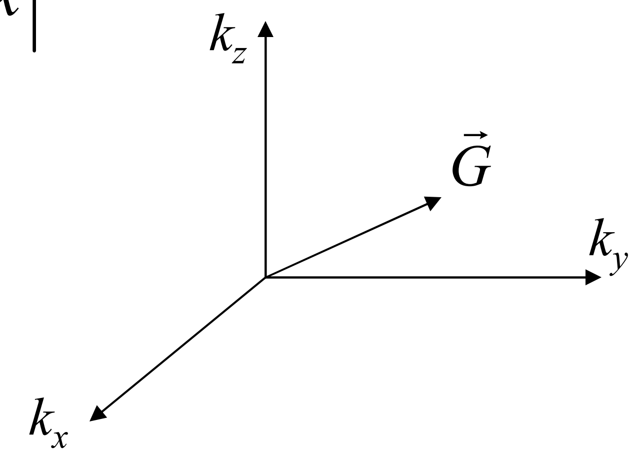
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

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

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

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

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



Plane wave:

$$\exp(i\vec{G}\cdot\vec{r}) = \cos(G_x x + G_y y + G_z z) + i\sin(G_x x + G_y y + G_z z)$$

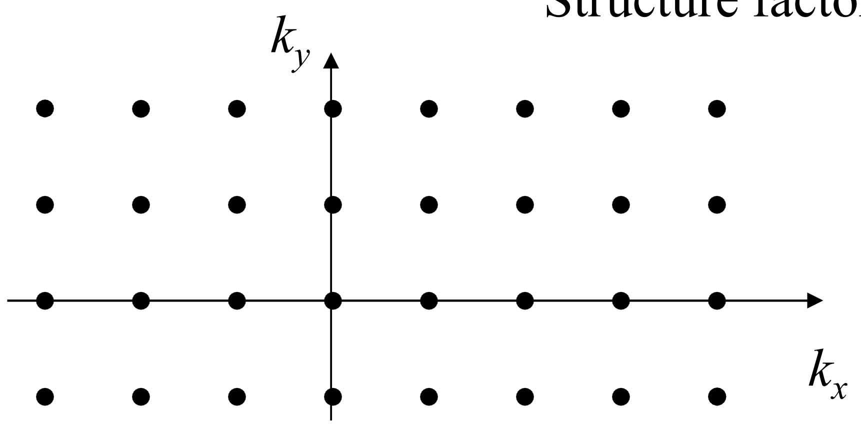
Reciprocal lattice (Reziprokes Gitter)

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



$$\vec{G} = \upsilon_1 \vec{b}_1 + \upsilon_2 \vec{b}_2 + \upsilon_3 \vec{b}_3$$

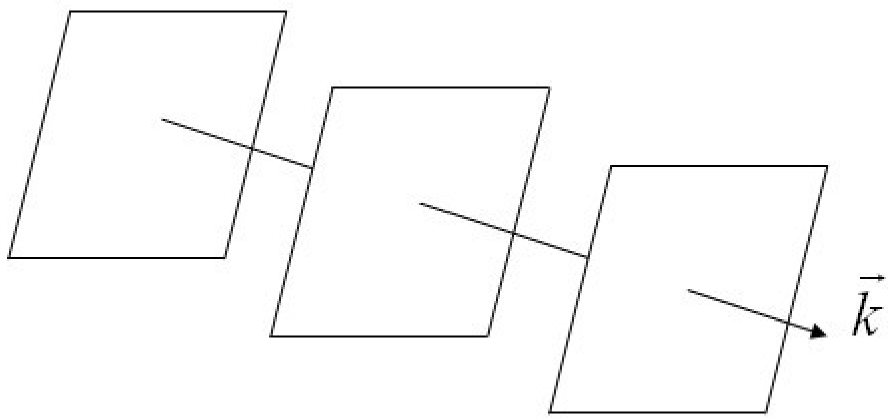
v_i integers

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

Plane waves (Ebene Wellen)

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

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



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

Most functions can be expressed in terms of plane waves

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

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

Determine the structure factors in 1-D

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

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

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

$$= \sum_G \int_{unit\ cell} \cos((G-G')x) + i\sin(G-G')x)dx = f_{G'}a$$

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

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

Fourier transforms

Most functions can be expressed in terms of plane waves

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

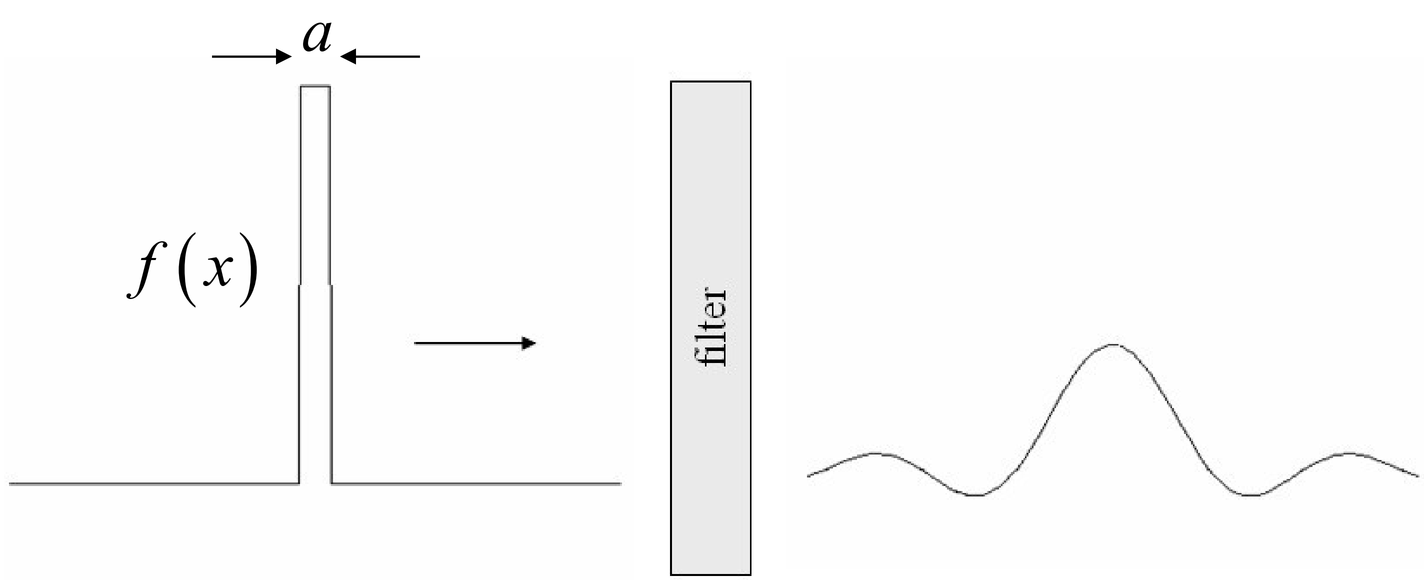
This can be inverted for $F(k)$

$$F\left(\vec{k}\right) = \frac{1}{\left(2\pi\right)^d} \int f(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} d\vec{r}$$

Fourier transform of $f(r)$

http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/ft/ft.php

Fourier transforms



Fourier transform: $F(k) = \frac{1}{2\pi} \int_{-a/2}^{a/2} e^{-ikx} dx = \frac{\sin(ka/2)}{\pi k}$

Inverse transform: $f(x) = \int_{-\infty}^{\infty} \frac{\sin(ka/2)}{\pi k} e^{ikx} dk$

Sine integral

Transmitted pulse: $f'(x) = \int_{-k_0}^{k_0} \frac{\sin(ka/2)}{\pi k} e^{ikx} dk = \frac{\mathrm{Si}(k_0 x + \frac{1}{2}) + \mathrm{Si}(k_0 x - \frac{1}{2})}{\pi}$

Notations for Fourier Transforms

$$F_{a,b}\left(\vec{k}\right) = \mathcal{F}_{a,b}\{f\left(\vec{r}\right)\} = \sqrt{\frac{|b|^d}{(2\pi)^{d\left(1-a\right)}}} \int_{-\infty}^{\infty} f\left(\vec{r}\right) e^{ib\vec{k}\cdot\vec{r}} d\vec{r}$$

$$f\left(\vec{r}\right) = \mathcal{F}_{a,b}^{-1}\{F\left(\vec{k}\right)\} = \sqrt{\frac{|b|^d}{(2\pi)^{d\left(1+a\right)}}} \int_{-\infty}^{\infty} F_{a,b}\left(\vec{k}\right) e^{-ib\vec{k}\cdot\vec{r}} d\vec{k}$$

d = number of dimensions 1,2,3
a,b = constants

Notations for Fourier Transforms

$$F_{-1,-1}\left(\vec{k}\right) = \frac{1}{\left(2\pi\right)^{d}} \int f\left(\vec{r}\right) e^{-i\vec{k}\cdot\vec{r}}\, d\vec{r}\,.$$

$$f\left(\vec{r}\right) = \int F_{-1,-1}\left(\vec{k}\right) e^{i\vec{k}\cdot\vec{r}}\, d\vec{k}\,.$$

$f(r)$ is built of plane waves

Notations for Fourier Transforms

$$F_{1,-1}\left(\vec{k}\right) = \int f\left(\vec{r}\right) e^{-i\vec{k}\cdot\vec{r}}\, d\vec{r}\,.$$

$$f\left(\vec{r}\right) = \frac{1}{\left(2\pi\right)^{d}} \int F_{1,-1}\left(\vec{k}\right) e^{i\vec{k}\cdot\vec{r}}\, d\vec{k}.$$

Matlab

Notations for Fourier Transforms

$$F_{0,-1}\left(\vec{k}\right) = \frac{1}{(2\pi)^{d/2}} \int f(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} d\vec{r}.$$

$$f(\vec{r}) = \frac{1}{(2\pi)^{d/2}} \int F_{0,-1}\left(\vec{k}\right) e^{i\vec{k}\cdot\vec{r}} d\vec{k}.$$

Mathematica

Notations for Fourier Transforms

$$F_{0,-2\pi}\left(\vec{q}\right) = \int f\left(\vec{r}\right) e^{-i2\pi\vec{q}\cdot\vec{r}}\, d\vec{r}\,.$$

$$f\left(\vec{r}\right) = \int F_{0,-2\pi}\left(\vec{q}\right) e^{i2\pi\vec{q}\cdot\vec{r}}\, d\vec{q}\,.$$

Engineering literature, usually on the 1-d case is considered.

$\exp(-\lvert a\rvert x)$	$\frac{\lvert a\rvert}{\pi(a^2+k^2)}$	$\frac{2\lvert a\rvert}{a^2+k^2}$
$\operatorname{sgn}(x)$ $\operatorname{sgn}(x)=-1$ for $x<0$ and $\operatorname{sgn}(x)=1$ for $x>0$	$\frac{-i}{\pi\omega}$	$\frac{-2i}{\omega}$
$\operatorname{sgn}(x)\exp(-\lvert a\rvert x)$	$\frac{-ik}{\pi(a^2+k^2)}$	$\frac{-i2k}{a^2+k^2}$
$H(x)\exp(-\lvert a\rvert x)$	$\frac{\lvert a\rvert-ik}{2\pi(a^2+k^2)}$	$\frac{\lvert a\rvert-ik}{a^2+k^2}$
$\sqcap(x)=H\left(x+\frac{1}{2}\right)H\left(\frac{1}{2}-x\right)$ Square pulse: height = 1, width = 1, centered at $x=0$.	$\frac{\sin(k/2)}{\pi k}$	$\frac{2\sin(k/2)}{k}$
$\sqcap\left(\frac{x-x_0}{a}\right)$ Square pulse: height = 1, width = a, centered at x_0.	$\frac{\sin(ka/2)}{\pi k}\exp(-ikx_0)$	$\frac{2\sin(ka/2)}{k}\exp(-ikx_0)$
$\exp\left(i\vec{k}_0\cdot\vec{r}\right)$ Plane wave	$\delta\left(\vec{k}-\vec{k}_0\right)$	$(2\pi)^d\delta\left(\vec{k}-\vec{k}_0\right)$
1	$\delta(k)$	$2\pi\delta(k)$
$\delta(x)$ $\delta\left(\frac{\vec{r}-\vec{r}_0}{a}\right)$	$\frac{1}{2\pi}$ $\left(\frac{a}{2\pi}\right)^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	1 $a^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$\exp\left(-\frac{\lvert\vec{r}-\vec{r}_0\rvert^2}{a^2}\right)$	$\left(\frac{a}{2\sqrt{\pi}}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$(a\sqrt{\pi})^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$H(R-\lvert\vec{r}-\vec{r}_0\rvert)$ Disc of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^2$ $H(R-\lvert\vec{r}-\vec{r}_0\rvert)$ Sphere of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^3$	$\frac{R}{2\pi\lvert\vec{k}\rvert}J_1(\lvert\vec{k}\rvert R)\exp(-i\vec{k}\cdot\vec{r}_0)$ $\frac{1}{(2\pi)^3\lvert\vec{k}\rvert^3}\left(\sin(\lvert\vec{k}\rvert R)-\lvert\vec{k}\rvert R\cos(\lvert\vec{k}\rvert R)\right)\exp(-i\vec{k}\cdot\vec{r}_0)$	$\frac{2\pi R}{\lvert\vec{k}\rvert}J_1(\lvert\vec{k}\rvert R)\exp(-i\vec{k}\cdot\vec{r}_0)$ $\frac{4\pi}{\lvert\vec{k}\rvert^3}\left(\sin(\lvert\vec{k}\rvert R)-\lvert\vec{k}\rvert R\cos(\lvert\vec{k}\rvert R)\right)\exp(-i\vec{k}\cdot$

Here $H(x)$ is the Heaviside step function, $\delta(x)$ is the Dirac delta function, $J_1(x)$ is the first order Bessel function of the first kind, and d is the number of dimensio

Calculate a Fourier transform numerically.

http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/ft/ft.php

Discrete Fourier Transforms

The Discrete Fourier Transform (DFT) is an algorithm that takes a discrete sequence of points and returns the Fourier components of a continuous periodic function that passes through all of those points. It is widely used in data analysis and digital signal processing. The standard form of the discrete Fourier transform of a sequence of N points $(f_0, f_1, \cdots, f_{N-1})$ is,[1]

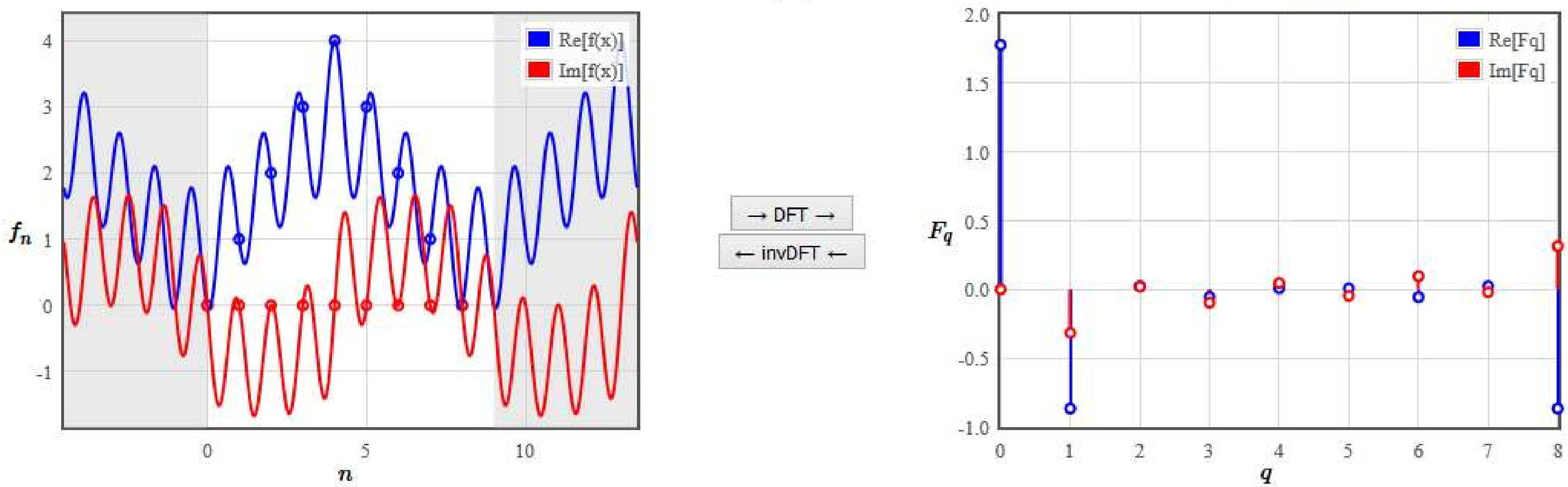
$$F_q = \frac{1}{N}\sum_{n=0}^{N-1} f_n e^{-i2\pi qn/N} \qquad q = 0, 1, \cdots, N-1.$$

The original sequence of points can be recovered via the inverse transform,

$$f_n = \sum_{q=0}^{N-1} F_q e^{i2\pi qn/N}.$$

A continuous periodic function $f(x)$ that passes through the points f_0 at $x = 0$, f_1 at $x = 1$, etc. is,

$$f(x) = \sum_{q=0}^{N-1} F_q e^{i2\pi qx/N}.$$



http://lampx.tugraz.at/~hadley/ss2/linearresponse/dft/dft0.php

Properties of Fourier transforms

Linearity and superposition

$\mathcal{F}\{\alpha f(\vec{r}) + \beta g(\vec{r})\} = \alpha\mathcal{F}\{f(\vec{r})\} + \beta\mathcal{F}\{g(\vec{r})\}$ where α and β are any constants.

Similarity

$\mathcal{F}\{f\left(\frac{\vec{r}}{a}\right)\} = |a|^d\mathcal{F}\{f(\vec{r})\}.$

Shift

$\mathcal{F}\{f(\vec{r} - \vec{r}_0)\} = \mathcal{F}\{f(\vec{r})\}\exp\left(-i\vec{k}\cdot\vec{r}_0\right).$

Convolution (Faltung)

$$f(\vec{r}) * g(\vec{r}) = \int f(\vec{r}')g(\vec{r}-\vec{r}')d\vec{r}$$

Notation [-1,-1]: $\mathcal{F}\{fg\} = \mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{2\pi}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Notation [1,-1]: $\mathcal{F}\{fg\} = \frac{1}{2\pi}\mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Notation [0,-1]: $\mathcal{F}\{fg\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Notation [0,-2π]: $\mathcal{F}\{fg\} = \mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

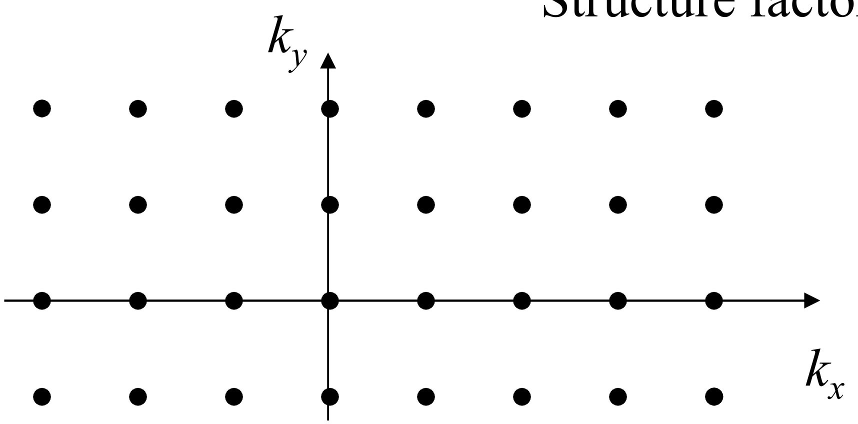
Reciprocal lattice (Reziprokes Gitter)

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

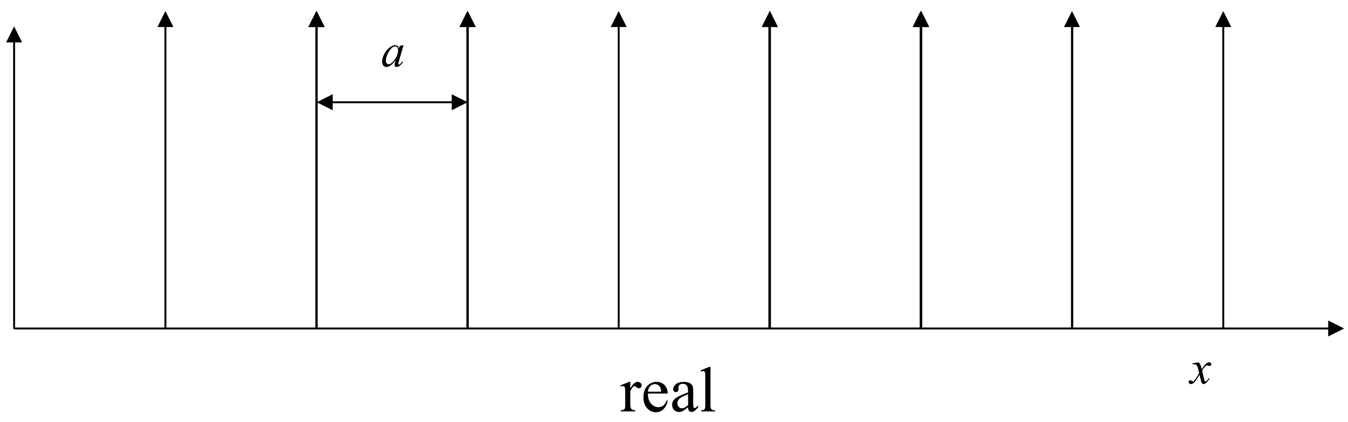


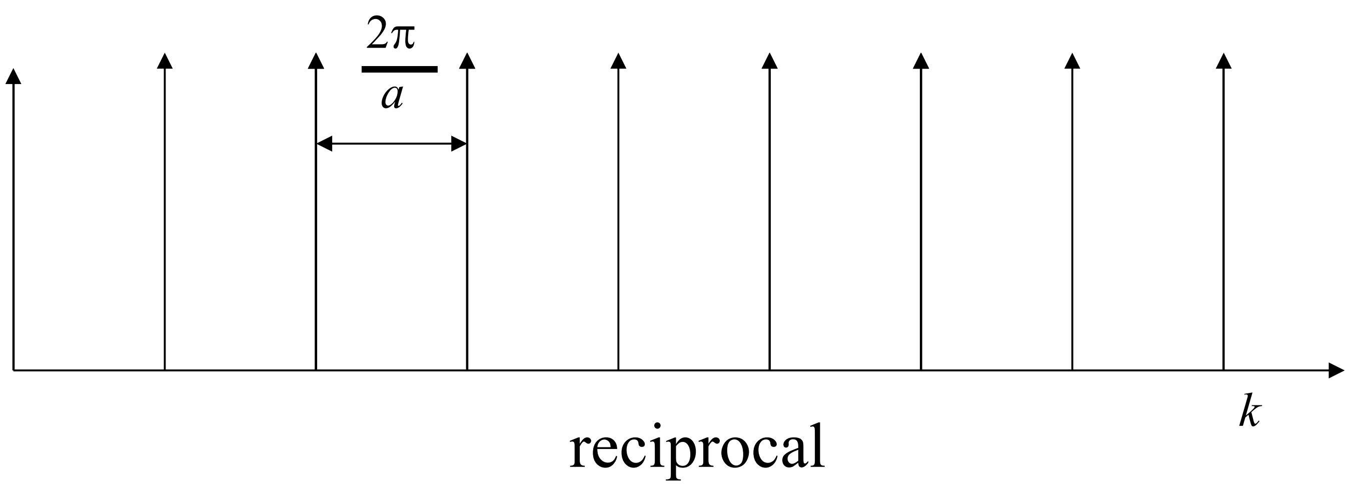
$$\vec{G} = \upsilon_1 \vec{b}_1 + \upsilon_2 \vec{b}_2 + \upsilon_3 \vec{b}_3$$

v_i integers

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

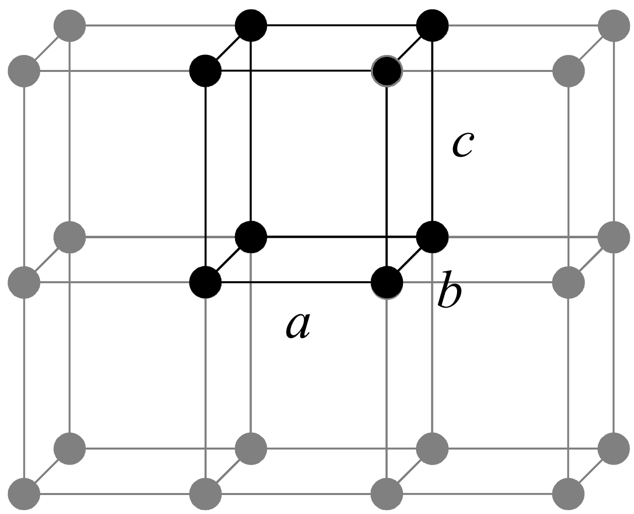
Bravais lattice and reciprocal lattice in 1-D

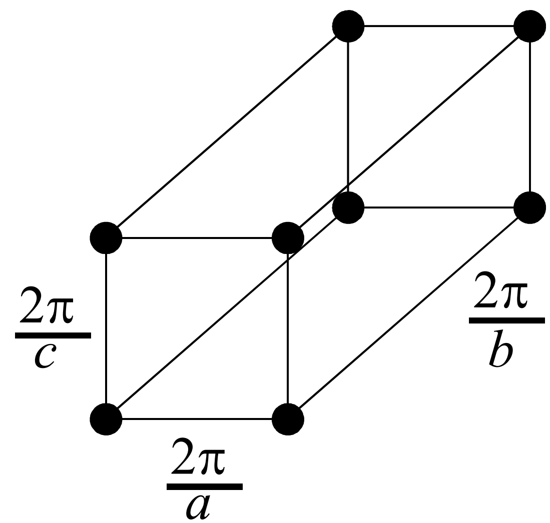




$$\cos\left(\frac{2\pi p x}{a}\right) \Rightarrow \cos(Gx) \qquad G = p\frac{2\pi}{a}$$

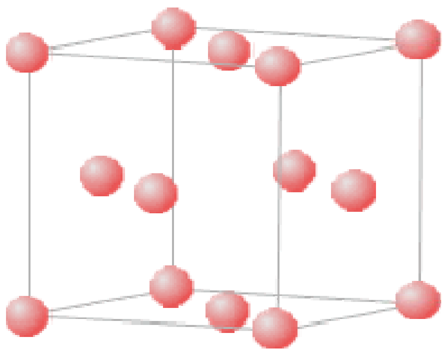
Reciprocal lattice of an orthorhombic lattice is an orthorhombic lattice



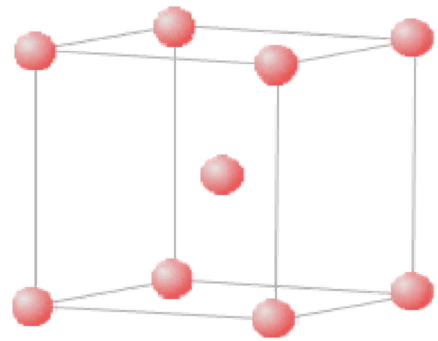


reciprocal lattice

The reciprocal lattice of an fcc lattice is a bcc lattice



a



$\frac{4\pi}{a}$

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

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

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

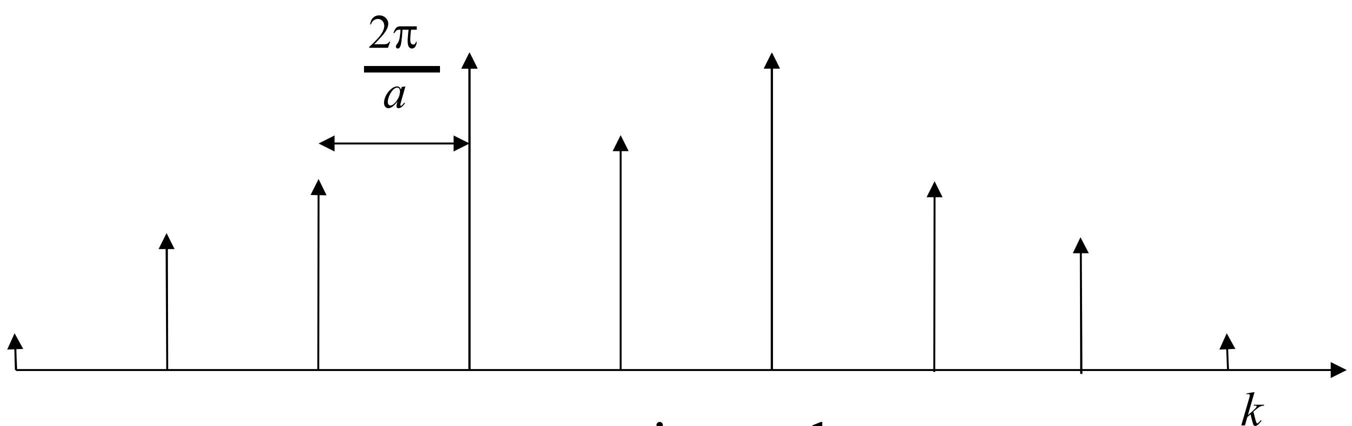
$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \left(\vec{a}_2 \times \vec{a}_3\right)}$$

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

The reciprocal lattice is the Fourier transform of the real space lattice

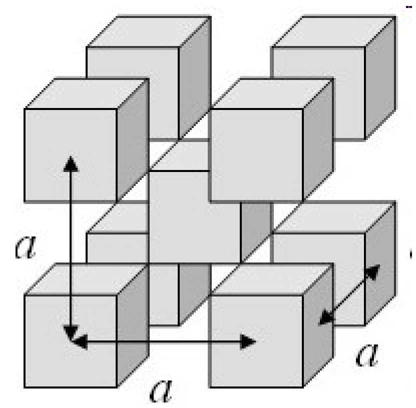
crystal = Bravais_lattice(r) * unit_cell(r)

$\mathcal{F}$(crystal) = $\mathcal{F}$(Bravais_lattice(r))$\mathcal{F}$(unit_cell(r))



reciprocal

Cubes on a bcc lattice



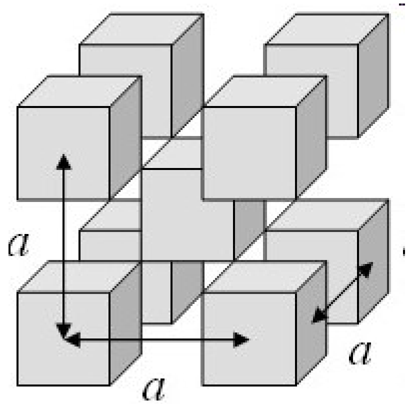
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

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.

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

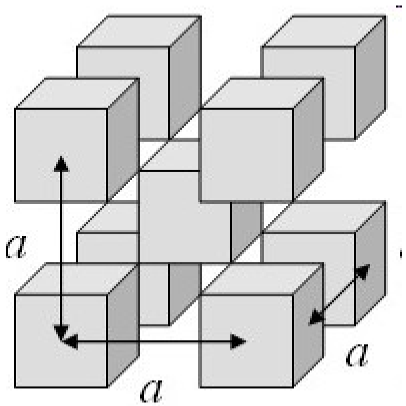
f_G is the Fourier transform of f_{cell} evaluated at *G*.
f_{cell} is zero outside the primitive unit cell.

$$f_{\vec{G}} = \frac{1}{V}\int f_{cell}(\vec{r})\exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r = \frac{2C}{a^3}\int_{\frac{-a}{4}}^{\frac{a}{4}}\int_{\frac{-a}{4}}^{\frac{a}{4}}\int_{\frac{-a}{4}}^{\frac{a}{4}}\exp\left(-iG_xx\right)\exp\left(-iG_yy\right)\exp\left(-iG_zz\right)dxdydz$$

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

Cubes on a bcc lattice

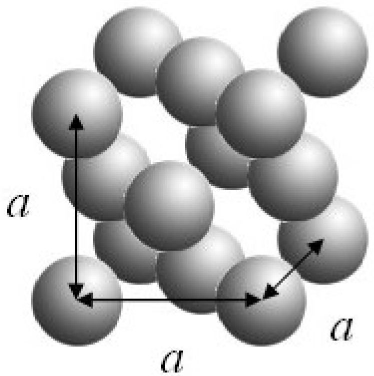
$$\int_{-\frac{a}{4}}^{\frac{a}{4}} \exp(-iG_x x)dx = \left.\frac{\exp(-iG_x x)}{-iG_x}\right|_{-\frac{a}{4}}^{\frac{a}{4}} = \left.\frac{\cos(-G_x x) + i\sin(-G_x x)}{-iG_x}\right|_{-\frac{a}{4}}^{\frac{a}{4}} = \frac{2\sin\left(\frac{G_x a}{4}\right)}{G_x}$$



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

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:

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



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.

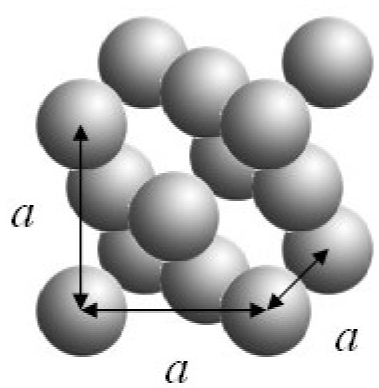
$$f_{\vec{G}} = \frac{1}{V}\int f_{cell}(\vec{r})\exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r = \frac{C}{V}\int_{\text{sphere}} \exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r.$$

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

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

Integrate over φ

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



Spheres on an fcc lattice

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

Both terms are perfect differentials

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

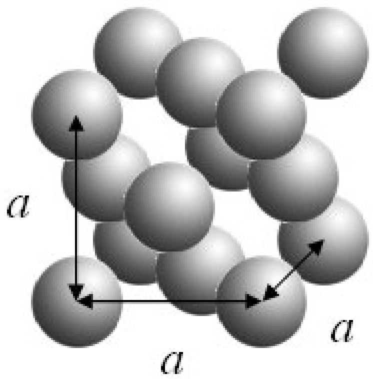
$$\frac{d}{d\theta}\sin\left(|G| r\cos\theta\right) = -|G| r \cos\left(|G| r\cos\theta\right)\sin\theta,$$

Integrate over θ:

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

0

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



Spheres on any lattice

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

Integrate over r

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

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

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

Molecular orbital potential

$$U(\vec{r}) = \frac{-Ze^2}{4\pi\varepsilon_0} \sum_{r_j} \frac{1}{\left|\vec{r} - \vec{r}_j\right|}$$

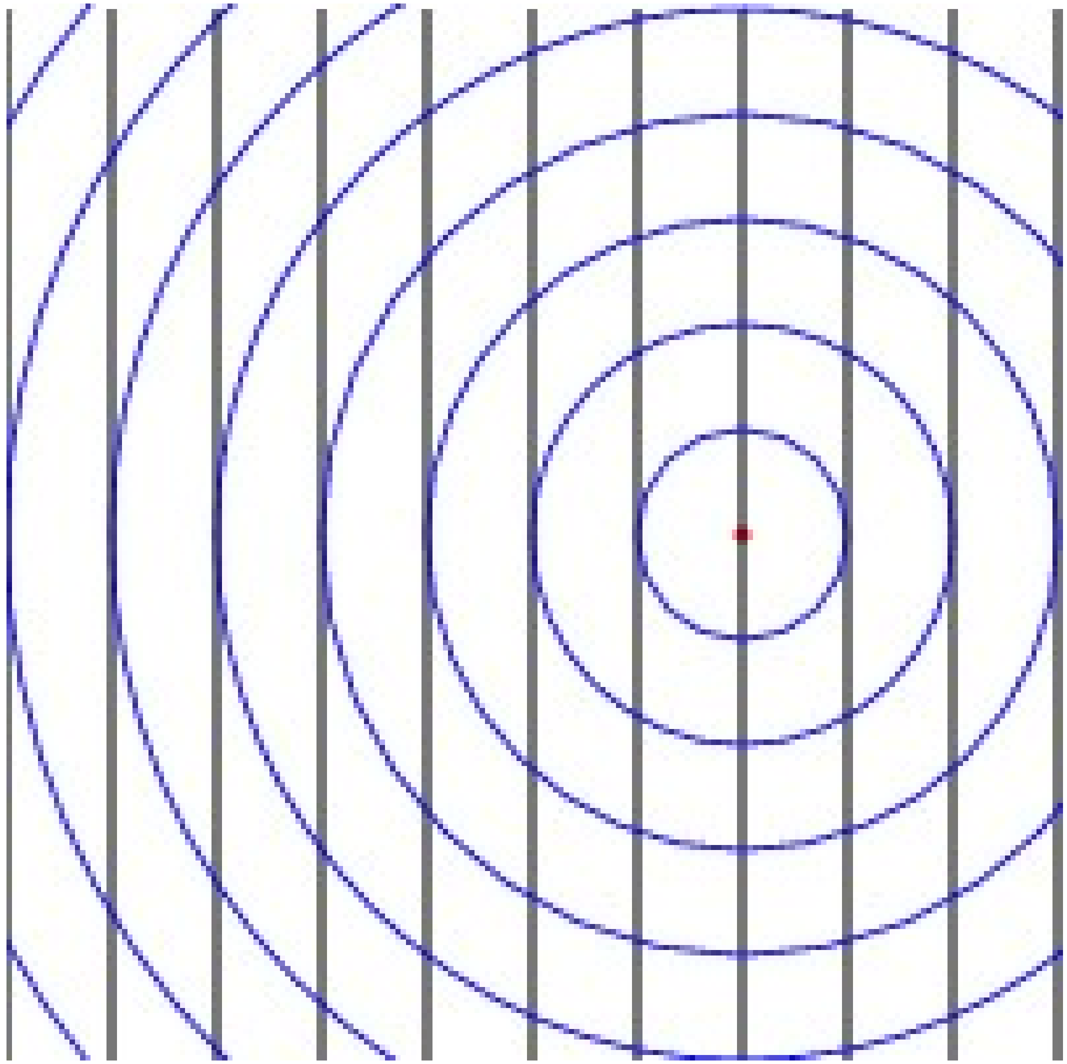
position of atom j

The Fourier series for any molecular orbital potential is:

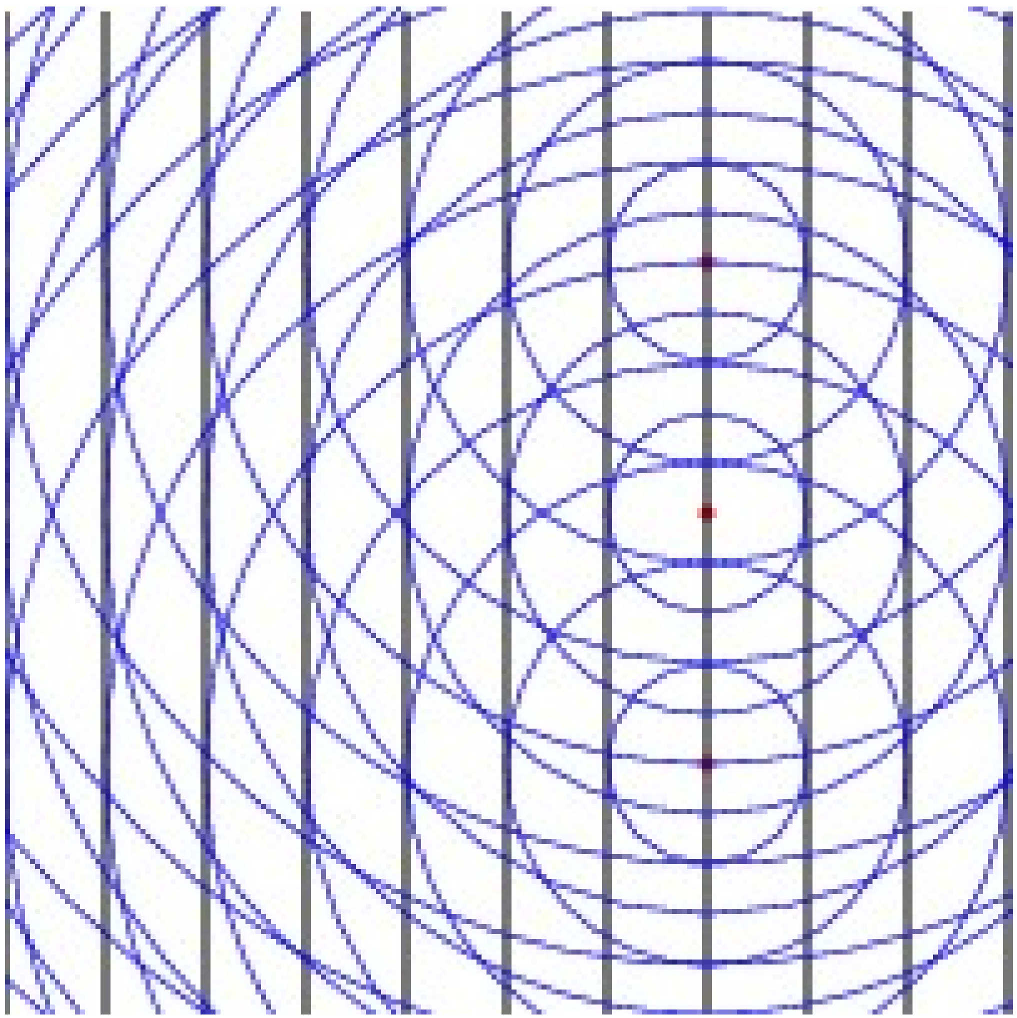
$$U(\vec{r}) = \frac{-Ze^2}{V\varepsilon_0} \sum_{\vec{G}} \frac{\exp\left(i\vec{G}\cdot\vec{r}\right)}{\left|G\right|^2}$$

Volume of the primitive unit cell

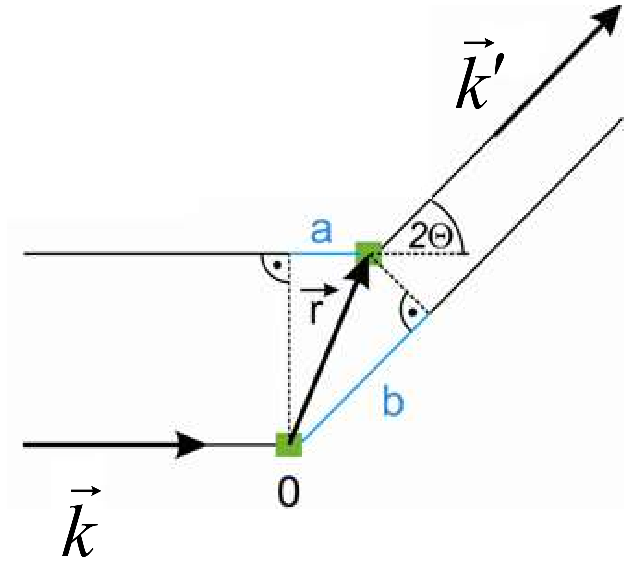
Interference



Interference



Interference



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

elastic scattering

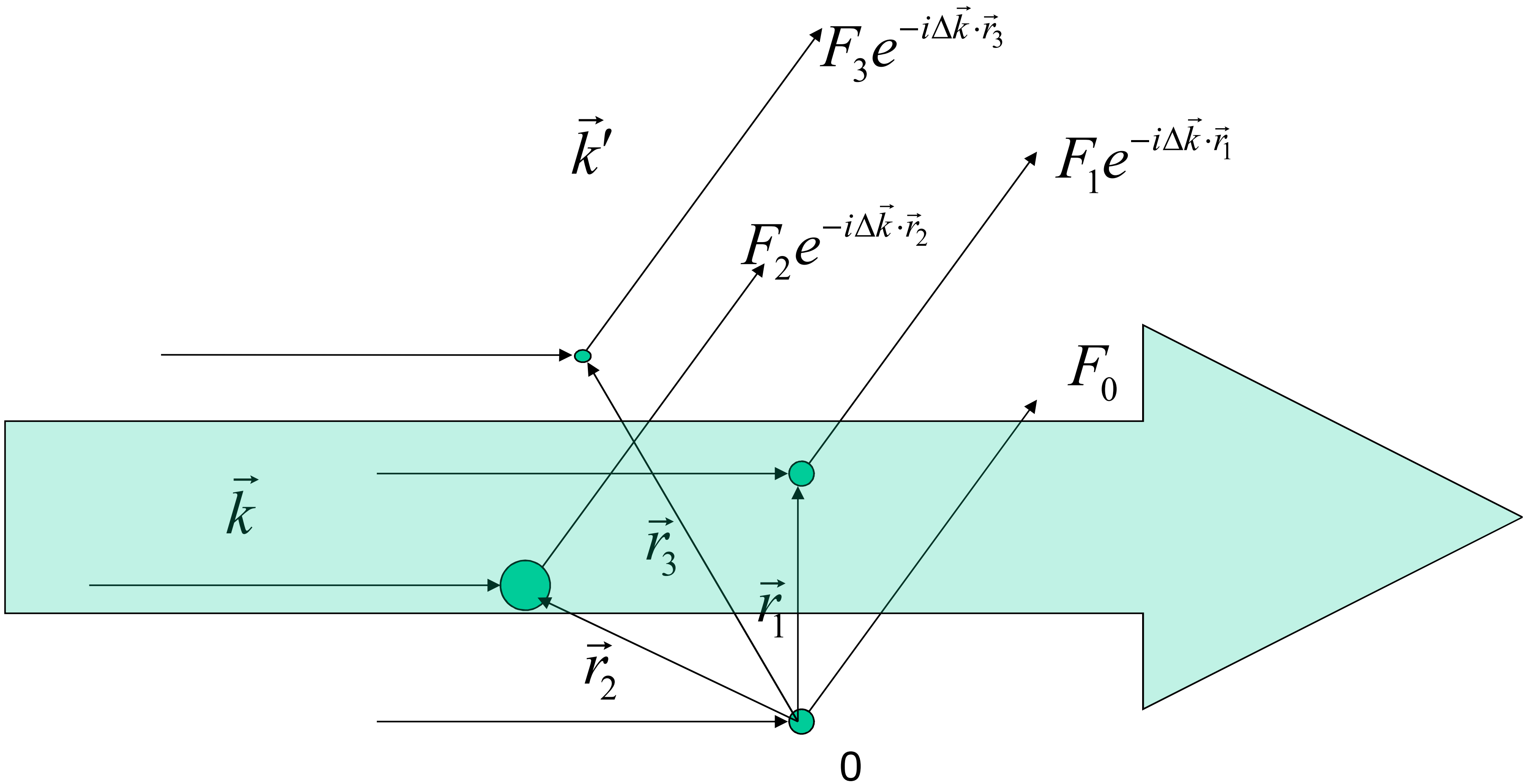
$$|k| = |k'|$$

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

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

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

Interference



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