V. Elastic Scattering of Waves

Roadmap

- A "narrower" question: How to determine crystal structure?

  X-ray diffraction

  - What do we know? "$2d\sin\theta = n\lambda$"

    We also know that inside a crystal, there are many sets of planes (labelled by (hkl))

    $$2\,d(hkl)\sin\theta = n\lambda$$

    ↳ key equation for seeing constructive interference [which angle(s) for given λ, etc.]

- A "broader" question:

  What are the properties of waves scattered by a periodic structure?

  Related questions

  - $2d(hkl)\sin\theta = n\lambda$ gives where to look for bright spots, is there a way to know the intensity of the spots?

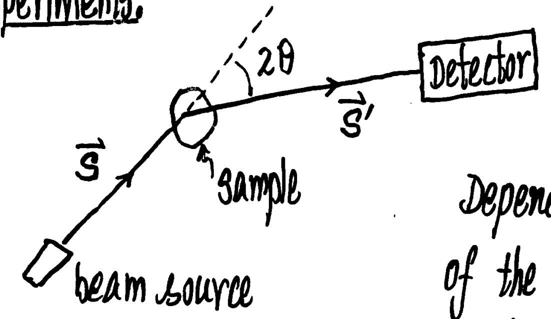
- Besides X-ray, one can also use neutron scattering to study magnetic ordering in a solid. Is X-ray scattering very different from neutron scattering?
- Why is the reciprocal space useful?
- One can also use scattering techniques to probe excitations of a solid, e.g. lattice vibrations. How does it work? [This is obviously inelastic, as energy and momentum are given to or taken from the solid.]
- Here, we introduce the basic formalism for elastic scattering of waves in a solid.

V. Elastic Scattering of waves

A. Motivation

To probe a solid, we must do something to it, e.g. heat it up, send in a beam of light and see what will come out, etc.

A usual and useful method is to perform scattering experiments.



Depends on the aim of the exp't, the beam may be X-rays, neutrons, electrons

$\vec{s}$ = propagation vector (wavevector) of incident wave[†]

$\vec{s}'$ = propagation vector of scattered wave[†]

[†] $\vec{s}$ is the wavevector. In EM theory, the symbols $\vec{k}$ and $\vec{k}'$ are used. However, there will be many $\vec{k}$ vectors in SSP (e.g., labelling electron waves).

Refs: Kittel Ch. 2 ; Christman Ch. 4; Hook & Hall: Sec 1.4 + Ch. 11

X-rays (EM wave, photon)

- scattered by atomic electrons
- gives crystal structure

$$\varepsilon = h\nu = \text{energy} = \frac{hc}{\lambda} \qquad h = 6.62 \times 10^{-34}\ \text{J}\cdot\text{s} = \text{Planck's constant}$$

In practical units, $\lambda(\text{Å}) = \dfrac{12.4}{\varepsilon(\text{keV})}$ (X-rays)

Neutrons

- have magnetic moment ⇒ can interact with entities with spin (electrons, nuclei)
- useful in studying magnetic properties of solids

de Broglie (matter wave) wavelength

$$\lambda = \frac{h}{p}$$

$$\frac{p^2}{2M_n} = \varepsilon = \text{k.e. of neutron} \Rightarrow \varepsilon = \frac{h^2}{2M_n\lambda^2}$$

↖ neutron mass = 1.675×10^{-27} Kg

In practical units,

$$\lambda(\text{Å}) \cong \frac{0.28}{\sqrt{\varepsilon(\text{eV})}} \quad \text{(neutrons)}$$

Electrons

- have charge, can't penetrate deep into solid
- useful in studying surfaces, films, etc.

de Broglie wavelength $\lambda = \frac{h}{p}$

$$\mathcal{E} = \frac{h^2}{2\underset{\uparrow}{m_e}\lambda^2}$$

electron mass = 9.11×10^{-31} Kg

In practical units,

$$\lambda(\text{Å}) \cong \frac{12}{\sqrt{\mathcal{E}(eV)}} \quad \text{(electrons)}$$

B. General Idea

- In exp'ts, what we detect is the resultant wave obtained by considering the <u>interference of the scattered waves from each scatterer</u>[+] (atom) in the solid.
- The discussion here is good for scattering of EM waves, electrons, neutrons. We shall say more on X-ray scattering[+], as it is useful in determining crystal structures.

[+] The idea is due to Max von Laue (1914 Nobel Physics Prize)

Incident and Scattered Waves

Consider monochromatic <u>incident</u> plane wave[+]: (see figure on p. V-⑤)

$$\xi_{inc}(\vec{r},t) = A\,\underbrace{e^{i\vec{s}\cdot\vec{r}}\,e^{-i\omega t}}_{\text{traveling, propagating in the direction of } \vec{s}}$$

- $\xi_{inc}(\vec{r},t)$ may represent:

  EM wave : Electric field component of X-ray (Maxwell eq'ns)

  Neutron/electron : wavefunction (Schrödinger eq'n)

- Let's focus on X-ray scattering, then ξ is a component of the electric field.

$$s = |\vec{s}| = \frac{2\pi}{\lambda}$$

s : wave number

$\vec{s}$: wave vector

- Consider <u>elastic scattering</u>:

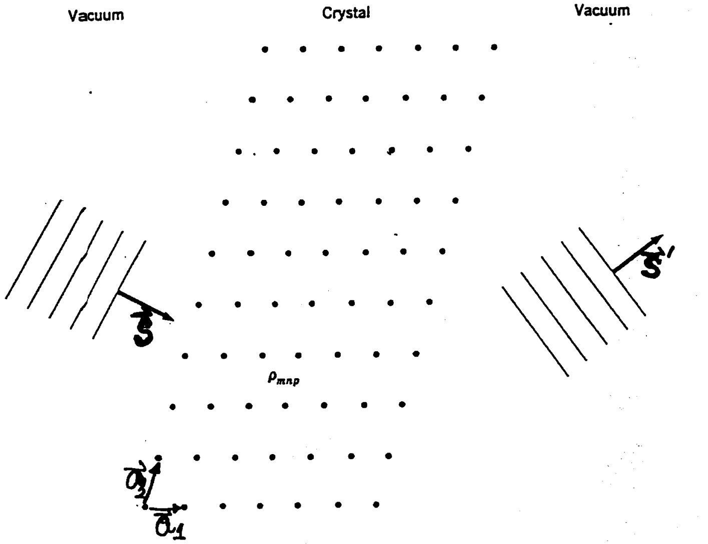
  it means: $|\vec{s}| = |\vec{s}'| = s$

  $$\omega = \omega'$$

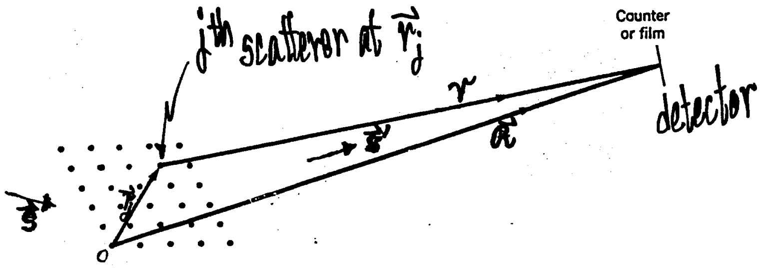
  But $\vec{s} \neq \vec{s}'$ (changed in direction)

- Laue: Add up contributions of the waves scattered from each volume <u>element</u> of the crystal.

[+] We haven't specified whether A is a vector or a scalar. For EM waves, A represents the amplitude (and gives the polarization) of the electric field. Hence, A becomes a vector in that case.



An electromagnetic wave of wavevector $\vec{s}$ is incident upon a crystal. We want to find the wavevectors $\vec{s}'$ of the outgoing waves created by diffraction by the atoms of the crystal.



There are many atoms (scatterers) in a solid.

$\vec{r}_j$ = position vector of the j^{th} scatterer

$\vec{R}$ = position vector of detector

One scatterer

- Consider the scattering from a particular scatterer in the sample. The scatterer is at $\vec{r}_j$. The detector is at $\vec{R}$ (see figure) and it is far away from sample.

$|\vec{R}| >>$ sample size

(*)

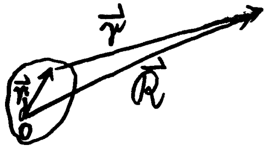
$\xi^{(j)}_{scatt}(\vec{R},t)$ = scattered wave by scatterer at $\vec{r}_j$ as observed at position $\vec{R}$ and at time t

$$= \underbrace{\left(A e^{i\vec{s}\cdot\vec{r}_j}\right)}_{\text{proportional to incident wave at the scatterer's location}} \cdot f_j \cdot \underbrace{\frac{e^{isr}}{r} e^{-i\omega t}}_{\text{outgoing spherical wave centered at } \vec{r}_j \ (|\vec{s}'| = s \text{ used})}$$

f_j = a factor that involves the details (e.g. which kind of atom? Si? Na?) of the scatterer

= $f_j(\vec{s}'-\vec{s})$ in general

= atomic form factor of the scatterer at $\vec{r}_j$



$$\vec{r} = \vec{R} - \vec{r}_j$$

$$r^2 = |\vec{R} - \vec{r}_j|^2 = R^2 - 2\vec{R}\cdot\vec{r}_j + r_j^2$$

$$\therefore\ r = R\left[1 - \frac{2\vec{R}\cdot\vec{r}_j}{R^2} + \frac{r_j^2}{R^2}\right]^{1/2}$$

$$\approx R\left(1 - \frac{\vec{R}}{R}\cdot\frac{\vec{r}_j}{R}\right) \qquad R >> \text{sample size} \Rightarrow \frac{r_j}{R} \ll 1 \quad \therefore \text{neglect } \frac{r_j^2}{R^2}$$

$$= R - \underset{\uparrow}{\hat{R}}\cdot\vec{r}_j$$

a <u>unit vector</u> in the direction of $\vec{R}$

In (*),

(i) Approximate $\frac{1}{r} \cong \frac{1}{R}$

(ii) r also appears in e^{isr}. Exponential function is rapidly changing with its argument. We need to make a better approximation.

$$e^{i\vec{s}\cdot\vec{r}_j} e^{isr} \approx e^{i\vec{s}\cdot\vec{r}_j} e^{isR} e^{-is\hat{R}\cdot\vec{r}_j}$$
$$= e^{isR} e^{-i(s\hat{R}-\vec{s})\cdot\vec{r}_j}$$

Recall $\vec{s}$ = incident propagation vector

Look at $s\hat{R}$: It is a vector of magnitude s and direction that points from the sample to the detector.

Since the detector is far far away from the sample, the direction $\hat{R}$ can be taken to be the direction of the propagation vector $\vec{s}'$ of the scattered wave.

Elastic scattering: $|\vec{s}'| = |\vec{s}| = s$

$$\therefore\ \vec{s}' = s\hat{R}$$

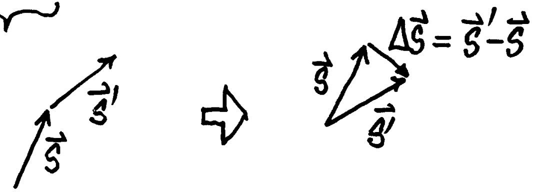
- Putting the two approximations together,

$$e^{i\vec{s}\cdot\vec{r}_j}\frac{e^{isr}}{r} \approx \frac{e^{isR}}{R} e^{-i(\vec{s}'-\vec{s})\cdot\vec{r}_j}$$

We pick up $\underbrace{\vec{s}'-\vec{s}}$

Define:

$$\Delta\vec{s} \equiv \vec{s}' - \vec{s}$$



= change in propagation vector

due to change in direction for elastic scattering

$\therefore$ The scattered wave due to one scatterer becomes (*) on p.V-6)

$$\boxed{\xi^{(j)}_{scatt}(\vec{R},t) = \underbrace{\left(\frac{A}{R} e^{isR} e^{-i\omega t}\right)}_{\text{outgoing spherical wave}} \cdot f_j\, e^{-i\Delta\vec{s}\cdot\vec{r}_j}}$$

Many scatterers

Add up the contributions from the scatterers.

$$\xi_{\text{scatt.}}(\vec{\mathcal{R}},t) = \frac{A}{\mathcal{R}} e^{is\mathcal{R}} e^{-i\omega t} \cdot \left(\sum_j f_j \, e^{-i\Delta\vec{s}\cdot\vec{r}_j} \right)$$

sum over all scatterers

$f_j = f_j(\Delta\vec{s})$ in general

This is a general expression for elastic scattering of waves off a collection of scatterers. The scatterers may or may not be ordered in an array. They may even be different scatterers. Thus, it is good for crystalline and amorphous solids.

Remark

When the scattering is due to a spatial distribution of electrons described by the electron concentration $n(\vec{r})$, the term $\sum_j f_j \, e^{-i\Delta\vec{s}\cdot\vec{r}_j}$ is replaced by an integral over the sample $\int d^3x \; n(\vec{r}) \, e^{-i\Delta\vec{s}\cdot\vec{r}}$.

C. Elastic Scattering by Crystals

Crystal = Lattice + Basis

To treat $\sum_j f_j \, e^{-i\Delta\vec{s}\cdot\vec{r}_j}$ ⇒ we need a way to specify the position of the atoms

Specify $\vec{r}_j$ by
- (i) specifying which primitive cell the atom is in by a lattice vector $\vec{R}$
- (ii) specifying which atom in the basis.

- Each lattice point has its associated primitive cell
  - ⇒ can use a lattice vector $\vec{R}$ to specify the location of a primitive cell
- Let there be α atoms in the basis. Relative to a lattice point, these α atoms are at the locations given by $\vec{\rho}_1, \vec{\rho}_2, \cdots, \vec{\rho}_\alpha$.

∴ The positions of the atoms of the ℓ-type are:

$$\vec{R} + \vec{\rho}_\ell = \left(u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3\right) + \vec{\rho}_\ell$$

⌜e.g.

CsCl,

$\vec{R}$'s are those for a sc lattice. Basis of 2 atoms.

$\vec{\rho}_{Cs} = \vec{0}$, $\vec{\rho}_{Cl} = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$ ⌟

- The scattered wave has a factor $\sum_j f_j e^{-i\Delta\vec{s}\cdot\vec{r}_j}$

(i) $\Delta\vec{s}\cdot\vec{r}_j \rightarrow \Delta\vec{s}\cdot(\vec{R}+\vec{\rho}_\ell)$

(ii) $\sum_{\substack{\text{atoms}\\ j}} \rightarrow \sum_{\vec{R}} \sum_{\ell=1}^{\alpha}$

all atoms ↗ j

↗ sum over every primitive (unit) cells

↖ sum over the α atoms in the basis

Hence, $\sum_j f_j e^{-i\Delta\vec{s}\cdot\vec{r}_j} = \sum_{\vec{R}}\sum_{\ell=1}^{\alpha} e^{-i\Delta\vec{s}\cdot\vec{R}} f_\ell(\Delta\vec{s}) e^{-i\Delta\vec{s}\cdot\vec{\rho}_\ell}$

$$= \underbrace{\left(\sum_{\vec{R}} e^{-i\Delta\vec{s}\cdot\vec{R}}\right)}_{\text{relate to the lattice only (nothing to do with the atoms in the basis) (geometric factor)}} \cdot \underbrace{\left(\sum_{\ell=1}^{\alpha} f_\ell(\Delta\vec{s}) e^{-i\Delta\vec{s}\cdot\vec{\rho}_\ell}\right)}_{\text{over atoms in the basis, relate to the atoms in the crystal (material)}}$$

$$\sum_{j\,(\text{all atoms})} f_j e^{-i\Delta\vec{s}\cdot\vec{r}_j} = \left(\sum_{\vec{R}} e^{-i\Delta\vec{s}\cdot\vec{R}}\right)\cdot\left(\sum_{\ell=1}^{\alpha} f_\ell(\Delta\vec{s}) e^{-i\Delta\vec{s}\cdot\vec{\rho}_\ell}\right)$$

= Geometrical term (lattice) × term related to materia (basis)

= $a(\Delta\vec{s}) \cdot \mathcal{S}(\Delta\vec{s})$ <u>for crystals</u>

where $a(\Delta\vec{s}) \equiv \sum_{\vec{R}} e^{-i\Delta\vec{s}\cdot\vec{R}}$

↖ over all $\vec{R}$'s (i.e., <u>all</u> lattice vectors)

↑ infinitely many in principle

Structure factor of the basis ↘ $\mathcal{S}(\Delta\vec{s}) \equiv \sum_{\ell=1}^{\alpha} f_\ell(\Delta\vec{s}) e^{-i\Delta\vec{s}\cdot\vec{\rho}_\ell}$

↖ over the atoms in the basis

Thus, $\boxed{\xi_{scatt}(\vec{R},t) = \frac{A}{R} e^{isR} e^{-i\omega t} \; a(\Delta\vec{s})\, \mathcal{S}(\Delta\vec{s})}$

- Experimentally, the pattern (bright spots) is related to the <u>intensity</u> of the scattered wave at the detector

$$\boxed{I = |\xi_{scatt}(\vec{R},t)|^2 = \underset{\substack{\uparrow\\ \text{a constant when detector is fixed}}}{\frac{|A|^2}{R^2}} \cdot |a(\Delta\vec{s})|^2 \cdot |\mathcal{S}(\Delta\vec{s})|^2}$$

- $I \neq 0$ only when $|a(\Delta\vec{s})|^2 \neq 0$ and $|\mathcal{S}(\Delta\vec{s})|^2 \neq 0$.

<u>Consider</u> $a(\Delta\vec{s}) = \sum_{\vec{R}} e^{-i\Delta\vec{s}\cdot\vec{R}}$

- It is a sum over many phase-factors which are highly sensitive to the argument. <u>For most $\Delta\vec{s}$, the terms tend to cancel and $a(\Delta\vec{s})$ vanishes.</u>

- <u>But</u>, there are some (in fact many, infinitely many) $\Delta\vec{s}$ that $a(\Delta\vec{s})$ is huge ($\neq 0$)!

<u>Recall</u>: $\underset{\uparrow}{\vec{G}}\cdot\vec{R} = 2\pi \cdot \text{integer}$ for all $\vec{R}$

a reciprocal lattice vector

<u>Key Point</u>:

note: There are many $\vec{G}$'s.

If $\Delta\vec{s} = \vec{G}$, then $e^{-i\Delta\vec{s}\cdot\vec{R}} = 1$ and a is huge.

If $\Delta\vec{s} \neq \vec{G}$, $a = 0$ and $I = 0$.

If $\Delta\vec{s} = \vec{G}$, $I \neq 0$ if $|\mathcal{S}(\vec{G})|^2 \neq 0$

Thus one needs to tune $\Delta\vec{s}$ (magnitude through the wavelength and direction through detector location) in clever ways to see $I \neq 0$ (bright spots), which result from constructive interference.

$\therefore$ An extremely intense scattered wave becomes possible when $\underbrace{\Delta\vec{s} = \vec{G}}$.

This condition is called the <u>Laue condition</u>.

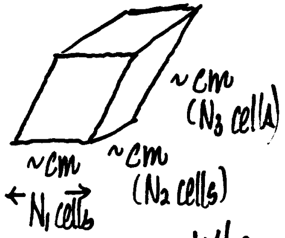
In expt's, the observations give information about the reciprocal lattice vectors $\vec{G}$'s, thus the reciprocal lattices, and thus the direct lattice. This is why an understanding of the concept of reciprocal lattice is important.

Remark:

In more elementary treatments (e.g. easier books), the previous result ($\Delta\vec{s}=\vec{G}$ for possible $I\neq 0$) can be illustrated as follows.

Consider a big crystal with (big but finite)

$$\mathcal{N} = \underset{\substack{\uparrow \\ N_1 \text{ lattice pts.} \\ \text{in } \vec{a}_1 \text{ direction}}}{N_1} \cdot \underset{\substack{\uparrow \\ N_2 \text{ lattice pts.} \\ \text{in } \vec{a}_2 \text{ direction}}}{N_2} \cdot N_3 \text{ primitive unit cells} \quad \xleftarrow{} N_3 \text{ lattice pts. in } \vec{a}_3 \text{ direction}$$



$$\underbrace{N_1,\ N_2,\ N_3}_{\sim 10^8 \text{ each for a crystal of } \sim 1\,\text{cm}^3} \gg 1$$

When $\Delta\vec{s}=\vec{G}$,

$$a(\Delta\vec{s}=\vec{G}) = \left(\sum_{u_1=0}^{N_1} 1\right)\left(\sum_{u_2=0}^{N_2} 1\right)\left(\sum_{u_3=0}^{N_3} 1\right)$$

$$= N_1 \cdot N_2 \cdot N_3 = \mathcal{N} = \underset{\substack{\uparrow \\ \sim 10^{24} \text{ for} \\ \text{a crystal} \sim 1\text{cm}^3}}{\overset{\text{a}}{\text{huge number}}}$$

How about arbitrary $\Delta\vec{s}$?

Note that the lattice vectors $\vec{R}$ can be written as:

$$\vec{R} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3\,, \quad \begin{cases} u_1 = 0,1,\cdots,N_1-1 \\ u_2 = 0,1,\cdots,N_2-1 \\ u_3 = 0,1,\cdots,N_3-1 \end{cases}$$

$$a(\Delta\vec{s}) = \sum_{\vec{R}} e^{-i\Delta\vec{s}\cdot\vec{R}} = \sum_{u_1=0}^{N_1-1}\sum_{u_2=0}^{N_2-1}\sum_{u_3=0}^{N_3-1} e^{-iu_1\Delta\vec{s}\cdot\vec{a}_1} e^{-iu_2\Delta\vec{s}\cdot\vec{a}_2} e^{-iu_3\Delta\vec{s}\cdot\vec{a}_3}$$

$$= \left(\sum_{u_1=0}^{N_1-1} e^{-iu_1\vec{a}_1\cdot\Delta\vec{s}}\right)\cdot\left(\sum_{u_2=0}^{N_2-1} e^{-iu_2\vec{a}_2\cdot\Delta\vec{s}}\right)\cdot\left(\sum_{u_3=0}^{N_3-1} e^{-iu_3\vec{a}_3\cdot\Delta\vec{s}}\right)$$

$$= \underbrace{\left(\frac{1-e^{-iN_1\vec{a}_1\cdot\Delta\vec{s}}}{1-e^{-i\vec{a}_1\cdot\Delta\vec{s}}}\right)}_{\frac{e^{-\frac{i}{2}N_1\vec{a}_1\cdot\Delta\vec{s}}}{e^{-\frac{i}{2}\vec{a}_1\cdot\Delta\vec{s}}}\cdot\frac{\sin\left(\frac{N_1}{2}\vec{a}_1\cdot\Delta\vec{s}\right)}{\sin\left(\frac{1}{2}\vec{a}_1\cdot\Delta\vec{s}\right)}}\cdot\left(\frac{1-e^{-iN_2\vec{a}_2\cdot\Delta\vec{s}}}{1-e^{-i\vec{a}_2\cdot\Delta\vec{s}}}\right)\cdot\left(\frac{1-e^{-iN_3\vec{a}_3\cdot\Delta\vec{s}}}{1-e^{-i\vec{a}_3\cdot\Delta\vec{s}}}\right)$$

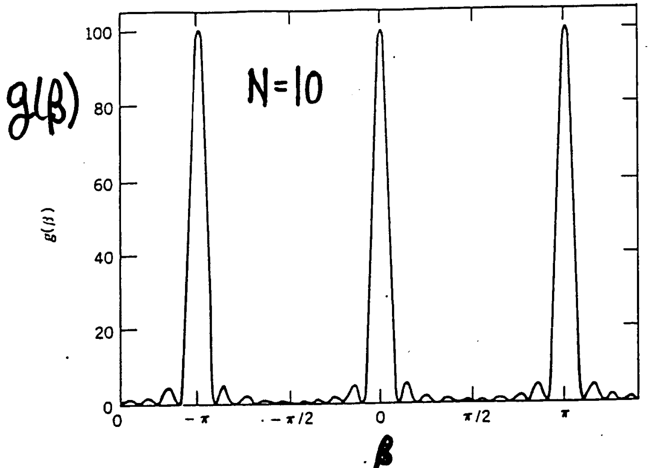
$$I \propto |a(\Delta\vec{s})|^2$$

$$= \left(\frac{\sin\left(\frac{N_1}{2}\vec{a}_1\cdot\Delta\vec{s}\right)}{\sin\left(\frac{1}{2}\vec{a}_1\cdot\Delta\vec{s}\right)}\right)^2\cdot\left(\frac{\sin\left(\frac{N_2}{2}\vec{a}_2\cdot\Delta\vec{s}\right)}{\sin\left(\frac{1}{2}\vec{a}_2\cdot\Delta\vec{s}\right)}\right)^2\cdot\left(\frac{\sin\left(\frac{N_3}{2}\vec{a}_3\cdot\Delta\vec{s}\right)}{\sin\left(\frac{1}{2}\vec{a}_3\cdot\Delta\vec{s}\right)}\right)^2$$

Thus, I exhibits the behaviour of the function

$$g(\beta) = \left(\frac{\sin(N\beta)}{\sin\beta}\right)^2 \quad \text{for } N\sim 10^8$$

Let's see how $g(\beta)$ behaves.



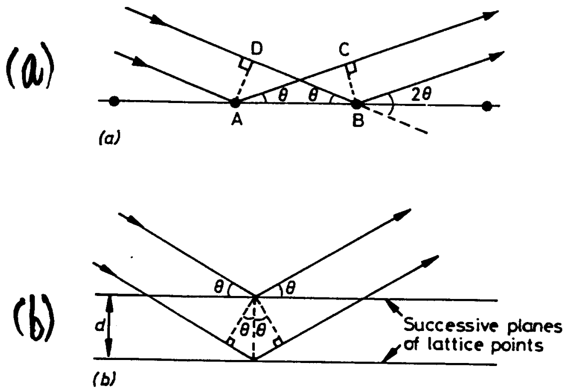
The function $g(\beta) = \sin^2(N\beta)/\sin^2(\beta)$ for $N = 10$. It is periodic with period π and has principal maxima at $\beta = \ell\pi$, where ℓ is an integer. $N - 2$ secondary maxima occur between adjacent principal maxima. As N increases the principal maxima become higher and narrower and secondary maxima become less prominent.

Note:
$N \sim 10^8$
in crystals

- sharply peaked at $\beta = \pi \cdot$ integer (gives $\Delta\vec{s} = \vec{G}$)
- drops rapidly away from peaks
- As N increases, peaks ($\sim N^2$) get sharper
- $N \sim 10^8$, only sharp peaks remain.
- This illustrates that we need to satisfy the Laue condition $\Delta\vec{s} = \vec{G}$ to get $I \neq 0$.

D. The Laue Condition and the Bragg Condition

Bragg (~1913) derived the condition for constructive interference of the X-rays scattered from a set of parallel lattice planes.



Proof of Bragg's law. (*a*) Scattering of x-rays from the adjacent lattice points A and B in the plane will be in phase if AC = DB and thus if the scattered beam makes the same angle θ to the plane as the incident beam. (*b*) Scattering of x-rays off successive planes is in phase if the path difference $2d \sin\theta$ is an integral number of wavelengths $n\lambda$

(a) From one plane: A and B are adjacent lattice points. For constructive interference of waves scattered from A and B, we need $\underbrace{AC = BD}$, true if the scattered wave makes the same angle ϑ to the plane as the incident wave

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Remark: ϑ here is the glancing angle (different from the angle of incidence in optics). It is also called the Bragg angle.

- Note that the result  is <u>similar</u> to that in the law of reflection in optics

⇒ { The diffracted wave looks <u>as if</u> it has been <u>reflected</u> from the crystal plane }

notes: (i) these planes have nothing to do with the surface planes bounding the specimen, as X-rays or neutrons see all!

(ii) Because of this result, people often talk about X-ray diffraction in solids as <u>Bragg reflection</u>.

(b) <u>From planes</u>:

To obtain diffraction maximum, <u>successive planes should scatter in phase</u>.

Consider path difference: d = spacing of parallel planes

$$\boxed{2d\sin\theta = n\lambda \quad \text{where } n \text{ is an integer}}$$

↳ <u>Bragg's law</u> or <u>Bragg's condition</u>

<u>Remark</u>:

$$\underbrace{2d(hkl)\sin\theta = n\lambda}_{\text{a condition that requires } \underline{\theta \text{ and } \lambda \text{ be matched}}} \qquad \text{Bragg's condition}$$

$n = 1, 2, 3, \cdots$

- If $2d(hkl)\sin\theta = n\lambda$, the constructive beam is identified by the statements "<u>n^{th}-order reflection from the (hkl) planes</u>"

<u>OR</u> by convention as

"the (nh, nk, nl) reflection"

[e.g., 3rd order reflection from (111) planes is described as the (333) reflection in X-ray crystallography.

- Smallest n is $n=1$,

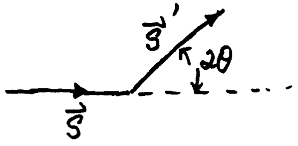
∴ need $\lambda \leq 2d$ (that's why we need to use X-rays)

- Bragg's argument does not say anything about the intensity of the beam. Also, it does not involve the basis atoms. These effects are included in $|S(\vec{G})|^2$ in the earlier derivation

The Laue Condition and the Bragg Condition

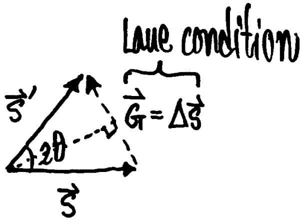
Laue condition: $\Delta\vec{s} = \vec{s}' - \vec{s} = \vec{G}$

Elastic scattering: $|\vec{s}| = |\vec{s}'| = s \qquad s = \frac{2\pi}{\lambda}$



$$|\vec{G}|^2 = s'^2 + s^2 - 2|\vec{s}||\vec{s}'|\cos 2\theta$$

$$\boxed{2\theta = \text{angle between } \vec{s} \text{ and } \vec{s}'}$$



$$|\vec{G}|^2 = 2s^2(1 - \cos 2\theta)$$
$$= 4s^2 \sin^2\theta$$

$$\boxed{\theta = \text{Bragg angle}}$$

$$|\vec{G}| = 2s\sin\theta = 2\cdot\left(\frac{2\pi}{\lambda}\right)\cdot\sin\theta$$

- Now consider a reciprocal lattice vector:

$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3 = \vec{G}(v_1v_2v_3), \quad v_1, v_2, v_3 = \text{integers}$$

We can find the common divisor, n, of v_1, v_2, v_3.

$$\vec{G} = n(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3) = n\vec{G}(hkl)$$

where n = positive integer,

and h, k, l are integers which do not have common divisor.

$\vec{G}(v_1v_2v_3)$ and $\vec{G}(hkl)$ are in the same direction. <u>$\vec{G}(hkl)$ is the shortest reciprocal lattice vector in that direction.</u>

$$|\vec{G}| = 2\cdot\frac{2\pi}{\lambda}\cdot\sin\theta$$

$$\Rightarrow n\cdot|\vec{G}(hkl)| = 2\cdot\frac{2\pi}{\lambda}\cdot\sin\theta \qquad \vec{G}(hkl) = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$\Rightarrow n\lambda = 2\cdot\frac{2\pi}{|\vec{G}(hkl)|}\cdot\sin\theta$$

$$\Rightarrow \boxed{2\cdot d(hkl)\cdot\sin\theta = n\lambda} \quad \text{Bragg condition (Bragg 1913)}$$

where $d(hkl)$ = spacing of adjacent lattice planes speified by the Miller indices (hkl).

n = positive integer

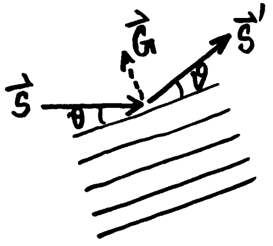
Note that: $\lambda \leq 2d$

typically $d \sim$ a few Å

$\Rightarrow \lambda \sim$ few Å

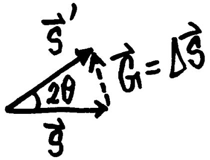
$\Rightarrow$ for EM waves, we need X-ray.

$$\therefore \boxed{\text{The Laue condition } \Delta\vec{s} = \vec{G} \text{ gives the Bragg condition } 2\cdot d(hkl)\cdot\sin\theta = n\lambda.}$$



Bragg

$\Rightarrow$



Laue