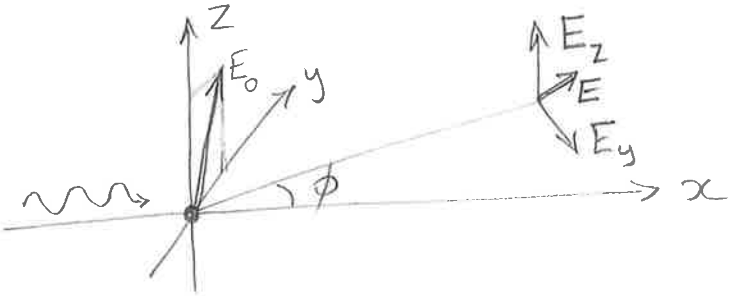
Lecture 1

1. Classical Scattering of EM wave by an electron.

EM wave accelerates electron (plane wave)

Moving electron radiates EM wave (spherical wave)



$\vec{a} = \vec{E}_0 \frac{e}{m}$ Newton's Law with Lorentz force.

Radiated E-field $|\vec{E}| = \frac{e|\vec{a}| \sin\alpha}{c^2 R}$

using cgs units (convenient)

$\vec{E}$ is in plane of $\vec{a}$ and $\vec{R}$

Combining:

$$\left.\begin{aligned} E_y &= E_{oy} \frac{e^2}{mc^2 R} \cos\phi \\ E_z &= E_{oz} \frac{e^2}{mc^2 R} \end{aligned}\right\}$$

Resultant $E^2 = E_y^2 + E_z^2 = \frac{e^4}{m^2 c^4 R^2} \left(E_{oy}^2 \cos^2\phi + E_{oz}^2 \right)$

Observed intensity (counts per second) $I \propto E^2$

i) If radiation is unpolarized $\langle E_{oy}^2 \rangle = \langle E_{oz}^2 \rangle$

$$I = I_0 \frac{e^4}{m^2 c^4 R^2} \left(\frac{1 + \cos^2\phi}{2} \right)$$

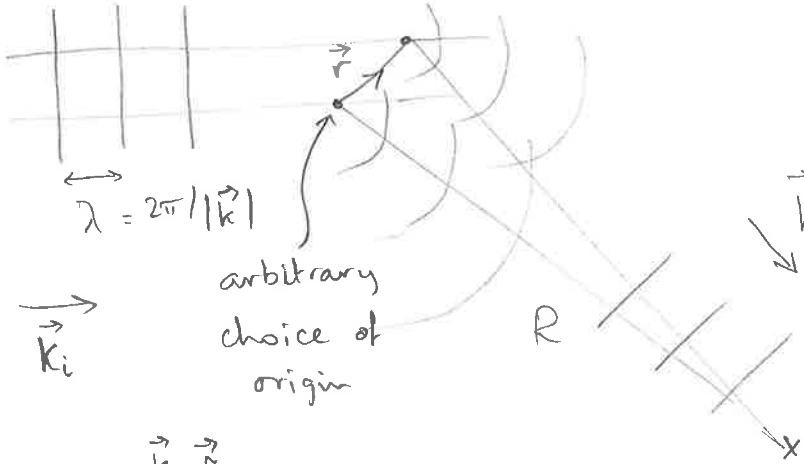
ii) If radiation is polarized (S.R.), need to keep track of y & z components separately.

$\frac{e^2}{mc^2}$ is a length = 'classical electron radius'
= 'scattering length' = 2.8×10^{-15} m

1 m away from a single electron $I/I_0 = 10^{-29}$ = small!

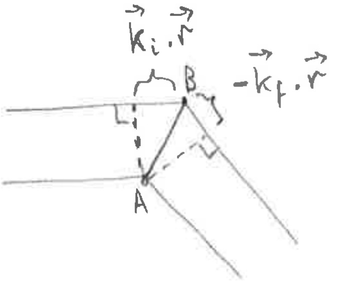
2. Interference between nearby scattering events.

Plane wave, $e^{-i\vec{k}\cdot\vec{r}}$ $\vec{k}$ = wavevector.



Looks like a plane wave when $R \gg |\vec{r}|$

Spherical waves interfere



Phase of scattering from particle A = ϕ_A
(= π for electron)

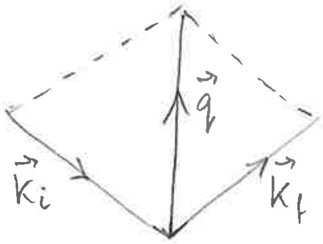
Phase .... B = $\phi_B + \vec{k}_i\cdot\vec{r} - \vec{k}_f\cdot\vec{r}$

$\phi_A = \phi_B$ if identical.

Outgoing (scattered) wave at large distance is superposition

$$\text{Amplitude} \propto e^{-i\phi_A} + e^{-i\phi_B - i\vec{k}_i\cdot\vec{r} + i\vec{k}_f\cdot\vec{r}} = e^{-\phi_A}\left(1 + e^{i(\vec{k}_f-\vec{k}_i)\cdot\vec{r}}\right)$$

$$= e^{-i\phi_A}\sum_{j=1}^{N} e^{i\underbrace{(\vec{k}_f-\vec{k}_i)}_{\text{call this } \vec{q} \text{ = momentum transfer}}\cdot\vec{r}_j}$$ for N particles at $\vec{r}_j$



Note Warren uses $\vec{S}$ with $\boxed{\vec{q} = \frac{2\pi}{\lambda}\vec{S}}$

$\vec{S}$ is dimensionless 'crystallographic notatio

$\vec{q}$ is in inverse Å^{-1} 'physics notation'

3. Scattering by an atom.

Needs Q.M. treatment instead of classical.

(i) electrons not at single points.

(ii) electronic excitation (absorption) possible.

Ignore (ii) for now → 'resonance' effects later.

Consequences of (i) are { Form factor of atom
Compton scattering
= 'Modified' scattering in Warren.

Electron in atom described by (Hartree-Fock) wavefunction with $\rho(r)$ = probability density $= |\Psi(r)|^2$

Amplitude = Weighted sum over positions

$$= \int \rho(r)\, e^{i\vec{q}\cdot\vec{r}}\, d^3\vec{r}$$

Integrate in cylindrical coords along $\vec{q}$

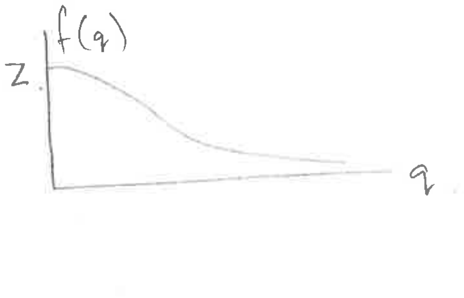
$$\vec{q}\cdot\vec{r} = qr\cos\phi\,, \quad d^3\vec{r} = 2\pi r^2 \sin\phi\, d\phi\, dr$$

$$f_e(q) = \int \rho_n(r)\, e^{iqr\cos\phi}\, 2\pi r^2 \sin\phi\, d\phi\, dr$$

$$= \int_0^\infty 4\pi r^2 \rho_n(r)\, \frac{\sin qr}{qr}\, dr \quad = \text{form factor of electron } n$$

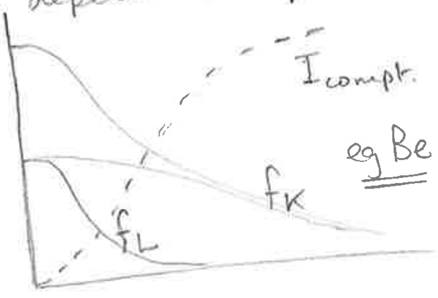
$$f(q) = \sum_{n=1}^{Z} \int_0^\infty 4\pi r^2 \rho_n(r)\, \frac{\sin qr}{qr}\, dr \quad = \text{form factor of atom.}$$

Limit of $q \to 0$ $\quad f(q) = \sum_{n=1}^{Z} \int 4\pi r^2 \rho_n(r)\, dr = Z$



4. Compton Scattering.

Full Q.M. scattering theory not discussed.
Important result is that the total scattered intensity from an electron = classical result, which does not depend on q.



$$f_e(q)^2 + I_{Compt}(q) = 1$$

$$\Rightarrow I_{compt} = 1 - f_e(q)^2 \quad \text{electron}$$

$$= Z - \sum_1^Z f_e(q)^2 \quad \text{atom}$$

Compton scattering is inelastic, hence incoherent
Total is a sum of intensities from all electrons in sample
⇒ no diffraction effects enter.

5. Crystal Lattice

Crystal = Lattice $*$ Basis (convolution).

Lattice = mathematical array of points with translational symmetry

Basis = real, physical distribution of matter: atoms / electron

1D example

combination = crystal

6. Bravais Lattice.

14 possible ways of making space translationally invariant

(i) Infinite array of discrete pts, which appears idendical (pos + orientation), viewed from any pt.

(ii) $\vec{R} = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3$ with $\vec{a}_1\ \vec{a}_2\ \vec{a}_3$ non coplanar

Enumeration of 14 Bravais Lattices in 3D.

Highest → Lowest symmetry approximately.

$a = |\vec{a}_1| \quad b = |\vec{a}_2| \quad c = |\vec{a}_3|$

$\alpha = \angle^{a_3}_{a_2} \quad \beta = \angle^{a_1}_{a_3} \quad \gamma = \angle^{a_2}_{a_1}$

System			# Bravais Latts
Cubic (SC, FCC, BCC)	$a=b=c$	$\alpha=\beta=\gamma=90°$	3
Tetragonal (ST, BCT)	$a=b\neq c$	$\alpha=\beta=\gamma=90°$	2
Orthorhombic (+body, base, face)	$a\neq b\neq c$	$\alpha=\beta=\gamma=90°$	4
Monoclinic (+ base)	$a\neq b\neq c$	$\alpha=\gamma=90°$ $\beta\neq 90$	2
Triclinic	$a\neq b\neq c$	$\alpha\neq\beta\neq\gamma$	1
Rhombohedral (= Trigonal)	$a=b=c$	$\alpha=\beta=\gamma\neq 90$	1
Hexagonal	$a=b\neq c$	$\alpha=\beta=90$ $\gamma=120°$	1

Several important lattices are not Bravais latts eg HCP, honeycomb and diamond.

All crystals can be classified as one of the above.

7. Primitive unit cell.

Volume of space which, when translated by all possible $\vec{R}$'s, fills space completely without overlap.

Not unique definition, but common to choose parallelapiped formed by $\vec{a}_1$ $\vec{a}_2$ $\vec{a}_3$

For any choice Volume of cell $V_{cell} = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

8. Reciprocal Lattice

The set of all possible plane wavevectors which have the periodicity of a given lattice.

Crystallographic Notation	Physics Notation
$e^{2\pi i \vec{H}\cdot\vec{r}}$ has periodicity of $\vec{R} = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3$	$e^{i\vec{K}\cdot\vec{r}}$ ....
$\Rightarrow e^{2\pi i \vec{H}\cdot\vec{R}} = 1 \quad \in \vec{R}$	$\Rightarrow e^{i\vec{K}\cdot\vec{r}} = 1$
$\Rightarrow \vec{H}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$	$\vec{K} = ...$
with $\vec{b}_1 = \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1\cdot\vec{a}_2\times\vec{a}_3}$ etc no 2π	$b_1 = 2\pi \frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot\vec{a}_2\times\vec{a}_3}$
$= \frac{1}{V_{cell}}\vec{a}_2\times\vec{a}_3$	$= \frac{2\pi}{V_{cell}}\vec{a}_2\times\vec{a}_3$

'Physics' reciprocal lattice is bigger by 2π in all directions.

In this course we will use crystallographic notation part of the time, but always retain $\vec{q}$ for momentum transfe

Thus Bragg condition for diffraction will be:

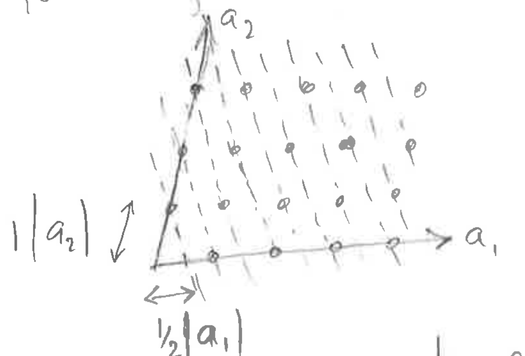
$$2\pi\vec{q} = \vec{H}_{hkl} \qquad \text{or} \qquad \vec{q} = \vec{K}$$

Orthogonality relation:

$$\vec{a}_i\cdot\vec{b}_j = \delta_{ij} \qquad\qquad \vec{a}_i\cdot\vec{b}_j = 2\pi\,\delta_{ij}$$

9. Relation to Lattice planes.

Any real space lattice can be sectioned into planes following the Miller Index rule:



Every lattice point lies on one of the planes.

Intercepts with the axes will always be a simple fraction

In general $\frac{a_1}{h}, \frac{a_2}{k}, \frac{a_3}{l}$ will be intercepts

Construct a pair of vectors to define this plane:

$\left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}\right)$ and $\left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_3}{l}\right)$

Consider product will $\vec{H}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

$$\left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}\right) \cdot \left(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3\right) = 1 - 1 = 0 \quad \text{etc.}$$

Proves that the vector $\vec{H}_{hkl}$ is perpendicular to the plane.

Now consider the 'd-spacing' d_{hkl} between the planes

$$d_{hkl} = \frac{\vec{a}_1}{h} \cdot \hat{n} \qquad \hat{n} = \text{unit vector normal to planes} = \frac{\vec{H}_{hkl}}{|H_{hkl}|}$$

$$= \frac{\vec{a}_1}{h}\left(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3\right)\frac{1}{|H_{hkl}|} = \frac{1}{|H_{hkl}|}$$

In physics notation, the result is $d_{hkl} = \frac{2\pi}{|K|}$

10. Diffraction

Amplitude scattered by a lattice of points:

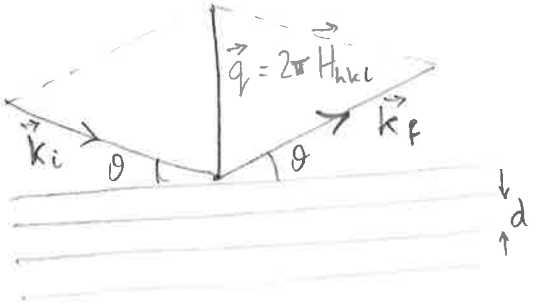
$$A = \sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r}_j} \qquad \vec{r}_j = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3 \in \vec{R}$$

$$= \sum_{m_1 m_2 m_3} e^{i\vec{q}\cdot(m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3)}$$

If the lattice is large enough (eg infinite), this will always add to zero except when:

$$e^{i\vec{q}\cdot\vec{R}} = 1 \quad \in \vec{R} \quad \text{definition of reciprocal lattice}$$

$$\Rightarrow \vec{q} = 2\pi \vec{H}_{hkl} \quad (\text{or } \vec{q} = \vec{K})$$



Implies

i) $\vec{q} \perp$ planes with Miller indices hkl.

ii) $\vec{k}_i$ & $\vec{k}_f$ are symmetric, making angle θ to planes

iii) $|q| = 2|k|\sin\theta = 2\frac{2\pi}{\lambda}\sin\theta = \frac{2\pi}{d_{hk}}$

Bragg's law. $\Rightarrow \boxed{2d_{hkl}\sin\theta = \lambda}$

This provides an elegant pictorial view of diffraction: the x-rays are seen to specularly 'reflect' from the lattice planes.

Every possible set of planes gives a different 'Bragg reflection'.