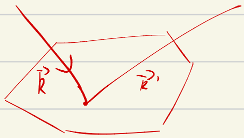


- Amplitude @ r_j: $\vec{E}_\alpha = \vec{E}_0 \exp(i[\vec{k}\cdot\vec{r}_j - \omega t]) = \vec{E}_\beta e^{-i\omega t}$, $\vec{E}_\beta = \vec{E}_0 \exp(\vec{k}\cdot\vec{r}_j)$

- An oscillating $\vec{E}$ field causes displacement of charges: $\vec{d} = \frac{eE}{m\omega^2}$

$$d(t) = \frac{e\vec{E}_\beta}{m\omega^2} e^{-i\omega t}$$

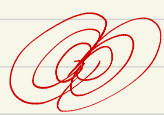
Note we assume $E(\vec{r}_j, t) = E(r_j + \alpha\vec{d}, t)$, $\alpha \in [-1,1]$.

- Leads to dipole oscillator, $\vec{p} = -e\vec{d} = \vec{p_0} e^{-i\omega t}$, $\vec{p_0} = -ed$

Accel

- Charge generates $\vec{E}$-field: $\frac{q}{4\pi\epsilon_0|\vec{r}|^2}\hat{r}$

- For a dipole oscillating of dipole we have: oscillating E field. $p_0 e^{-i\omega t}\frac{k^2 e^{ikR}}{4\pi\epsilon_0 R}(\hat{R}\times\hat{p_0}\times\hat{R})$



Contains that stuff

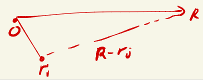
- An atom of Atomic No Z, will have Z e^-'s.

So $\vec{E}$ field due to the impact of the incident x-rays is: $\vec{E}_j = \vec{E}_0 \exp(i[\vec{k}\cdot\vec{r}_j - \omega t]) \times f_j \times \frac{e^{ik|R-r_j|}}{|\vec{R}-\vec{r}_j|}$

$\sim \frac{1}{k}$

Spherical wave

Far field approximation for dipole radiation. as $\|\vec{R}\| \gg 1$



Looking here at: $|\vec{R} - \vec{r}_j|$

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

Now we take $\|R\| \gg \|r_j\|$ so

$$\approx R^2 - 2\vec{R}\cdot\vec{r}_j ,$$

$$|\vec{R} - \vec{r}_j| \approx R\sqrt{1 - \frac{2\vec{R}\cdot\vec{r}_j}{R}}$$

Taking $\sqrt{1-x} \approx 1 - \frac{x}{2}$

$$\approx R\left(1 - \frac{\vec{R}\cdot\vec{r}_j}{R^2}\right)$$

$$\approx R - \frac{\vec{R}}{R}\cdot r_j$$

$$\approx R - \hat{R}\cdot\vec{r}_j$$

Applying this to we get:

$$\vec{E}_j = \vec{E}_0 \exp(i[\vec{k}\cdot\vec{r}_j - \omega t]) \times f_j \times \frac{e^{ik|R - r_j|}}{|\vec{R} - \vec{r}_j|} \longrightarrow \frac{\exp(ik[\|R\| - \hat{R}\cdot\vec{r}_j])}{\|R\| - \vec{r}_j\cdot\hat{R} \approx \|R\|}$$

Note we drop the r_j term here as it has a lesser effect than in the $\exp(i\cdots)$ term.

@ Detector

$$\vec{E}_j = \overbrace{E_0 \exp(i[\vec{k}\cdot\vec{r}_j - \omega t])}^{\text{Incident at atom}} \times \overbrace{f_j}^{\text{Atomic scattering factor}} \times \frac{\exp(ik[R - \hat{R}\cdot r_j])}{R} \longrightarrow \vec{k}\hat{R} = \vec{k}' \text{ as } \|\vec{k}'\| = \|\vec{k}\|$$

$$E_j = E_0 \exp\left(i\left[\vec{k}\cdot\vec{r}_j - \omega t\right]\right) \times f_j \times \exp(ikR)\, \exp\left(-i\vec{k}'\cdot\vec{r}_j\right)$$

$$= E_0 \frac{\exp\left(i\left[kR - \omega t\right]\right)}{R} \times f_j \times \exp\left(i\left[\left(\vec{k}' - \vec{k}\right)\cdot\vec{r}_j\right]\right)$$

Three step process:

$$A_j = \underbrace{A \exp\left(i\left[\vec{k}\cdot\vec{r}_j - \omega t\right]\right)}_{\text{Incident rad @ } r_j} \times \underbrace{f_j}_{\text{Atomic factor}} \times \underbrace{\frac{\exp\left(ik|\vec{R} - \vec{r}_j|\right)}{|\vec{R} - \vec{r}_j|}}_{\text{Amplitude at detector of wave emitted by atom.}}$$

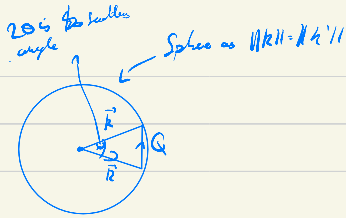
If detector is a long way from crystal:

$$A_j = \underbrace{A\, \frac{\exp\left(i\left[kR - \omega t\right]\right)}{R}}_{\text{Constant for all atoms in crystal}} \times \underbrace{f_j}_{\text{Dep on type of atom @ } r_j} \times \frac{\exp\left(ik'|\vec{R} - \vec{r}_j|\right)}{|\vec{R} - \vec{r}_j|}$$

Dep on location of atom r_j.

Now considering the total Amplitude:

$$A_{TOT} = \underbrace{C}_{\text{Same for all atoms}} \sum_j f_j \exp\left(-i\left[\vec{Q} \cdot \vec{r}_j\right]\right), \quad \vec{Q} = \vec{k}' - \vec{k}$$



$$|\vec{Q}| = 2k \sin\theta$$

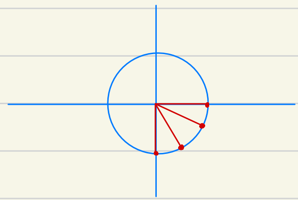
θ: Bragg angle.

For a simplified example we consider:

$$A(\vec{Q}) = C f \; f(\vec{Q}\cdot\vec{a})\, f(\vec{Q}\cdot\vec{b})\, f(\vec{Q}\cdot\vec{c})$$

$$f(c) = \sum_{n\in\mathbb{Z}} e^{-i n \cdot c}$$

$$= \sum \left[\exp(-i\cdot c)\right]^n$$



As per the discussion on [roots of unity]]