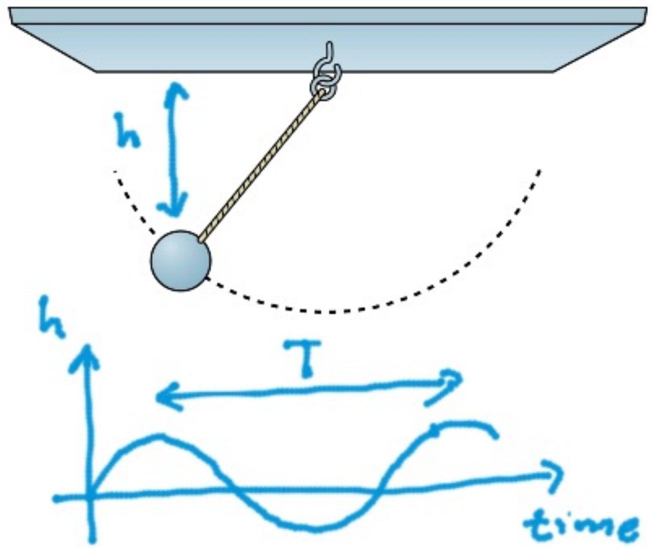
REAL TIME:

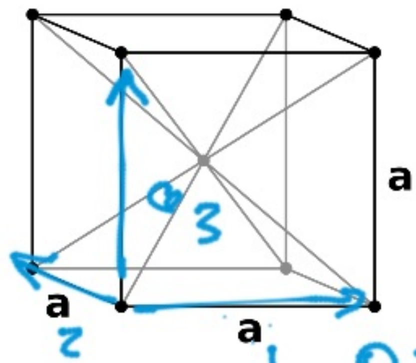


RECIPROCAL TIME:

ANGULAR FREQUENCY

$$\omega = \frac{2\pi}{T} \quad [1/s]$$

REAL SPACE:



Units

[Å]

Dimension

3

$$r = \mu_1 \vec{a}_1 + \mu_2 \vec{a}_2 + \mu_3 \vec{a}_3$$

μ_i = real numbers

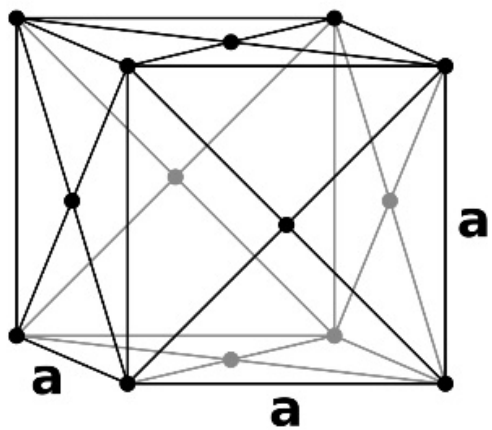
RECIPROCAL SPACE:

$\frac{2\pi}{a}$ [$Å^{-1}$]

3

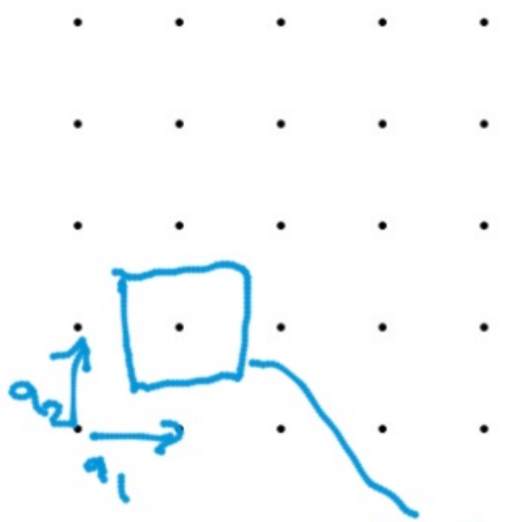
$$\vec{r} = \mu_1 \vec{b}_1 + \mu_2 \vec{b}_2 + \mu_3 \vec{b}_3$$

LATTICE VECTORS:



RECIPROCAL LATTICE VECTORS

REAL SPACE SQUARE LATTICE:



Wigner-Seitz

$\vec{a}_1 = (1,0)\,a$

$\vec{a}_2 = (0,1)\,a$

RECIPROCAL LATTICE:

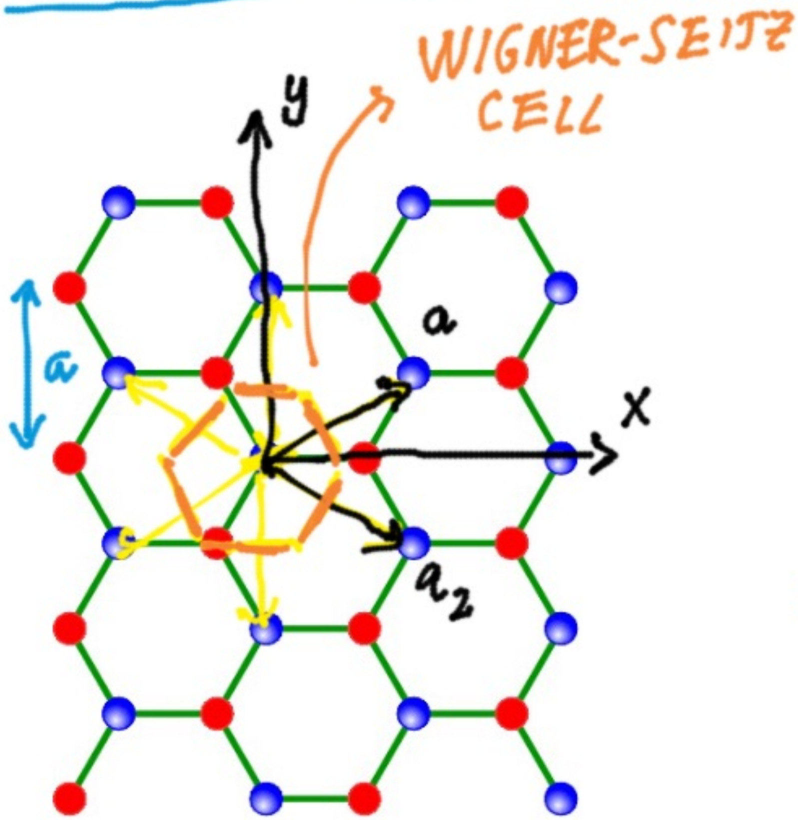
Brillouin Zone

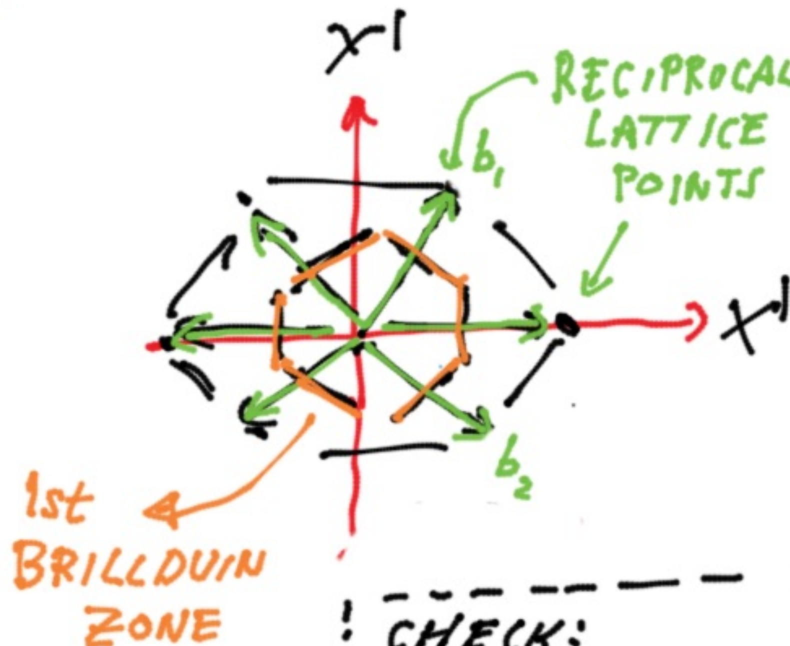
$\vec{b}_1 = \frac{2\pi}{a}(1,0)$

$\vec{b}_2 = \frac{2\pi}{a}(0,1)$

GRAPHENE:

RECIPROCAL LATTICE





LATTICE VECTORS (LV)

$a_1 = (\sqrt{3}, 1)\frac{a}{2}$

$a_2 = (\sqrt{3}, -1)\frac{a}{2}$

$\longleftrightarrow$

RECIPROCAL LV

$b_1 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, 1\right)$

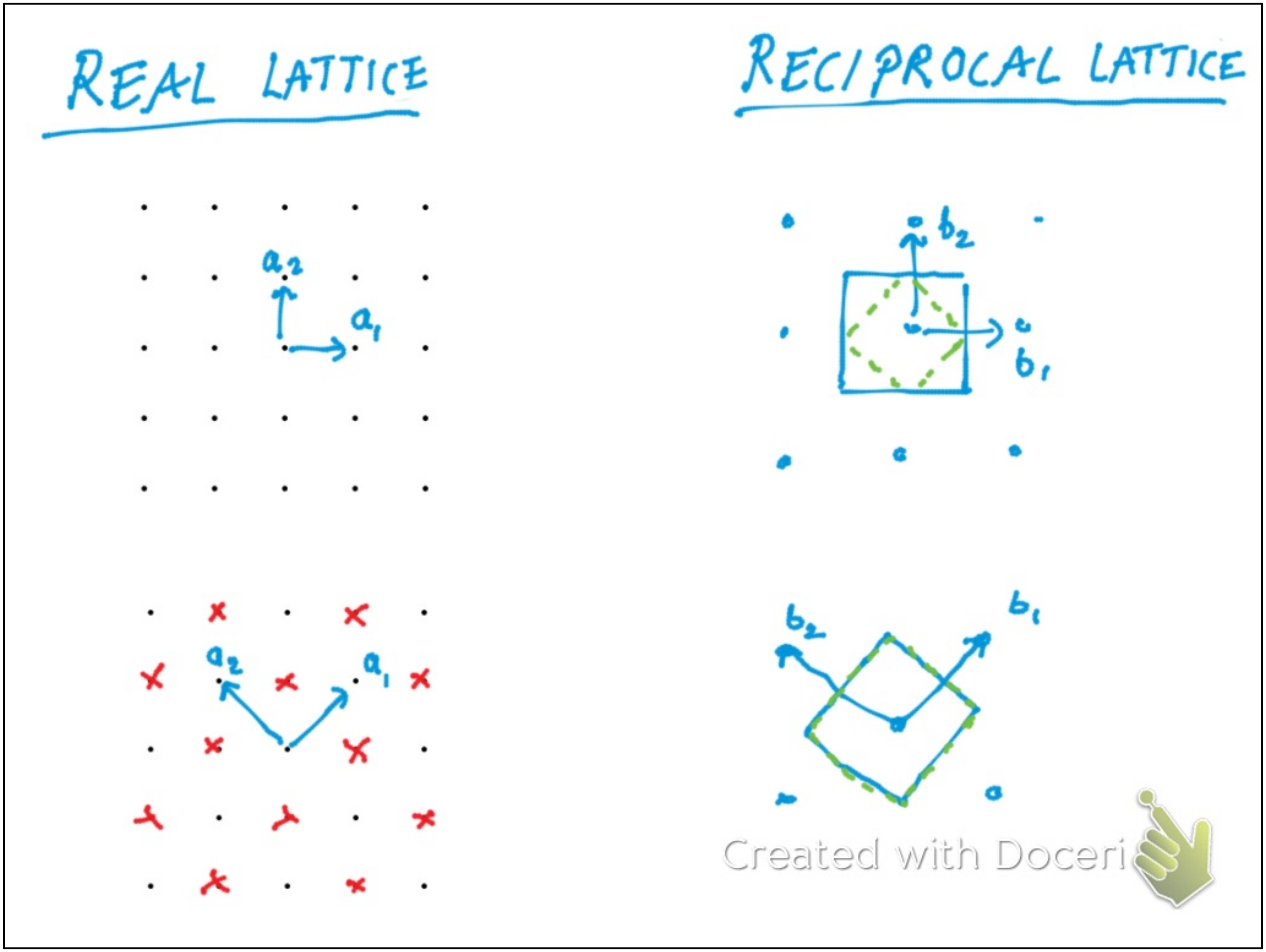
$b_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, -1\right)$

CHECK:

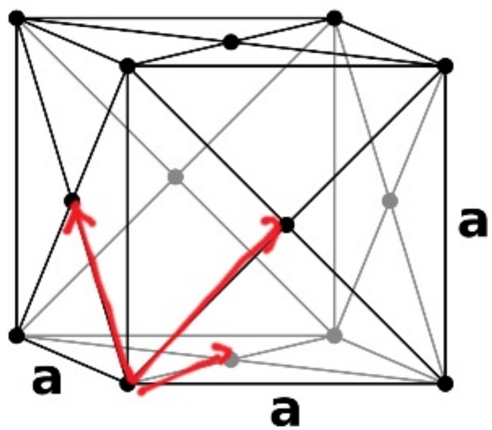
$$\bar{a}_1 \cdot \bar{b}_1 = \frac{2\pi}{a}\frac{a}{2}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix}\cdot\begin{pmatrix}\frac{1}{\sqrt{3}}\\1\end{pmatrix}$$

$$= \pi(1+1)$$

$$= 2\pi$$


REAL LATTICE
RECIPROCAL LATTICE
a2
a1
b2
b1
a2
a1
b2
b1
Created with Doceri

LATTICE VECTORS:

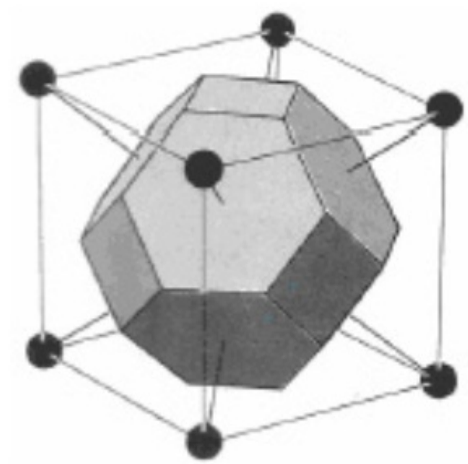


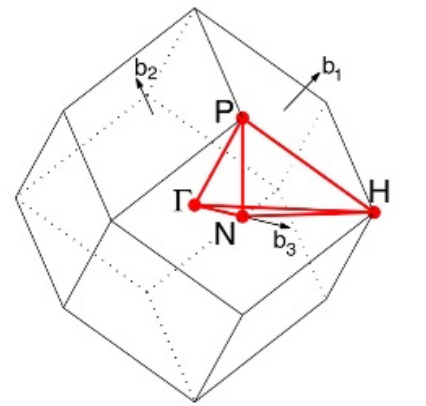
RECIPROCAL LATTICE VECTORS

EXERCISE SHEET 2
EXERCISE 2

WIGNER-SEITZ CELL ⟷ BRILLOUIN ZONE

BCC

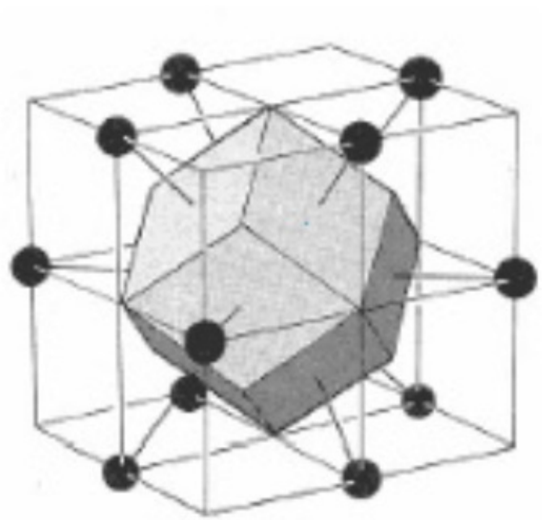


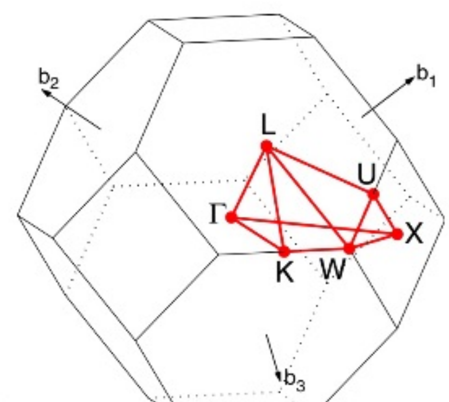


BCC path: Γ-H-N-Γ-P-H|P-N

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

FCC

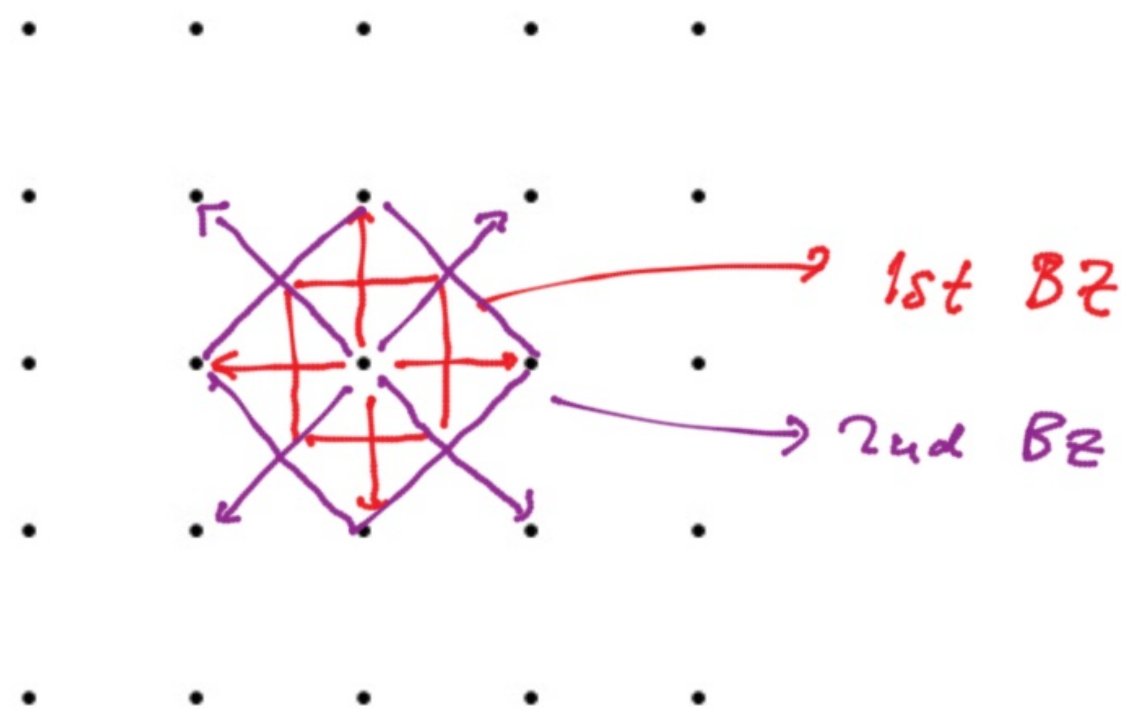




FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

HIGHER ORDER BRILLOUIN ZONES::



SCATTERING THEORY:

DETECTOR

FINAL ENERGY E_f

INCIDENT ENERGY E_i

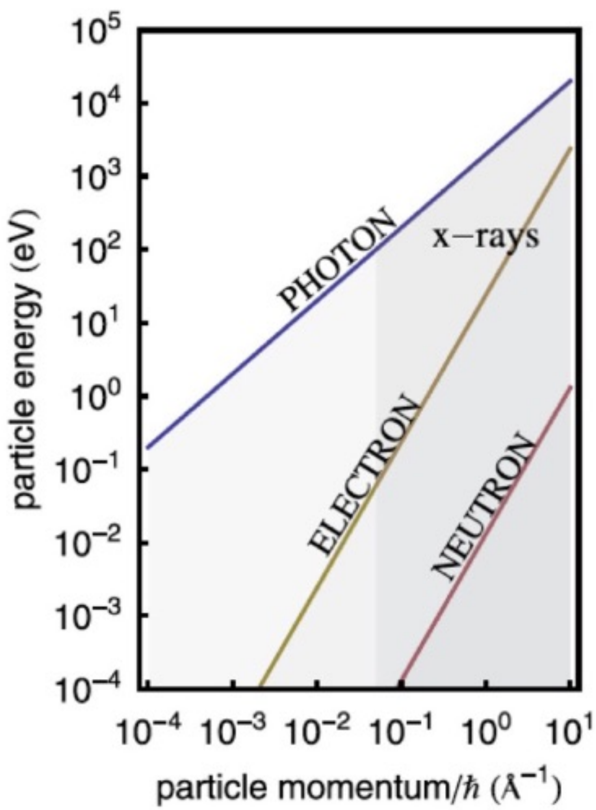
ELECTRON
NEUTRON
PHOTON

OBJECT
ATOM
ELECTRON

ELASTIC SCATTERING MEANS:

$$E_i = E_f$$

DISPERSION RELATION:



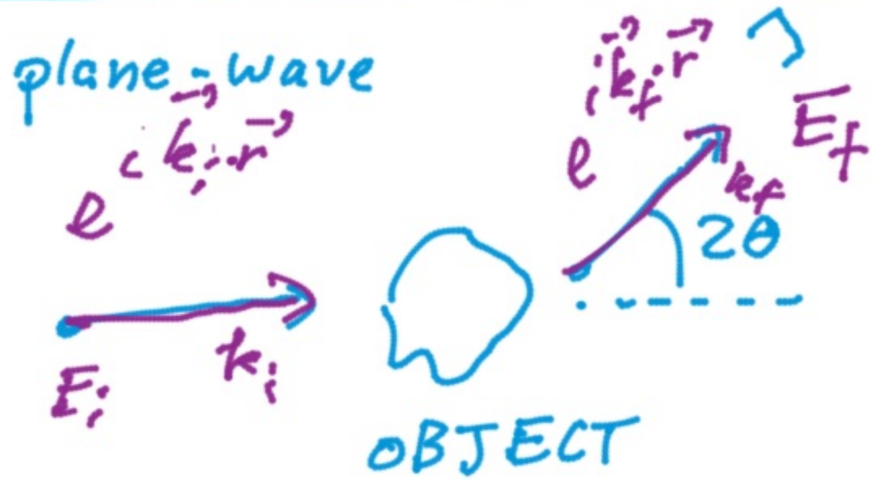
Neutron or Electron

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

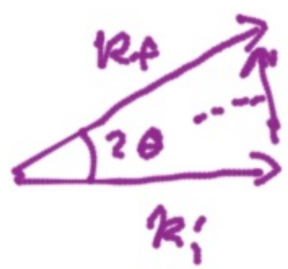
Photon

$$E = \hbar c k$$

SCATTERING TRIANGLE:



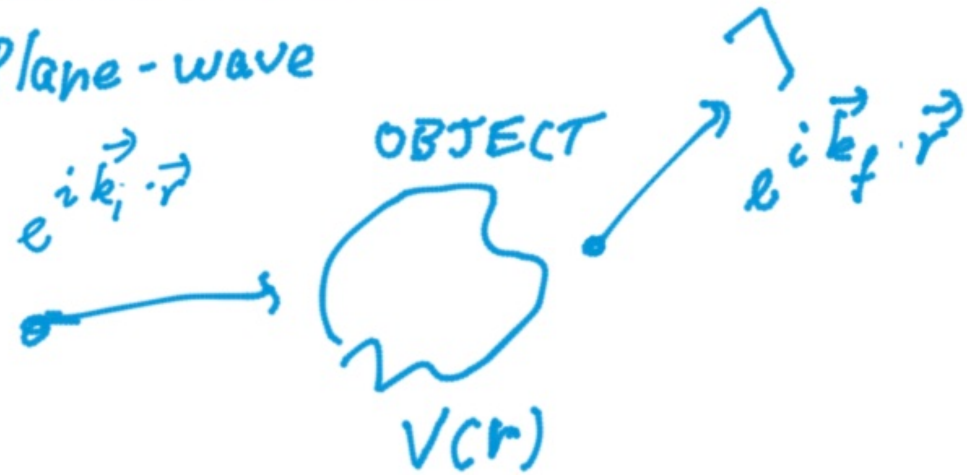
WE CONSIDER ELASTIC SCATTERING: $E_i = E_f$



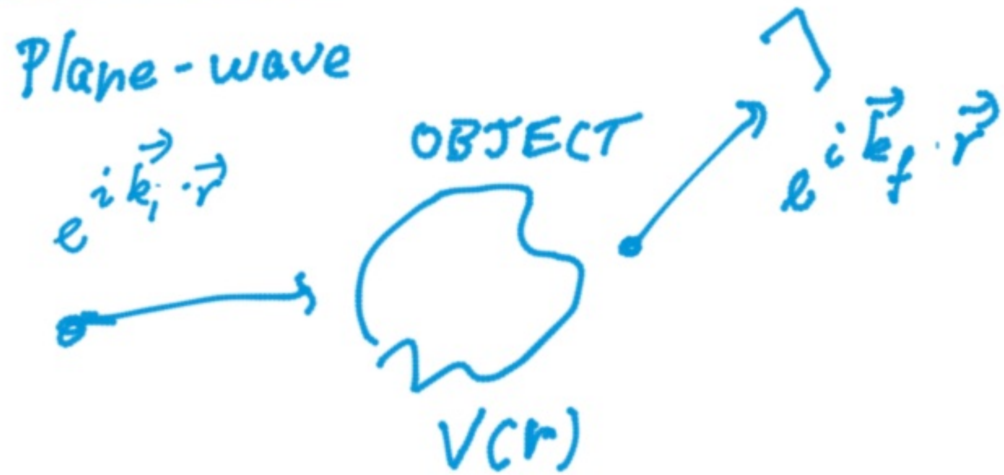
$$\vec{\Delta k} = \vec{q} = \vec{k}_f - \vec{k}_i$$

$$|q| = 2|k_i| \sin\theta$$

SCATTERING POTENTIAL:



SCATTERING POTENTIAL:



FERMI GOLDEN RULE:

$$P = 2\pi \left| \langle k_f | V(r) | k_i \rangle \right|^2 \delta(E_f - E_i)$$

FORM FACTOR:

$$F(q) = \langle k_f | V(r) | k_i \rangle$$

$$= \int e^{-i\vec{k}_f\cdot\vec{r}}\, V(r)\, e^{+i\vec{k}_i\cdot\vec{r}}\, dr$$

$$= \int V(r)\, e^{-i(\vec{k}_f-\vec{k}_i)\cdot\vec{r}}\, dr$$

$$= \int V(r)\, e^{-i\vec{q}\cdot\vec{r}}\, dr = V(q)$$

SUMMARY

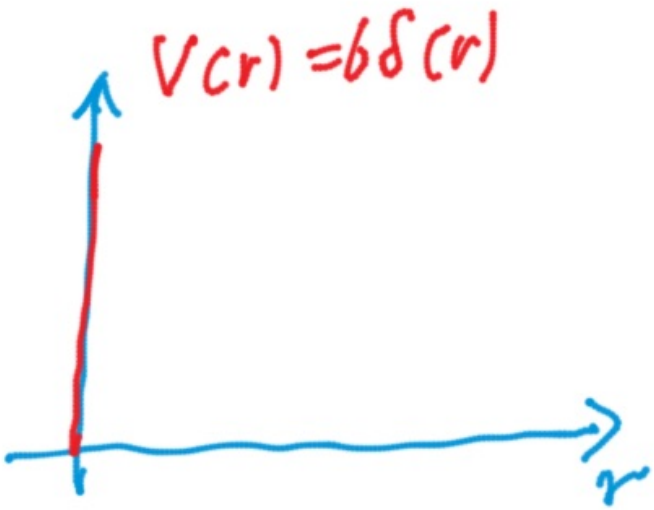
$$\text{Intensity} \propto P \propto F^2(q)$$

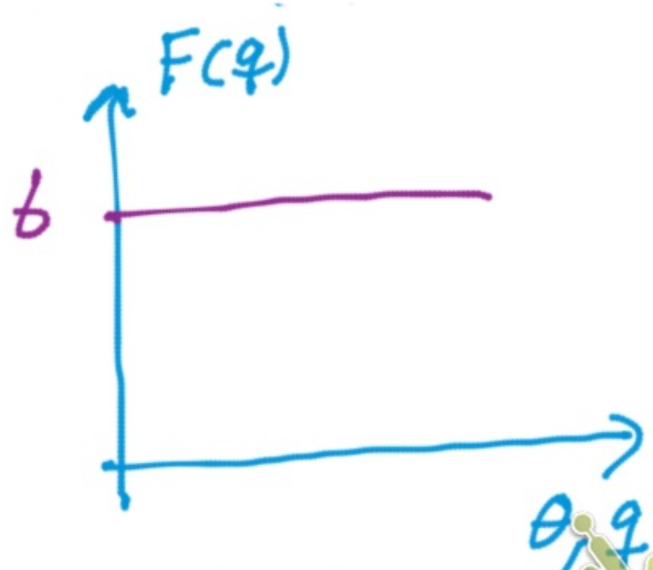
FROM SCATTERING TRIANGLE:

$$|q| = 2|k_i| \sin\theta$$

EXAMPLE 1:

NEUTRON SCATTERNG ON AN ATOMIC NEUCLEUS.





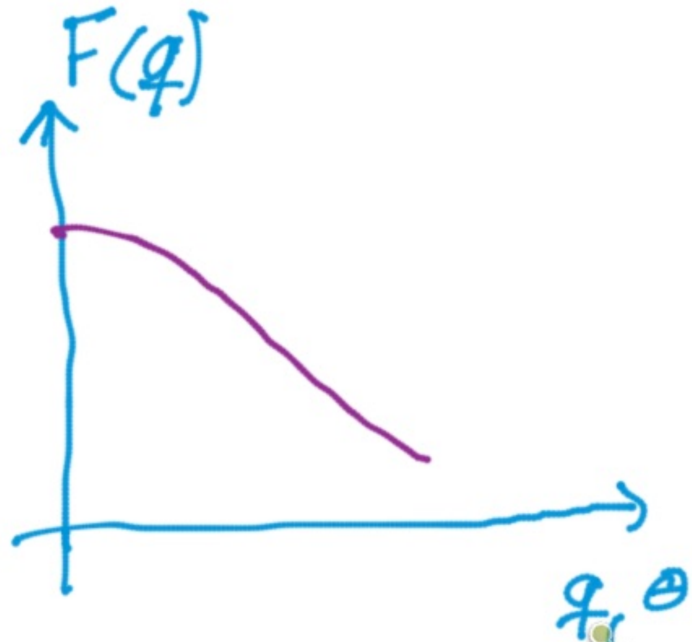
EXAMPLE 2:

Electron scattering on an atom

$$V(r) = \frac{V_0 e^{-\mu r}}{\mu r}$$

Screened Coulomb potential

(Yukawa potential)



Scattering on a CRYSTAL:

$$V(r) = \sum_i V_i(r - r_i)$$

Scattering on a CRYSTAL:

$$V(r) = \sum_i V_i(r - r_i)$$

FERMI GOLDEN RULE:

$$P = 2\pi \, |\langle k_f | V(r) | k_i \rangle|^2 \, \delta(E_i - E_f)$$

SCATTERED INTENSITY:

$$\langle k_f | V(r) | k_i \rangle = \int e^{i\vec{k}_f\cdot\vec{r}} \sum_i V_i(r - r_i)\, e^{-i\vec{k}_i\cdot\vec{r}}\, dr$$

change var.

$r' = r - r_i$

$r = r' + r_i$

$dr = dr'$

$$= \sum_i \int e^{-ik_f r'} V(r')\, e^{+ik_i r'}\, dr'\, e^{-i\bar{k}_f \bar{r}_i}\, e^{i\bar{k}_i \bar{r}_i}$$

$$= F(q) \sum_i e^{-i(\bar{k}_f - \bar{k}_i)\cdot\bar{r}_i}$$

$$= F(q) \sum_i e^{-i\vec{q}\cdot\vec{r}_i}$$

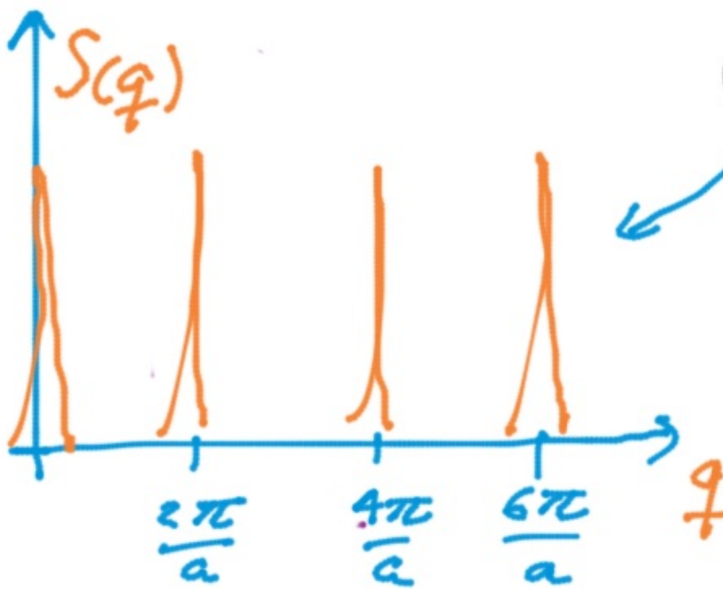
$$= F(q)\, S(q)$$

WHERE STRUCTURE FACTOR: $S(q) = \sum_i e^{\cdots}$

STRUCTURE FACTOR:

LINEAR CHAIN EXAMPLE

$$S(q) = \sum_i e^{-iqr}$$



BRAGG'S LAW

$$\lambda = 2d\sin\theta$$

$$|q| = n\frac{2\pi}{a} = 2|k_i|\sin\theta$$

Scattering TRIANGLE

$$\Downarrow$$

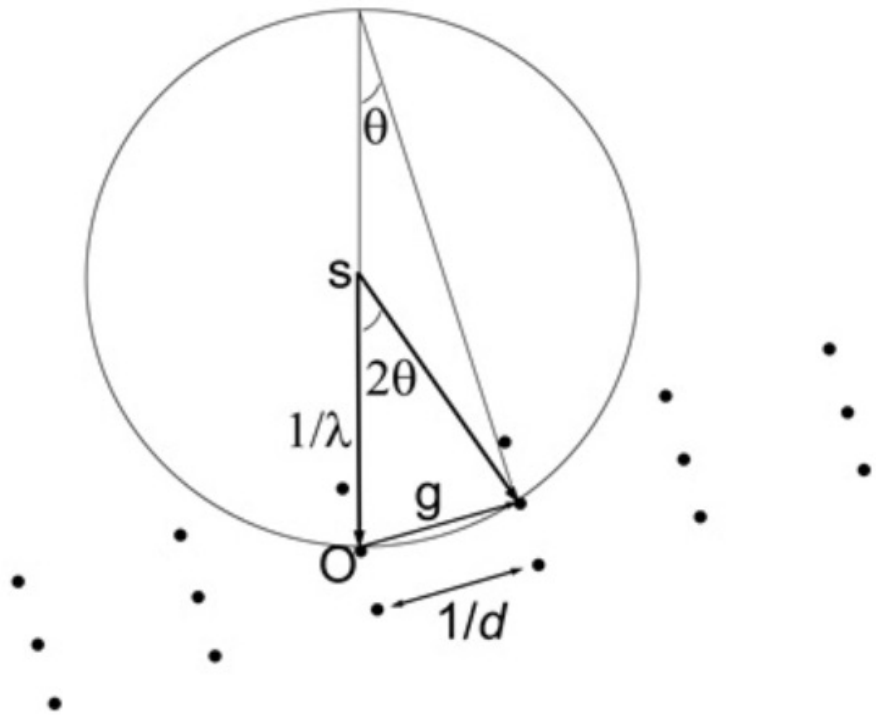
$$n\frac{2\pi}{|k_i|} = 2a\sin\theta$$

$$\Downarrow$$

$$n\lambda = 2a\sin\theta$$

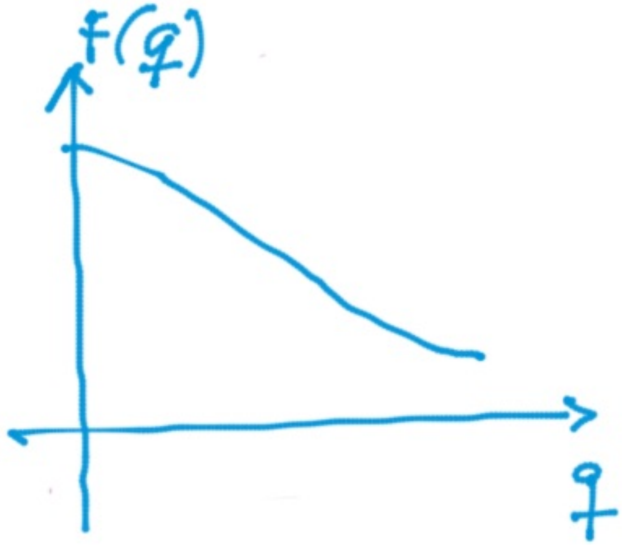
ANOTHER WAY TO EXPRESS BRAGG'S LAW

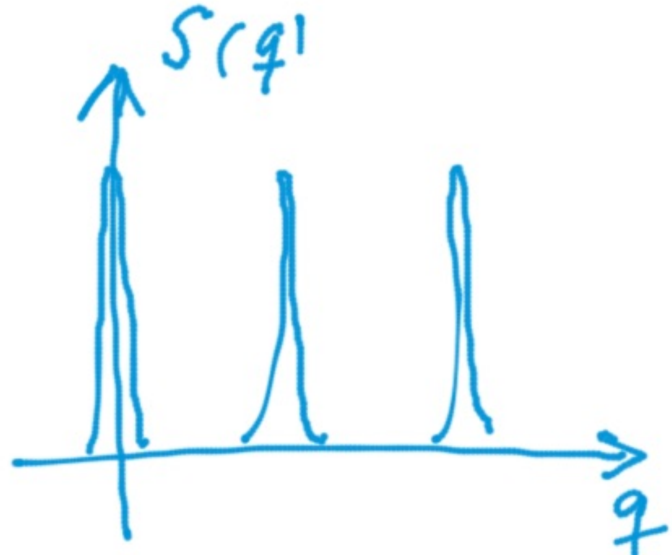
EWALD'S SPHERE:



OVERVIEW

SCATTERED INTENSITY $\propto F(q)\, S(q)$





STRUCTURE FACTOR:

$$S(q) = \sum_i e^{-i\vec{q}\cdot\vec{r}}$$

$$= N \sum_i^{BASIS} e^{-i\vec{q}\cdot\vec{r}_i}$$

$$\propto \sum_i^{BASIS} e^{-2\pi i(hx_i + ky_i + \ell z_i)}$$

RECIPROCAL LATTICE POINTS

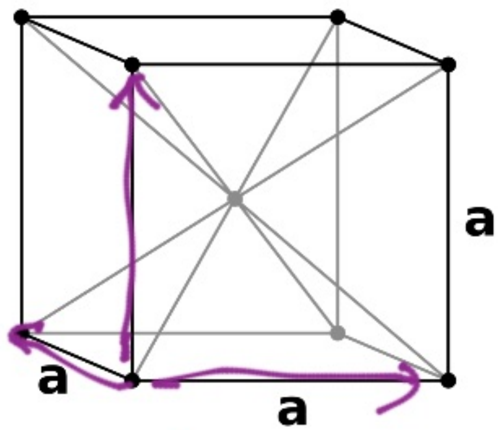
$$q = (h, k, \ell)\frac{2\pi}{a}$$

with h, k, ℓ integers

BASIS NOTATION

$$r_i = (x_i, y_i, z_i)\, a$$

STRUCTURE FACTOR: BCC



$a_1 = (1,0,0)\,a$

$a_2 = (0,1,0)\,a$

$a_3 = (0,0,1)\,a$

Basis

$(0,0,0)\quad \left(\tfrac{1}{2}\,\tfrac{1}{2}\,\tfrac{1}{2}\right) a$

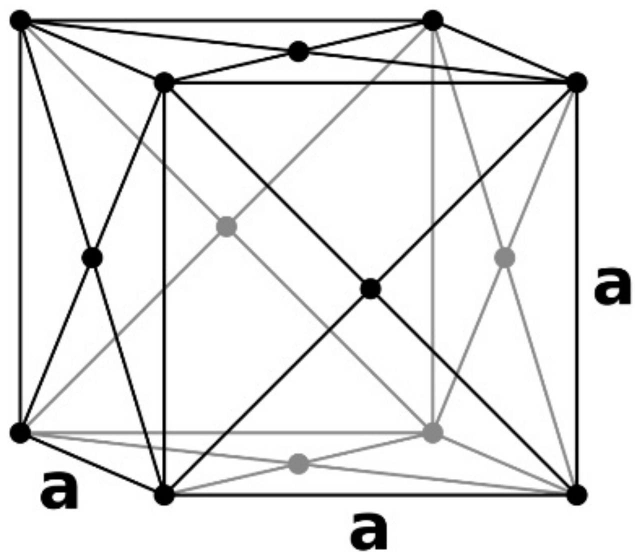
Reciprocal lattice

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

$(1,0)\,\frac{2\pi}{a}$

$(h,k,l)\,\frac{2\pi}{a}$

STRUCTURE FACTOR: FCC



FT

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x \xi}\, dx$$

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(t)\, e^{-2\pi i t \omega}\, dt.$$

$$\hat{f}(y) = \int_{-\infty}^{\infty} f(x)\, e^{2\pi i x y}\, dx$$

$y \to$

$$f(x) = a_0 + \sum_{k=0}^{n} a_n \sin(nx) +$$

$$\int \delta(x-a) f(x)\, dx = f(a)$$

$$\mathcal{F}^{(2)}\left(f(x)\right) = f(-x)$$

$$\mathcal{F}^{(4)}\left(f(x)\right) = f(x)$$

$$\mathcal{F}^{(3)}(f) = \mathcal{F}^{-1}(f)$$