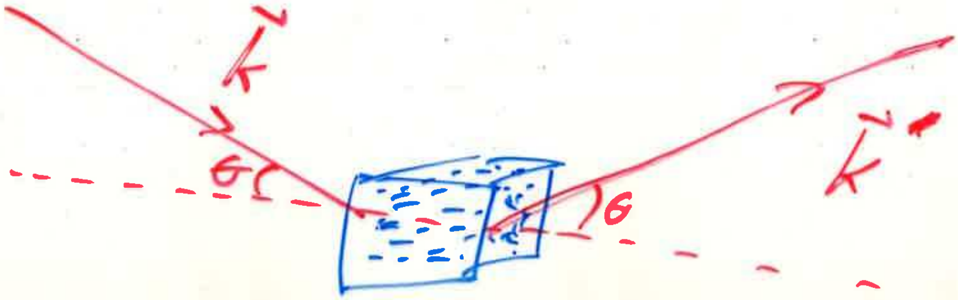
Diffraction from Xtals



elastic scattering
(no recoil)

$$|\vec{k}| = |\vec{k}'|$$

$$\Delta \vec{k} = \vec{k}' - \vec{k}$$

Direct lattice vector $\vec{T} = \sum_{j=1}^{3} n_j \vec{a}_j$

Reciprocal lattice vector $\vec{G} = \sum_{j=1}^{3} p_j \vec{b}_j$

$$\vec{b}_1 = \frac{2\pi\, \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad , \quad \vec{a}_1 \cdot \vec{b}_1 = 2\pi$$

Electron number density

$$n(\vec{r}) = \sum_{\vec{p}} \tilde{n}_{\vec{p}}\, e^{i\vec{G}\cdot\vec{r}}$$

$\sum_{\vec{p}} = \sum_{p_1 = -\infty}^{+\infty} \sum_{p_2} \sum_{p_3}$

$\tilde{n}_{\vec{p}}$: p_1, p_2, p_3

$\vec{G}$: p's in here

$$\tilde{n}_{\vec{p}} = \frac{1}{V} \iiint_{cell} n(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dV$$

Scattering Amplitude   Intensity $\propto F^*F = |F|^2$

$$F \equiv \iiint n(\vec{r})\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\, dV$$

$$\frac{\text{path difference}}{\text{wavelength} - \lambda} = \text{phase difference}$$

Some particular R.L. vector

$$F = \sum_{\vec{p}} \iiint \hat{n}_{\vec{p}}\, e^{i(\vec{G}-\Delta\vec{k})\cdot r}\, dV = \begin{cases} V\hat{n}_{\vec{p}_0}, & \Delta\vec{k} = \vec{G}_0 \\ \sim 0, & \Delta\vec{k} \neq \vec{G}_0 \end{cases}$$

$$\Delta\vec{k} = \vec{G}_0 \Rightarrow \vec{k} + \vec{G}_0 = \vec{k}'$$

dot product both sides

$$(\vec{k}+\vec{G}_0)\cdot(\vec{k}+\vec{G}_0) = \vec{k}'\cdot\vec{k}'$$

$$k^2 + G_0^2 + 2\vec{k}\cdot\vec{G}_0 = (k')^2 = k^2$$

$\vec{G}_0 \rightarrow -\vec{G}_0$

$$\Rightarrow \boxed{2\vec{k}\cdot\vec{G}_0 = G_0^2}$$

divide by 4

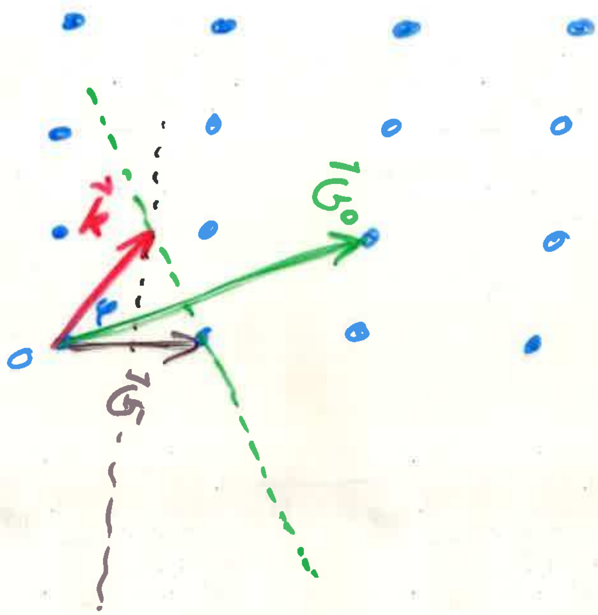
$$\Rightarrow \vec{k}\cdot\left(\frac{\vec{G}_0}{2}\right) = \left(\frac{G_0}{2}\right)^2$$

Brillouin Zone

$\vec{k}$ can be scattered by xtal

Reciprocal Lattice

If $\vec{k}$ ends on the plane that is the perpendicular bisector of $\vec{G}_0$, then

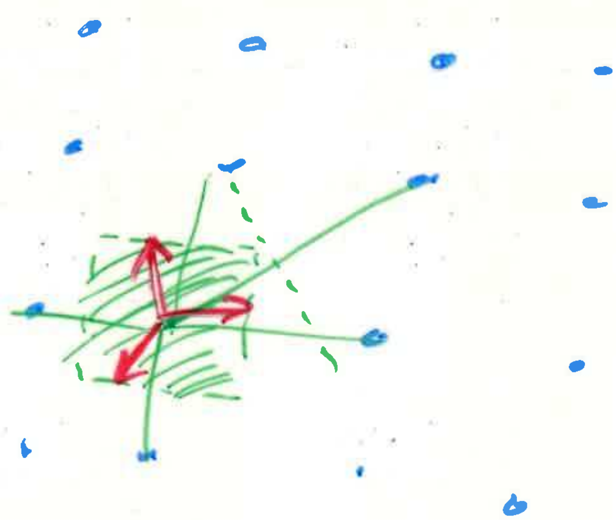


$$\vec{k}\cdot\left(\frac{\vec{G}_0}{2}\right) = \left|\frac{\vec{G}_0}{2}\right| \left|\vec{k}\right| \cos\varphi$$

$$= \left|\frac{\vec{G}_0}{2}\right| \left|\frac{\vec{G}_0}{2}\right|$$

Wigner-Seitz cell in the Reciprocal Lattice
$\Rightarrow$ Brillouin zone

$\vec{k}$ and $\vec{k}'$ must end on the boundary of the B.Z.



Structure Factors

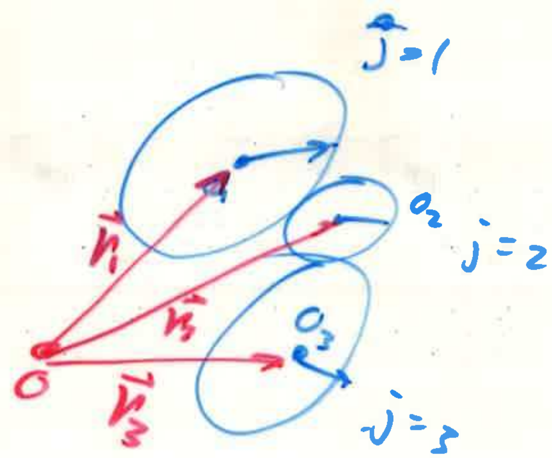
$$F_{\vec{G}_0} = N \iiint n(\vec{r})\, e^{-i\vec{G}_0 \cdot \vec{r}}\, dV$$

Fourier Transform of $n(\vec{r})$

$$\equiv N S_{\vec{G}_0}$$

s atoms in the basis

$$n(\vec{r}) = \sum_{j=1}^{s} n_j(\vec{r} - \vec{r}_j)$$

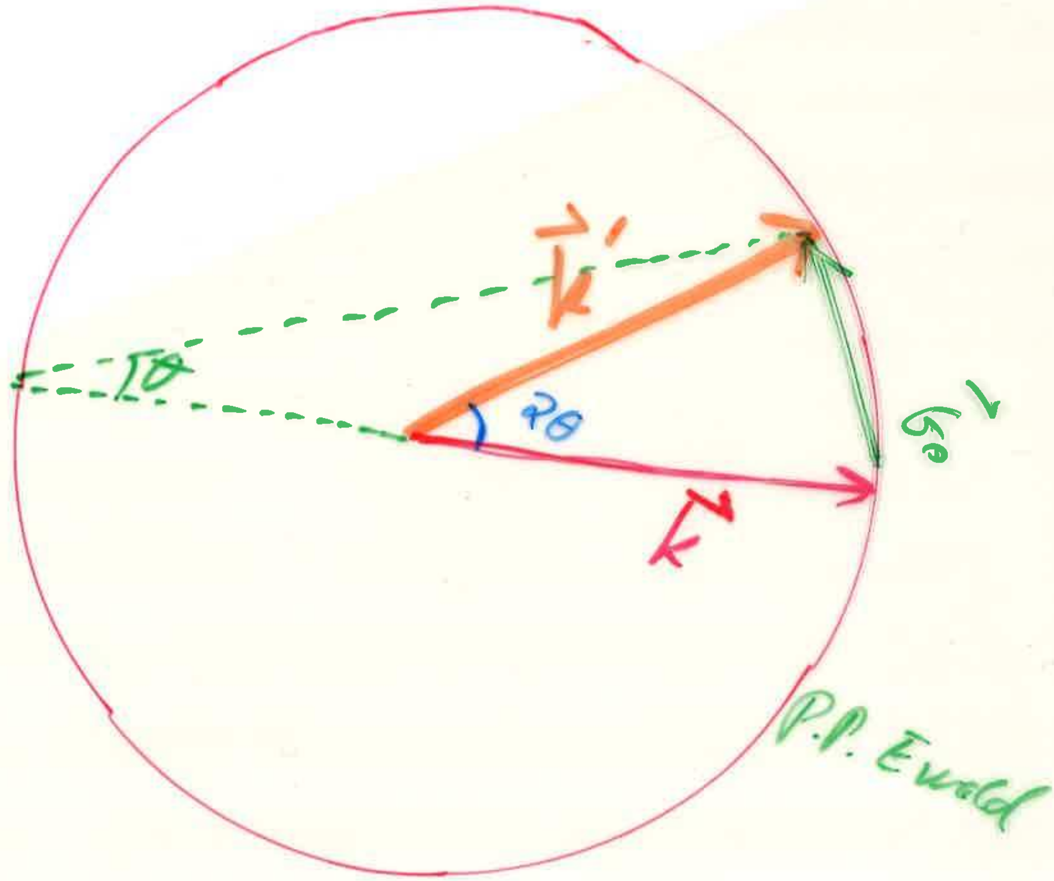


$$S_{\vec{G}_0} = \sum_{j=1}^{s} \iiint n_j(\vec{r} - \vec{r}_j)\, e^{-i\vec{G}_0 \cdot \vec{r}}\, dV$$

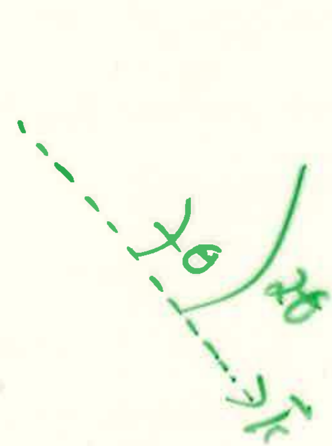
change variable

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

$$= \sum_{j=1}^{s} e^{-i\vec{G}_0 \cdot \vec{r}_j} \iiint n_j(\vec{\rho}_j)\, e^{-i\vec{G}_0 \cdot \vec{\rho}_j}\, dV$$



$\vec{k}'$
2θ
$\vec{G}_0$
$\vec{k}$
P.P. Ewald



$\vec{k}$