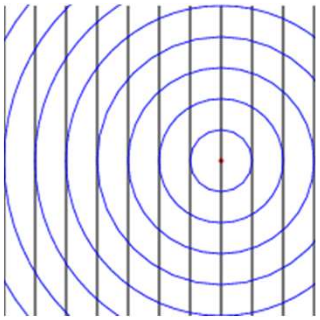
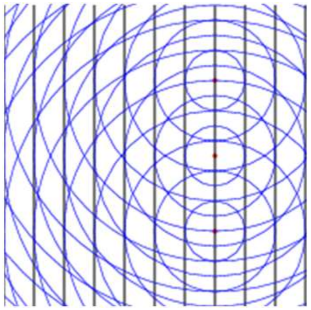
Diffraction

Crystal diffraction (Beugung)

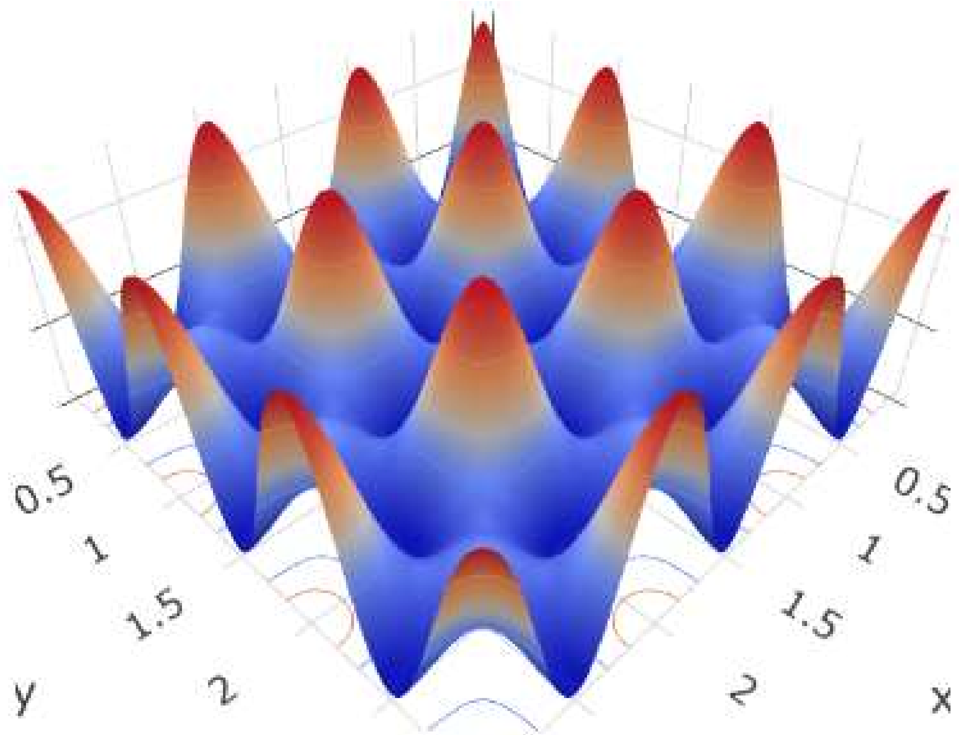
Everything moves like a wave but exchanges energy and momentum as a particle

light	photons
sound	phonons
electron waves	electrons
neutron waves	neutrons
positron waves	positrons
plasma waves	plasmons



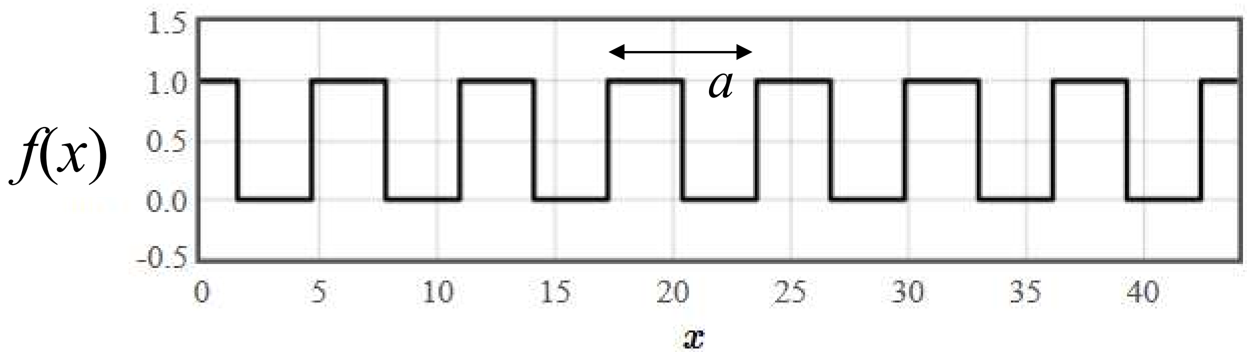


Periodic functions



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.

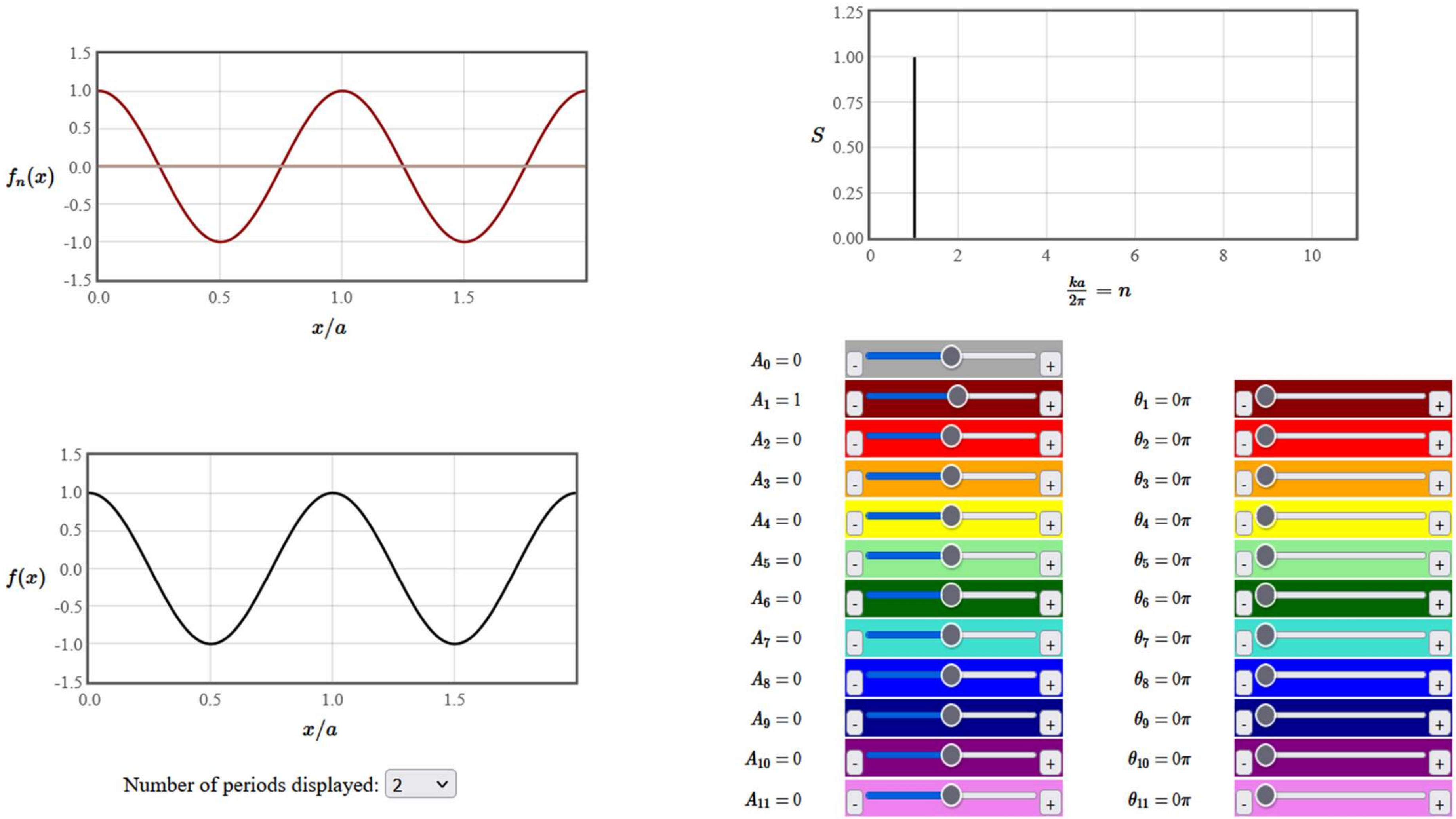
$$\int_0^a f(x)\cos\left(2\pi p'x/a\right)dx = c_p \int_0^a \cos\left(2\pi p'x/a\right)\cos\left(2\pi p'x/a\right)dx = \frac{ac_{p'}}{2}$$

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

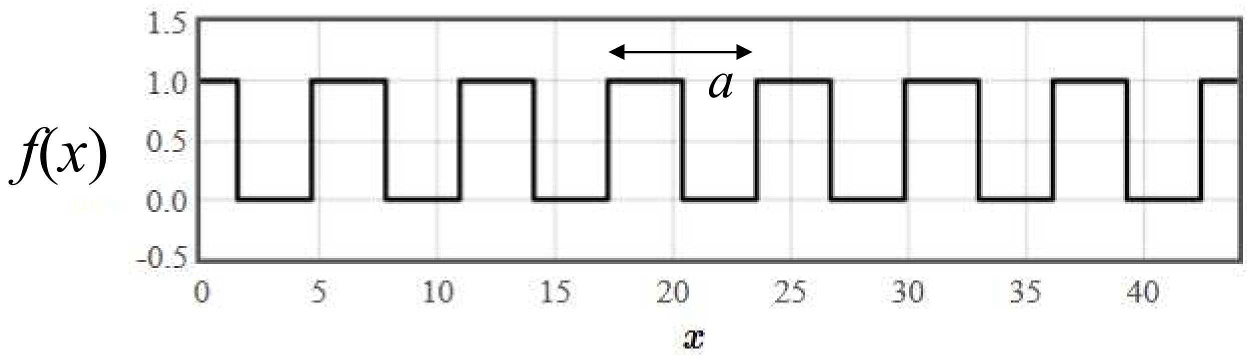
Fourier synthesis

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

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



Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

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

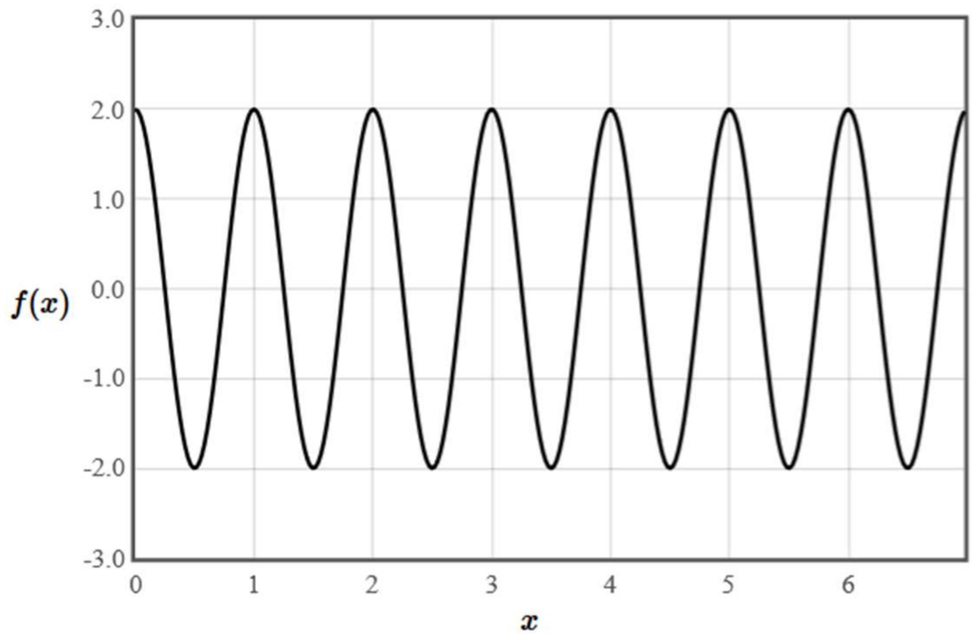
$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

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

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

reciprocal lattice vector

Fourier series in 1-D



square triangle sawtooth comb

$f_0 = 0$ - +

$f_1 = f^*_{-1} = 1$ - + $+i\ (0)$ - +

$f_2 = f^*_{-2} = 0$ - + $+i\ (0)$ - +

$f_3 = f^*_{-3} = 0$ - + $+i\ (0)$ - +

$f_4 = f^*_{-4} = 0$ - + $+i\ (0)$ - +

$f_5 = f^*_{-5} = 0$ - + $+i\ (0)$ - +

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

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

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

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)

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

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

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

Reciprocal lattice (Reziprokes Gitter)

Any periodic function can be written as a Fourier series

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

Reciprocal lattice vector *G*

Structure factor

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

v_i integers

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

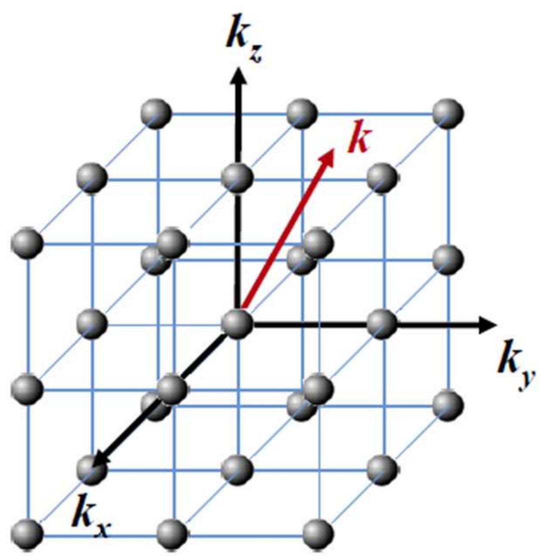
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}, \qquad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

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



Reciprocal lattice (Reziprokes Gitter)

$$\text{sc:} \qquad \vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\hat{y}, \quad \vec{a}_3 = a\hat{z},$$

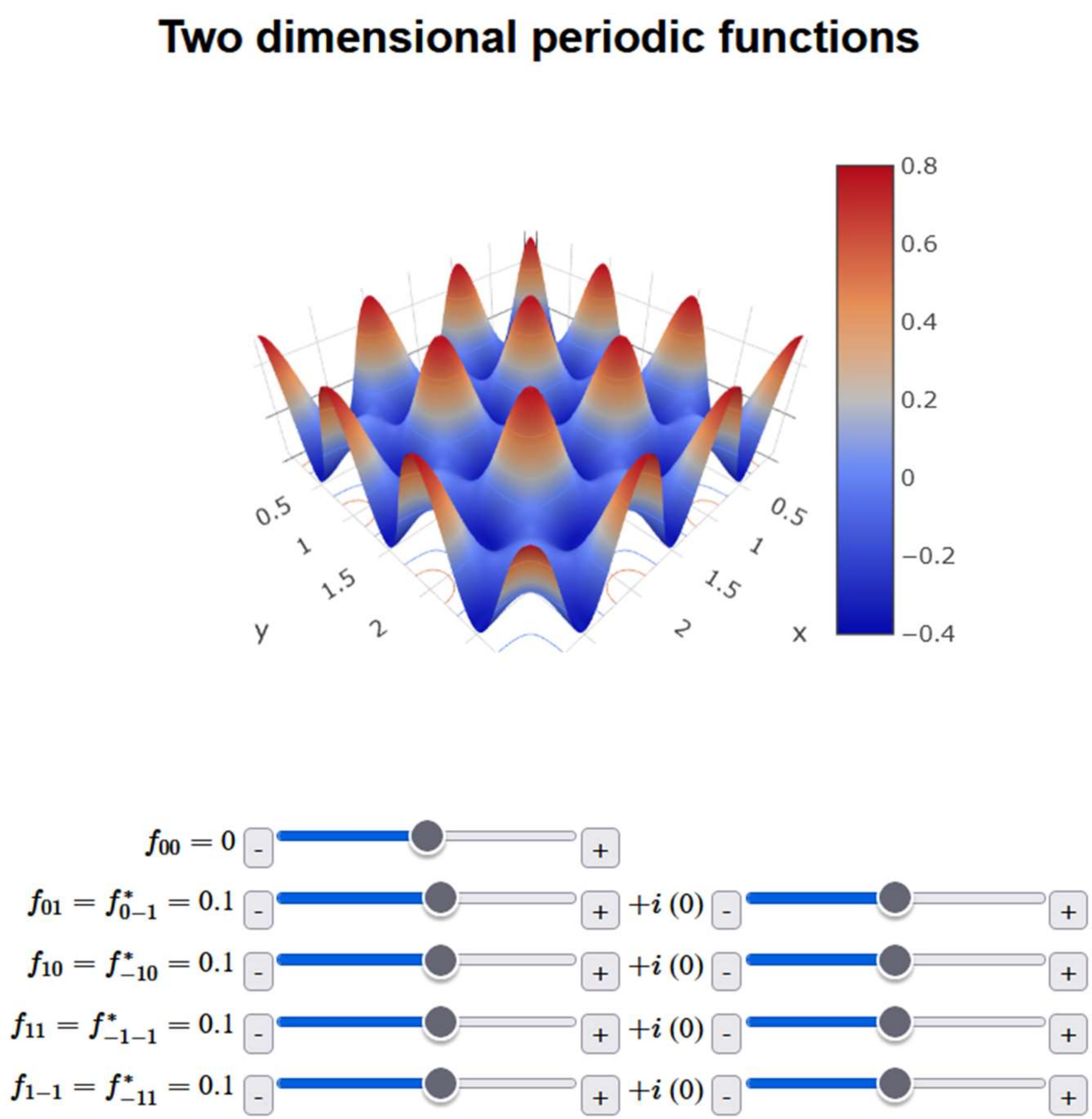
$$\vec{b}_1 = \frac{2\pi}{a}\hat{k}_x, \quad \vec{b}_2 = \frac{2\pi}{a}\hat{k}_y, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{k}_z.$$

$$\text{fcc:} \qquad \vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{z}), \quad \vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{y}), \quad \vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z}),$$

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

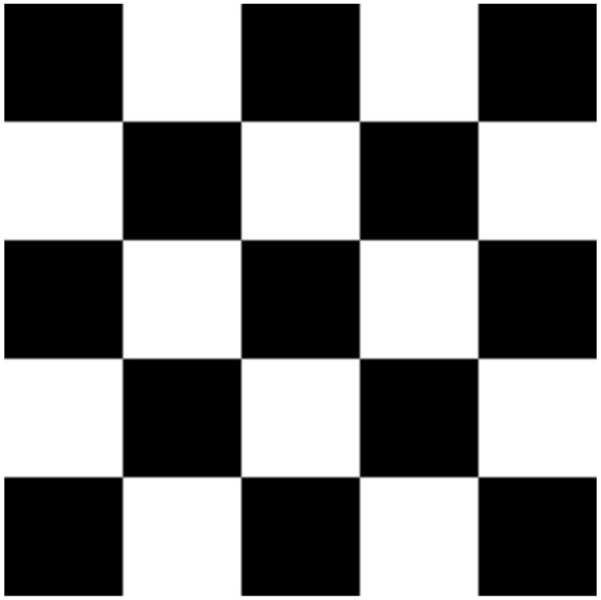
$$\text{bcc:} \qquad \vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}), \quad \vec{a}_2 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}), \quad \vec{a}_3 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z}),$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_y), \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{k}_y + \hat{k}_z), \quad \vec{b}_3 = \frac{2\pi}{a}(\hat{k}_x + \hat{k}_z).$$



2D comb function

Determine the Fourier coefficients



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

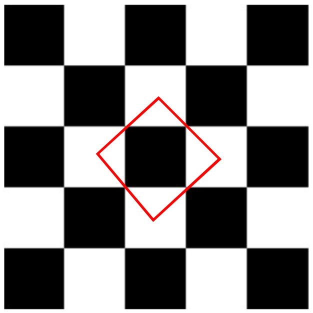
Determine the Fourier coefficients

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

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

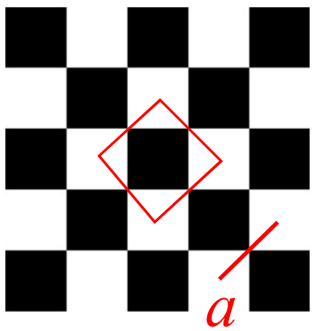
$$\int\limits_{\text{unit cell}} f(\vec{r})\exp(-i\vec{G}'\cdot\vec{r})d\vec{r} = \sum_{\vec{G}}\int\limits_{\text{unit cell}} f_{\vec{G}}\exp(-i\vec{G}'\cdot\vec{r})\exp(i\vec{G}\cdot\vec{r})d\vec{r}$$

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



Determine the Fourier coefficients

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



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

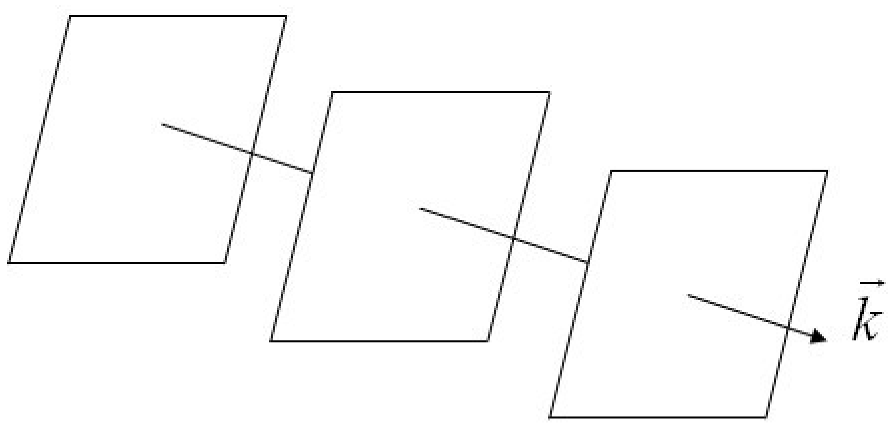
$$f_{\vec{G}} = \frac{C}{a^2} \frac{\left(\exp(-iG_x\sqrt{2}a/4) - \exp(iG_x\sqrt{2}a/4)\right)\left(\exp(-iG_y\sqrt{2}a/4) - \exp(iG_y\sqrt{2}a/4)\right)}{-G_xG_y}$$

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

Plane waves (Ebene Wellen)

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

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

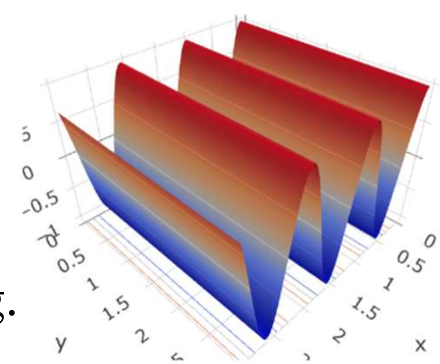


$$\exp\left(i\vec{k}\cdot(\vec{r}+\vec{r}_{\perp})\right) = \exp\left(i\vec{k}\cdot\vec{r}\right)$$

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

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

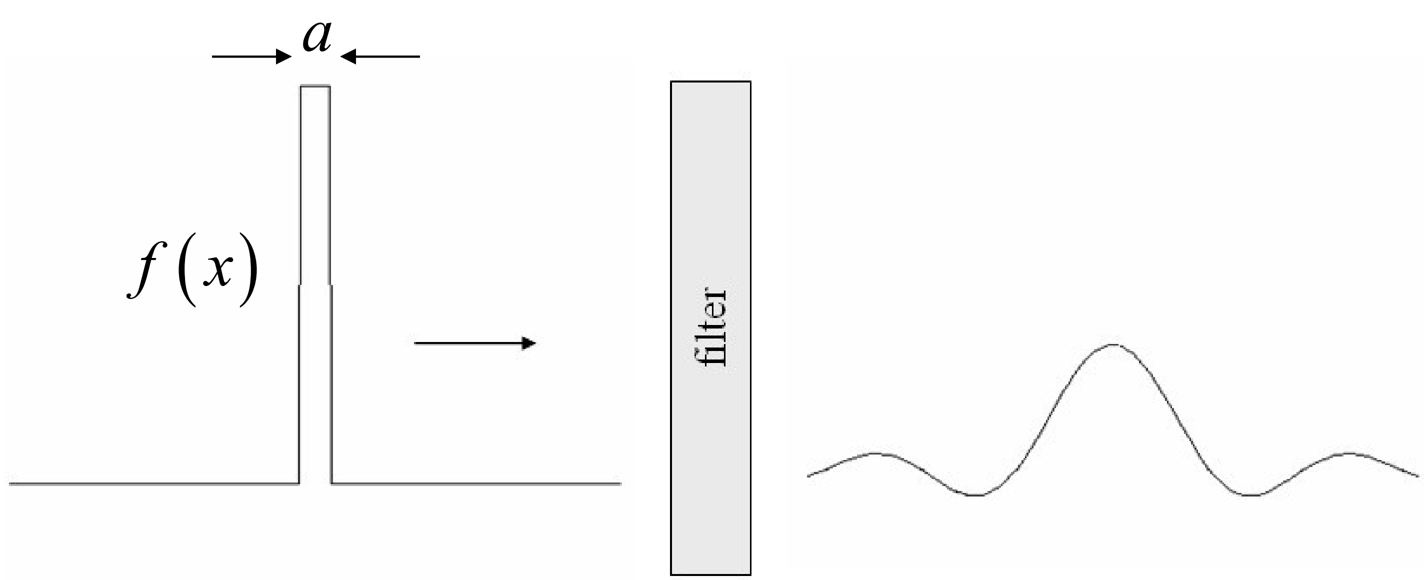
This can be inverted for $F(k)$

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

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

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

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

$f(r)$ 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

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

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

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.

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

Notations for Fourier Transforms

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

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

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

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

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