Phys 460/560 Lecture 8

The Reciprocal Lattice

Crystals are structures which are periodic with respect to all translations of the Bravais lattice:

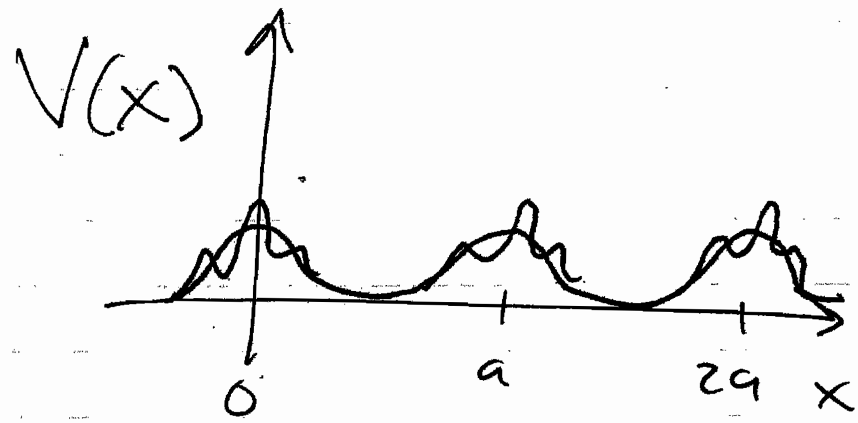
BL: $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

Thus the electron density $\rho(\vec{r})$ and the electrostatic potential $V(\vec{r})$ are periodic

$$\rho(\vec{r} + \vec{R}) = \rho(\vec{r}) \qquad \forall \vec{R} \in BL$$
$$V(\vec{r} + \vec{R}) = V(\vec{r})$$

Periodic functions can be represented by <u>Fourier series</u>.

Let's start with a 1D example:



$$V(x+na) = V(x)$$

$$\Rightarrow V(x) = \sum_{m=-\infty}^{\infty} V_m \, e^{i \frac{2\pi m}{a} x}$$

$$V(x+a) = \sum_{m=-\infty}^{\infty} V_m \underbrace{e^{i \frac{2\pi m}{a}(x+a)}}_{e^{i 2\pi \frac{m x}{a}} \underbrace{e^{i 2\pi}}_{1}}$$

Here $$V_m = \frac{1}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx \; e^{-\frac{2\pi m x i}{a}} V(x)$$

Notice that the factor in the exponent $\frac{2\pi m}{a} = G$ has dimensions of a wave number.

We could write

$$V(x) = \sum_G \tilde{V}_G \, e^{iGx}$$

where $\tilde{V}_G = V_m$.

Now for a function with the periodicity of our 3D Bravais lattice, we must find the vectors $\vec{G}$ s.t.

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

requirement:

$$V(\vec{r}+\vec{R}) = \left(\sum_{\vec{G}} \tilde{V}_{\vec{G}} \, e^{i\vec{G}\cdot\vec{r}} \right) e^{i\vec{G}\cdot\vec{R}} = V(\vec{r}) \quad \forall \vec{R} \in BL$$

$$\Rightarrow \boxed{e^{i\vec{G}\cdot\vec{R}} = \underline{1} \quad \forall \vec{R} \in BL}$$

The set of all vectors $\{\vec{G}\}$ satisfying this constraint is the <u>reciprocal lattice</u> of $\{\vec{R}\}$.

$$e^{i\vec{G}\cdot(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)} = \underline{1}$$

$$\forall n_i \in \mathbb{Z}$$

Clearly a necessary and sufficient condition on $\vec{G}$ is

$$e^{i\vec{G}\cdot\vec{a}_1} = e^{i\vec{G}\cdot\vec{a}_2} = e^{i\vec{G}\cdot\vec{a}_3} = \underline{1}$$

These conditions can be satisfied iff $\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$

where $v_i \in \mathbb{Z}$ and

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

The basis vectors of the reciprocal lattice are

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \qquad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$$

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

It is clear that $\vec{a}_i \cdot \vec{b}_j = 0$ if $i \neq j$ and $\vec{a}_i \cdot \vec{b}_i = 2\pi$.

The reciprocal lattice $\{\vec{G}\}$ is itself a Bravais lattice.

- The reciprocal lattice to $\{\vec{G}\}$, i.e., all vectors $\vec{K}$ satisfying $e^{i\vec{K}\cdot\vec{G}} = 1 \quad \forall \vec{G}$ is evidently the original Bravais lattice $\{\vec{R}\}$.

- The coefficient $\tilde{V}_{\vec{G}}$ in the Fourier series $V(\vec{r}) = \sum_{\vec{G}} \tilde{V}_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$ is determined by
$$\tilde{V}_{\vec{G}} = \frac{1}{V_c} \int_{\text{cell}} d^3r \; e^{-i\vec{G}\cdot\vec{r}} \, V(\vec{r}),$$

analogous to the inverse Fourier transform in 1D.

Verify:

$$\tilde{V}_{\vec{G}} = \frac{1}{V_c} \int_{\text{cell}} d^3r \, e^{-i\vec{G}\cdot\vec{r}} \left\{ \sum_{\vec{G}'} \tilde{V}_{\vec{G}'} \, e^{i\vec{G}'\cdot\vec{r}} \right\}$$

$$= \sum_{\vec{G}'} \tilde{V}_{\vec{G}'} \left\{ \frac{1}{V_c} \int_{\text{cell}} d^3r \, e^{i(\vec{G}'-\vec{G})\cdot\vec{r}} \right\}$$

The term in brackets is clearly 1 if $\vec{G}=\vec{G}'$. If $\vec{G}\neq\vec{G}'$, then $\vec{G}'-\vec{G}=\vec{K}$, where $\vec{K}\neq 0$ is a vector in the reciprocal lattice. Now

$$\int_{\text{all space}} d^3r \, e^{i\vec{K}\cdot\vec{r}} = 0 \qquad \text{and}$$

$e^{i\vec{K}\cdot\vec{r}}$ is a periodic function on the Bravais lattice, so its integral over any unit cell is equal to its integral over any other unit cell. Since the whole of space can be divided into unit cells, we must have

$$\int_{\text{cell}} d^3r \; e^{i\vec{K}\cdot\vec{r}} = 0 \,. \qquad \text{QED.}$$

<u>Scattering</u> Let us now consider how the periodic potential $V(\vec{r})$ scatters electrons, photons, etc.

If we have an electron of

momentum $\vec{p} = \hbar\vec{k}$ incident on the crystal, how is it scattered?

$$\psi_{in}(\vec{r}) = A e^{i\vec{k}\cdot\vec{r}}$$

$$\psi_{out}(\vec{r}) = \int d^3\vec{k}' \; \phi(\vec{k}') \, e^{i\vec{k}'\cdot\vec{r}}$$

The amplitude $\phi(\vec{k}')$ will be nonzero if the matrix element

$$0 \neq \langle \vec{k}' | V | \vec{k} \rangle \propto \int d^3\vec{r} \; e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} \; V(\vec{r})$$

$$= \int d^3\vec{r} \, e^{-i\Delta\vec{k}\cdot\vec{r}} \sum_{\vec{G}} \tilde{V}_G \, e^{i\vec{G}\cdot\vec{r}}$$

$$= \sum_{\vec{G}} \tilde{V}_{\vec{G}} \int d^3\vec{r} \; e^{i(\vec{G}-\Delta\vec{k})\cdot\vec{r}}$$

i.e., if $\Delta \vec{k} = \vec{G}$, a reciprocal lattice vector.

Thus a plane wave $e^{i\vec{k}\cdot\vec{r}}$ is not an eigenstate in the presence of a lattice potential, but is mixed with all states of momentum

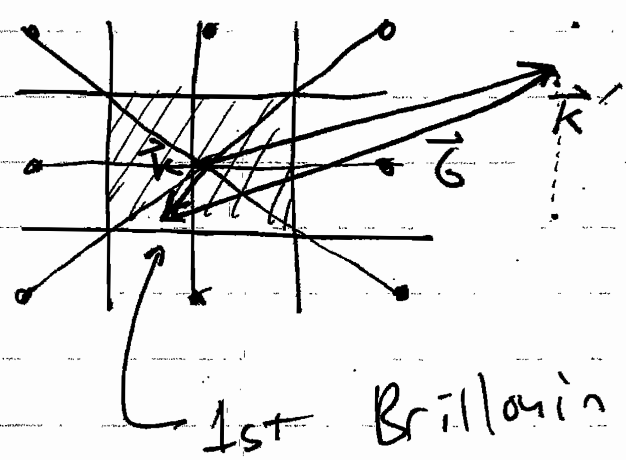
$\vec{k} + \vec{G}$, where $\vec{G}$ is a reciprocal lattice vector.

The momentum is only defined <u>modulo a reciprocal lattice vector</u>

This is a consequence of the broken translational invariance.

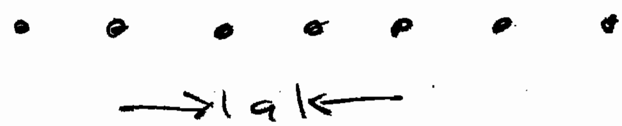
Since momentum is only defined modulo a reciprocal lattice vector, it is conventional to choose $\vec{k}$ to lie in the Wigner-Seitz cell of the reciprocal lattice, known as the <u>1st Brillouin Zone</u>.

Reciprocal lattice:

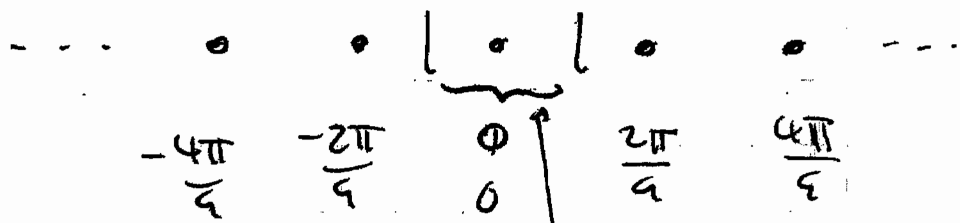


Ex. 1D

lattice: $x = na$

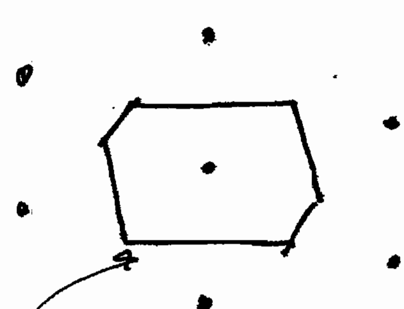


reciprocal lattice: $G = \frac{2\pi m}{a}$



1st Brillouin zone $= \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$

Ex. oblique 2D lattice



reciprocal lattice

1st Brillouin zone

Ex. Reciprocal to sc lattice:

sc lattice $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, $\vec{a}_3 = a\hat{z}$

recip. $\vec{b}_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$, $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

volume of unit cell

$$V_c = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = a^3$$

1st Brillouin zone = cube
bounded by planes

$$k_x = \pm\frac{\pi}{a} \quad k_y = \pm\frac{\pi}{a} \quad k_z = \pm\frac{\pi}{a}$$

volume $\left(\frac{2\pi}{a}\right)^3$

- Quite generally, one can show from the definition of $\vec{b}_i$ in terms of $\vec{a}_j$ that the volume of the 1st

Brillouin zone

$$|\vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3| = \frac{(2\pi)^3}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|} = \frac{(2\pi)^3}{V_{cell}}$$

Ex. Reciprocal to bcc lattice

bcc lattice:

$$\vec{a}_1 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}) \qquad \vec{a}_2 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$$

$$V_{cell} = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = \frac{a^3}{2}$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}) \qquad \vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z})$$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$$

$\Rightarrow$ fcc lattice

$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$

$$= \frac{2\pi}{a}\left[(v_2+v_3)\hat{x} + (v_1+v_3)\hat{y} + (v_1+v_2)\hat{z}\right]$$

The shortest $\vec{G}$'s are the 12

$$\frac{2\pi}{a}(\pm\hat{y} \pm \hat{z}) \qquad \frac{2\pi}{a}(\pm\hat{x} \pm \hat{y}) \qquad \frac{2\pi}{a}(\pm\hat{x} \pm \hat{z})$$

where all signs are independent.

$\Rightarrow$ See figure from pg. 41
1st Brillouin Zone is regular 12-sided polygon.

Ex. <u>Reciprocal to fcc lattice</u>

fcc lattice: $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$$

$$V_c = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = \frac{a^3}{4}$$

reciprocal lattice:

$\vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$ $\qquad$ $\vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \Rightarrow bcc$$

Shortest $\vec{G}$s are 8 vectors

$$\frac{2\pi}{a}(\pm\hat{x}\pm\hat{y}\pm\hat{z})$$

→ 1st Brillouin zone is truncated octahedron.

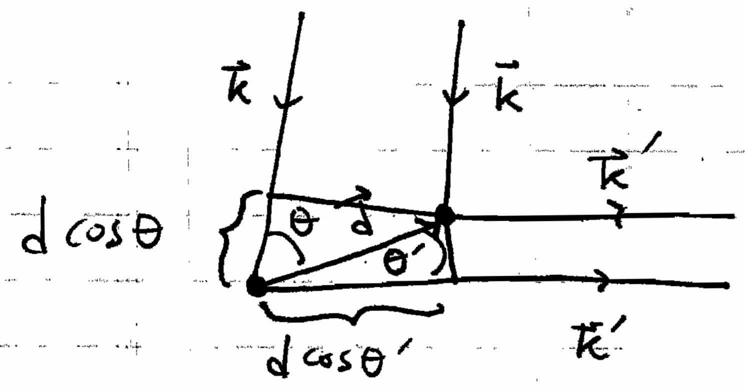
See figs. 14 and 15 pg. 42-43

X-Ray diffraction

Photons, like electrons, are scattered by a crystal:

$$\vec{k} \longrightarrow \vec{k}+\vec{G}$$

Scattering from two atoms:



Constructive interference if

$$d\cos\theta + d\cos\theta' = m\lambda$$

m ← integer

$$\frac{2\pi d\cos\theta}{\lambda} = -\vec{d}\cdot\vec{k}$$

($\lambda = \lambda'$ elastic scattering dominates)

$$\frac{2\pi d\cos\theta'}{\lambda} = \vec{d}\cdot\vec{k}'$$

$$\vec{d}\cdot(\vec{k}'-\vec{k}) = 2\pi m$$

$$\vec{d}\cdot\Delta\vec{k} = 2\pi m$$

or $$e^{i\Delta\vec{k}\cdot\vec{d}} = 1$$

Scattering from a Bravais lattice $\{\vec{R}\}$ will thus give constructive interference if

$$e^{i\Delta\vec{k}\cdot\vec{R}} = 1 \quad \forall\ \vec{R} \in BL$$

This is true provided

$\Delta\vec{k} = \vec{G} \in$ reciprocal lattice

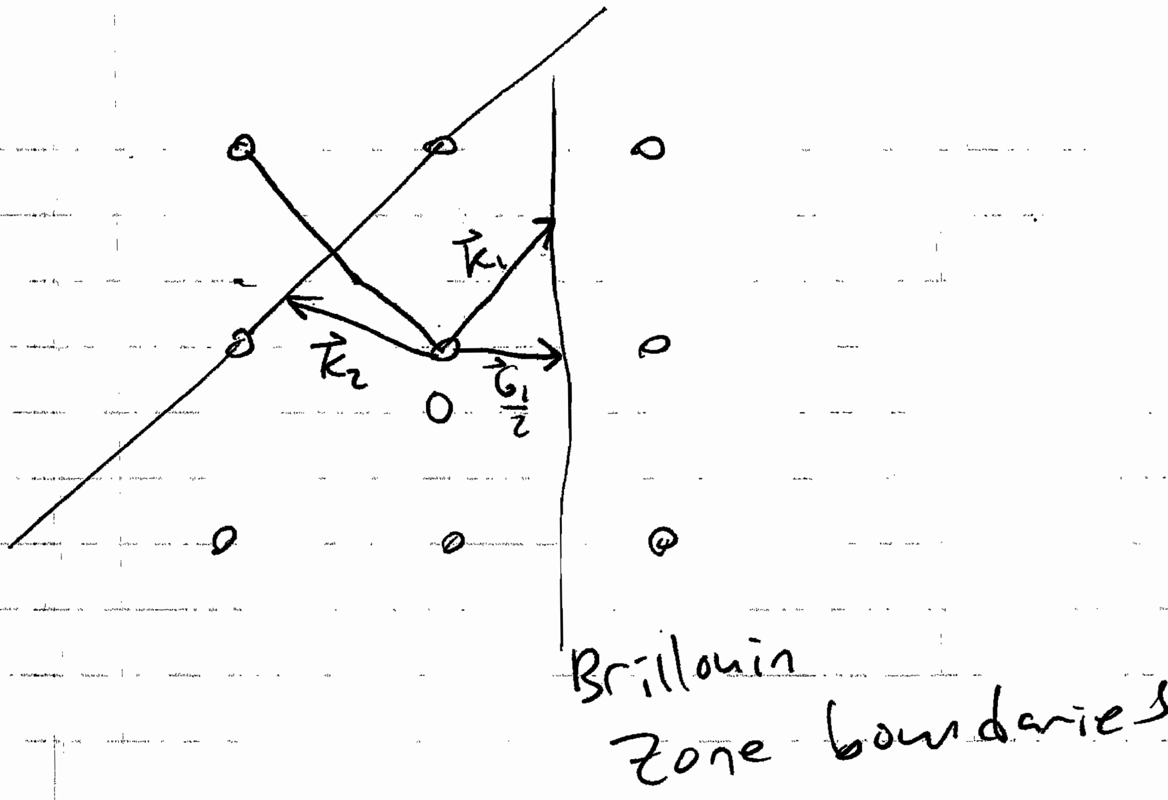
Elastic condition

$$\vec{k}'^2 = \vec{k}^2$$

$$(\vec{k}+\vec{G})^2 = \vec{k}^2 \quad \Rightarrow \quad 2\vec{k}\cdot\vec{G} + \vec{G}^2 = 0$$

$-\vec{G}$ also a reciprocal lattice vector

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



If $\vec{k}$ lies on a Brillouin zone boundary, it will be diffracted. The smallest region enclosed by Brillouin zone boundaries is the 1st Brillouin Zone.