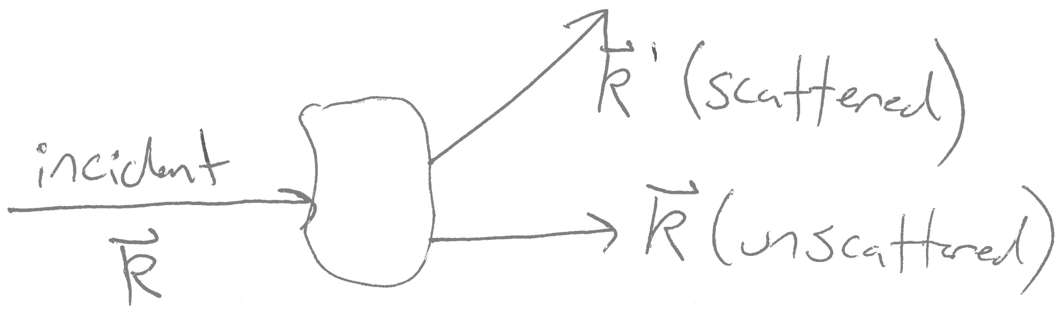
Fri. Oct. 26

- Last time we started with the Laue condition for crystal wave scattering



- the transition rate per unit time

$$\Gamma(\vec{k}', \vec{k}) = \frac{2\pi}{\hbar} |\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle|^2 \delta(E_{\vec{k}'} - E_{\vec{k}})$$

$V(\vec{r}) \rightarrow$ potential of sample

$\delta(E_{\vec{k}'} - E_{\vec{k}}) \rightarrow \rho \rightarrow$ density of final states

"Fermi's golden rule"

- what we are interested in is the matrix element

$$\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle$$

$$\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle = \int d\vec{r} \frac{e^{-i\vec{k}'\cdot\vec{r}}}{\sqrt{L^3}} V(\vec{r}) \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}}$$

$$= \frac{1}{L^3} \int d\vec{r}\, e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}} V(\vec{r}),$$ which is the F.T. of $V(\vec{r})$

- let's see what happens when $V(\vec{r})$ is periodic, like in a crystal

- choose some position $\vec{r} = \vec{R} + \vec{x}$, where $\vec{R}$ is a real lattice vector + $\vec{x}$ is a vector within a unit cell

- now we have

$$\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle =$$

$$\frac{1}{L^3} \sum_{\vec{R}} \int_{\text{unit cell}} d\vec{x}\, e^{-i(\vec{k}'-\vec{k})\cdot(\vec{x}+\vec{R})} V(\vec{x}+\vec{R})$$

- by periodicity $V(\vec{x}+\vec{R}) = V(\vec{x})$

$$\Rightarrow \langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle$$

$$= \frac{1}{L^3} \left[\sum_{\vec{R}} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} \right] \left[\int d\vec{x}\, e^{-i(\vec{k}'-\vec{k})\cdot\vec{x}}\, V(x) \right]$$

- recall $\sum_{\vec{R}} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = 0$, unless $\vec{k}' - \vec{k} = \vec{G}$

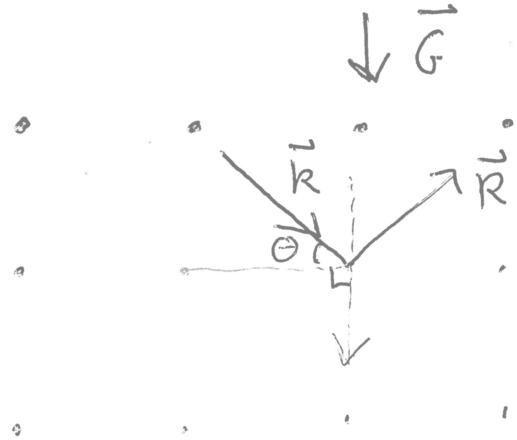
where $\vec{G}$ = rec. lattice vector

- we can see this by recalling

$$\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} = \frac{(2\pi)^D}{\text{vol.}} \sum_{\vec{G}} \delta^D(\vec{k}-\vec{G})$$

- $\vec{k}' - \vec{k} = \vec{G}$ is called the Laue condition

- Equivalence of Bragg + Laue conditions



$$\vec{k} = k\hat{k}$$
$$\vec{k}' = k'\hat{k}'$$
$$\vec{G} = G\hat{G}$$

$$\hat{k}\cdot\hat{G} = \sin\theta = \cos(\theta + 90^\circ)$$
$$= \hat{k}'\cdot\hat{G}$$

- note $k = k' = 2\pi/\lambda \Rightarrow \frac{2\pi}{\lambda}(\hat{k} - \hat{k}') = \hat{G}G = \vec{G}$

$$\Rightarrow \frac{2\pi}{\lambda}\hat{G}\cdot(\hat{k} - \hat{k}') = \hat{G}\cdot\vec{G}$$
$$= \frac{2\pi}{\lambda}(\sin\theta - \sin\theta') = G$$
$$\Rightarrow \frac{2\pi}{G}(2\sin\theta) = \lambda$$
$$\uparrow$$
$$\frac{2\pi}{G} = d \Rightarrow 2d\sin\theta = \lambda \checkmark$$

- let's look at the matrix element

$$\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle, \quad \text{for the periodic function}$$

$$= \left[\frac{1}{L^3} \sum_{\vec{R}} e^{-i(\vec{k}'-\vec{k})\cdot\vec{R}} \right] \left[\int_{\text{unit-cell}} d\vec{x}\, e^{-i(\vec{k}'-\vec{k})\cdot\vec{x}}\, V(x) \right]$$

- first term $=0$ unless Laue condition is met

$$\text{So } S(\vec{G}) = \int_{\text{unit-cell}} d\vec{x}\, e^{i\vec{G}\cdot\vec{x}}\, V(x) \; ; \; \vec{G} = \vec{k} - \vec{k}'$$

- $S(\vec{G})$ is called the "structure factor"
- So what is important about S?
- the intensity of scattering is

$$I(hkl) \propto |S(hkl)|^2$$

assume the potential is the sum over all atoms

$$V(\vec{x}) = \sum_j V_j(\vec{x}-\vec{x}_j), \quad j = \text{atoms in unit cell}$$

• for X-rays,

e.g.

$$V_j(\vec{x}-\vec{x}_j) = Z_j\, g_j(\vec{x}-\vec{x}_j)$$

V → sum of pot. at atom at corner + center

$Z_j \equiv$ atomic # + thus # electrons

$g_j \equiv$ short-range function on order of atomic size

• from which we obtain

$$S(\vec{G}) = \sum_j f_j(\vec{G})\, e^{i\vec{G}\cdot\vec{x}_j}$$

↑ unit cell atoms

$$f_j(\vec{G}) = \int d\vec{x}\, e^{i\vec{G}\cdot\vec{x}}\, V_j(x) \rightarrow \text{F.T. of potential}$$