Fourier Series,
Fourier transforms

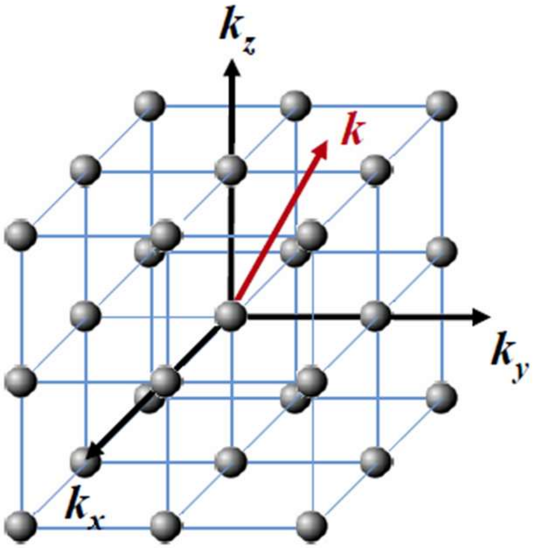
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

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

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

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

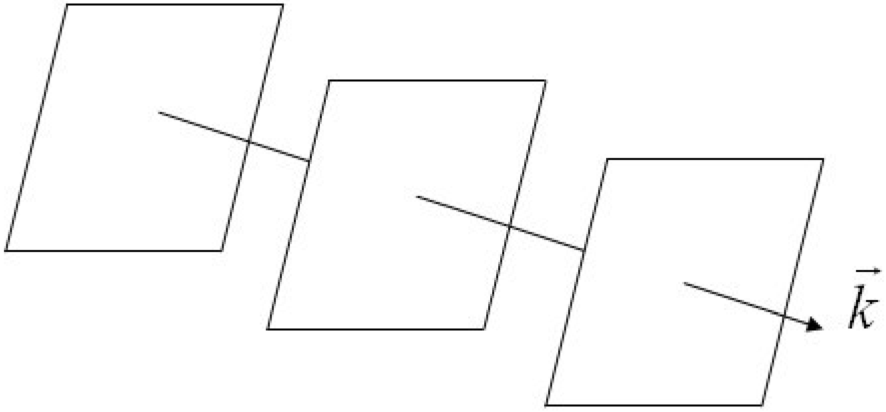
momentum: $\vec{p} = \hbar \vec{k}$



Plane waves (Ebene Wellen)

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

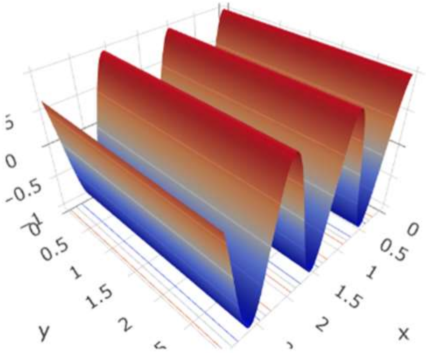
$$\lambda = \frac{2\pi}{\left|\vec{k}\right|}$$



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

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.

Fourier transforms

Most functions can be expressed in terms of plane waves

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

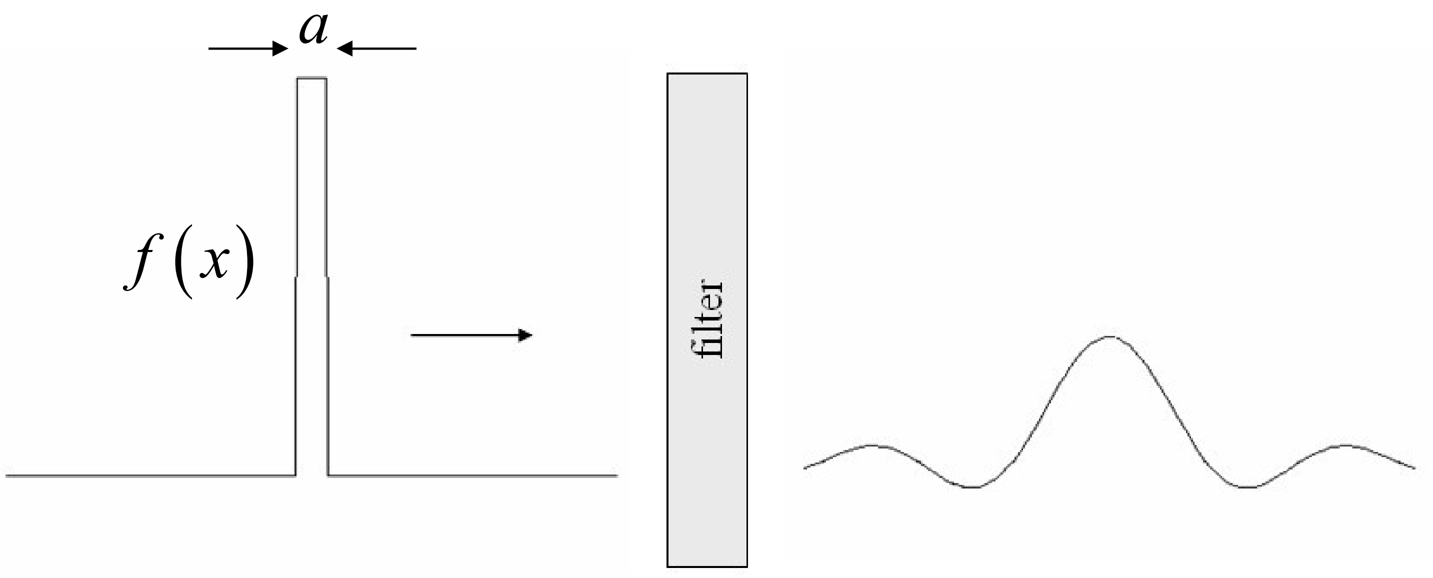
This can be inverted for $F(k)$

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

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: $f'(x)=\int_{-k_0}^{k_0}\frac{\sin(ka/2)}{\pi k}e^{ikx}dk=\frac{\mathrm{Si}(k_0x+\frac{1}{2})+\mathrm{Si}(k_0x-\frac{1}{2})}{\pi}$

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

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

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

Matlab

Notations for Fourier Transforms

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

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

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.

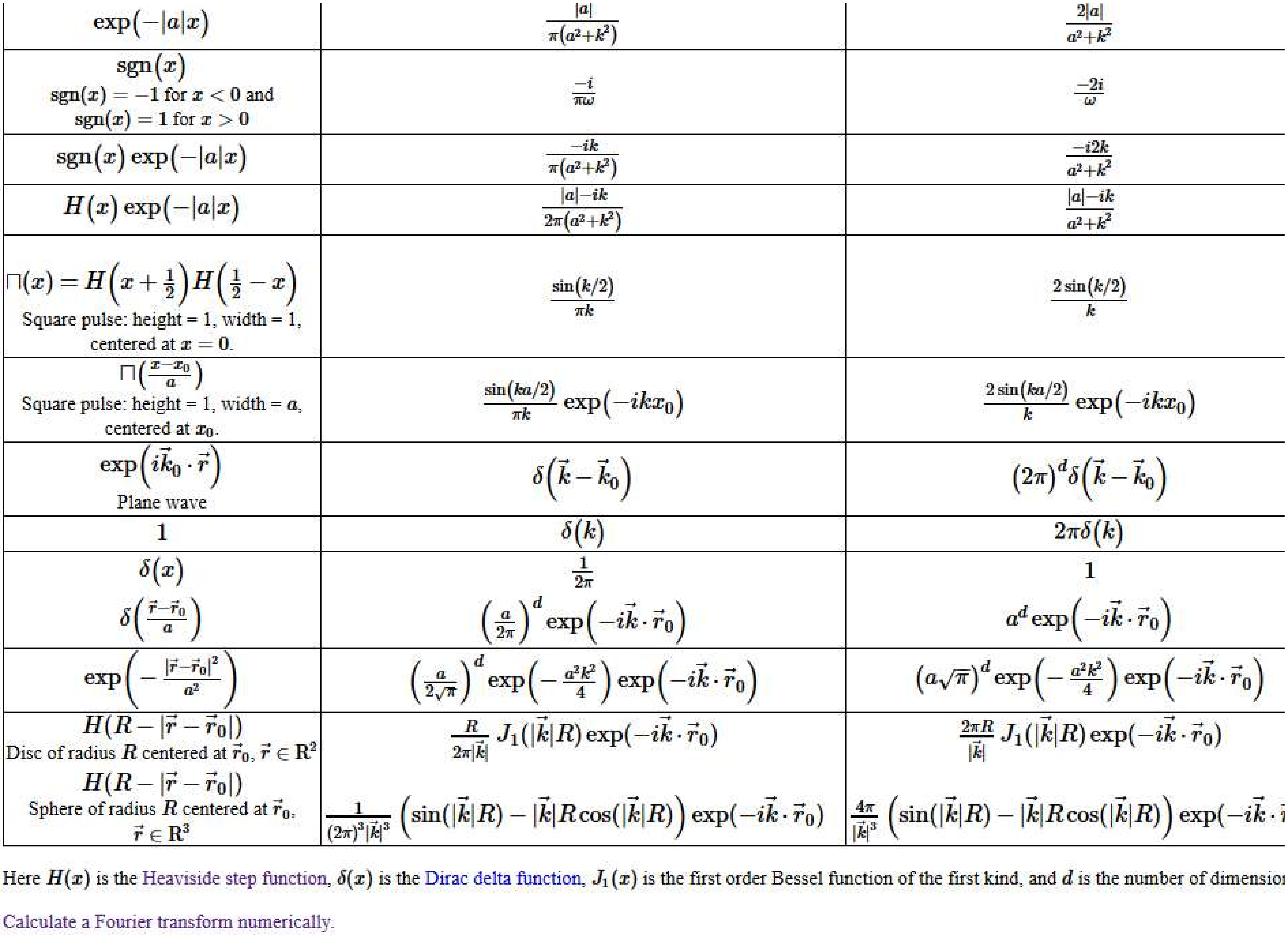
https://online.stanford.edu/courses/ee261-fourier-transform-and-its-applications

Notations for Fourier Transforms

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

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

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



$\exp(-\|a\|x)$	$\frac{\|a\|}{\pi(a^2+k^2)}$	$\frac{2\|a\|}{a^2+k^2}$
$\mathrm{sgn}(x)$ $\mathrm{sgn}(x)=-1$ for $x<0$ and $\mathrm{sgn}(x)=1$ for $x>0$	$\frac{-i}{\pi\omega}$	$\frac{-2i}{\omega}$
$\mathrm{sgn}(x)\exp(-\|a\|x)$	$\frac{-ik}{\pi(a^2+k^2)}$	$\frac{-i2k}{a^2+k^2}$
$H(x)\exp(-\|a\|x)$	$\frac{\|a\|-ik}{2\pi(a^2+k^2)}$	$\frac{\|a\|-ik}{a^2+k^2}$
$\sqcap(x)=H\left(x+\frac{1}{2}\right)H\left(\frac{1}{2}-x\right)$ 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 $a^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$\exp\left(-\frac{\|\vec{r}-\vec{r}_0\|^2}{a^2}\right)$	$\left(\frac{a}{2\sqrt{\pi}}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$(a\sqrt{\pi})^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$H(R-\|\vec{r}-\vec{r}_0\|)$ Disc of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^2$ $H(R-\|\vec{r}-\vec{r}_0\|)$ Sphere of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^3$	$\frac{R}{2\pi\|\vec{k}\|}J_1(\|\vec{k}\|R)\exp(-i\vec{k}\cdot\vec{r}_0)$ $\frac{1}{(2\pi)^3\|\vec{k}\|^3}\left(\sin(\|\vec{k}\|R)-\|\vec{k}\|R\cos(\|\vec{k}\|R)\right)\exp(-i\vec{k}\cdot\vec{r}_0)$	$\frac{2\pi R}{\|\vec{k}\|}J_1(\|\vec{k}\|R)\exp(-i\vec{k}\cdot\vec{r}_0)$ $\frac{4\pi}{\|\vec{k}\|^3}\left(\sin(\|\vec{k}\|R)-\|\vec{k}\|R\cos(\|\vec{k}\|R)\right)\exp(-i\vec{k}\cdot$

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

Fourier transforms

The Fourier transform of a function $f(t)$ using the [1,-1] notation is,

$$\mathcal{F}(\omega) = \int\limits_{-\infty}^{\infty} f(t) e^{-i\omega t} dt.$$

Using Euler's formula, you can think of this as the projecting $f(t)$ onto its cosine components and its sine components.

$$\mathcal{F}(\omega) = \int\limits_{-\infty}^{\infty} f(t)\cos(\omega t) dt + i \int\limits_{-\infty}^{\infty} f(t)\sin(\omega t) dt.$$

Consider a function that is nonzero only in the interval $t_1 < t < t_2$. The Fourier transform in this case is,

$$\mathcal{F}(\omega) = \int\limits_{t_1}^{t_2} f(t) e^{-i\omega t} dt.$$

The following form can be used to define $f(t)$ between t_1 and t_2. The function $f(t)$ as well as its Fourier transform $\mathcal{F}(\omega)$ are tabulated and plotted.

$f(t) =$ H(t+0.5)*H(0.5-t) ?+ ?-

Calculate Fourier Transform where $t_1 =$ -4 and $t_2 =$ 4 for frequencies $|\omega| <$ 24.

sine | cosine | Gaussian | Gaussian derivative | sech | square | shifted square | triangle | beats | even pulse | odd pulse | exp(-|t|/τ) | sgn(t)exp(-|t|/τ) | H(t)exp(-t/τ) | H(t)exp(-t/τ)sin(ωt)

t $f(t)$

```
-1       -3.6739403974420594e-16
-0.998   -0.01884943189667738
-0.996   -0.03769811965005851
-0.994   -0.056545319146225376
-0.992   -0.07539028633001343
-0.99    -0.09423227723438471
-0.988   -0.1130705480098036
-0.986   -0.13190435495359484
-0.984   -0.150732954539309
-0.982   -0.16955560344607404
-0.98    -0.18837155858794075
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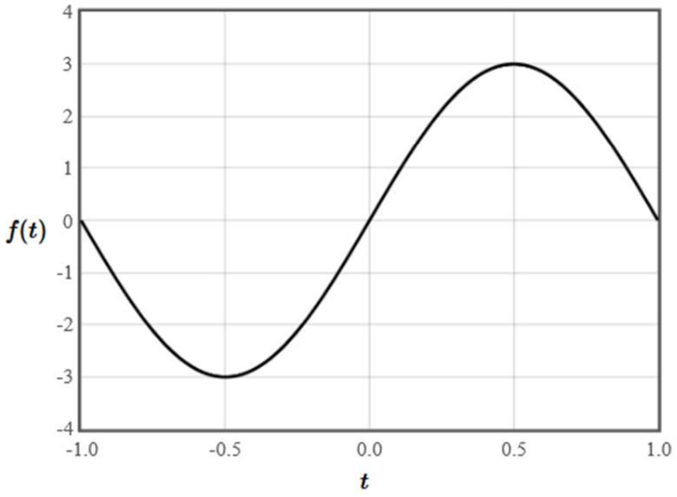


Properties of Fourier transforms

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

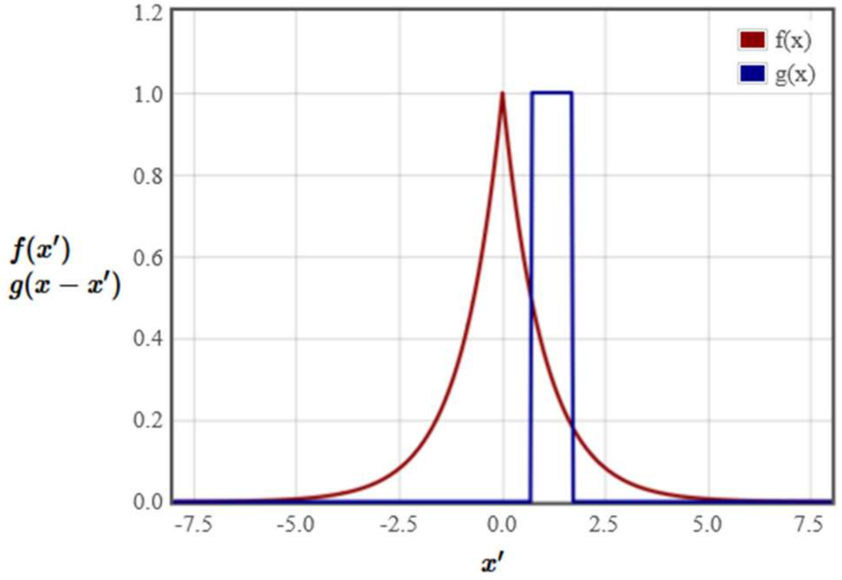
$\mathcal{F}\{f\left(\frac{\vec{r}}{a}\right)\} = |a|^d F\left(a\vec{k}\right).$

Shift

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

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

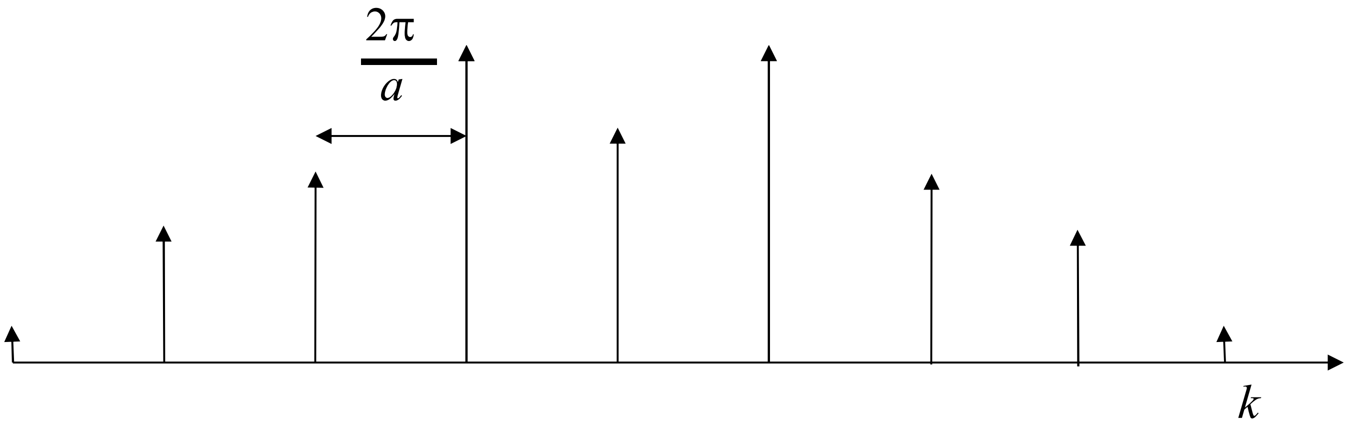
Notation [0,-1]: $\mathcal{F}\{fg\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

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

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))



$\mathcal{F}$(Bravais_lattice(r)) = reciprocal lattice

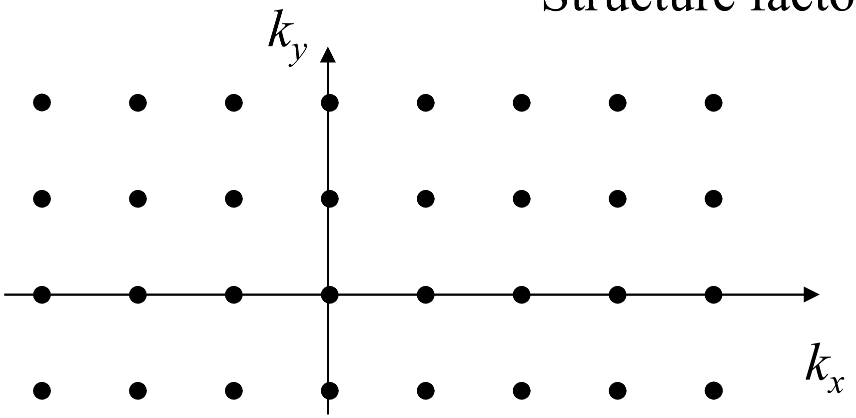
Reciprocal lattice (Reziprokes Gitter)

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



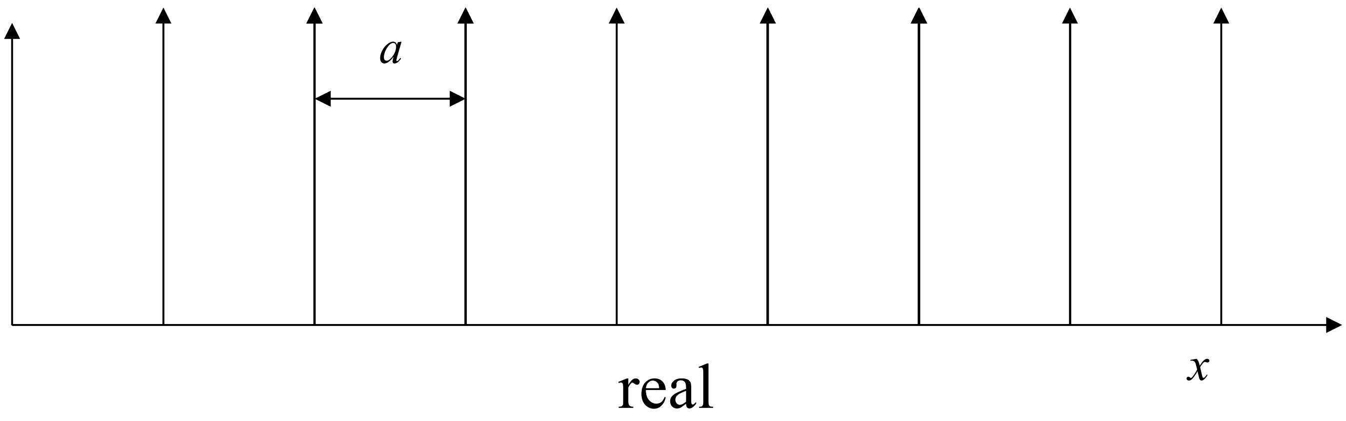
$$\vec{G} = \upsilon_1\vec{b}_1 + \upsilon_2\vec{b}_2 + \upsilon_3\vec{b}_3$$

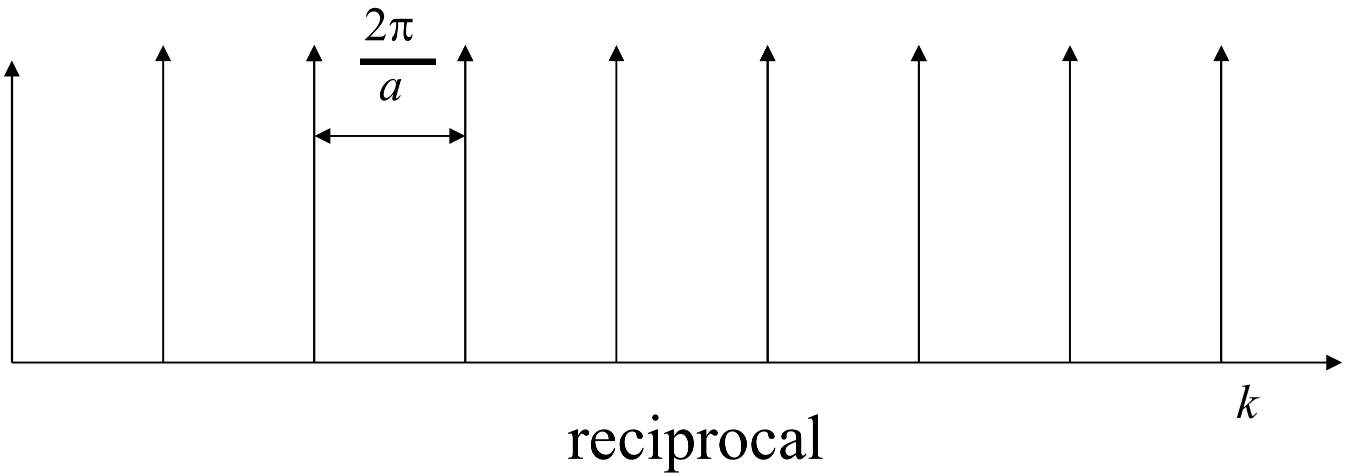
v_i integers

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

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

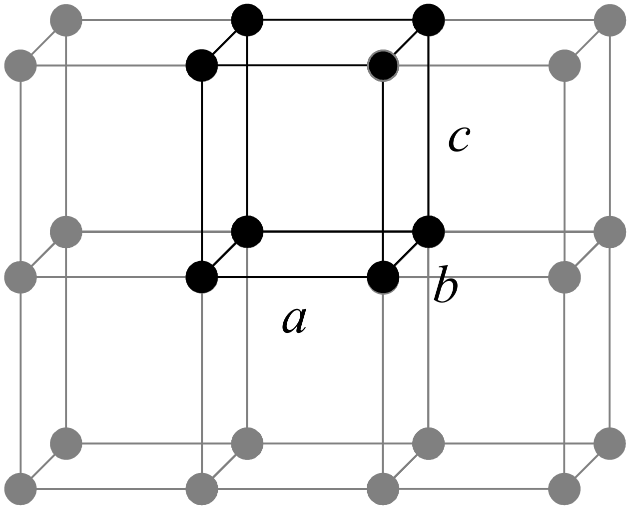
Bravais lattice and reciprocal lattice in 1-D

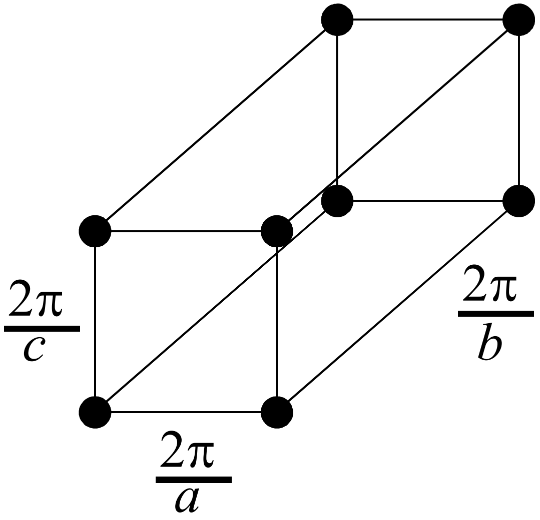




$$\cos\left(\frac{2\pi px}{a}\right) \Rightarrow \cos(Gx) \qquad G = p\frac{2\pi}{a}$$

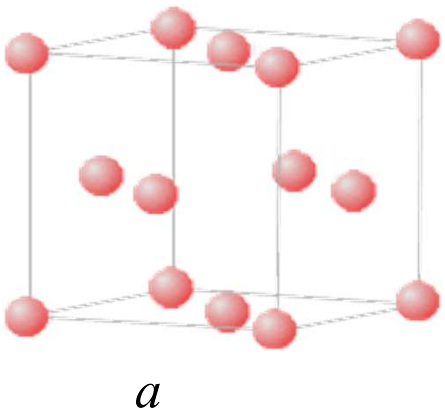
Reciprocal lattice of an orthorhombic lattice is an orthorhombic lattice

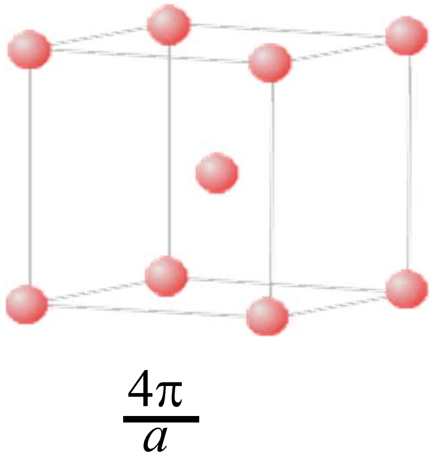




reciprocal lattice

The reciprocal lattice of an fcc lattice is a bcc lattice





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

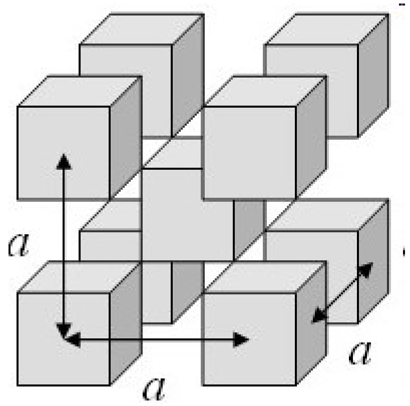
$$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{z}$$

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

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

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

Cubes on a bcc lattice



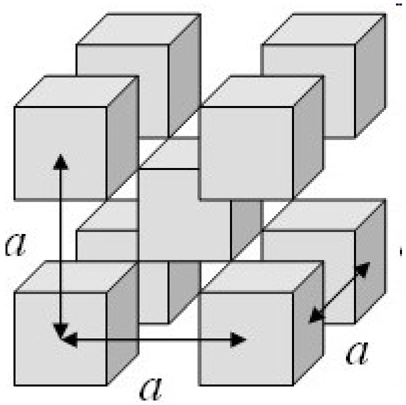
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

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.

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

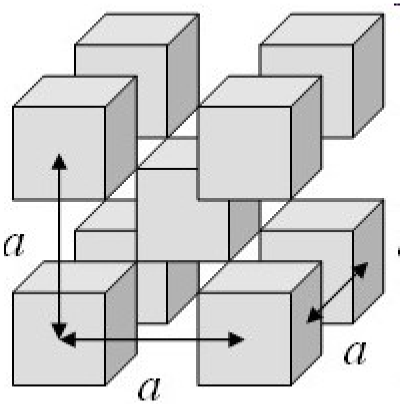
f_G is the Fourier transform of f_{cell} evaluated at G.
f_{cell} is zero outside the primitive unit cell.

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

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

Cubes on a bcc lattice

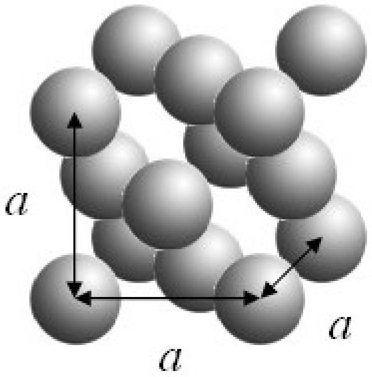
$$\int_{-\frac{a}{4}}^{\frac{a}{4}} \exp\left(-iG_x x\right) dx = \left.\frac{\exp\left(-iG_x x\right)}{-iG_x}\right|_{\frac{-a}{4}}^{\frac{a}{4}} = \left.\frac{\cos\left(-G_x x\right)+i\sin\left(-G_x x\right)}{-iG_x}\right|_{\frac{-a}{4}}^{\frac{a}{4}} = \frac{2\sin\left(\frac{G_x a}{4}\right)}{G_x}$$



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

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.

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

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

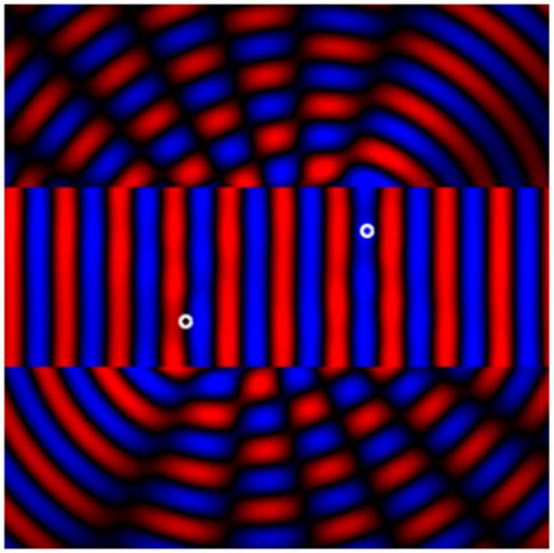
Muffin tin potential

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.

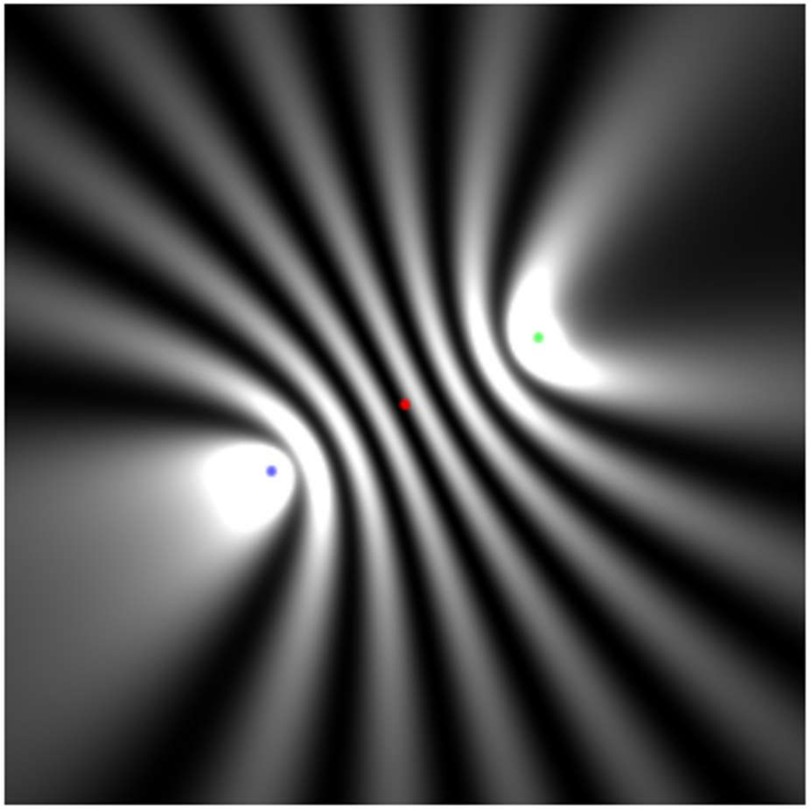
$$U(\vec{r}) = \frac{Ze^2}{V\epsilon_0}\sum_{\vec{G}}\left(\frac{\cos(|G|R)-1}{|G|^2} + \frac{\sin(|G|R)-|G|R\cos(|G|R)}{R|G|^3}\right)\exp\left(i\vec{G}\cdot\vec{r}\right).$$

Intensity of the scattered waves



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

Intensity of the scattered waves



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