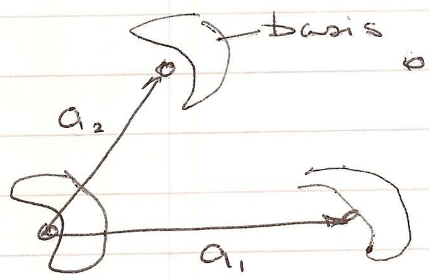
Structure of Periodic Solids

xtal : Infinite repeat of identical units.
Basis : Repeating unit
Lattice : Translation vector

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

primitive translation vector.

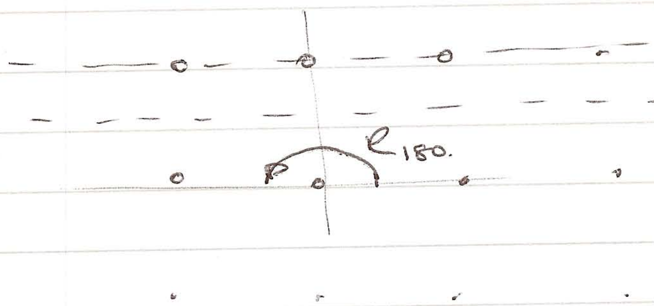
$\{R\} \Rightarrow$ Bravais lattice.



Symmetries: — $T = \sum_i n_i \vec{a}_i$

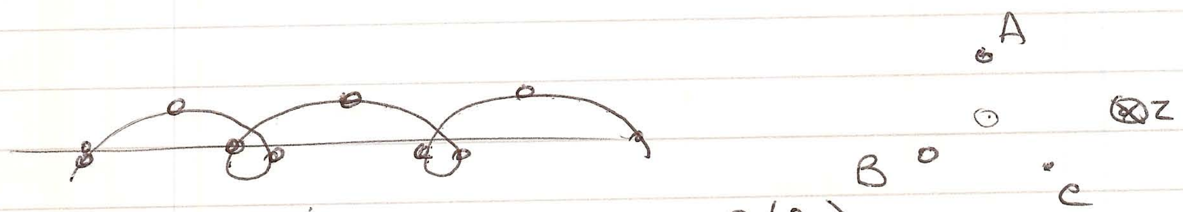
Point group symm. $R \equiv$ Rotations / Reflections.

2D ▭ lattice



mirror planes

Space group — All possible T+R
[N.B. Maybe T+R symm, T, R separately not.



$\Rightarrow T\left(\frac{1}{3}\text{ latt const}\right) + R\left(\frac{2\pi}{3}\right)$

[Se]

3D Lattices.

7 distinct point groups — crystal symmetries

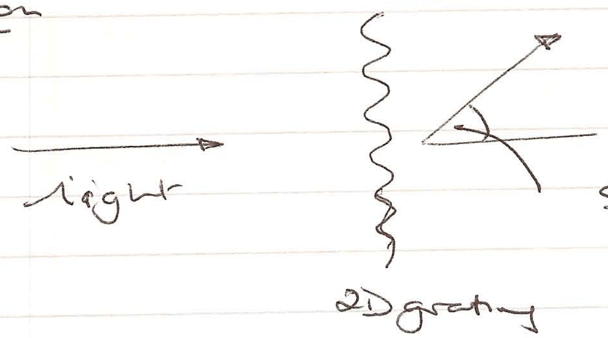
→ 14 Bravais lattices

[Simple cubic → bcc → fcc]

32 distinct point groups

230 different space groups ....

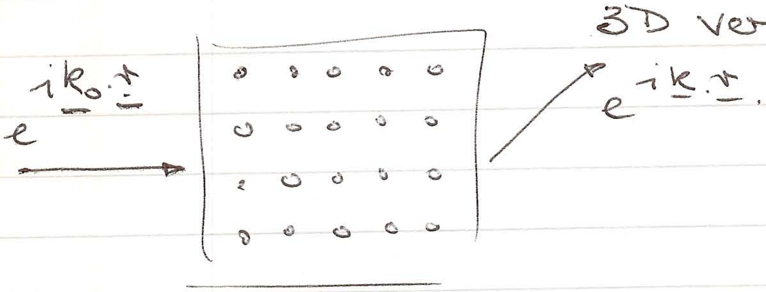
<u>Diffraction</u>



fraunhofer diffraction pattern.

$$\sin\theta = \frac{\lambda}{d}.$$

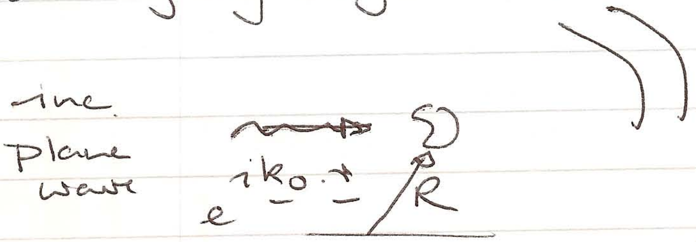
3D version.



Scattering by single atom.

$$\frac{e^{ik_0 r}}{r}$$

$$k_0 = \frac{\omega}{c} = \frac{2\pi}{\lambda}$$



Weak scattering — 1st Born Approx

$$\psi \propto e^{i\underline{k}_0 \cdot \underline{r}} + f(\theta)\, \frac{e^{ik_0|r-R|}}{|r-R|}\, e^{i\underline{k}_0 \cdot \underline{R}}$$

Now $|r| \gg |R|$

$$k_0|r-R| = k_0\sqrt{[r^2 + R^2 - 2\underline{r}\cdot\underline{R}]}^{1/2}$$

$$\simeq k_0 r - k_0 \frac{\underline{r}\cdot\underline{R}}{r}$$

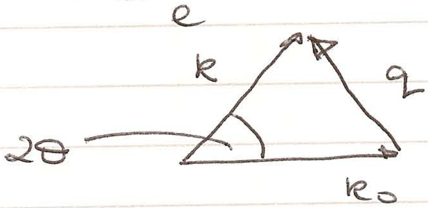
$$= k_0 \underline{r} - \underline{k}\cdot\underline{R}$$

scattered wave

$\underline{k} = \; = k_0 \underline{r}/|r|$

Scattered wave

ψ_{scatt} $\quad f(\theta)\frac{e^{ik_0 r}}{r} e^{-i\underline{k}\cdot\underline{R}} e^{i\underline{k}_0\cdot\underline{R}}$



Many scatterers:

$$\psi_{Scatt} = f(\theta)\frac{e^{ik_0 r}}{r} \underbrace{\sum_{\underline{R}} e^{i\underline{q}\cdot\underline{R}}}_{\text{in general varies in phase } \Sigma \to 0}$$

<u>Except</u> if $\underline{q}\cdot\underline{R}_i = 2\pi m_i$

Set of vectors $\underline{G}$ that satisfy

$\underline{G}\cdot\underline{R} = 2\pi \times \text{integer} \Rightarrow$ recip lattice.

<u>Ans:</u> $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \wedge \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \wedge \vec{a}_3}$ + cyclic perm.

By inspection. $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$

~~Form~~ Lattice of $\vec{b}$'s just like lattice of $\vec{a}$'s.

Qu 8, 9.

Brillouin zones & Bragg's Law

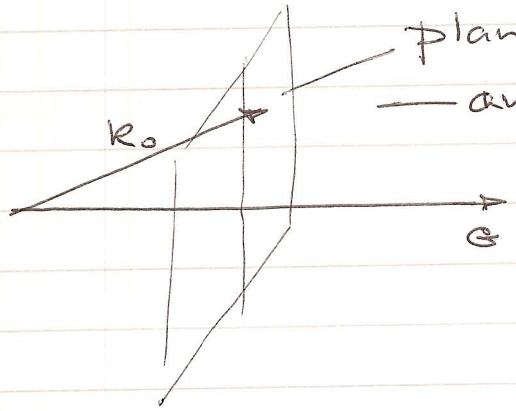
$|k| = |k_0|$ Cons of Energy

$k = k_0 + G$ diffr^n cond^n.

$\therefore \cancel{k^2} = \cancel{k_0^2} + G^2 + 2k_0 \cdot G$

) send $G \to -G$, still in set.

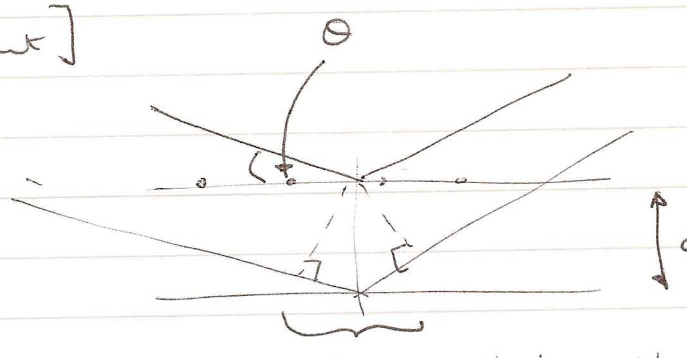
$\therefore \underline{k_0} \cdot \frac{1}{2}\underline{G} = \left|\frac{1}{2}G\right|^2$



plane ⊥ to & bisecting G
— any k_0 will satisfy this condition.

Bragg's law.

[Baby argument]



extra path length. $2d\sin\theta$

constructive interference
if $2d\sin\theta = n\lambda$

Qu 10

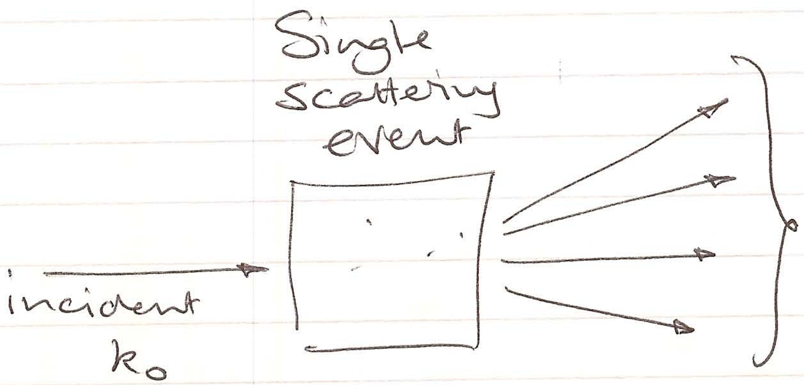
Consistent:

$|G| = \frac{2\pi}{d} \cdot n \qquad |k_0| = \frac{2\pi}{\lambda}.$

$\underline{k_0} \cdot \frac{1}{2}\underline{G} = \frac{2\pi}{\lambda}\sin\theta \cdot \left|\frac{1}{2}G\right| = \left|\frac{1}{2}G\right|^2$

ie $\frac{2\pi}{\lambda}\sin\theta = \left|\frac{1}{2}G\right| = \frac{\pi n}{d}.$

X-ray determination of xtal structure



Outgoing set of waves

$$\sum_G a_G e^{i(\underline{k}_0 - \underline{G}) \cdot \underline{r}}$$

— measure G's → reciprocal lattice → lattice

— measure a_G → "form factors" — detailed structure of "basis".

Electrons — single scattering approx no good

→ multiple scattering (complicated)

BUT $k \longrightarrow k+G \longrightarrow k+G' \longrightarrow \ldots$

Always momentum changes in units of $\underline{G}$ — "fractional" part of k is a good quantum number

— fundamental symmetry, Bloch's Th$^{\underline{m}}$.