II. The Reciprocal Lattices

e.g. $\vec{a}_1$ has units of length

A. Every Bravais Lattice (for crystals in real or direct space) has a corresponding Reciprocal Lattice (forming the reciprocal space)

$\vec{a}_1, \vec{a}_2, \vec{a}_3$: Bravais Lattice (14 of them)

Define

$$\vec{b}_1 \equiv 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \; ; \; \vec{b}_2 \equiv 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \; ; \; \vec{b}_3 \equiv 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad (1)$$

Ω_c = volume of primitive unit cell (length^3)

Numerators: (length)^2

$\therefore |\vec{b}_1|, |\vec{b}_2|, |\vec{b}_3|$ have units of $\frac{1}{\text{length}}$

Use $\vec{b}_1, \vec{b}_2, \vec{b}_3$ as Primitive Translation Vectors, map out the Reciprocal Lattice (2)

Define $\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$ (3)

n_1, n_2, n_3: integers $(0, \pm 1, \pm 2, \cdots)$

$\vec{G}$: Reciprocal Lattice Vectors

(Key Concept)

All $\vec{G}$'s dot out the Reciprocal Lattice

$\vec{a}_1, \vec{a}_2, \vec{a}_3$	$\vec{b}_1, \vec{b}_2, \vec{b}_3$
$\vec{R} = l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3$	$\vec{G} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$
(Direct)	(Reciprocal)

← "dual lattice of each other" →

Ex: Show that the reciprocal lattice of a reciprocal lattice is the Direct Lattice

Logic

- 14 Bravais Lattices in 3D
- $\vec{a}_1, \vec{a}_2, \vec{a}_3$ map out a 3D lattice
- $\vec{b}_1, \vec{b}_2, \vec{b}_3$ map out the reciprocal lattice, which is also a 3D lattice
- Reciprocal Lattice is also one of the 14 Bravais lattice

  only that $\vec{b}$'s are $\frac{1}{\text{length}}$
- Every Bravais lattice has a reciprocal lattice, which is one of the Bravais lattices

  [a pair of Dual Lattices]

E.g. Simple Cubic $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, $\vec{a}_3 = a\hat{z}$

Then $\vec{b}_1 = \frac{2\pi}{a^3}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a^3} \cdot a^2(\hat{y} \times \hat{z}) = \frac{2\pi}{a}\hat{x}$

$\vec{b}_2 = \frac{2\pi}{a}\hat{y}$; $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

∴ $\vec{b}_1, \vec{b}_2, \vec{b}_3$ also map out a simple cubic lattice

[$a \sim$ few Å $\sim$ few 10^{-10} m] [$\frac{2\pi}{a} \sim 10^{10}\ m^{-1}$]

$\Omega_c = a^3$; Volume of primitive unit cell of reciprocal lattice

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

$$\Omega_c \cdot \Omega_G = (2\pi)^3 \qquad (4)$$

Ω_c: Volume of primitive unit cell in direct space

Ω_G: Volume of primitive unit cell in reciprocal space

Ex: { What are $\vec{b}_1, \vec{b}_2, \vec{b}_3$ for real space FCC lattice?
{ What is the reciprocal space of FCC lattice?

{ What are $\vec{b}_1, \vec{b}_2, \vec{b}_3$ for real space hexagonal lattice?
{ What is the reciprocal space of hexagonal lattice?

Direct	Reciprocal
FCC (Semiconductors)	BCC
BCC	FCC
SC ← (Self-Dual) →	SC

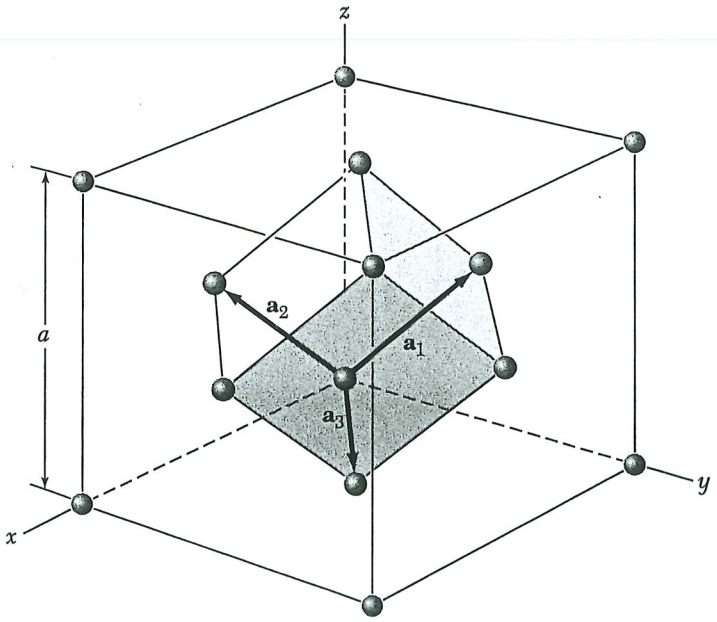
FCC is the (Direct) Lattice for Si, Ge, GaAs, ...
(Most important for Semiconductors)

$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}) \; ; \quad \vec{a}_2 = \frac{a}{2}(\hat{y}+\hat{z}) \; ; \quad \vec{a}_3 = \frac{a}{2}(\hat{z}+\hat{x})$$

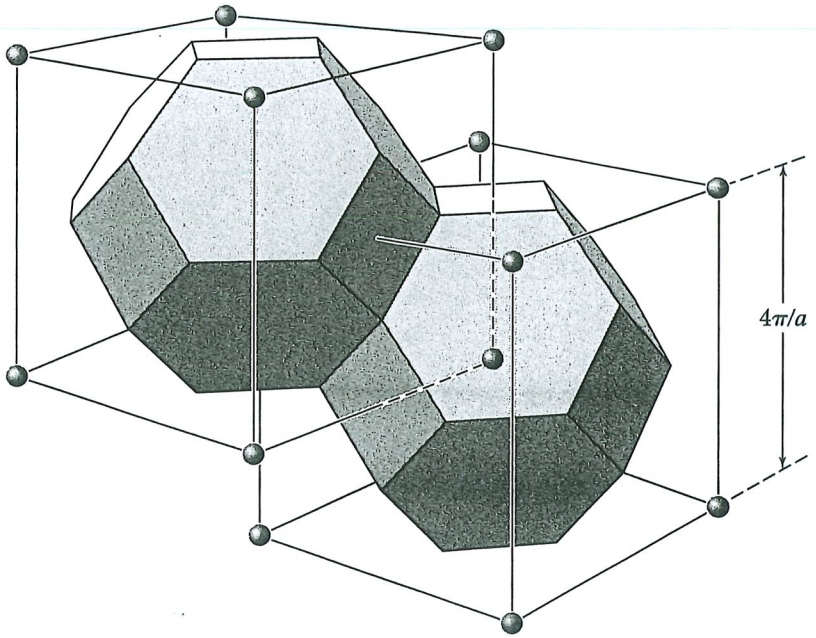
From definition:

$$\begin{cases} \vec{b}_1 = \frac{2\pi}{a}(\hat{x}+\hat{y}+\hat{z}) \\ \vec{b}_2 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{b}_3 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}) \end{cases} \qquad (5) \quad (Ex)$$

→ Map out a Body-centered cubic Reciprocal Lattice, with a conventional unit cell of cube edge $\left(\frac{4\pi}{a}\right)$.



FCC Lattice (Direct Lattice)



(See Eq.(5)) $\vec{b}_1, \vec{b}_2, \vec{b}_3$ give a reciprocal lattice which is BCC

The region in reciprocal space bounded by the polyhedron is called the Brillouin Zone (an important concept) (See Sec. D)

B. Why bother with all these? What for?

- Most important concept in handling crystalline solids
  periodic
- Need it to understand X-ray diffraction patterns
  Not taking picture of Direct Lattice
  But map out Reciprocal Lattice!
- Need it to understand waves in solids
  lives in reciprocal space
  - Electron Waves in Solids [Band Structure] $E(\vec{k})$
  - Elastic Waves in Solids [lattice vibrations, phonon dispersion]
    $\omega(\vec{q})$
    lives in reciprocal space
  - electrons scattered by phonons (resistivity)

Why so?

- Much to do with Fourier Series (Analysis) of Periodic Functions

  Many of them in crystalline solids!

- Life is easier if we only have cubic structure
  (always $\hat{x}$, $\hat{y}$, $\hat{z}$ (orthogonal, same edge length)
- But in solids, we need the formal $\vec{b}_1, \vec{b}_2, \vec{b}_3$ (for $\vec{a}_1, \vec{a}_2, \vec{a}_3$)
  to get ready for any of the 14 Bravais Lattices

[Those interested only in semiconductors can focus on FCC and its reciprocal lattice]

Relations between $(\vec{b}_1, \vec{b}_2, \vec{b}_3)$ and $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$

- $\vec{a}_1 \cdot \vec{b}_1 = \vec{a}_1 \cdot \frac{2\pi}{\Omega_c} (\vec{a}_2 \times \vec{a}_3) = 2\pi = 2\pi \delta_{11}$

  ($\vec{a}_1$ ① $\vec{b}_1$ ①)

- $\vec{a}_1 \cdot \vec{b}_2 = \vec{a}_1 \cdot \frac{2\pi}{\Omega_c} \underbrace{(\vec{a}_3 \times \vec{a}_1)}_{\perp \vec{a}_1} = 0 = 2\pi \underbrace{\delta_{12}}_{\text{"0"}}$

$$\therefore \boxed{\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}} \quad (6)$$

(Key Result)

$\{\vec{b}_i\}$ are intentionally defined to obey these relations

What for?

Consider $\vec{R} \cdot \vec{G} = (l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3) \cdot (n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3)$

$= 2\pi (l_1 n_1 + l_2 n_2 + l_3 n_3) = 2\pi \cdot (\text{integer})$ (Key Result)

$\vec{R}$: any lattice vector

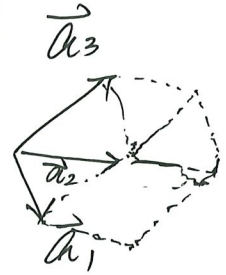
$\vec{G}$: any reciprocal lattice vector

$$\therefore \quad \boxed{e^{i\vec{G}\cdot\vec{R}} = e^{i\,2\pi\cdot(\text{integer})} = 1} \qquad (7) \qquad \text{(Key Result)}$$

Appreciation: $\vec{G}$ (infinitely many, any one of them)

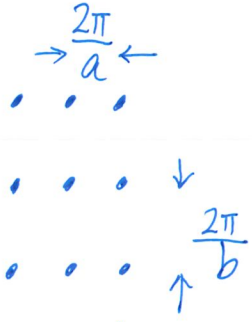
$\vec{R}$ (infinitely many, any one of them)

$\vec{a}_i$ (not necessarily orthogonal to each other)



$\vec{b}_i$ (constructed to be $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$)

Direct



Reciprocal

(X-ray diffraction of Direct lattice pattern gives spots with pattern of the Reciprocal lattice)

A quick application

$\frac{\Omega_c}{2\pi}\vec{b}_1$

(hkl) planes $\quad \vec{g} = h(\vec{a}_2 \times \vec{a}_3) + k(\vec{a}_3 \times \vec{a}_1) + l(\vec{a}_1 \times \vec{a}_2)$

$\perp$ (hkl) planes

$$d(hkl) = \frac{\Omega_c}{|\vec{g}|}$$

no common divisor

With Reciprocal Lattice Vectors $\vec{G}$, $\vec{G}(hkl) = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is normal to (hkl) planes

$$d(hkl) = \frac{\Omega_c}{|\vec{g}|} = \frac{\Omega_c}{\frac{\Omega_c}{2\pi}|\vec{G}(hkl)|} = \frac{2\pi}{|\vec{G}(hkl)|} \qquad (8)$$

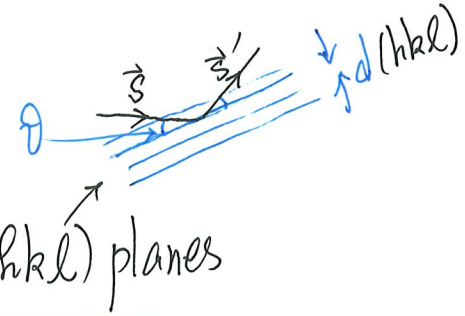
separation between adjacent crystal planes (real space quantity)

length of $\vec{G}(hkl)$ $\perp$ planes

reciprocal space quantity

C. Emergence of Notion of Reciprocal Lattice in X-ray (EM waves) diffraction

Elementary Level



$\vec{S}$ = wave vector

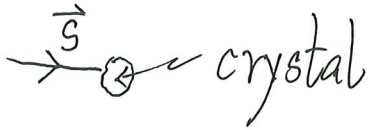
$|\vec{S}| = \frac{2\pi}{\lambda}$

$|\vec{S}'| = \frac{2\pi}{\lambda}$ (Elastic scattering)

$$2\, d(hkl) \sin\theta = n\lambda \quad (9)$$

Bragg condition (n = positive integer)

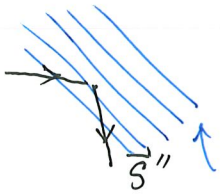
Meaning: Incident Light $\vec{S}$



look for sets of planes that satisfy Bragg condition for some angle

(is it possible?)

Are there



?

planes of proper d

How about

?

Etc.

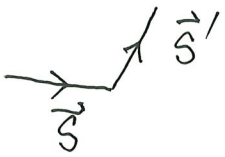
Equivalent to ask whether $\vec{S}' - \vec{S} = \vec{G}_T$ or Not!

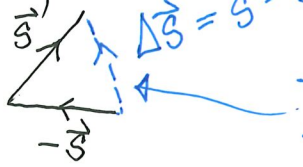
$\vec{S}'$: coming out; $\vec{S}$: incident; $\vec{G}_T$: some reciprocal lattice vector

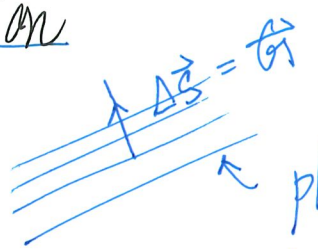
if yes, see bright spot (at least possible) in $\vec{S}'$ direction

$$\boxed{\Delta\vec{S} \equiv \vec{S}' - \vec{S} = \vec{G}_T} \quad (10)$$ is called the Laue Condition

Meaning:







Is this a $\vec{G}_T$ vector in reciprocal lattice?

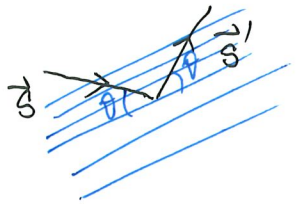
Recall: $\vec{G}_T$ is $\perp$ to a set of planes

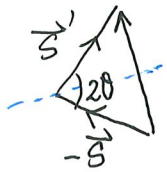
e.g. $\vec{G}(hkl) \perp (hkl)$ planes

$h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

no divisor (corresponds to $n=1$)

$\Delta\vec{S} = \vec{G}$ and $2d\sin\theta = n\lambda$





$\Delta\vec{S} = \vec{s}' - \vec{s} = \vec{G}$ ← some $\vec{G}$ (Laue condition)

$$|\vec{G}|^2 = s'^2 + s^2 - 2|\vec{s}||\vec{s}'|\cos 2\theta$$
$$= 2s^2(1-\cos 2\theta) = 4s^2\sin^2\theta$$

$$|\vec{G}| = 2s\sin\theta = 2\cdot\left(\frac{2\pi}{\lambda}\right)\sin\theta$$

$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3 \qquad (v_1, v_2, v_3 \text{ integers})$$
$$= n(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)$$

↑ common divisor of v_1, v_2, v_3 (thus h, k, l have no common divisor)

$$n\,|\vec{G}(hkl)| = |\vec{G}(v_1, v_2, v_3)| = 2\cdot\frac{2\pi}{\lambda}\sin\theta$$

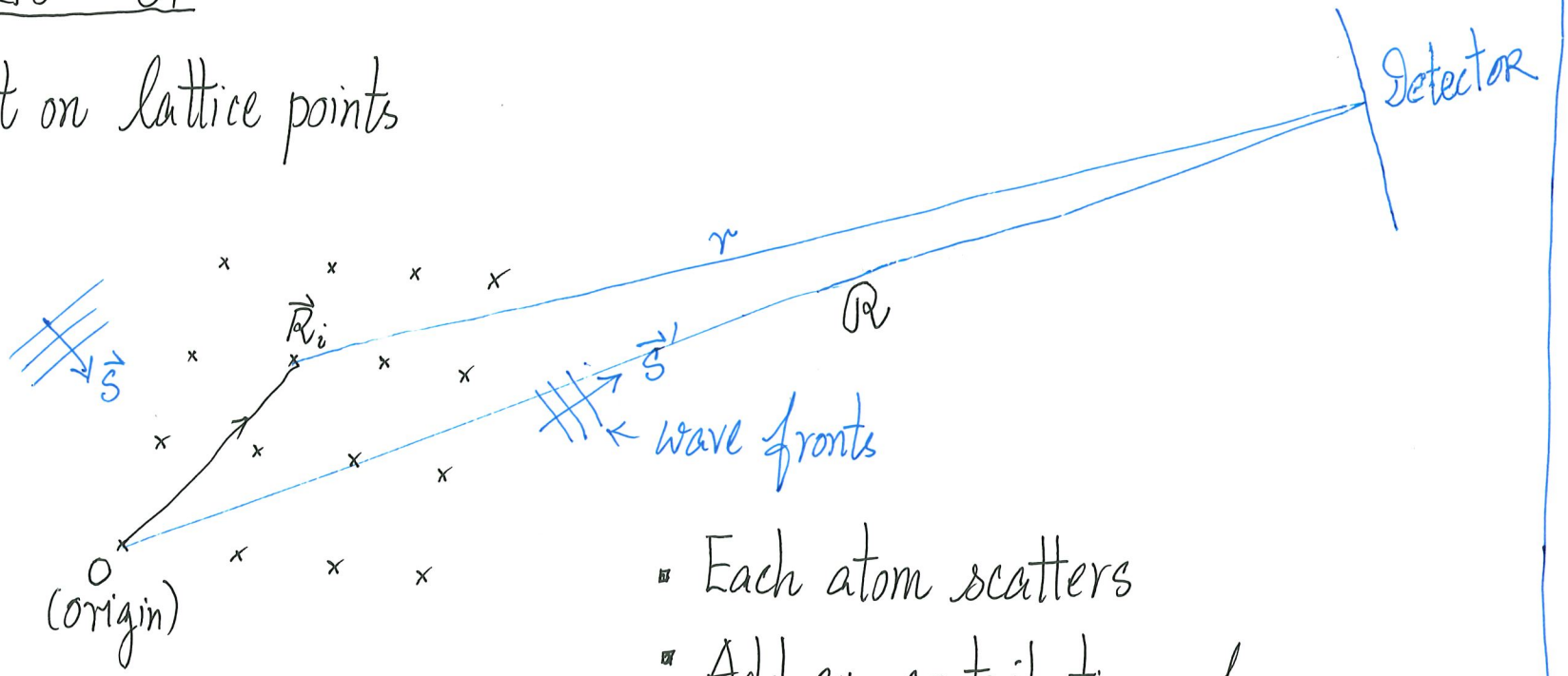
$$\Rightarrow n\lambda = 2\cdot\frac{2\pi}{|G(hkl)|}\sin\theta = 2\,d(hkl)\sin\theta$$

∴ The Laue Condition $\Delta\vec{S} = \vec{G}$ gives the Bragg condition $2d(hkl)\sin\theta = n\lambda$

spots map out reciprocal lattice!

Aside: $\Delta\vec{s} = \vec{G}$

Atoms sit on lattice points



- Each atom scatters
- Add up contributions from regular array of atoms gives what is detected

From Atom at $\vec{R}_i$:

$$\text{Scattered field at detector} \propto \frac{e^{isR}}{R} f\, e^{-i\Delta\vec{s}\cdot\vec{R}_i}$$

spherical outgoing

f: what atom is there

Adding up all atoms: Scattered field at detector

$$\propto \sum_i e^{-i\Delta\vec{s}\cdot\vec{R}_i}$$

$i \leftarrow$ sum over all atoms in solid

Recall: $\vec{G}\cdot\vec{R} = 2\pi\cdot(\text{integer})$ and $e^{i\vec{G}\cdot\vec{R}} = 1$

If $\Delta\vec{s} \neq \vec{G}$, then we have "random phases" that tend to cancel (sum to zero)

If $\Delta\vec{s} = \vec{G}$, then $\sum_i e^{-i\Delta\vec{s}\cdot\vec{R}} = \sum_i 1 =$ # of lattice points in solid

this gives the Laue Condition

10^{23} in solid of cm^3 (or ∞ for infinite system)

[Same idea works for neutron scattering]

We see a good reason to introduce the Reciprocal Lattice

Geometric Feature of Laue Condition

$\frac{2\pi}{\lambda}$

$|\vec{s}| = |\vec{s}'|$ (elastic)

$$\Delta\vec{s} = \vec{s}' - \vec{s} = \vec{G} \Rightarrow \vec{s} + \vec{G} = \vec{s}'$$

$$\Rightarrow s^2 + 2\vec{s}\cdot\vec{G} + G^2 = s'^2 \Rightarrow 2\vec{s}\cdot\vec{G} + G^2 = 0$$

Can rewrite this as $2\vec{s}\cdot\vec{G} = G^2$ ($\because -\vec{G}$ is a reciprocal lattice vector if $\vec{G}$ is one)

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

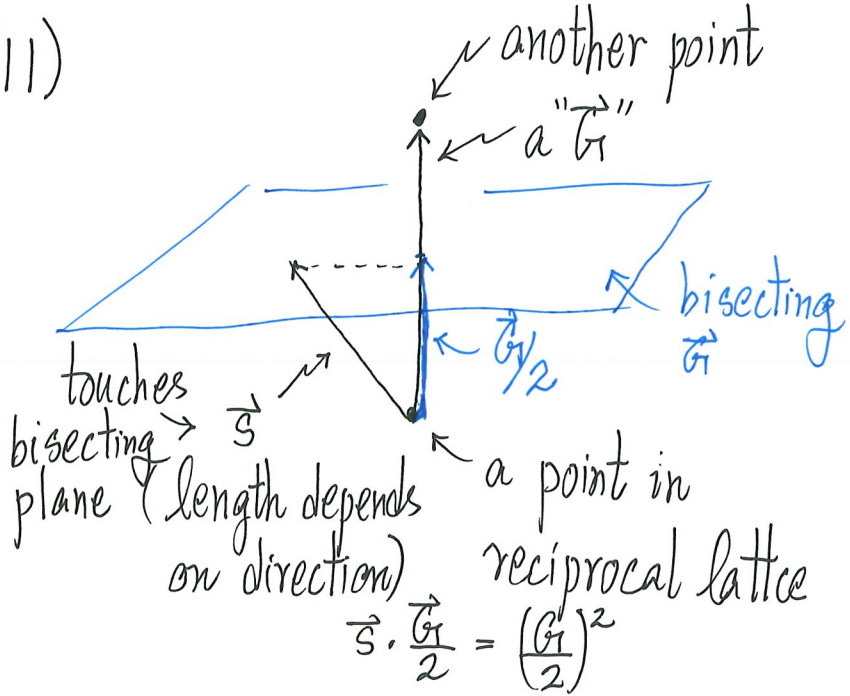
$$\Rightarrow \boxed{\vec{s}\cdot\left(\frac{\vec{G}}{2}\right) = \left(\frac{G}{2}\right)^2} \quad (11)$$

half of a reciprocal lattice vector

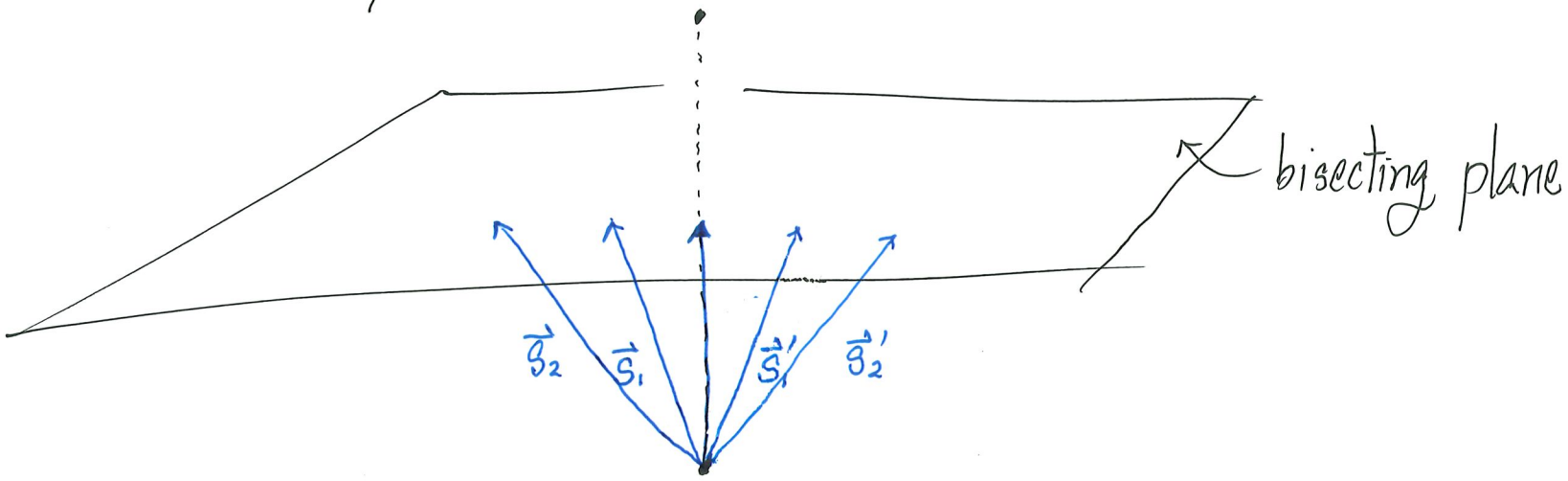
that halved vector's (magnitude)^2

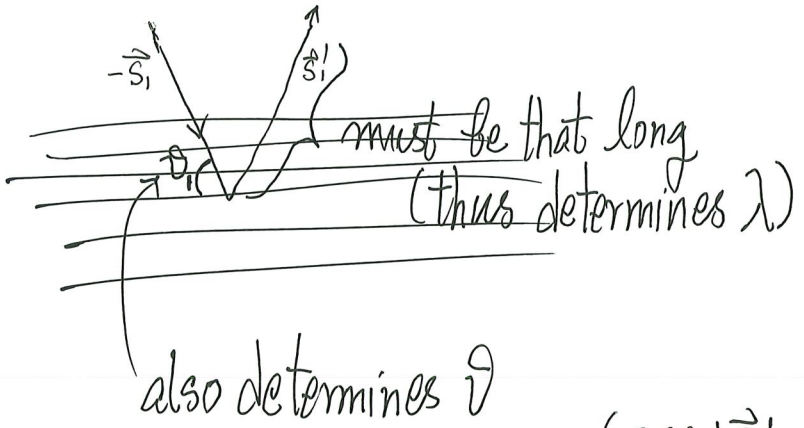
$\vec{s}\cdot\frac{\vec{G}}{2}$ — projecting $\vec{s}$ onto $\frac{\vec{G}}{2}$

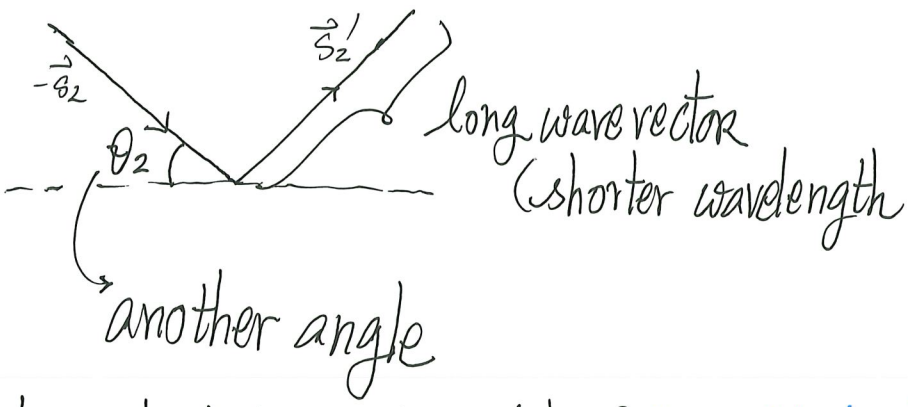
→ Picture



What does it say?







(see $|\vec{S}|$ can't be too short to meet condition) (λ can't be too long)

(another way of thinking about Bragg condition/Laue Condition)

D. Brillouin Zones

- Pick a point in Reciprocal Lattice
- Draw $\vec{G}$'s pointing to other points (from shorter $\vec{G}$'s to longer $\vec{G}$'s)
- Draw Bisecting Planes to every $\vec{G}$ drawn
- Planes enclosed a "volume" (region) nearest to starting point

1st Brillouin Zone (1st B.Z.)

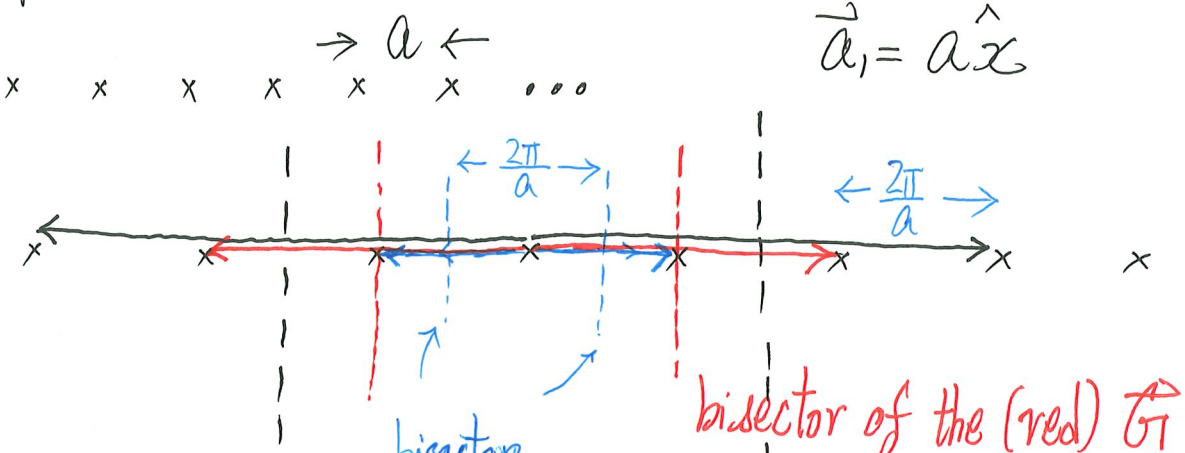
- a primitive unit cell of the reciprocal lattice
- best reflects the symmetry of the reciprocal lattice
- other primitive unit cells must of same volume
- Wigner-Seitz cell of Reciprocal Lattice

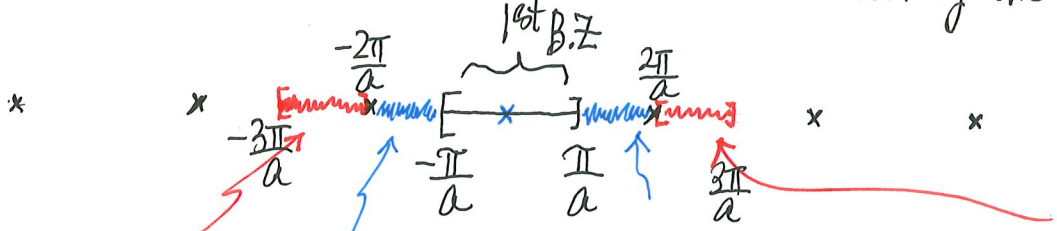
- There are pieces of disjoint volumes formed by the bisecting planes that are NEXT NEAREST to the starting point
  - Collectively the pieces form the 2nd Brillouin Zone
    (the pieces add up to the same volume as the 1st B.Z.)
  - Each piece can be translated (moved) into 1st B.Z. by a $\vec{G}$ vector
- 3rd B.Z., 4th B.Z., ... defined similarly

1D Example

Direct

Reciprocal





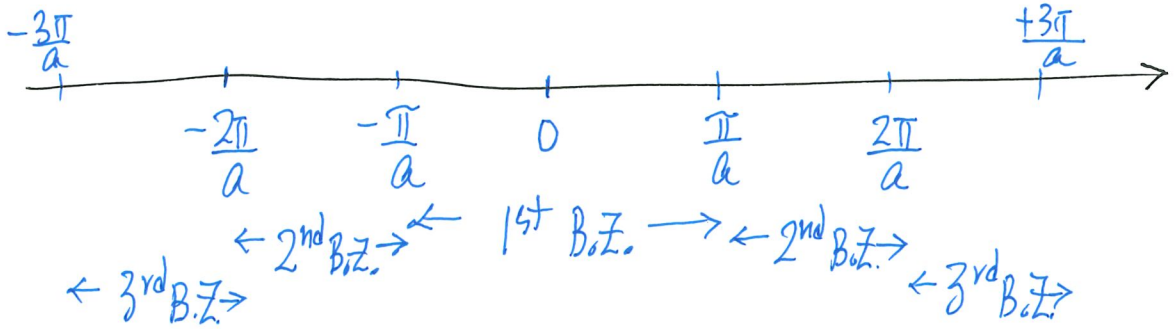
part of 3rd B.Z. can be moved into 1st B.Z. by $+\frac{2\pi}{a}\hat{x}$ (i.e. $+\vec{b}_1$)

part of 2nd B.Z. can be moved into 1st B.Z. by $+\frac{2\pi}{a}\hat{x}$ (i.e. $+\vec{b}_1$)

part of 2nd B.Z. can be moved into 1st B.Z. by $-\frac{2\pi}{a}\hat{x}$ (which is $-\vec{b}_1$)

part of 3rd B.Z. can be moved into 1st B.Z. by $-\frac{2\pi}{a}\hat{x}$ (i.e. $-\vec{b}_1$)

All we need is a $\vec{b}_1$ vector that gives $\vec{a}_1 \cdot \vec{b}_1 = 2\pi$. Orelse, you many introduce $\vec{a}_2 = \hat{y}$, $\vec{a}_3 = \hat{z}$.



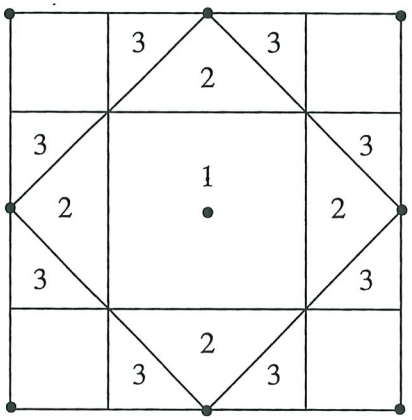
Reciprocal space
(or $\vec{k}$-space or $\vec{q}$-space)

Will be useful in understanding energy bands and band gaps

2D Square Lattice

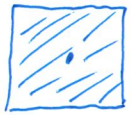
$\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$ (Reciprocal Lattice is also a Square Lattice, edge $\frac{2\pi}{a}$)



The first three Brillouin zones of a two-dimensional square lattice.

1st B.Z



$\frac{2\pi}{a}$

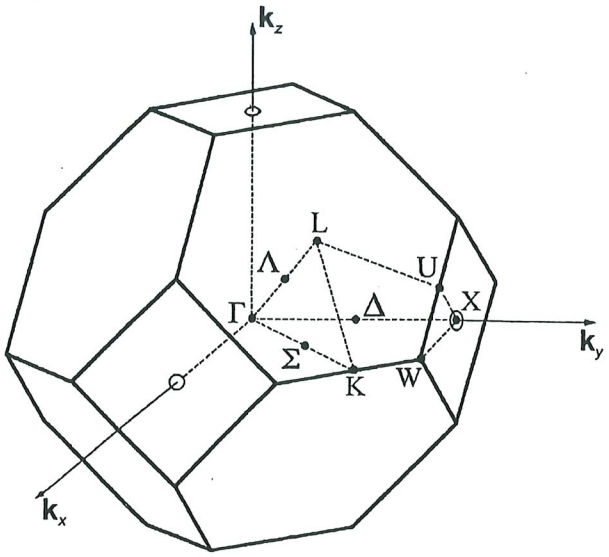
See how the four pieces of 2nd B.Z. add up to the correct area and can be moved into 1st B.Z. by some $\vec{G}$'s

Ex. Graphene has a hexagonal lattice. Work out the reciprocal lattice and identify the 1st, 2nd, 3rd B.Z.

3D Face-Centered Cubic Direct Lattice

- Reciprocal Lattice is BCC, cube edge $\frac{4\pi}{a}$

Gives the most important 1st B.Z. for semiconductors

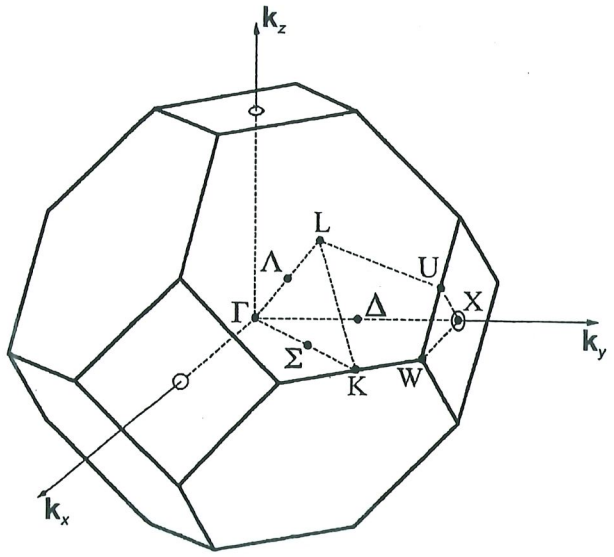


The first Brillouin zone of the diamond and zincblende-type structures. The important symmetry points and lines are indicated.

Γ point $\vec{k}=(0,0,0)$

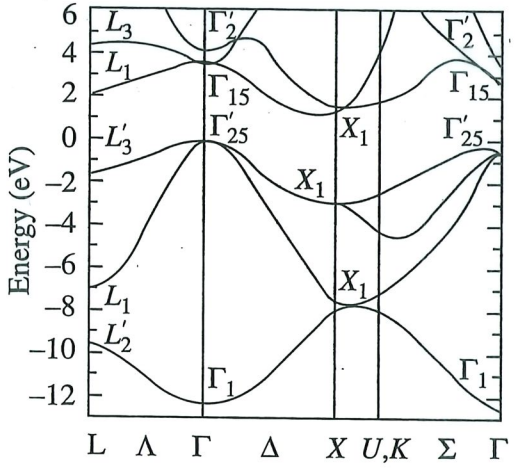
Later, when you see energy band diagram showing $E(\vec{k})$ from Γ to X, it means $\vec{k}$ starts from (0,0,0) to $(\frac{2\pi}{a}, 0, 0)$ along k_x

Appliable to Si, Ge, GaAs, ...
(diamond and zincblende crystal structure)



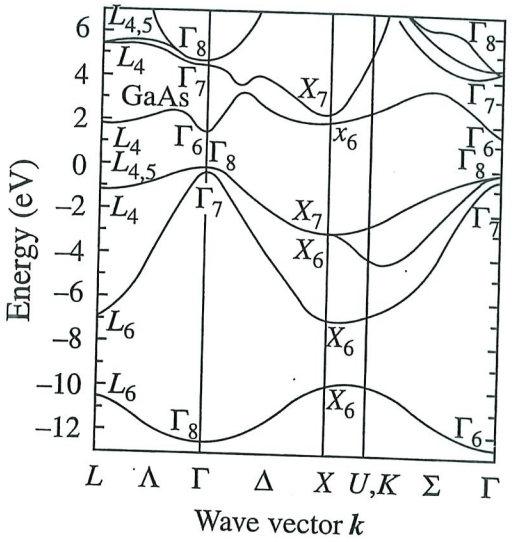
1st B.Z.

Silicon



Band structure of Si (after Chelikowsky and Cohen 1976).

GaAs



Band structure of GaAs (after Chelikowsky and Cohen 1976).

"Δ": a line from Γ to X

x-axis: trace some paths in B.Z

(line to edge (zone edge) and back)

[Why does 1st B.Z. play such an important role in semiconductor energy band studies?]

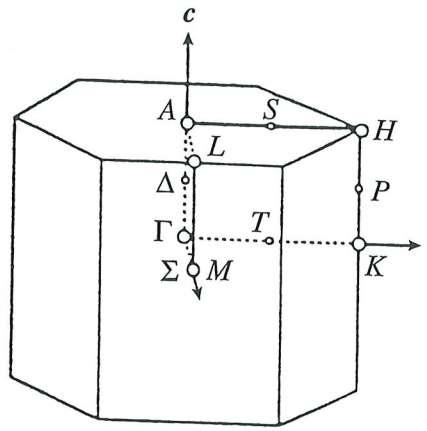
Chelikowsky and Cohen, Phys. Rev. B14, 556 (1976)

3D Hexagonal Lattice

Some II-VI compounds have the Wurtzite structure

hexagonal direct lattice

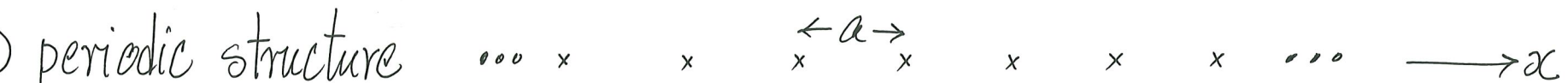
Reciprocal Lattice is also hexagonal. (Ex.)



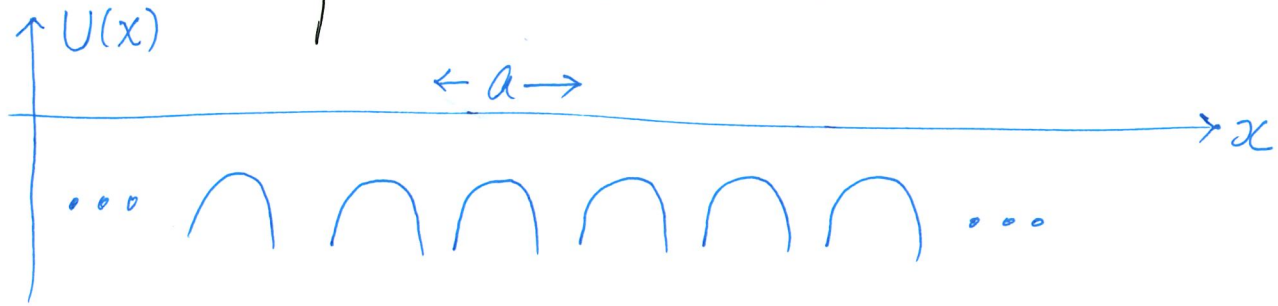
Brillouin zone for the hexagonal lattice.

E. Application of Reciprocal Lattice Vectors $\vec{G}$'s in Describing Periodic Functions

- 1D periodic structure



Some periodic functions† come up in such structure



$U(x + na) = U(x)$ mathematical expression of periodicity

n: integers

We will see a lot of such periodic functions in (3D) solids described by

$$f(\vec{r} + \vec{R}) = f(\vec{r}) \qquad (12)$$

$\vec{R}$: Lattice Vectors

† Another example is the electronic density $n(x)$

For studying energy bands, we need to solve the problem of allowed energies [energy eigenvalues] and allowed electronic states [eigenstates] for an electron under the influence of a periodic potential energy function

(1D) $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$

$U(x)$: periodic $[U(x+na) = U(x)]$

to solve for MANY $E \leftrightarrow \psi$ pairs!

$\psi(x,y,z) \rightarrow \psi(\vec{r})$

(3D) $$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + U(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

$U(\vec{r})$: periodic $U(\vec{r}+\vec{R}) = U(\vec{r})$

$\vec{R}$: any lattice vector (one of 14 Bravais lattices)

to solve for MANY $E \leftrightarrow \psi$ pairs!

In general, $f(\vec{r}) = \sum_{\vec{k}} f_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}$ ← plane waves (all $\vec{k}$'s are involved)

$f_{\vec{k}}$ ↑ weighting of $\vec{k}$-component

If $f(\vec{r})$ is periodic, $f(\vec{r}+\vec{R}) = \sum_{\vec{k}} f_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}\, e^{i\vec{k}\cdot\vec{R}} = f(\vec{r}) = \sum_{\vec{k}} f_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}}$

$\Updownarrow$ periodic (definition)

$\therefore$ needs $\vec{k}$ such that $e^{i\vec{k}\cdot\vec{R}} = 1$

true for $\vec{k} = \vec{G}$ (a reciprocal lattice vector)

$\therefore$

Key Result

If $f(\vec{r})$ is periodic,

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}} \qquad (13)$$

i.e. only plane waves $e^{i\vec{G}\cdot\vec{r}}$ are needed to construct a periodic function

Appreciation: $f_{\vec{k}} = 0$ for $\vec{k} \neq \vec{G}$ (excluded many components!)

In words, a periodic function carries only (still infinitely many in general) Fourier components corresponding to those with wavevectors EQUAL to reciprocal lattice vectors!

This is the key/starting point for many band structure calculations.

obtaining $E(\vec{k})$ for a material

F. Tie Things up

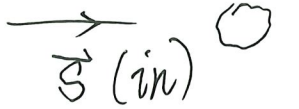
crystal sample (seemingly can do nothing)

Periodicity, e.g. charge (electron) density

$$n(\vec{r}) = n(\vec{r}+\vec{R})$$

$$n(\vec{r}) = \sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Scattering processes



Q.M. says

Prob. amplitude for this to happen $\propto$

$$\int \underbrace{e^{-i\vec{s}'\cdot\vec{r}}}_{\text{final state}} \overbrace{\left(\sum_{\vec{G}} n_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}\right)}^{\text{what could cause the scattering}} \underbrace{e^{i\vec{s}\cdot\vec{r}}}_{\text{initial state}} d^3r$$

Pick up $\int e^{-i(\vec{s}'-\vec{s})\cdot\vec{r}}\, e^{i\vec{G}\cdot\vec{r}}\, d^3r$

not negligible only for $\vec{s}'-\vec{s}=\vec{G}$ (Laue condition, X-ray)

a condition we saw

Stretching our imagination a bit... $e^{i\vec{G}\cdot\vec{r}} = e^{i(\hbar\vec{G})\cdot\vec{r}}$ ← like a momentum

So, a periodic function is good at providing or destroying discrete values $\hbar\vec{G}$ of momentum

Thus, $\vec{s}'-\vec{s}=\vec{G}$ is a way to express momentum change in scattering is compensated by that provided by the crystal.

Summary

- Easy to define $\vec{b}_1, \vec{b}_2, \vec{b}_3$ from $\vec{a}_1, \vec{a}_2, \vec{a}_3$ and map out the Reciprocal Lattice
- But why so needs more appreciation
  - $\vec{G}_1 \perp$ planes, Bragg condition as Laue Condition involves $\vec{G}$s
  - X-ray experiments map out reciprocal lattice
  - $\vec{S}\cdot\left(\frac{\vec{G}_1}{2}\right) = \left(\frac{G_1}{2}\right)^2$ is Laue Condition

    suggests bisecting planes are important for waves in periodic systems
  - 1st B.Z. and other Brillouin Zones
  - $f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$ involves $\vec{G}$'s only if $f(\vec{r}+\vec{R}) = f(\vec{r})$