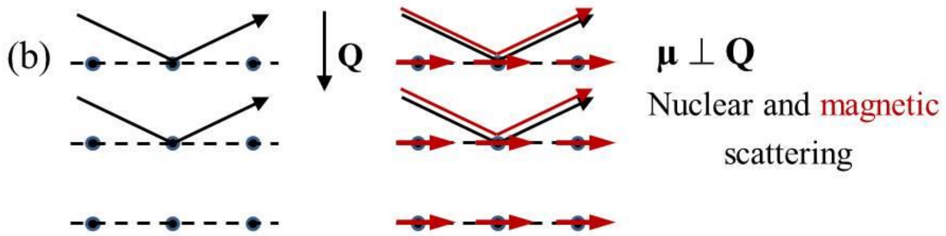
- Neutrons scatter from electrons in atomic orbitals :
  Smeared out in space
  $\rightarrow$ weaker scattering at higher angles
  (like Debye-Waller factor)
  Intensity fall-off described by a magnetic form factor
  (similar to atomic form factor used in x-ray diffraction)



Diffraction from a Magnetic Structure

1. Ferromagnet



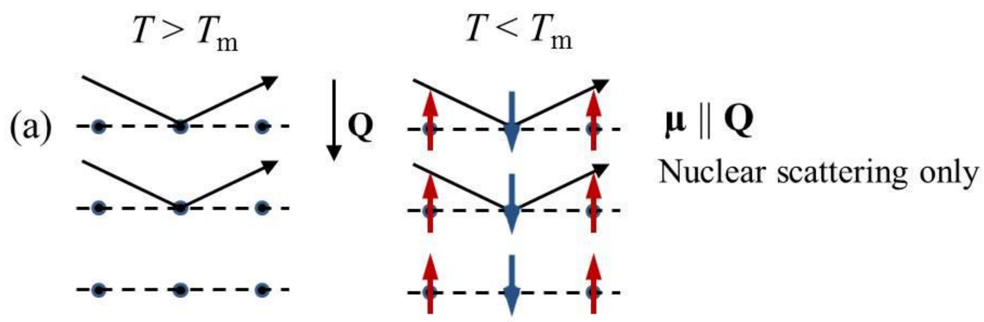


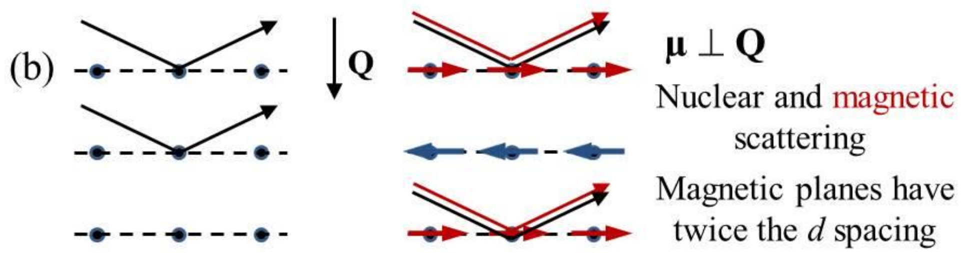
$I_M \propto \sin^2\theta \,|F_M|^2$ (θ is angle between $\boldsymbol{\mu}$ and $\mathbf{Q}$)

where,

$F_M = \sum_j f_j(Q)\, e^{-W_j} \mu_j \exp(\,i\mathbf{Q}.\mathbf{r}_j)$ *Magnetic structure factor (collinear)*

2. Antiferromagnet





Neutron Polarization

- Neutron has spin 1/2, so moment is ↑or ↓ relative to a magnetic field. Can have different scattering cross-sections according to the neutron spin state before and after scattering:

$$\begin{array}{ccc} \uparrow & \rightarrow & \uparrow \\ \uparrow & \rightarrow & \downarrow \\ \downarrow & \rightarrow & \uparrow \\ \downarrow & \rightarrow & \downarrow \end{array}$$

[or $\mathbf{P}_i \rightarrow \mathbf{P}_f$ if initial and final field directions different]

→ polarization analysis

- Torque on magnetic dipole moment in magnetic field **B** is

$$\mathbf{T} = \boldsymbol{\mu} \times \mathbf{B}$$

Eq. of motion:

Torque = rate of change of angular momentum

and angular momentum $\propto \boldsymbol{\mu}$

$$\rightarrow \qquad \frac{d\boldsymbol{\mu}}{dt} \propto \boldsymbol{\mu} \times \mathbf{B}$$

Consider 2 cases :

(i) $\boldsymbol{\mu}$ parallel to **B**

no change in neutron spin state ('non- spin-flip scattering')

(ii) $\boldsymbol{\mu}$ perpendicular to **B**

neutron spin precesses in field ('spin-flip scattering')

Neutron Inelastic Scattering

Kinematics (again)

Scattering triangle ($\mathbf{k}_i \neq \mathbf{k}_f$) :

$\mathbf{k}_i$ = incident wavevector
$\mathbf{k}_f$ = final scattered wavevector

$\mathbf{Q}$ = scattering vector

- Momentum transfer $\hbar\mathbf{Q} = \hbar(\mathbf{k}_i - \mathbf{k}_f)$
- Energy transfer $\hbar\omega = E_i - E_f = \dfrac{\hbar^2}{2m}(k_i^2 - k_f^2)$

A scattering event is characterised by $(\mathbf{Q}, \omega)$

Accessible region of $(\mathbf{Q}, \omega)$ space :

Neutron Cross-Section

Suppose detector can analyse energy of neutrons.

Define the *double differential scattering cross-section* :

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\begin{array}{l}\text{No. particles scattered per sec. into solid angle } d\Omega \\ \text{with final energies between } E_f \text{ and } E_f + dE_f\end{array}}{I_0 \times d\Omega \times dE_f}$$

Numerator depends implicitly on 5 factors :

(i) $d\Omega$

(ii) dE_f

(iii) speed of scattered neutrons, $v_f = \hbar k_f / m$

(iv) density of incident neutrons $|\psi_0|^2$

(v) $S(\mathbf{Q},\omega)$, the probability that system can change its energy by an amount $\hbar\omega$, accompanied by a momentum change $\hbar\mathbf{Q}$

In denominator, remember $I_0 = |\psi_0|^2 v_i = |\psi_0|^2 \hbar k_i / m$

Hence, these factors together give

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} S(\mathbf{Q},\omega)$$

<u>Notes :</u>

- $S(\mathbf{Q},\omega)$ contains all the physics of the system
  – scattering function/
  response function/
  dynamical structure factor

- the k_f/k_i factor is sometimes important, for example if the neutron loses a lot of energy ($k_f << k_i$) then the intensity is much reduced.

Scattering from lattice vibrations in a crystal

(Example of coherent inelastic scattering)

Phonon – quantum of lattice vibrational energy

Consider 1-*d* chain of identical atoms:

(1) Transverse vibrational mode

(2) Longitudinal vibrational mode (sound wave)

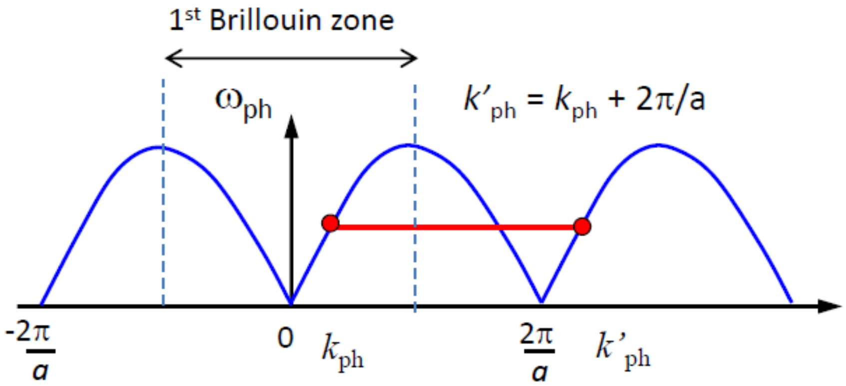
- Equivalent wavevectors

In general,

$\mathbf{k}_{ph}$ and $\mathbf{k}_{ph} + \mathbf{G}$ represent the same mode of vibration

- Phonon dispersion curve

Energy $\hbar\omega_{ph}$ of a phonon depends on $\boldsymbol{k}_{ph}$



- Scattering from phonons

Peaks occur when
$$\begin{cases} \hbar\omega = \hbar\omega_{ph} \\ \hbar\mathbf{Q} = \hbar(\mathbf{k}_{ph} + \mathbf{G}) \end{cases}$$

(1) Longitudinal :

(2) Transverse :

- Inelastic scattering cross-section for phonons

Consider a *static* sinusoidal distortion of the lattice:

Position of n^{th} atom $\quad x_n = na + u \sin(k_{\text{ph}} na)$

Elastic scattering cross-section :

$$\frac{d\sigma}{d\Omega} = \Big|\sum_n b_n \exp\{ i\mathbf{Q} \cdot \mathbf{r}_n \}\Big|^2$$

$$= \Big|\sum_n b \exp\{ iQ\,(na + u \sin(k_{\text{ph}} na) \}\Big|^2$$

Can make Taylor expansion in Qu when $Qu << 1$:

$$\rightarrow \quad \frac{d\sigma}{d\Omega} = \Big|\sum_n b\ [\underset{(1)}{1} + \underset{(2)}{iQu \sin(k_{\text{ph}} na)} + \ldots] \exp\{ iQ\, na \}\Big|^2$$

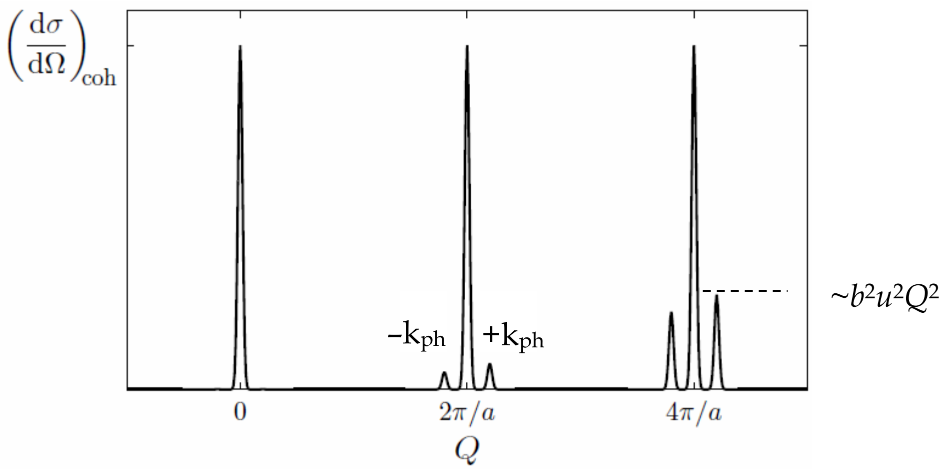
1st term (1)

$\rightarrow$ Bragg peak at $Q = m\,(2\pi/a)$ $\quad$ (m = integer)
Intensity $\propto b^2$

2nd term (2): write $\sin x = (e^{ix} - e^{-ix})/2i$

$$\rightarrow \quad \Big|\sum_n bQu\,[\exp\{ i(Q + k_{\text{ph}})na \} - \exp\{ i(Q - k_{\text{ph}})na \}]\Big|^2$$

$\rightarrow$ peaks at $Q = m\,(2\pi/a) \pm k_{\text{ph}}$
Intensity $\propto b^2 Q^2 u^2$



Lattice vibration – dynamic, sinusoidal distortion of the lattice

Inelastic scattering cross-section as for static case but conserve energy as well

$\rightarrow$ Peaks in $\frac{d^2\sigma}{d\Omega dE_f}$ when $\begin{cases} \hbar\omega = \pm\hbar\omega_{ph} \\ \hbar\mathbf{Q} = \hbar(\mathbf{G} \pm \mathbf{k}_{ph}) \end{cases}$

$$\text{Intensity} \quad \propto b^2Q^2u^2$$

$$\propto \frac{b^2(\mathbf{Q}\cdot\hat{\mathbf{u}})^2}{\omega_{ph}} \qquad (u^2 \propto 1/\omega_{ph})$$

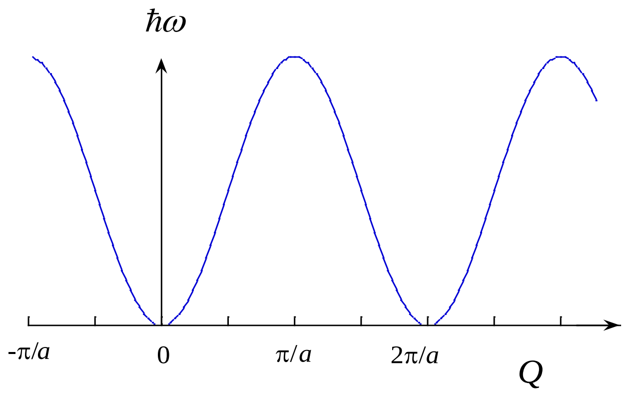
Spin Waves

Ground state of ferromagnet:

Displace one spin:

Displacement propagates through lattice as wave with wavevector k_{mag}

Magnon dispersion curve :



Notes

- Angular momentum (spin) of the crystal is reduced by 1 unit (of $\hbar$)
  $\rightarrow$ spin of neutron changes by 1 unit to conserve angular momentum

  $\rightarrow$ spin flip scattering

- Intensity varies with magnetic form factor – decreases with $|\mathbf{Q}|$.

Principle of Detailed Balance

General property of $S(\mathbf{Q},\omega)$

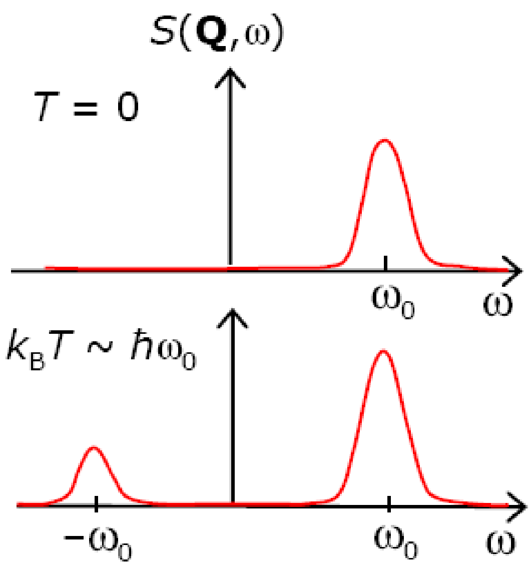
Consider neutron energy loss and energy gain processes:

For <u>any</u> neutron inelastic scattering process,

$$S(\mathbf{Q}, -\omega) \quad = \quad \exp(-\hbar\omega/k_BT) \times S(\mathbf{Q}, \omega)$$

neutron energy gain neutron energy loss

Principle of Detailed Balance



Summary of Coherent Inelastic Scattering

- Double differential scattering cross-section :

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} S(\mathbf{Q},\omega)$$

- Propagating excitations (e.g. lattice vibs., spin waves) $S(\mathbf{Q},\omega)$ has peaks

$$\text{when} \quad \begin{cases} \hbar\omega = \pm\hbar\omega_{ph} \\ \hbar\mathbf{Q} = \hbar(\mathbf{G} \pm \mathbf{k}_{ph}) \end{cases}$$

- The size of the peaks in $S(\mathbf{Q},\omega)$ varies according to

  (i) Phonons

$$S(\mathbf{Q},\omega) \propto \exp\{-2W(Q,T)\} \times |F_{ph}(\mathbf{Q})|^2 \times [\,n(\omega_{ph}) + 1\,] \times \frac{1}{\omega_{ph}} \times (\mathbf{Q}.\hat{\boldsymbol{u}})^2$$

  (ii) Spin waves

$$S(\mathbf{Q},\omega) \propto \exp\{-2W(Q,T)\} \times |F_{mag}(\mathbf{Q})|^2 \times [\,n(\omega_{mag}) + 1\,] \times \frac{1}{\omega_{mag}} \times f^2(Q)$$

- Excitations can be measured in neutron energy loss or neutron energy gain, but remember that $S(\mathbf{Q},\omega)$ has the property,

$$S(\mathbf{Q},-\omega) = \exp(-\hbar\omega/k_B T) \times S(\mathbf{Q},\omega)$$