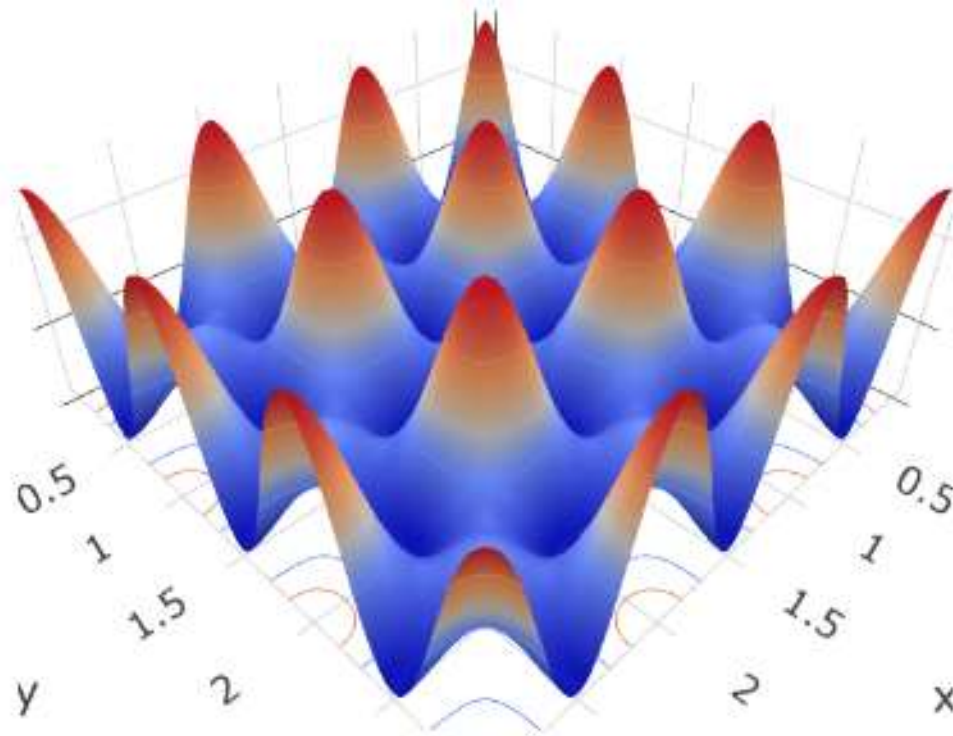
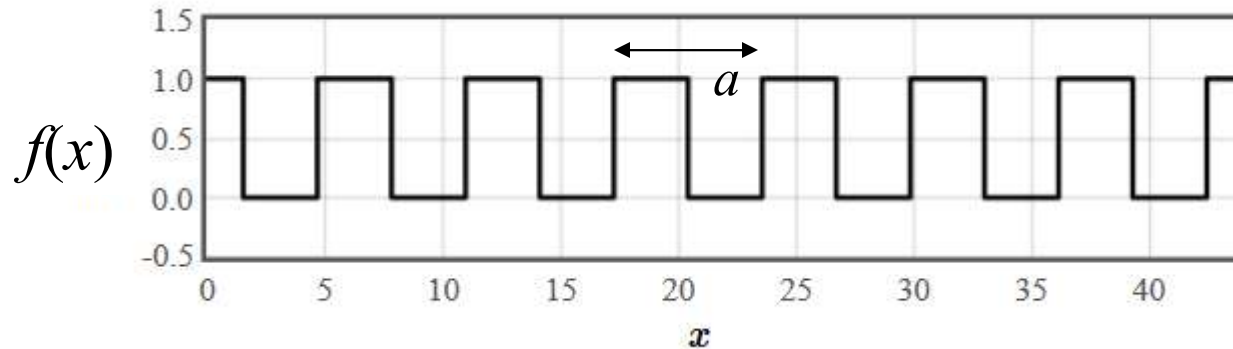


Periodic functions



Use a Fourier series to describe periodic functions

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

multiply by $\cos(2\pi p'x/a)$ and integrate over a period.

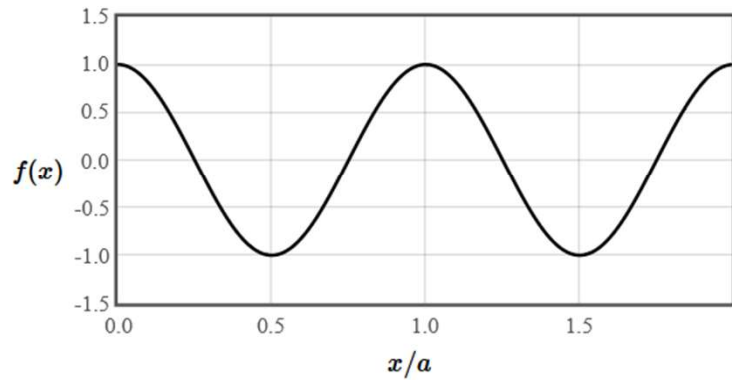
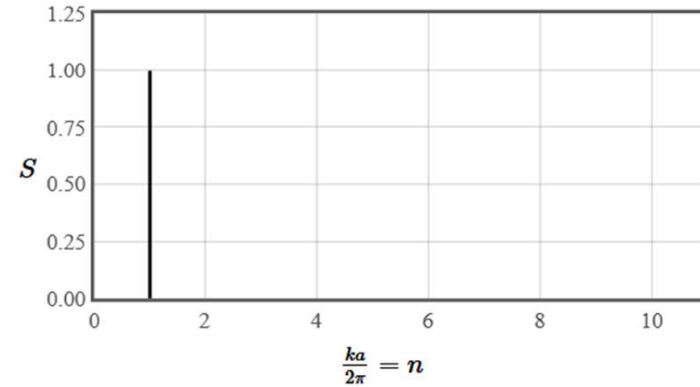
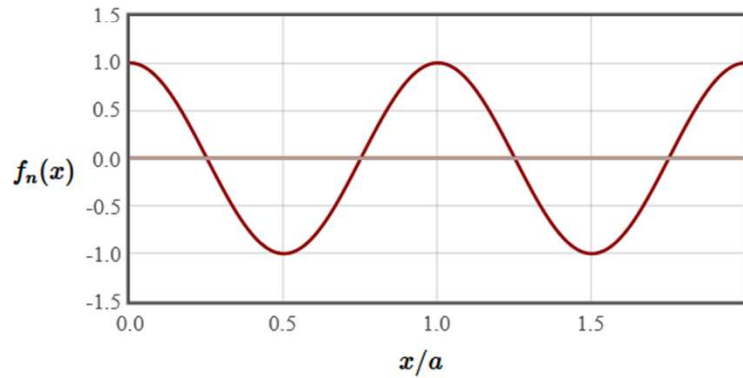
$$\int_0^a f(x) \cos(2\pi p'x/a) dx = c_p \int_0^a \cos(2\pi p'x/a) \cos(2\pi p'x/a) dx = \frac{ac_p}{2}$$

$$c_p = \frac{2}{a} \int_0^a f(x) \cos(2\pi px/a) dx$$

Fourier synthesis

A periodic function with period a can be written as a Fourier series of the form,

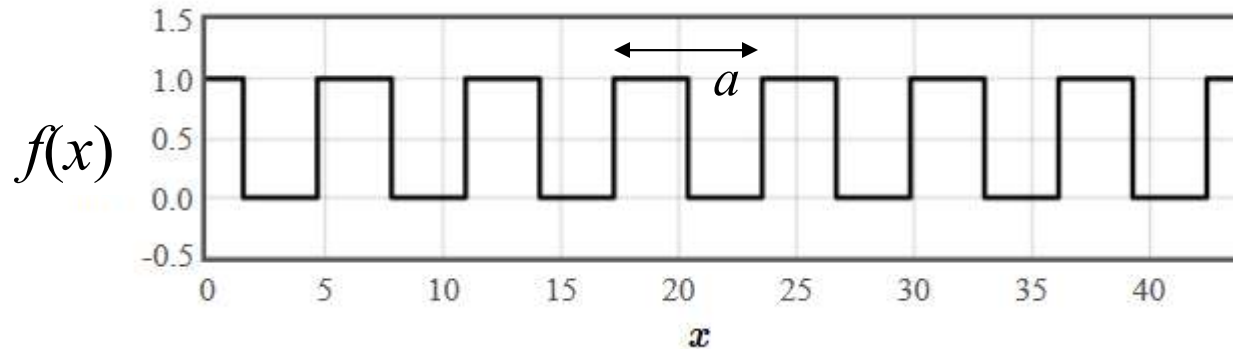
$$f(x) = A_0 + \sum_n A_n (\cos(\theta_n) \cos(2\pi n x/a) + \sin(\theta_n) \sin(2\pi n x/a)).$$



Number of periods displayed:

$A_0 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_1 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_1 = 1$	<input type="text" value="1"/> <input type="button" value="-"/> <input type="button" value="1"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_2 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_2 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_3 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_3 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_4 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_4 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_5 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_5 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_6 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_6 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_7 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_7 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_8 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_8 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_9 = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_9 = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_{10} = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_{10} = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>	$\theta_{11} = 0\pi$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>
$A_{11} = 0$	<input type="text" value="0"/> <input type="button" value="-"/> <input type="button" value="0"/> <input type="button" value="+"/> <input type="text" value="1"/>		

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

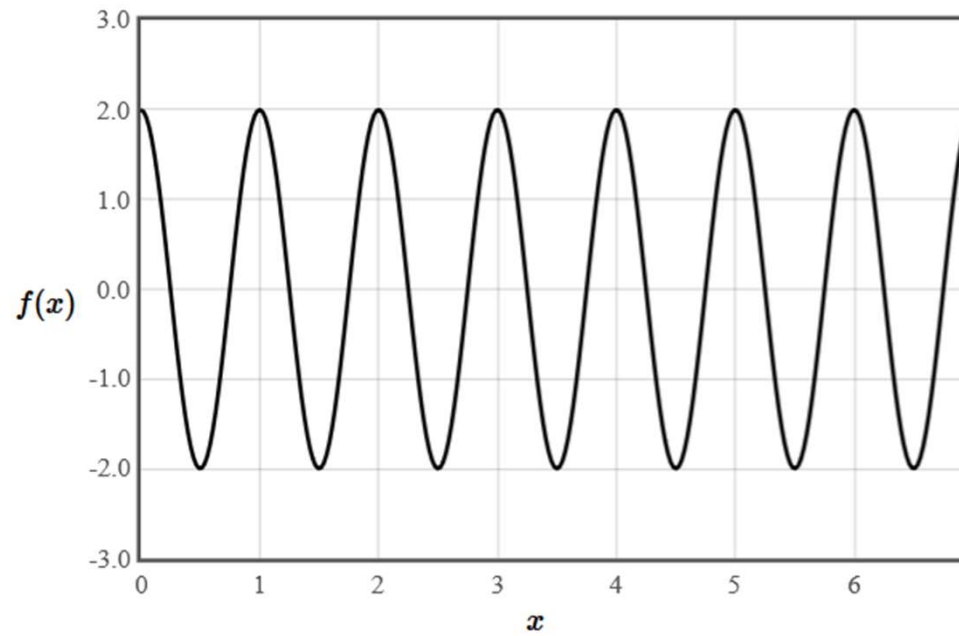
$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \quad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$f(x) = \sum_{G=-\infty}^{\infty} f_G e^{iGx} \quad f_G = \frac{c_p}{2} - i \frac{s_p}{2} \quad G = \frac{2\pi p}{a}$$

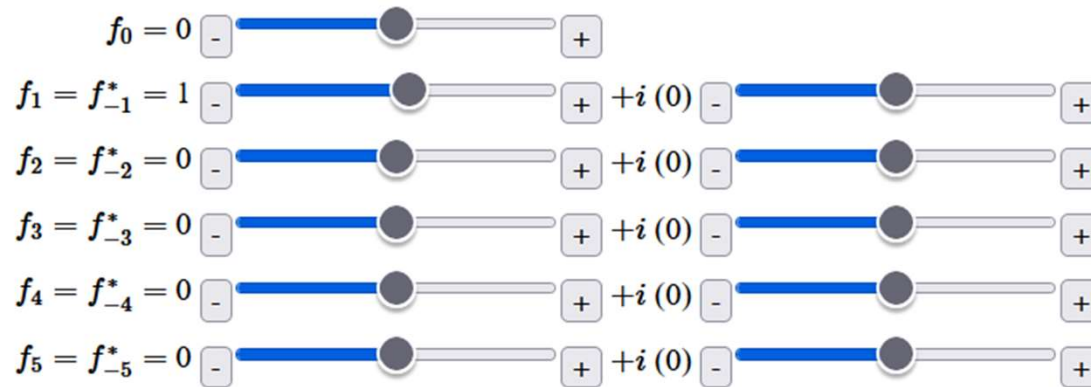
For real functions: $f_G^* = f_{-G}$

reciprocal lattice vector

Fourier series in 1-D



square triangle sawtooth comb



Determine the Fourier coefficients in 1-D

$$f(x) = \sum_G f_G e^{iGx}$$

Multiply by $e^{-iG'x}$ and integrate over a period a

$$\int_{\text{unit cell}} f(x) e^{-iG'x} dx = \int_{\text{unit cell}} \sum_G f_G e^{i(G-G')x} dx = f_{G'} a$$

$$f_G = \frac{1}{a} \int_{-\infty}^{\infty} f_{\text{cell}}(x) e^{-iGx} dx$$

The Fourier coefficient is proportional to the Fourier transform of the pattern that gets repeated on the Bravais lattice, evaluated at that G -vector.

Fourier series in 1-D, 2-D, or 3-D

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

Reciprocal lattice vectors G
(depend on the Bravais lattice)

Structure factors
(complex numbers)

$$\vec{T}_{hkl} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \quad \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0, & \text{for } i \neq j \end{cases}$$

$$\vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$$

Reciprocal lattice (Reziprokes Gitter)

Any periodic function can be written as a Fourier series

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

Structure factor ↑ Reciprocal lattice vector G

$$\vec{G} = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3$$

ν_i integers

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

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

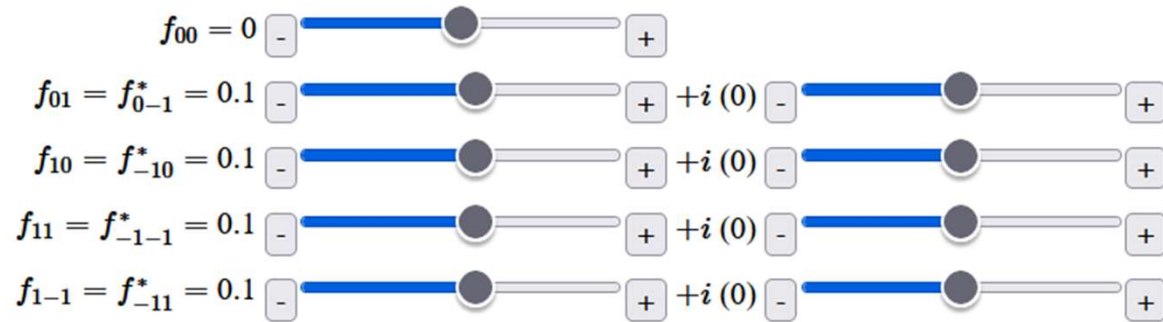
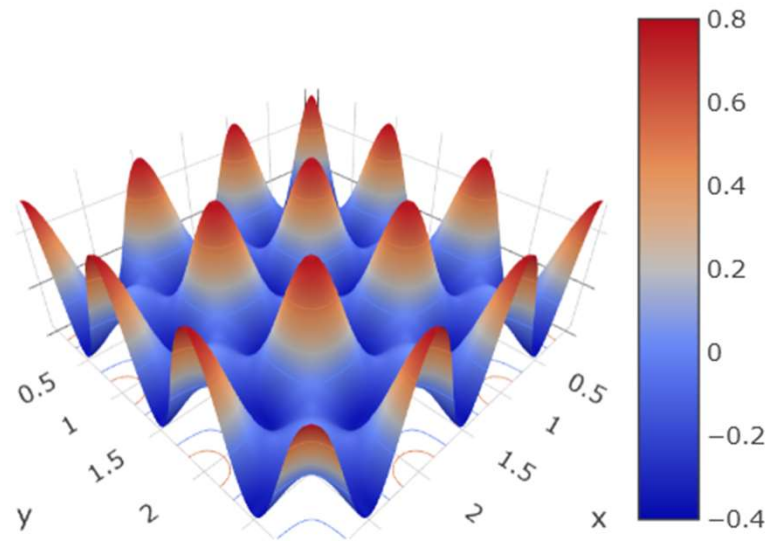
Reciprocal lattice (Reziprokes Gitter)

$$\text{sc:} \quad \vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\hat{y}, \quad \vec{a}_3 = a\hat{z},$$
$$\vec{b}_1 = \frac{2\pi}{a}\hat{k}_x, \quad \vec{b}_2 = \frac{2\pi}{a}\hat{k}_y, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{k}_z.$$

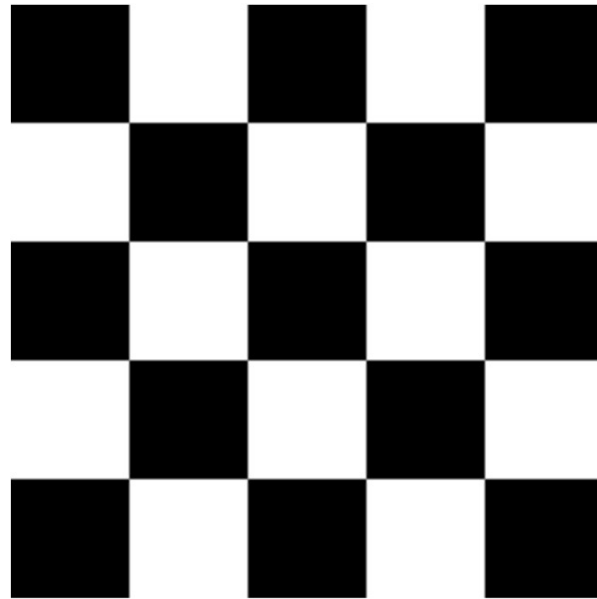
$$\text{fcc:} \quad \vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{z}), \quad \vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{y}), \quad \vec{a}_3 = \frac{a}{2}(\hat{y} + \hat{z}),$$
$$\vec{b}_1 = \frac{2\pi}{a}(\hat{k}_x - \hat{k}_y + \hat{k}_z), \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_y - \hat{k}_z), \quad \vec{b}_3 = \frac{2\pi}{a}(-\hat{k}_x + \hat{k}_y + \hat{k}_z).$$

$$\text{bcc:} \quad \vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}), \quad \vec{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}), \quad \vec{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}),$$
$$\vec{b}_1 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_y), \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{k}_y + \hat{k}_z), \quad \vec{b}_3 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_z).$$

Two dimensional periodic functions



Determine the Fourier coefficients



$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

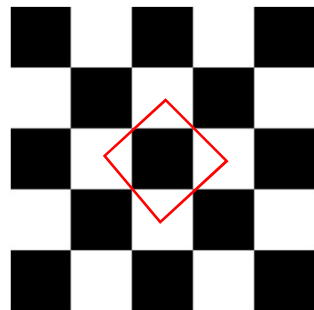
Determine the Fourier coefficients

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp(i\vec{G} \cdot \vec{r})$$

Multiply by $\exp(-i\vec{G}' \cdot \vec{r})$ and integrate over a unit cell

$$\int_{\text{unit cell}} f(\vec{r}) \exp(-i\vec{G}' \cdot \vec{r}) d\vec{r} = \sum_{\vec{G}} \int_{\text{unit cell}} f_{\vec{G}} \exp(-i\vec{G}' \cdot \vec{r}) \exp(i\vec{G} \cdot \vec{r}) d\vec{r}$$

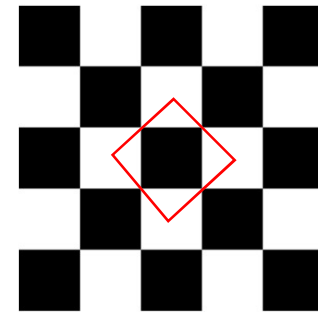
$$f_{\vec{G}} = \frac{1}{V_{\text{uc}}} \int_{\text{unit cell}} f(\vec{r}) \exp(-i\vec{G} \cdot \vec{r}) d\vec{r}$$



Determine the Fourier coefficients

$$f_{\vec{G}} = \frac{C}{a^2} \int_{-a/4}^{a/4} \int_{-a/4}^{a/4} \exp(-i\vec{G} \cdot \vec{r}) dx dy$$

$$f_{\vec{G}} = \frac{C}{a^2} \int_{-a/4}^{a/4} \int_{-a/4}^{a/4} \exp(-iG_x x) \exp(-iG_y y) dx dy$$



$$f_{\vec{G}} = \frac{C}{a^2} \frac{(\exp(-iG_x a/4) - \exp(iG_x a/4)) (\exp(-iG_y a/4) - \exp(iG_y a/4))}{-G_x G_y}$$

$$f_{\vec{G}} = \frac{4C}{a^2} \frac{\sin(G_x a/4) \sin(G_y a/4)}{G_x G_y}$$

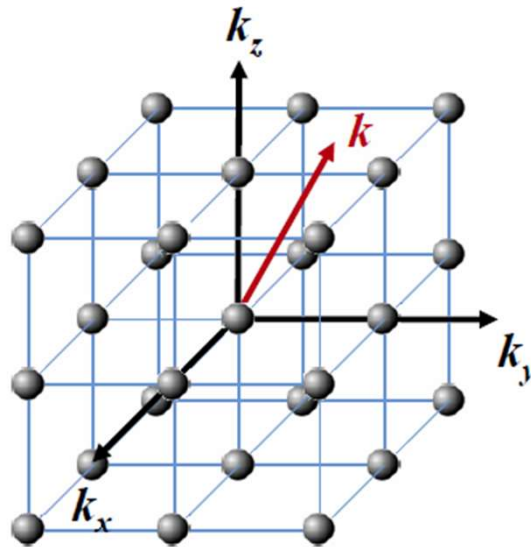
Reciprocal space (Reziproker Raum) k -space (k -Raum)

k -space is the space of all wave-vectors.

A k -vector points in the direction a wave is propagating.

wavelength: $\lambda = \frac{2\pi}{|\vec{k}|}$

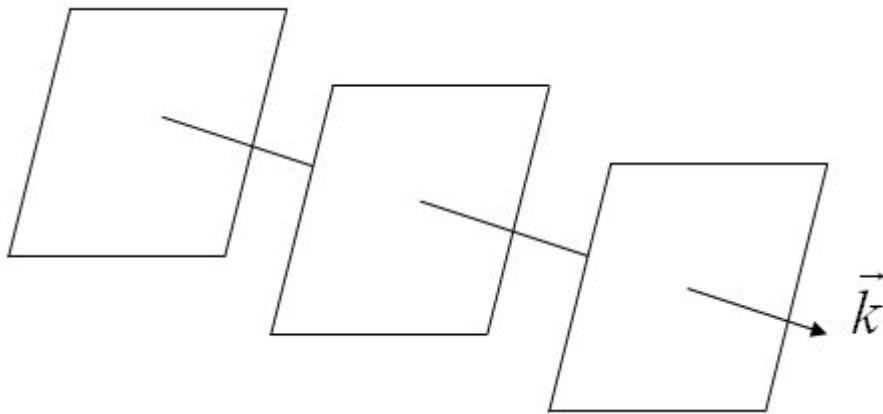
momentum: $\vec{p} = \hbar\vec{k}$



Plane waves (Ebene Wellen)

$$e^{i\vec{k}\cdot\vec{r}} = \cos(\vec{k}\cdot\vec{r}) + i\sin(\vec{k}\cdot\vec{r})$$

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

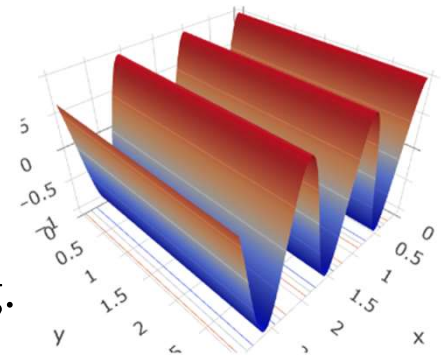


$$\exp(i\vec{k}\cdot(\vec{r} + \vec{r}_\perp)) = \exp(i\vec{k}\cdot\vec{r})$$

Most functions can be expressed in terms of plane waves

$$f(\vec{r}) = \int F(\vec{k}) e^{i\vec{k}\cdot\vec{r}} d\vec{k}$$

A k -vector points in the direction a wave is propagating.



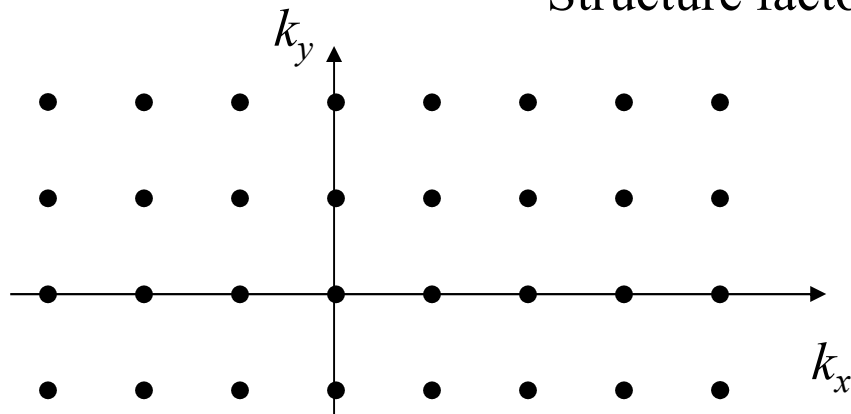
Reciprocal lattice (Reziprokes Gitter)

Any periodic function can be written as a Fourier series

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

↑
↑
Reciprocal lattice vector G

Structure factor



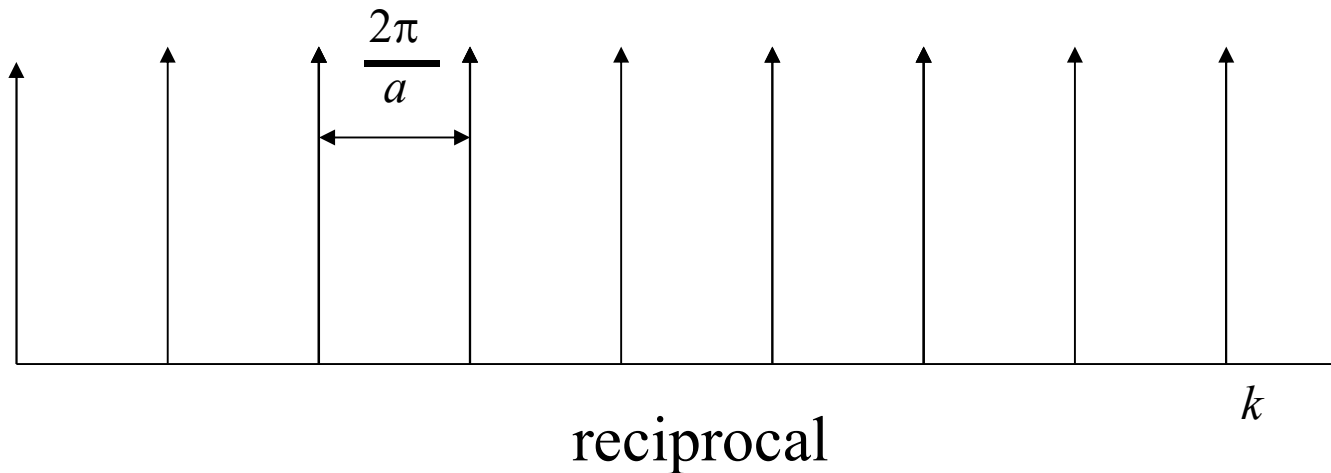
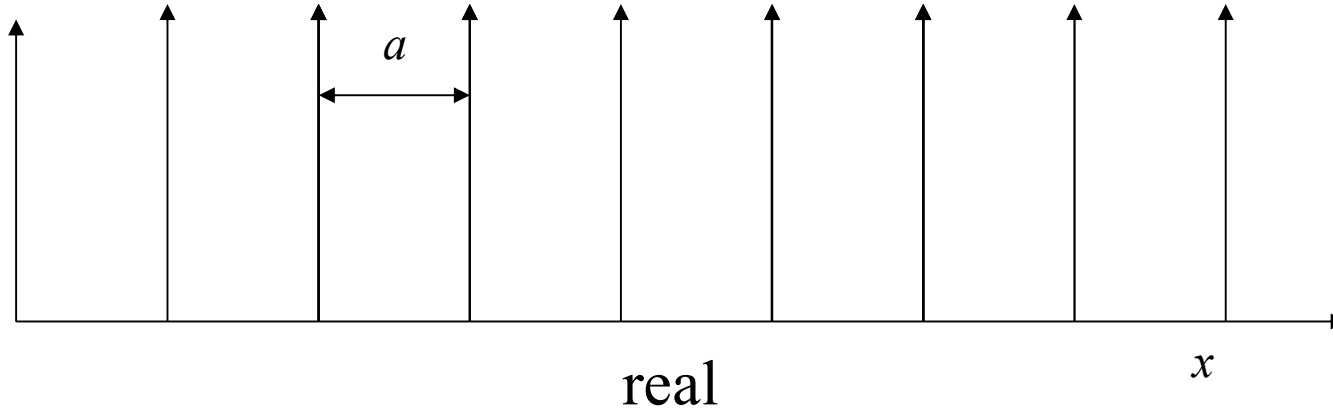
$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$$

v_i integers

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

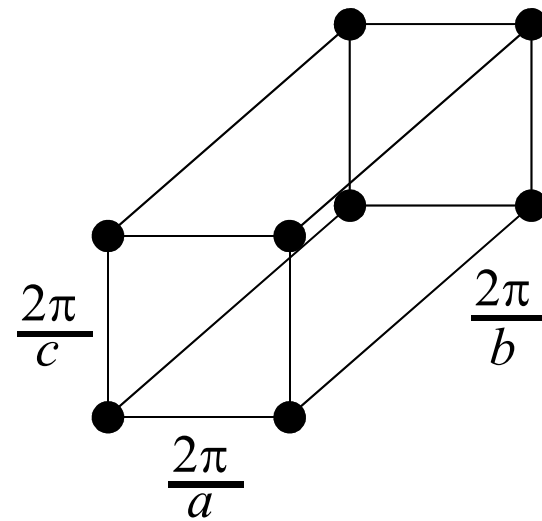
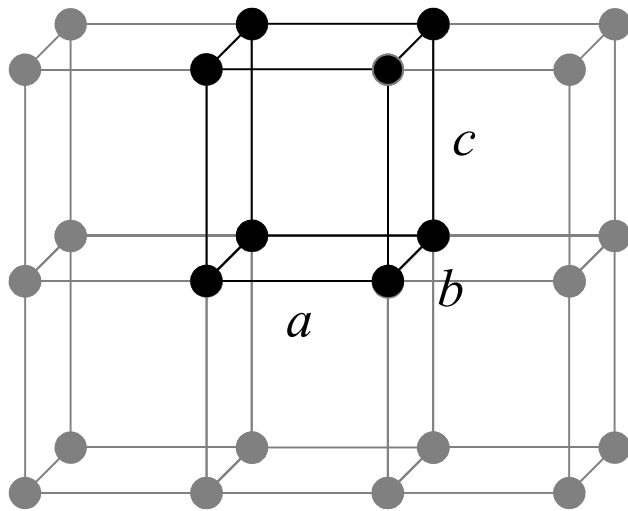
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Bravais lattice and reciprocal lattice in 1-D



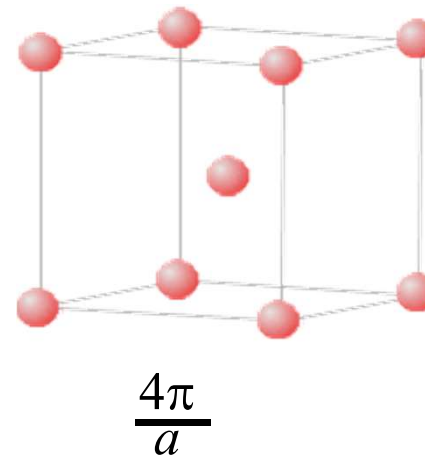
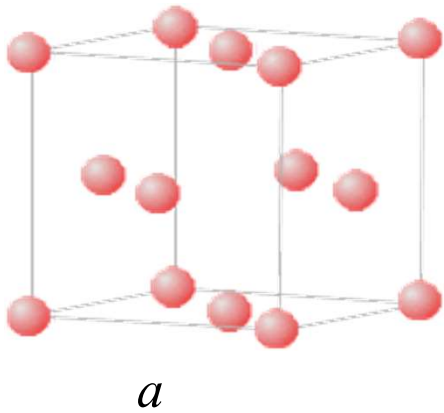
$$\cos\left(\frac{2\pi px}{a}\right) \Rightarrow \cos(Gx) \quad G = p \frac{2\pi}{a}$$

Reciprocal lattice of an orthorhombic lattice is an orthorhombic lattice



reciprocal lattice

The reciprocal lattice of an fcc lattice is a bcc lattice



$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

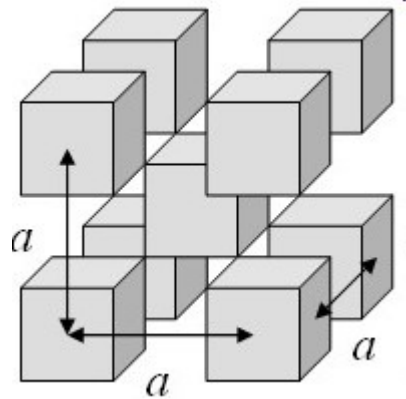
$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

$$\vec{a}_3 = \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}$$

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

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

Cubes on a bcc lattice



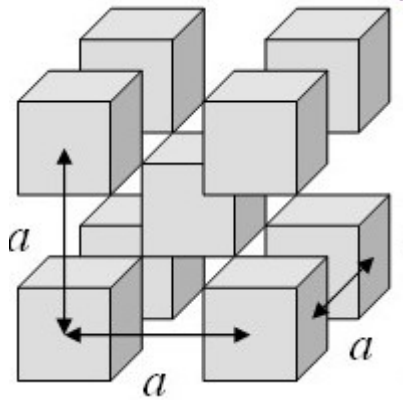
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Multiply by $e^{-i\vec{G}'\cdot\vec{r}}$ and integrate over a primitive unit cell.

$$\int_{\text{unit cell}} f(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3r = f_{\vec{G}} V$$

<http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/fourier.php>

Cubes on a bcc lattice



$$\int_{\text{unit cell}} f(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3r = f_{\vec{G}} V$$

V is the volume of the primitive unit cell.

$$f_{\vec{G}} = \frac{1}{V} \int f_{\text{cell}}(\vec{r}) \exp(-i\vec{G}\cdot\vec{r}) d^3r$$

$f_{\vec{G}}$ is the Fourier transform of f_{cell} evaluated at G .

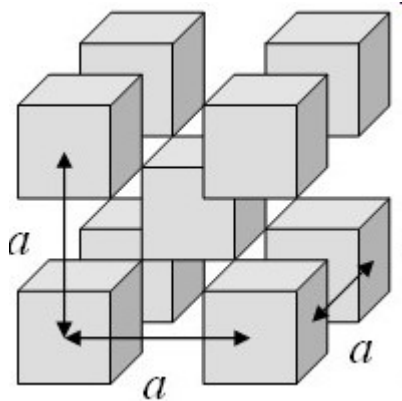
f_{cell} is zero outside the primitive unit cell.

$$f_{\vec{G}} = \frac{1}{V} \int f_{\text{cell}}(\vec{r}) \exp(-i\vec{G}\cdot\vec{r}) d^3r = \frac{2C}{a^3} \int_{-\frac{a}{4}}^{\frac{a}{4}} \int_{-\frac{a}{4}}^{\frac{a}{4}} \int_{-\frac{a}{4}}^{\frac{a}{4}} \exp(-iG_x x) \exp(-iG_y y) \exp(-iG_z z) dx dy dz$$

Volume of conventional u.c. a^3 . Two Bravais points per conventional u.c.

Cubes on a bcc lattice

$$\int_{-\frac{a}{4}}^{\frac{a}{4}} \exp(-iG_x x) dx = \frac{\exp(-iG_x x)}{-iG_x} \Big|_{-\frac{a}{4}}^{\frac{a}{4}} = \frac{\cos(-G_x x) + i \sin(-G_x x)}{-iG_x} \Big|_{-\frac{a}{4}}^{\frac{a}{4}} = \frac{2 \sin\left(\frac{G_x a}{4}\right)}{G_x}$$

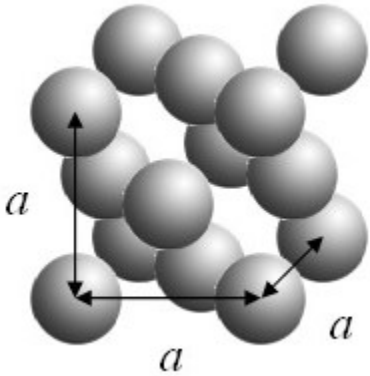


$$f_{\vec{G}} = \frac{16C \sin\left(\frac{G_x a}{4}\right) \sin\left(\frac{G_y a}{4}\right) \sin\left(\frac{G_z a}{4}\right)}{a^3 G_x G_y G_z}$$

The Fourier series for any rectangular cuboid with dimensions $L_x \times L_y \times L_z$ repeated on any three-dimensional Bravais lattice is:

$$f(\vec{r}) = \sum_{\vec{G}} \frac{8C \sin\left(\frac{G_x L_x}{2}\right) \sin\left(\frac{G_y L_y}{2}\right) \sin\left(\frac{G_z L_z}{2}\right)}{V G_x G_y G_z} \exp(i\vec{G} \cdot \vec{r})$$

Spheres on an fcc lattice



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

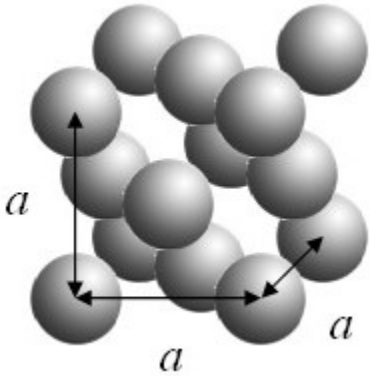
Multiply by $e^{-i\vec{G}'\cdot\vec{r}}$ and integrate over a primitive unit cell.

$$f_{\vec{G}} = \frac{1}{V} \int f_{\text{cell}}(\vec{r}) \exp(-i\vec{G}\cdot\vec{r}) d^3r = \frac{C}{V} \int_{\text{sphere}} \exp(-i\vec{G}\cdot\vec{r}) d^3r.$$

The Fourier series for non-overlapping spheres on any three-dimensional Bravais lattice is:

$$f(\vec{r}) = \frac{4\pi C}{V} \sum_{\vec{G}} \frac{\sin(|G|R) - |G|R \cos(|G|R)}{|G|^3} \exp(i\vec{G}\cdot\vec{r}).$$

Spheres on an fcc lattice



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

Multiply by $e^{-i\vec{G}'\cdot\vec{r}}$ and integrate over a primitive unit cell.

$$f_{\vec{G}} = \frac{1}{V} \int f_{cell}(\vec{r}) \exp(-i\vec{G}\cdot\vec{r}) d^3r = \frac{C}{V} \int_{\text{sphere}} \exp(-i\vec{G}\cdot\vec{r}) d^3r.$$

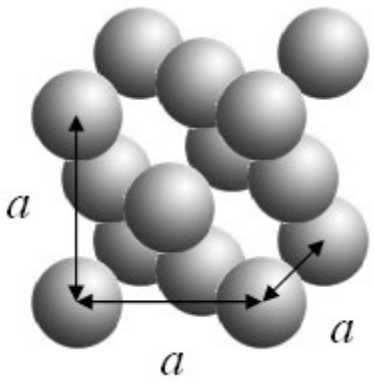
$$f_{\vec{G}} = \frac{C}{V} \int_0^R \int_0^\pi \int_{-\pi}^\pi \exp(-i\vec{G}\cdot\vec{r}) r^2 \sin\theta dr d\theta d\varphi$$

$$= \frac{C}{V} \int_0^R \int_0^\pi \int_{-\pi}^\pi \left(\cos(|G|r \cos\theta) - i \sin(|G|r \cos\theta) \right) r^2 \sin\theta dr d\theta d\varphi$$

Integrate over φ

$$f_{\vec{G}} = \frac{2\pi C}{V} \int_0^R \int_0^\pi \left(\cos(|G|r \cos\theta) - i \sin(|G|r \cos\theta) \right) r^2 \sin\theta dr d\theta$$

Spheres on an fcc lattice



$$f_{\vec{G}} = \frac{2\pi C}{V} \int_0^R \int_0^\pi \left(\cos(|G|r \cos \theta) - i \sin(|G|r \cos \theta) \right) r^2 \sin \theta dr d\theta$$

Both terms are perfect differentials

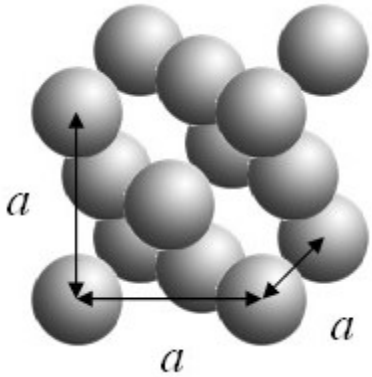
$$\frac{d}{d\theta} \cos(|G|r \cos \theta) = |G|r \sin(|G|r \cos \theta) \sin \theta \quad \text{and}$$

$$\frac{d}{d\theta} \sin(|G|r \cos \theta) = -|G|r \cos(|G|r \cos \theta) \sin \theta,$$

Integrate over θ :

$$f_{\vec{G}} = \frac{2\pi C}{V} \int_0^R \left(-\sin(|G|r \cos \theta) - i \cos(|G|r \cos \theta) \right) \Big|_0^\pi dr$$

$$f_{\vec{G}} = \frac{4\pi C}{V} \int_0^R \frac{\sin(|G|r)}{|G|} r dr$$



Spheres on any lattice

$$f_{\vec{G}} = \frac{4\pi C}{V} \int_0^R \frac{\sin(|G|r)}{|G|r} r^2 dr$$

Integrate over r

$$f_G = \frac{4\pi C}{V|G|^3} \left(\sin(|G|R) - |G|R \cos(|G|R) \right).$$

The Fourier series for non-overlapping spheres on any three-dimensional Bravais lattice is:

$$f(\vec{r}) = \frac{4\pi C}{V} \sum_{\vec{G}} \frac{\sin(|G|R) - |G|R \cos(|G|R)}{|G|^3} \exp(i\vec{G} \cdot \vec{r}).$$

Molecular orbital potential

$$U(\vec{r}) = \frac{-Ze^2}{4\pi\epsilon_0} \sum_{r_j} \frac{1}{|\vec{r} - \vec{r}_j|}$$

position of atom j

The Fourier series for any molecular orbital potential is:

$$U(\vec{r}) = \frac{-Ze^2}{V\epsilon_0} \sum_{\vec{G}} \frac{\exp(i\vec{G} \cdot \vec{r})}{|G|^2}$$

Volume of the primitive unit cell

Muffin tin potential

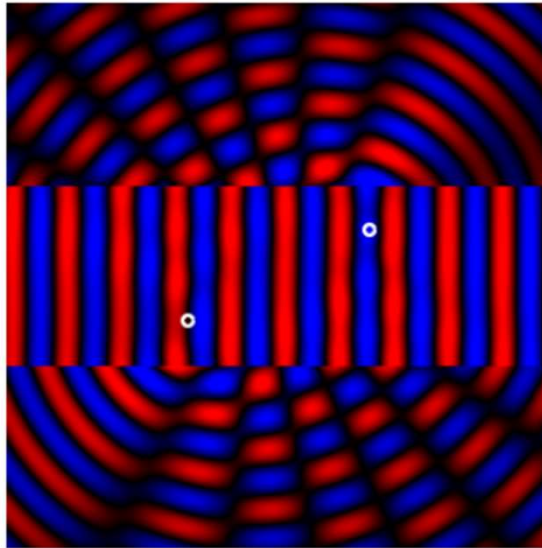


The potential is $U(\vec{r}) = -\frac{Ze^2}{4\pi\epsilon_0} \sum_j \frac{1}{|\vec{r} - \vec{r}_j|}$ around the Bravais lattice points

The potential is constant between the spheres.

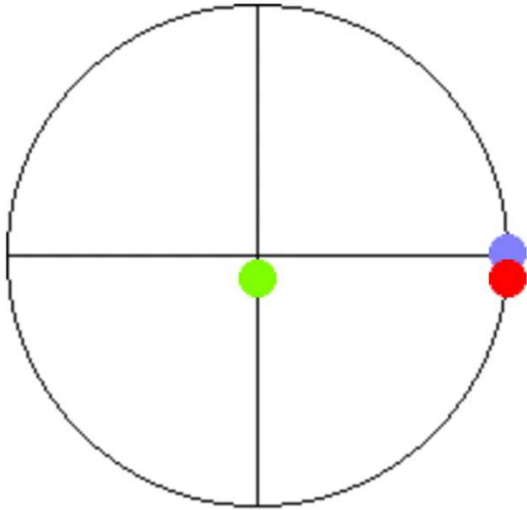
$$U(\vec{r}) = \frac{Ze^2}{V\epsilon_0} \sum_{\vec{G}} \left(\frac{\cos(|G|R) - 1}{|G|^2} + \frac{\sin(|G|R) - |G|R \cos(|G|R)}{R|G|^3} \right) \exp(i\vec{G} \cdot \vec{r}).$$

Intensity of the scattered waves

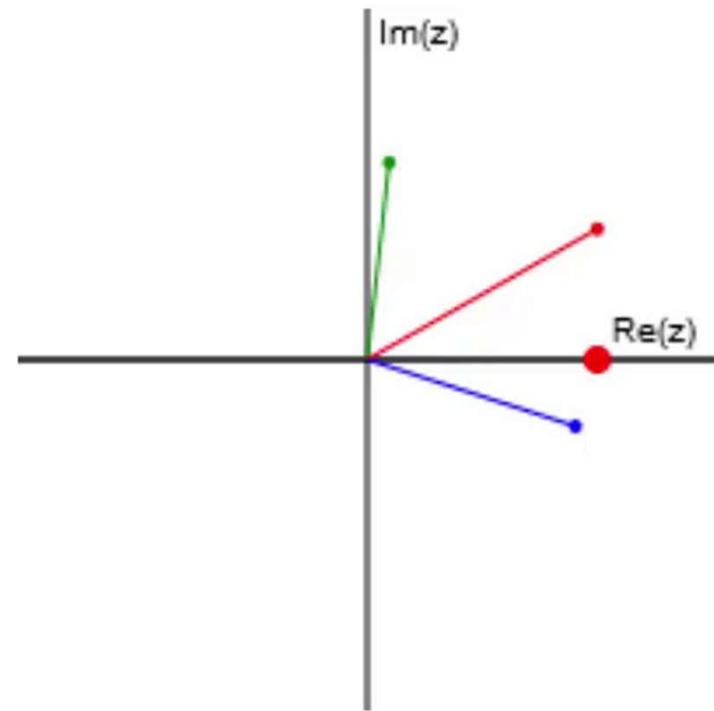


$$F_1 \frac{\cos(k|\vec{r} - \vec{r}_1| - \omega t + kx_1)}{\sqrt{|\vec{r} - \vec{r}_1|}} + F_2 \frac{\cos(k|\vec{r} - \vec{r}_2| - \omega t + kx_2)}{\sqrt{|\vec{r} - \vec{r}_2|}}.$$

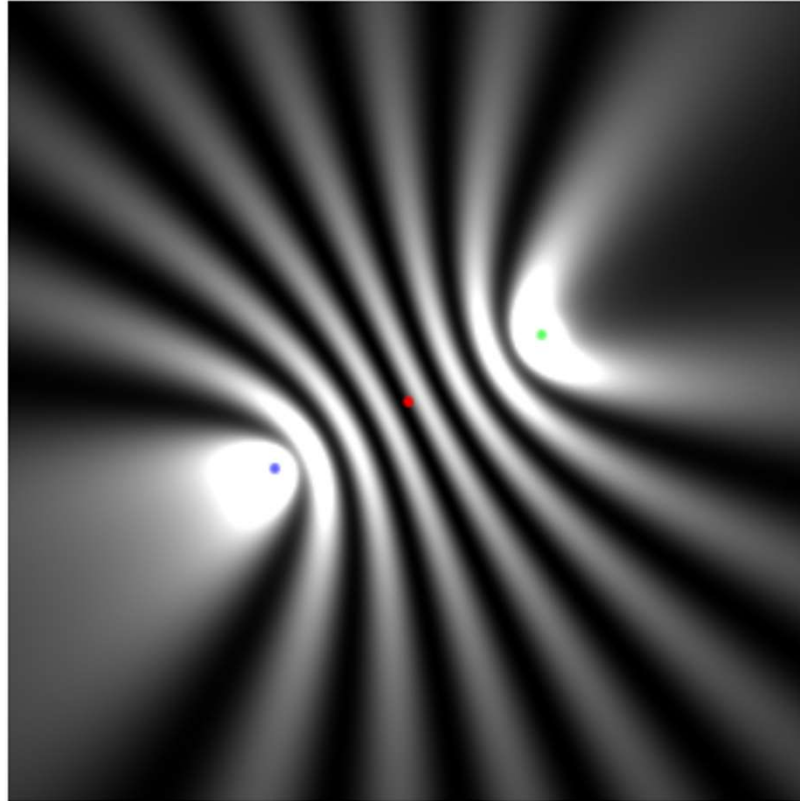
Using complex numbers to describe oscillations



$$e^{i\omega t} = \cos(\omega t) + i\sin(\omega t)$$

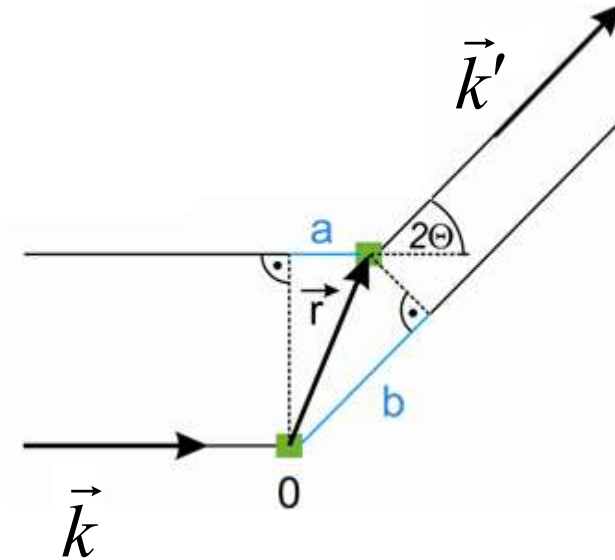


Intensity of the scattered waves



$$\left(\frac{F_1}{\sqrt{|\vec{r} - \vec{r}_1|}} e^{i(k|\vec{r} - \vec{r}_1| + kx_1)} + \frac{F_2}{\sqrt{|\vec{r} - \vec{r}_2|}} e^{i(k|\vec{r} - \vec{r}_2| + kx_2)} \right) e^{-i\omega t}$$

Interference



$$a = \frac{\vec{r} \cdot \vec{k}}{|\vec{k}|} \quad b = \frac{\vec{r} \cdot \vec{k}'}{|\vec{k}'|}$$

elastic scattering

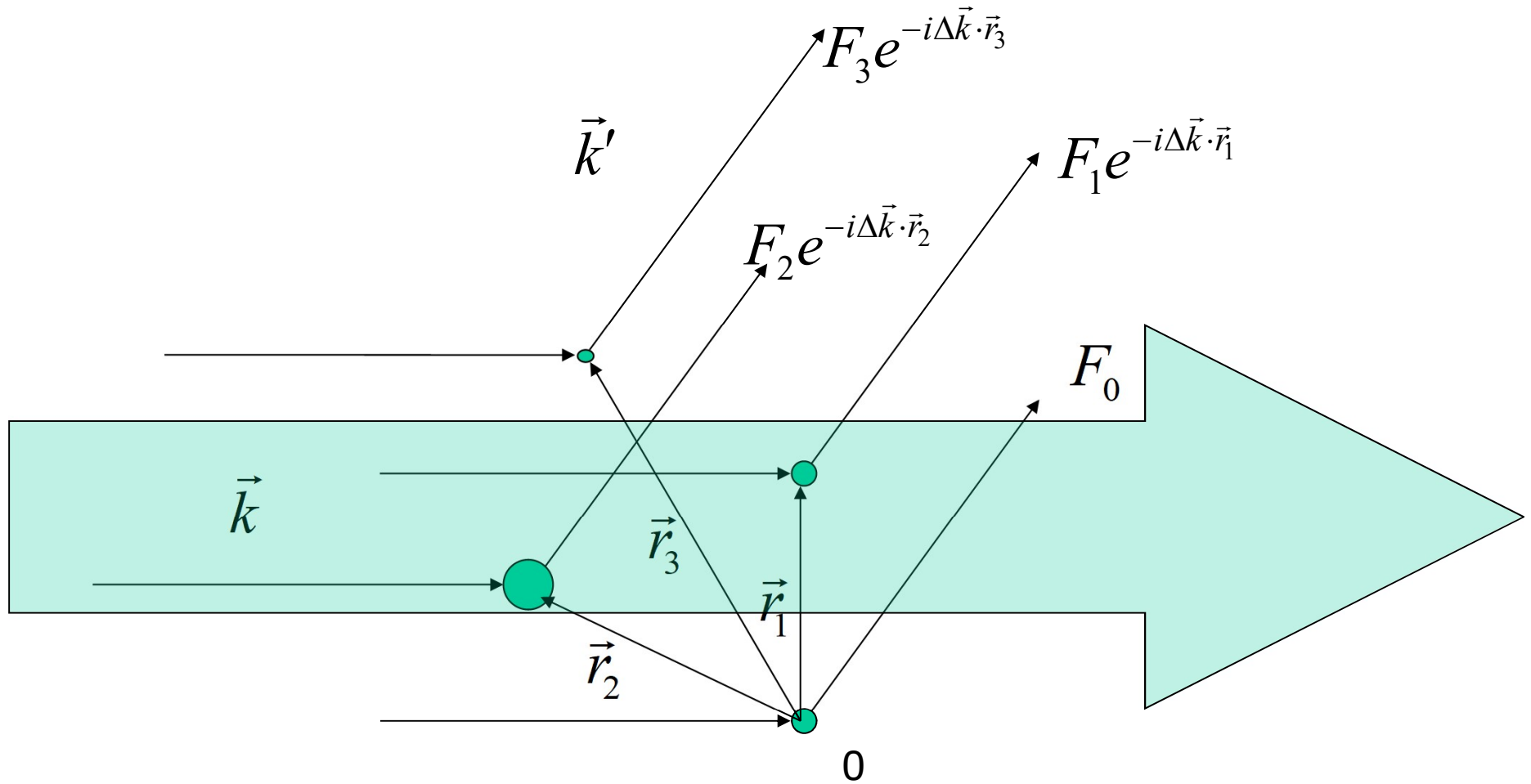
$$|\vec{k}| = |\vec{k}'|$$

path difference:
$$a - b = \frac{-\vec{r} \cdot (\vec{k}' - \vec{k})}{|\vec{k}|}$$

phase shift:
$$\varphi = 2\pi \frac{a - b}{\lambda} = 2\pi \frac{-\vec{r} \cdot (\vec{k}' - \vec{k})}{|\vec{k}| \lambda} = -\vec{r} \cdot (\vec{k}' - \vec{k}) = -\Delta\vec{k} \cdot \vec{r}$$

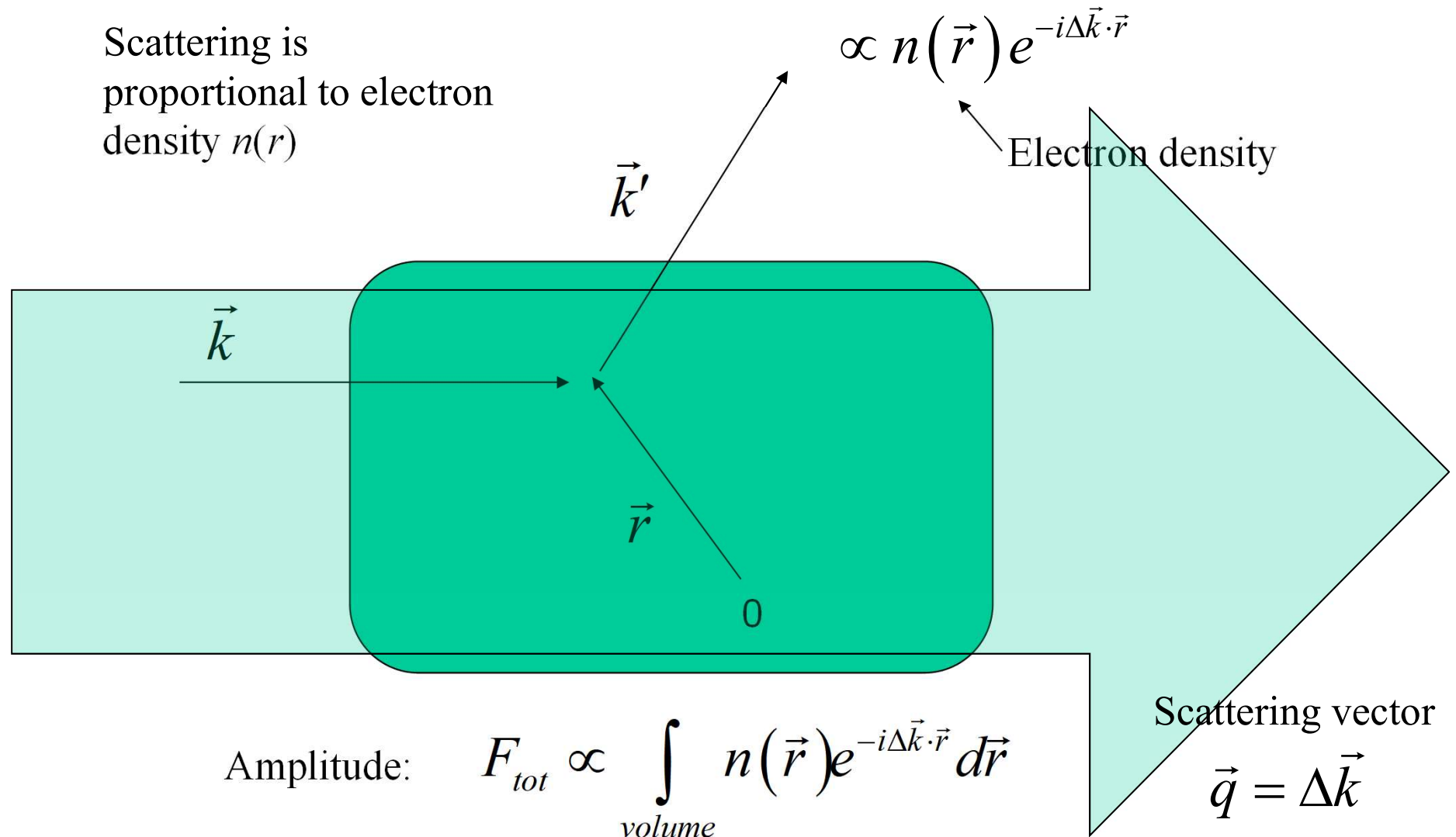
Amplitude:
$$F = F_0 + F_0 e^{-i\Delta\vec{k} \cdot \vec{r}}$$

Interference



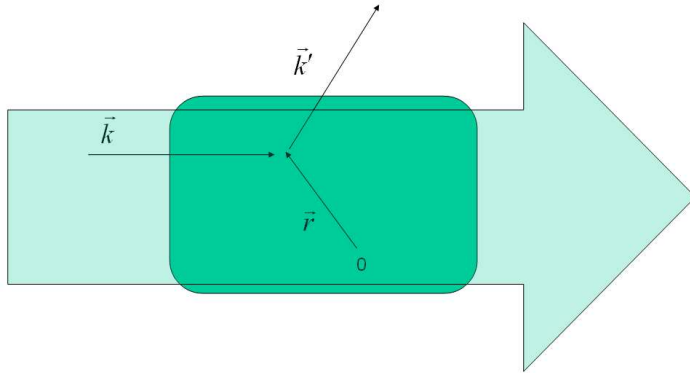
Amplitude:
$$F_{tot} = \sum_i F_i e^{-i\Delta\vec{k} \cdot \vec{r}_i}$$

Interference



The scattering amplitude is proportional to the Fourier transform of the electron density.

Scattering amplitude



$$F \propto \int n(\vec{r}) \exp(-i\Delta\vec{k} \cdot \vec{r}) dV$$

expand $n(r)$ in a Fourier series

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

$$F \propto \sum_{\vec{G}} \int n_{\vec{G}} \exp(i(\vec{G} - \Delta\vec{k}) \cdot \vec{r}) dV$$

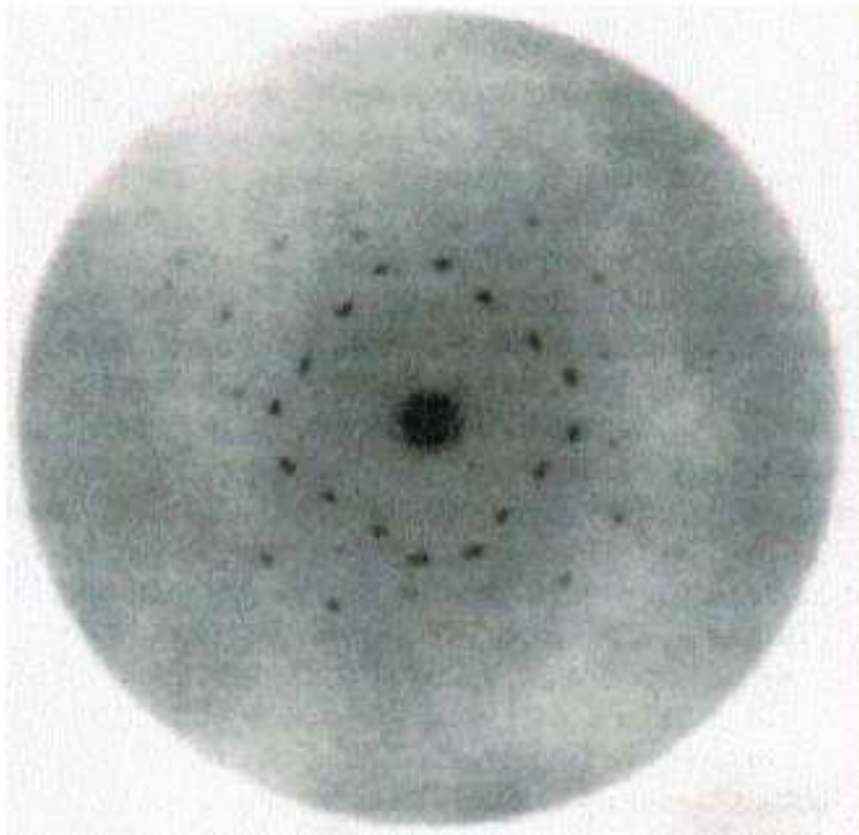
if $\vec{G} = \Delta\vec{k}$, all components add coherently

diffraction condition: $\vec{G} = \Delta\vec{k}$

The intensity of the peak at G is $|n_G|^2$

nobel prize 1914

first diffraction experiment of Max von Laue 1912
ZnS single crystal, exposure time 30'
the 5th diffraction pattern



M. von Laue (1879-1960)

$$\vec{G} = \Delta\vec{k}$$