



# 18th Oxford School on Neutron Scattering

3 to 13 September, 2024

## Introductory Theory

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*Oxford University*



# Books on Neutron Scattering

- General (with introductory theory)

Willis, B.T.M. and Carlile, C.G.

*Experimental Neutron Scattering*,

O.U.P., 2009, ~£58

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, ~£60

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, Free to you!

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, ~£95 and £68

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), ~£45;

More elementary than Lovesey, excellent for basic theory

Sivia, D.S.

*Elementary Scattering Theory for X-ray and Neutron Users*

O.U.P., 2011, ~£40

Basic principles of neutron scattering from a wave perspective

- Online: [www.neutronsources.org](http://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  $\Delta x$  to define  $\lambda$  better:

Decrease  $\Delta x$  to define position better,  
but lose information on  $\lambda$ .

Cannot define both  $\Delta x$  and  $\lambda$  to arbitrary precision  
(Heisenberg's Uncertainty Principle)

- Kinematics — Einstein, de Broglie

1) Energy:  $E = hf$   $h = \text{Planck's constant}$   
 $= \hbar\omega$   $f = \text{frequency}$   
 $\hbar = h/2\pi, \quad \omega = 2\pi f$

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

# 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:

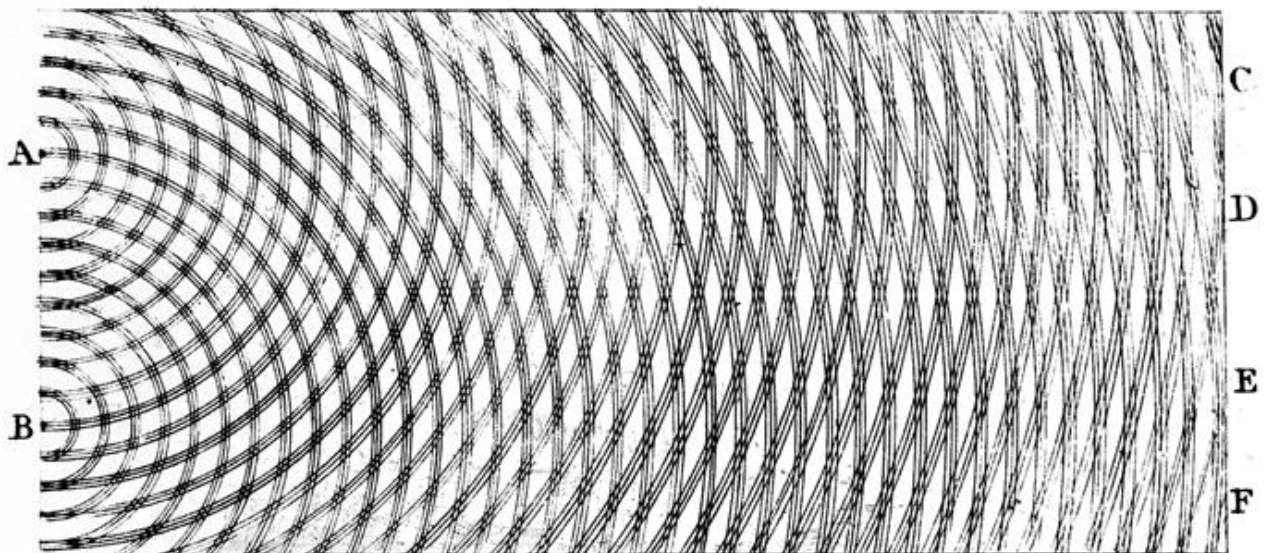
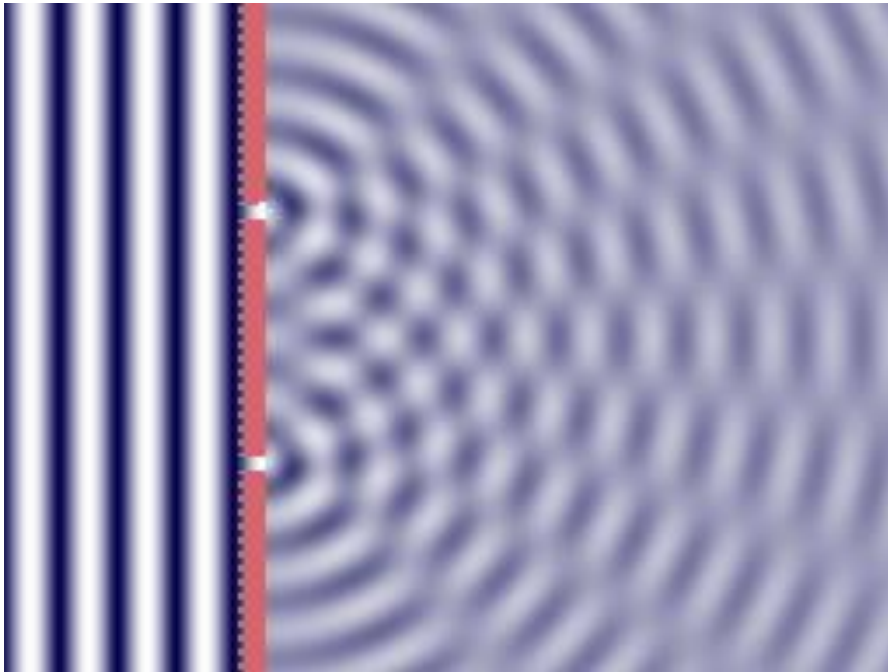
- Assumption – small fraction are scattered
- Justification – nuclear potential is short range  
most neutrons 'miss' nucleus

Born  
Approximation

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



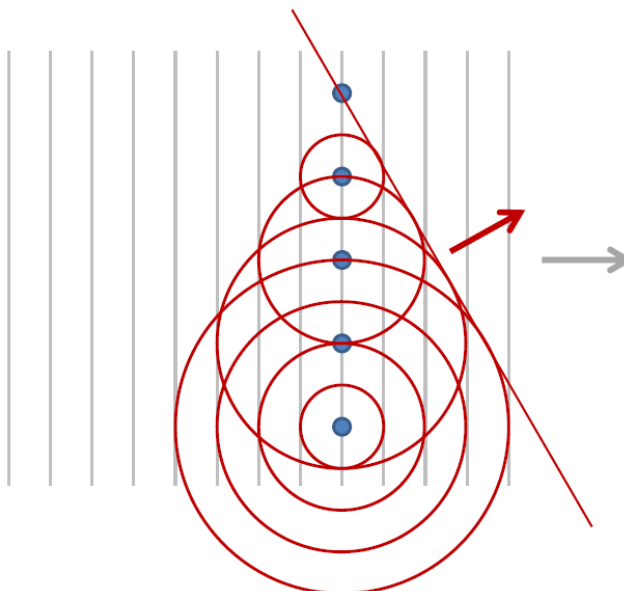
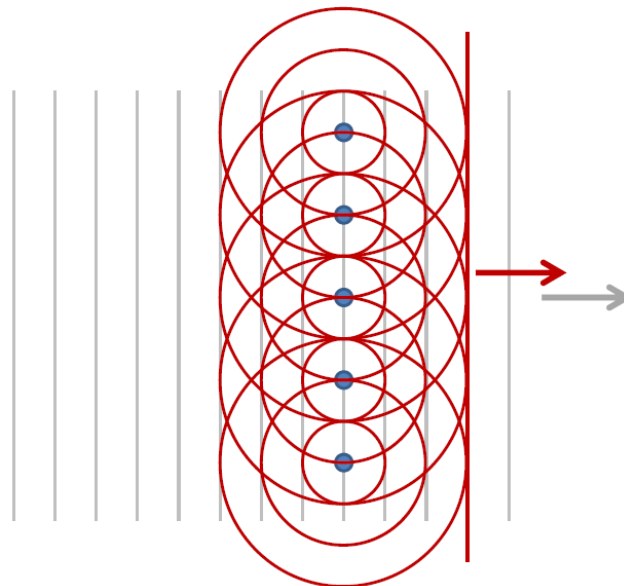
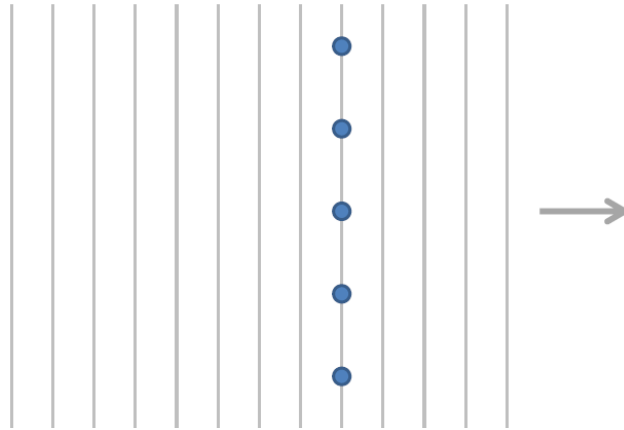
Wave interference from 2 slits:



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 =  $\lambda$

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

Suppose path difference =  $2\lambda$ :

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

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  $\sim N$   
elsewhere, amplitude  $\sim 1$



# Elastic Scattering from a Crystal

## a) Normal Incidence

In general,  $AA' \neq AB$ , 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

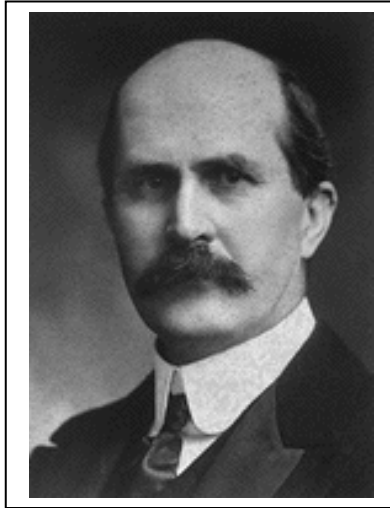
This time,  $AA' = BB'$ , so always achieve constructive interference from successive columns of atoms.

Hence, diffraction from a crystal occurs when

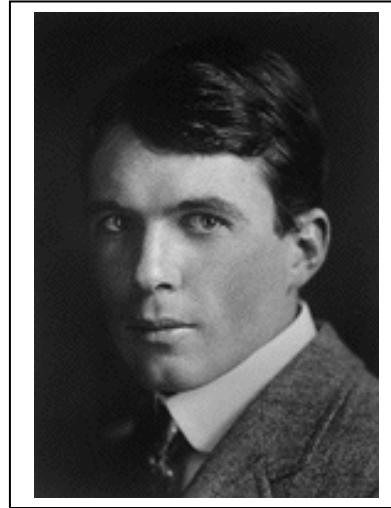
$$n\lambda = 2d \sin \theta \quad (\text{Bragg's Law})$$



# 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 →  $d$ -spacings  
→ crystal structure
- Braggs shared Nobel Prize in Physics (1915)

# Debye-Waller factor

In reality, nuclei are not stationary:

Instantaneous positions

Time-average

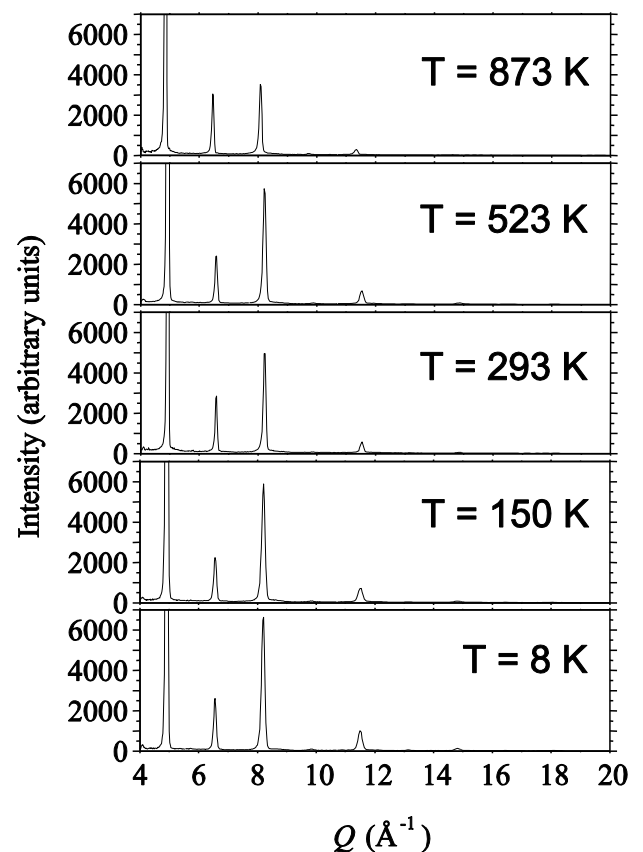
- causes decrease in intensity of diffracted beam because waves are not so well in phase.
- Effect worsens as  $k$  ( $=2\pi/\lambda$ ) and  $\theta$  increase

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

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

Debye-Waller  
Factor

Single crystal diffraction data from  $\text{Nd}_{0.5}\text{Pb}_{0.5}\text{MnO}_3$  taken on the SXD diffractometer, courtesy of Dr Dave Keen (ISIS).



# Particle Waves (again)

Two of the 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  $dV$  is  $|\psi(\mathbf{r})|^2 dV$ .

## Examples

(i) Infinite plane wave :

$$\begin{aligned}\psi &= \exp \{ ikz \} \quad (= \cos kz + i \sin kz) \\ |\psi|^2 &= \psi \psi^* \\ &= \exp \{ ikz \} \exp \{ -ikz \} \\ &= 1\end{aligned}$$

→ 1 particle per unit volume everywhere

(ii) Spherical wave :

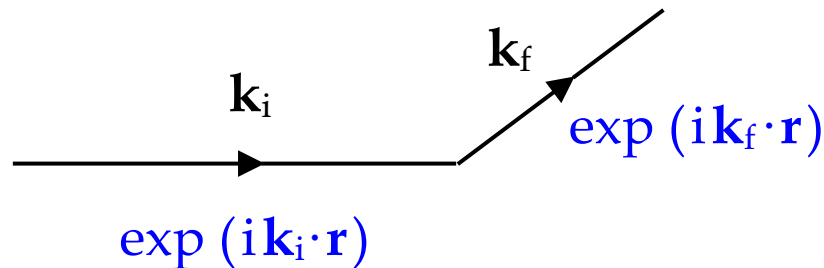
$$\begin{aligned}\psi &= -\frac{b \exp \{ ikr \}}{r} \\ |\psi|^2 &= b^2 / r^2\end{aligned}$$

→ 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:

$$\text{Scattering probability} \sim |M|^2$$

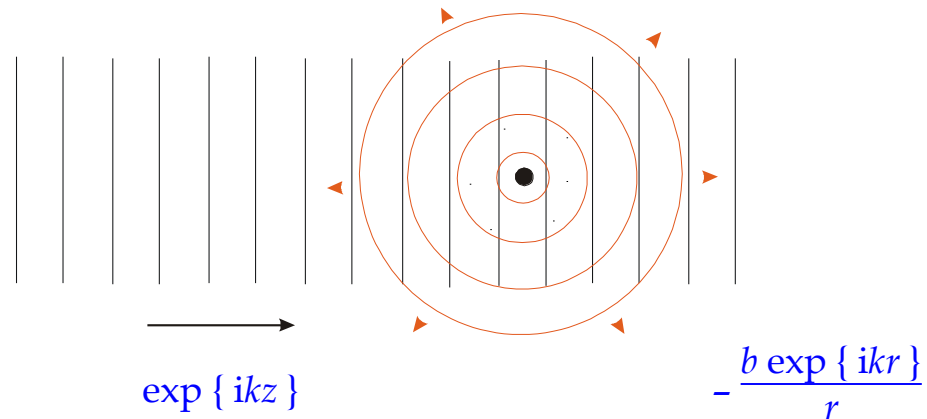
where

$$\begin{aligned} M &= \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}) V(\mathbf{r}) \exp(i\mathbf{k}_i \cdot \mathbf{r}) d^3\mathbf{r} \\ &= \int V(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r} \quad (\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f) \\ &= V(\mathbf{Q}) \quad \text{--- Fourier transform of } V(\mathbf{r}) \end{aligned}$$

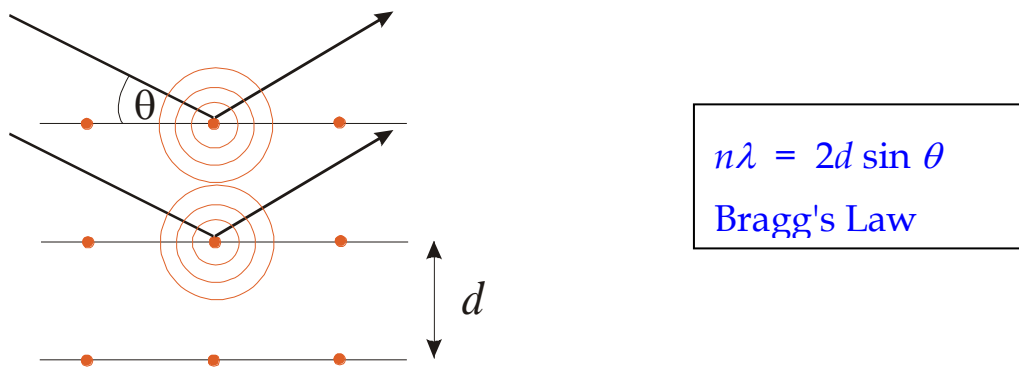
Neutron scattering is determined by the Fourier transform of the interaction potential (exception is reflectometry).

## 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:



$d$  = spacing between planes

$\theta$  = 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  $\sigma$  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  $a$

$$\text{No. particles scattered per sec.} = I_0 \times \pi a^2$$

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

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

$$\begin{aligned} \text{Incident wave, } \psi_0 &= \exp \{ ikz \} \\ \text{Incident flux, } I_0 &= |\psi_0|^2 v = v \end{aligned}$$

$$\text{Scattered wave, } \psi^{\text{sc}} = -\frac{b \exp \{ ikr \}}{r}$$

$$\begin{aligned} \text{Scattered flux, } I^{\text{sc}} &= |\psi^{\text{sc}}|^2 v = b^2 v / r^2 \\ &\text{at distance } r \end{aligned}$$

$$\begin{aligned} \text{Total no. particles scattered per sec.} &= I^{\text{sc}} \times \text{total area} \\ &= b^2 v / r^2 \times 4\pi r^2 \\ &= 4\pi b^2 v \end{aligned}$$

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

## Notes:

- $\sigma$  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  
       "      "  $\sigma$ : barn (b)      1 barn =  $10^{-28}$  m<sup>2</sup>

## Differential cross-section

Differential cross-section,  $\frac{d\sigma}{d\Omega}$  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  $\frac{d\sigma}{d\Omega}$ , no. particles detected per sec. =  $I_0 \Delta\Omega \frac{d\sigma}{d\Omega}$

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

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

Example: isolated nucleus

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

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

## Note:

- units of  $\frac{d\sigma}{d\Omega}$ : barns (steradian)<sup>-1</sup> (b sr<sup>-1</sup>)



## 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,

$$\begin{aligned}\psi_0^{sc} &= -\frac{b_o \exp\{ikL\}}{L} \\ \psi_n^{sc} &= -\frac{b_n \exp\{ik(L+\Delta L_n)\}}{(L+\Delta L_n)}\end{aligned}$$

What is  $\Delta L_n$  ?

$$\begin{aligned}\Delta L_n &= An + nB \\ &= \frac{\mathbf{k}_i \cdot \mathbf{r}_n}{k} - \frac{\mathbf{k}_f \cdot \mathbf{r}_n}{k}\end{aligned}$$

$$\begin{aligned}\rightarrow k\Delta L_n &= (\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}_n, \\ &= \mathbf{Q} \cdot \mathbf{r}_n,\end{aligned}$$

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

$$\mathbf{l} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}, \quad (n_1, n_2, n_3 \text{ integers})$$

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

**Unit cell** is a building block from which the crystal is constructed.

Usually, the unit cell is chosen to be a parallelepiped with edges **a**, **b**, **c**:

Cross-section :

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

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

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

$$\rightarrow \frac{d\sigma}{d\Omega} = \left| \sum_{\mathbf{l}} \exp \{ i\mathbf{Q} \cdot \mathbf{l} \} \sum_{\mathbf{d}} b_{\mathbf{d}} \exp \{ i\mathbf{Q} \cdot \mathbf{d} \} \right|^2$$

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

$$\exp \{ i\mathbf{Q} \cdot \mathbf{l} \} = 1 \quad \text{for all } \mathbf{l}$$

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

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

where,

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

and  $v_0 = \mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = \mathbf{b} \cdot \mathbf{c} \times \mathbf{a} = \mathbf{c} \cdot \mathbf{a} \times \mathbf{b}$ .

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

Proof:

Now consider summation over position vector  $\mathbf{d}$ .

Write  $\mathbf{d}$  in terms of fractional coordinates  $(x_d, y_d, z_d)$  of nucleus

$$\mathbf{d} = x_d \mathbf{a} + y_d \mathbf{b} + z_d \mathbf{c}$$

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

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= N^2 \left| \sum_{\mathbf{d}} b_d \exp \{ i (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \cdot (x_d \mathbf{a} + y_d \mathbf{b} + z_d \mathbf{c}) \} \right|^2 \\ &= N^2 |F_{hkl}|^2 \quad (N \text{ is the no. unit cells in the crystal}) \end{aligned}$$

where,

$$F_{hkl} = \sum_{\mathbf{d}} b_d \exp \{ 2\pi i (hx_d + ky_d + lz_d) \}$$

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

# Reciprocal Lattice

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



Strong elastic scattering occurs when

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

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**.



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

2 properties:

- (i)  $\mathbf{G}_{hkl}$  is normal to the plane  $(hkl)$ .
- (ii)  $|\mathbf{G}_{hkl}| = 2\pi/d_{hkl}$

Bragg  $\equiv$  Laue:

$$\begin{aligned} |\mathbf{Q}| &= |\mathbf{G}_{hkl}| && \text{Laue Condition} \\ \rightarrow \frac{4\pi}{\lambda} \sin \theta &= 2\pi/d_{hkl} \\ \rightarrow \lambda &= 2d \sin \theta && \text{Bragg's Law} \end{aligned}$$

## Summary of Lecture 2

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

- For nuclear 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

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

where,

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

The cross-section for nuclear Bragg scattering is given by

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

where,

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

- 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

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

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

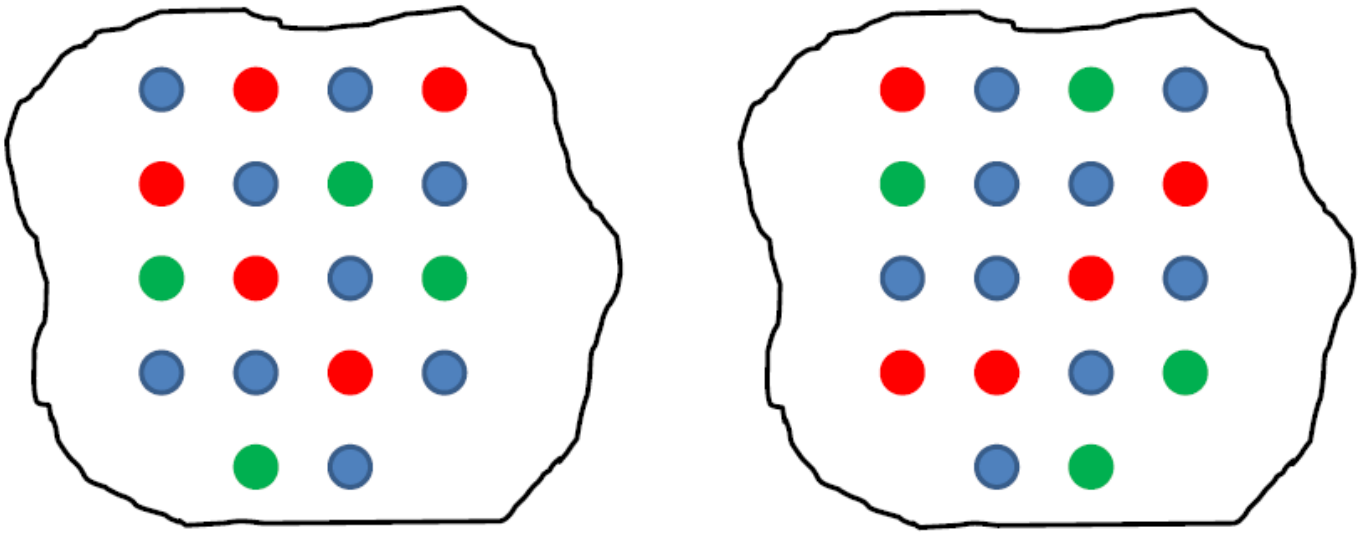
Assume that distribution of isotopes and spin states is **random** and **uncorrelated** between the sites.

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

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

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

## Ensemble averaging



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

isotope	natural abundance	scattering length
$r$	$c_r$	$b_r$
<span style="color: blue;">●</span>	50 %	$b_B$
<span style="color: red;">●</span>	25 %	$b_R$
<span style="color: green;">●</span>	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,

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \left| \sum_n b_n \exp \{ i\mathbf{Q} \cdot \mathbf{r}_n \} \right|^2 \\ &= \sum_n \sum_m b_n b_m \exp \{ i\mathbf{Q} \cdot (\mathbf{r}_n - \mathbf{r}_m) \}\end{aligned}$$

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

Sites uncorrelated  $\rightarrow$

$$\begin{aligned}\overline{b_n b_m} &= \bar{b}_n \bar{b}_m & \text{if } n \neq m \\ &= \bar{b}_n^2 & \text{if } n = m\end{aligned}$$

Therefore,

$$\begin{aligned}\overline{\frac{d\sigma}{d\Omega}} &= \sum_{n \neq m} \bar{b}_n \bar{b}_m \exp \{ i\mathbf{Q} \cdot (\mathbf{r}_n - \mathbf{r}_m) \} + \sum_{n=m} \bar{b}_n^2 \\ &= \sum_n \sum_m \bar{b}_n \bar{b}_m \exp \{ i\mathbf{Q} \cdot (\mathbf{r}_n - \mathbf{r}_m) \} + \sum_{n=m} (\bar{b}_n^2 - \bar{b}_n^2) \\ &= \underbrace{\left| \sum_n \bar{b}_n \exp \{ i\mathbf{Q} \cdot \mathbf{r}_n \} \right|^2}_{\text{coherent scattering}} + \underbrace{\sum_n (\sigma_{\text{inc}})_n / 4\pi}_{\text{incoherent scattering}}\end{aligned}$$

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  $\bar{b}^2$  are tabulated:

e.g. *Neutron News* vol. 3 No. 3 (1992) 29–37;

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

A. T. Boothroyd, *Principles of Neutron Scattering from Condensed Matter*, Appendix A.

Often written as  $\sigma_{\text{coh}} = 4\pi \bar{b}^2$   
and  $\sigma_{\text{inc}} = 4\pi (\bar{b}^2 - \bar{b}^2)$

### Examples

	$\sigma_{\text{coh}}$ (barns)	$\sigma_{\text{inc}}$ (barns)
hydrogen	1.8	80.3
carbon	5.6	0
vanadium	0.0	5

### Effect of coherent and incoherent scattering on data

(i) Bragg diffraction from a powdered crystal

(i) Elastic scattering from a liquid or glass

# Magnetic Scattering

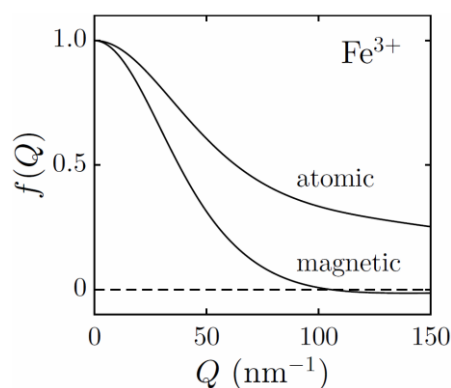
- Neutron is uncharged, but possesses a magnetic dipole moment  $\mu_n \sim 0.001\mu_B$  which can interact with magnetic fields from unpaired electrons via :
  - (i) the intrinsic spin dipole moment of the electron,
  - (ii) magnetic fields produced by orbital motion of electrons.
- Strength of magnetic 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**

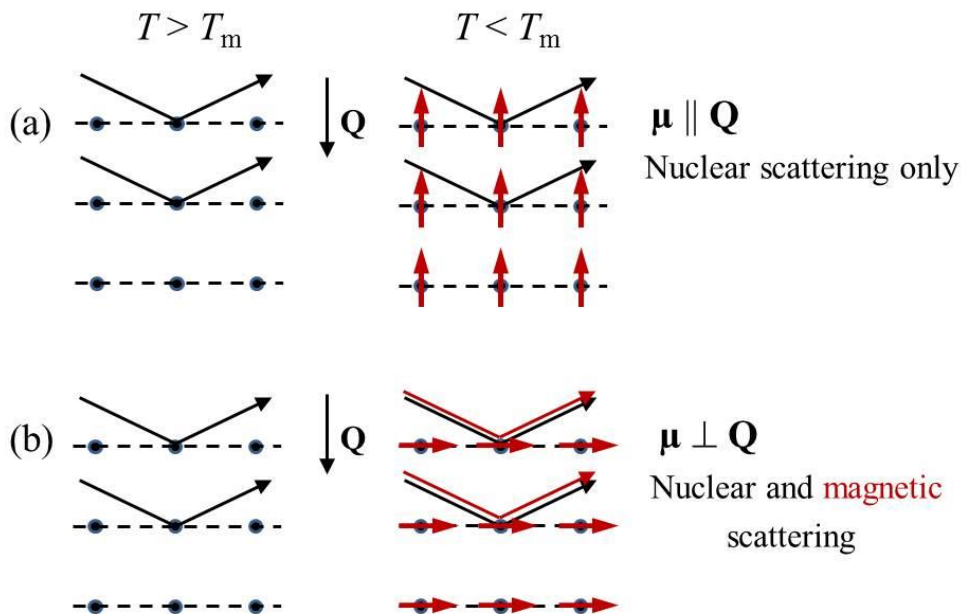
$$\begin{aligned} V_M(\mathbf{r}) &= -\boldsymbol{\mu}_n \cdot \mathbf{B}(\mathbf{r}) \\ V_M(\mathbf{Q}) &= -\boldsymbol{\mu}_n \cdot \mathbf{B}_\perp(\mathbf{Q}) \\ &= -\mu_0 \boldsymbol{\mu}_n \cdot \mathbf{M}_\perp(\mathbf{Q}) \end{aligned}$$

- Neutron probes component of the magnetization **perpendicular to  $\mathbf{Q}$** .
- Neutrons scatter from unpaired electrons in atomic orbitals :  
Smeared out in space  
→ 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



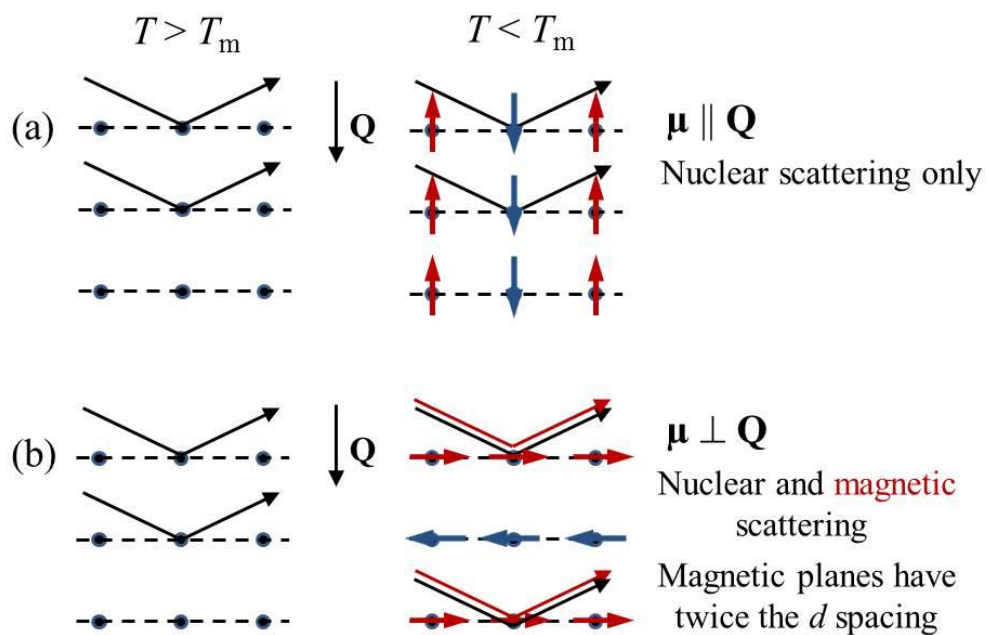
$$I_M \propto \sin^2 \beta |F_M|^2$$

( $\beta$  is angle between  $\mu_n$  and  $\mathbf{Q}$ )

where,

$$F_M = \sum_j f_j(\mathbf{Q}) e^{-i\mathbf{Q} \cdot \mathbf{r}_j} \mu_j \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \quad \text{Magnetic structure factor (collinear)}$$

## 2. Antiferromagnet



## Neutron Polarization

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

$$\begin{array}{ccc}
 \uparrow & \rightarrow & \uparrow \\
 \uparrow & \rightarrow & \downarrow \\
 \downarrow & \rightarrow & \uparrow \\
 \downarrow & \rightarrow & \downarrow \\
 \text{[ or } & \mathbf{P}_i & \rightarrow & \mathbf{P}_f \text{ if initial and final field directions different ]}
 \end{array}$$

→ polarization analysis

- Torque on magnetic dipole moment  $\boldsymbol{\mu}$  in magnetic field  $\mathbf{B}$  is

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

Eq. of motion:

Torque = rate of change of angular momentum

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

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

Consider 2 cases :

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

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

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

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  $\hbar\omega = E_i - E_f = \frac{\hbar^2}{2m} (k_i^2 - k_f^2)$

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

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

# Neutron inelastic scattering cross-section

Suppose detector can analyse energy of neutrons.

Define the *double differential scattering cross-section* :

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

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

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

Notes :

- $S(\mathbf{Q}, \omega)$  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 ( $k_f \ll k_i$ ) 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

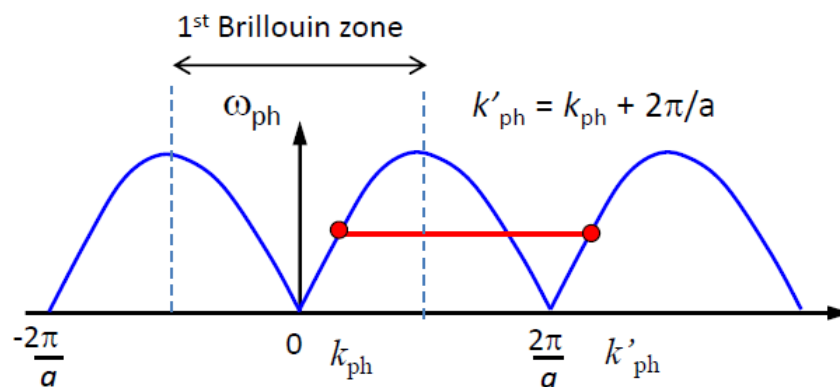
In general,

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

see [https://en.wikipedia.org/wiki/Phonon#/media/File:Phonon\\_k\\_3k.gif](https://en.wikipedia.org/wiki/Phonon#/media/File:Phonon_k_3k.gif)

- Phonon dispersion curve

Energy  $\hbar\omega_{\text{ph}}$  of a phonon depends on  $k_{\text{ph}}$



- Scattering from phonons

Peaks occur when

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

(1) Longitudinal :

(2) Transverse :

- Inelastic scattering cross-section for phonons

Consider a *static* sinusoidal distortion of the lattice:

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

Elastic scattering cross-section :

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \left| \sum_n b_n \exp \{ i\mathbf{Q} \cdot \mathbf{r}_n \} \right|^2 \\ &= \left| \sum_n b \exp \{ iQ (na + u \sin(k_{\text{ph}}na)) \} \right|^2\end{aligned}$$

Can make Taylor expansion in  $Qu$  when  $Qu \ll 1$  :

$$\rightarrow \frac{d\sigma}{d\Omega} = \left| \sum_n b \left[ 1 + iQu \sin(k_{\text{ph}}na) + \dots \right] \exp \{ iQ na \} \right|^2$$

(1)                      (2)

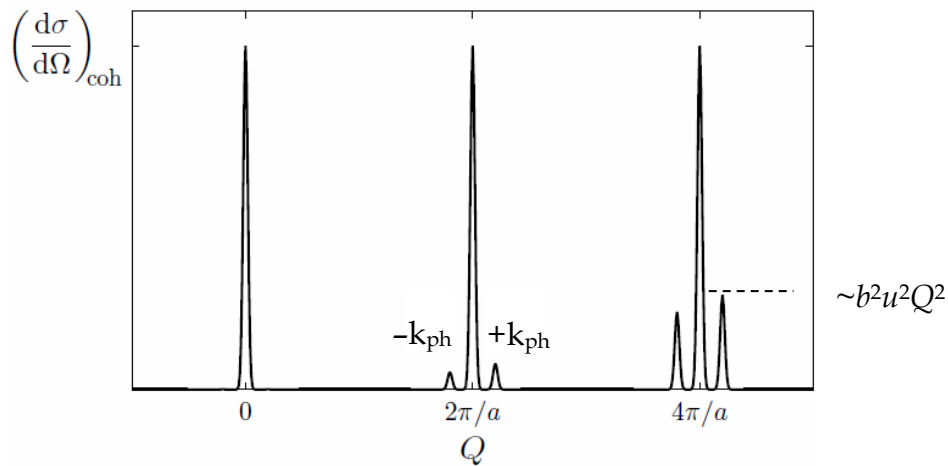
1st term (1)

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

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

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

$\rightarrow$  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

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

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

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

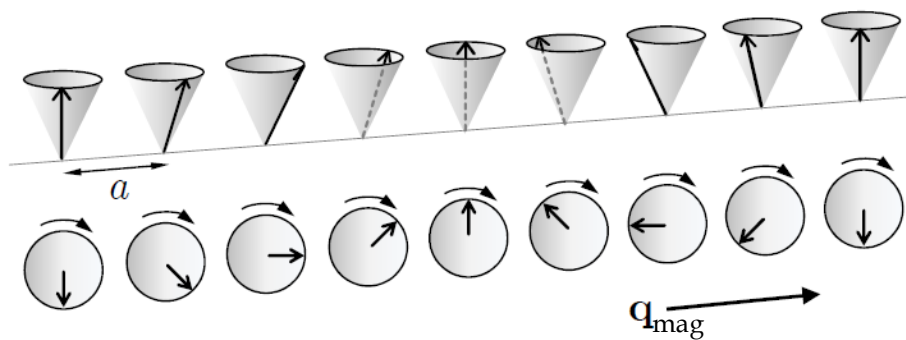
The intensity is also proportional to the square of a structure factor  $F_{\text{ph}}(\mathbf{Q})$  which depends on the relative amplitudes and phases of the vibrations of the atoms in the unit cell

# Spin Waves

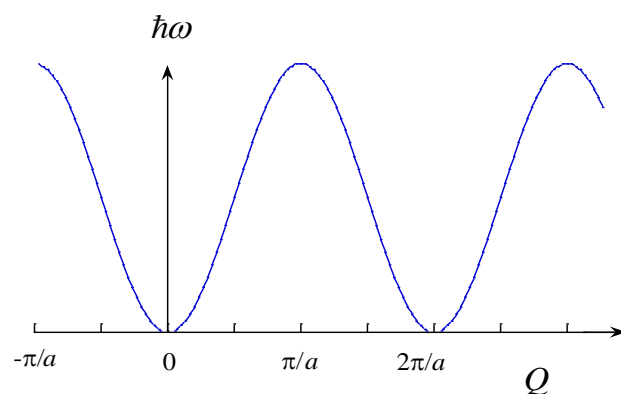
Ground state of ferromagnet:

Displace one spin:

Displacement propagates through lattice as wave with wavevector  $\mathbf{q}_{\text{mag}}$



Magnon dispersion curve :



## Notes

- Angular momentum (spin) of the crystal is reduced by 1 unit (of  $\hbar$ )  
→ spin of neutron changes by 1 unit to conserve angular momentum  
→ spin flip scattering
- Intensity varies with magnetic form factor – decreases with  $|\mathbf{Q}|$ .

## Principle of Detailed Balance

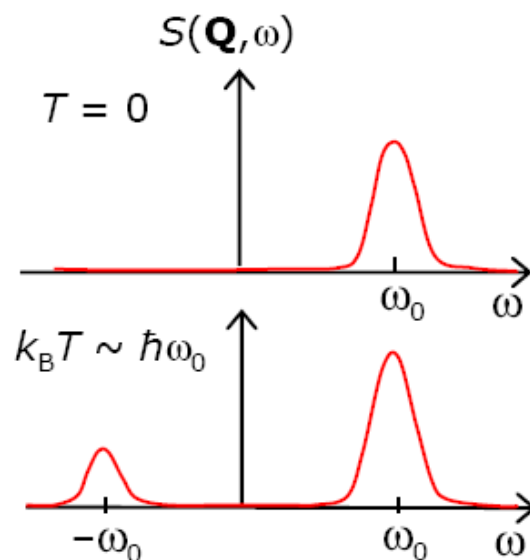
General property of  $S(\mathbf{Q}, \omega)$

Consider neutron energy loss and energy gain processes:

For any neutron inelastic scattering process,

$$\underbrace{S(\mathbf{Q}, -\omega)}_{\text{neutron energy gain}} = \exp(-\hbar\omega/k_{\text{B}}T) \times \underbrace{S(\mathbf{Q}, \omega)}_{\text{neutron energy loss}}$$

## 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 vibrations, spin waves)  $S(\mathbf{Q}, \omega)$  has peaks

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

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

(i) Phonons

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

(ii) Spin waves

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

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

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