# Periodic functions in 3-D

# 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)

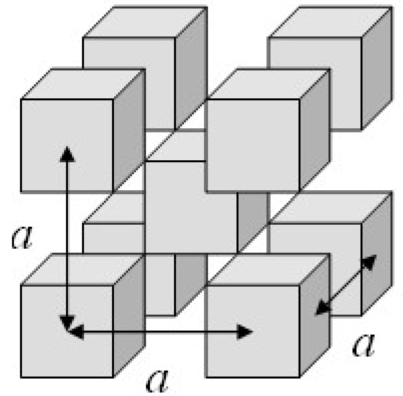
Structure factors
(complex numbers)

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

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

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

# Cubes on a bcc lattice



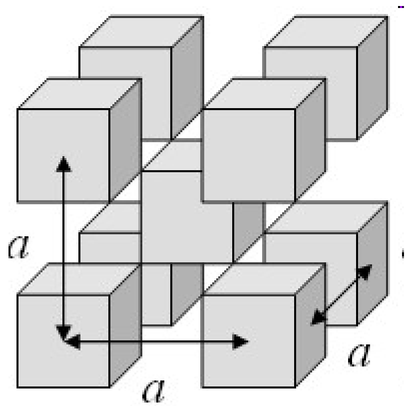

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

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.

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

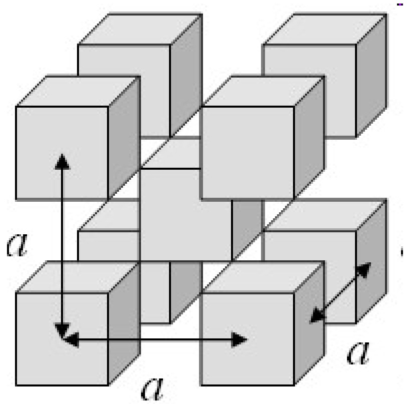
$f_G$ is the Fourier transform of $f_{cell}$ evaluated at $G$.
$f_{cell}$ is zero outside the primitive unit cell.

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

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

# Cubes on a bcc lattice

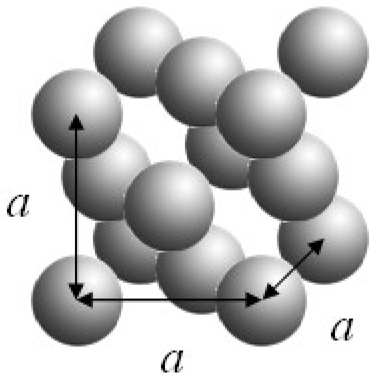
$$\int_{-\frac{a}{4}}^{\frac{a}{4}} \exp\left(-iG_x x\right) dx = \left.\frac{\exp\left(-iG_x x\right)}{-iG_x}\right|_{\frac{-a}{4}}^{\frac{a}{4}} = \left.\frac{\cos\left(-G_x x\right) + i\sin\left(-G_x x\right)}{-iG_x}\right|_{\frac{-a}{4}}^{\frac{a}{4}} = \frac{2\sin\left(\frac{G_x a}{4}\right)}{G_x}$$




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

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.

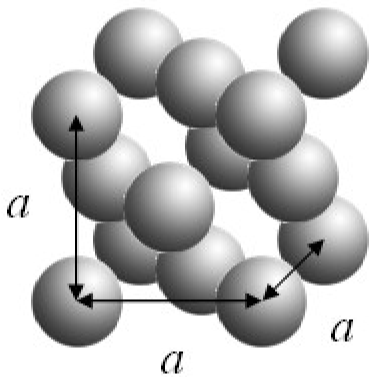
$$f_{\vec{G}} = \frac{1}{V}\int f_{cell}(\vec{r})\exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r = \frac{C}{V}\int_{\text{sphere}} \exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r.$$

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

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

Integrate over φ

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




# Spheres on an fcc lattice

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

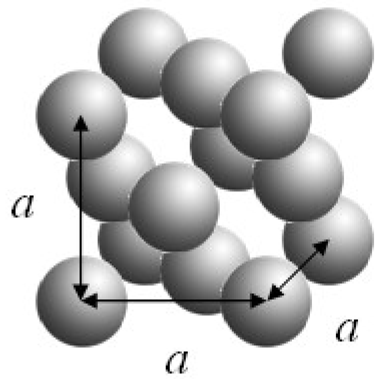
Both terms are perfect differentials

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

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

Integrate over θ: $$f_{\vec{G}} = \frac{2\pi C}{V}\int_0^R \left(-\sin\left(|G| r\cos\theta\right) - \cancelto{0}{i\cos\left(|G| r\cos\theta\right)}\right)\Big|_0^\pi dr$$

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




# Spheres on any lattice

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

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:

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

http://lampx.tugraz.at/~hadley/ss1/crystaldiffraction/fourier/fourier_examples.php



## Fourier series in 3-D

There are fourteen Bravais lattices in three dimensions. A three dimensional periodic function is can be described with a Fourier series of the form,

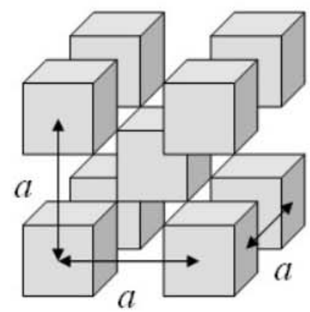
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp\left(i\vec{G}\cdot\vec{r}\right),$$

where the Fourier coefficients are given by,

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

**Example 1: cubes repeated on a bcc lattice**

Cubes are arranged on a bcc lattice such that the corners of the cubes just touch. This is a three dimensional analog to the square wave problem that was solved in one dimension.




A three-dimensional periodic function $f$ is defined such that it has a constant value $C$ inside the cubes and is zero outside the cubes. This function can be expressed as a Fourier series,

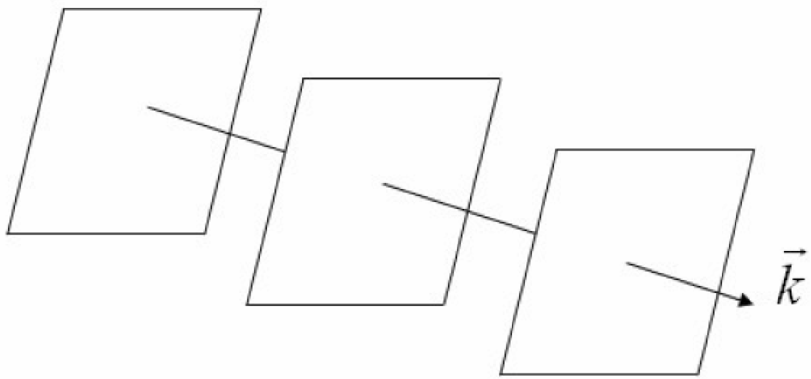
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp\left(i\vec{G}\cdot\vec{r}\right).$$

The Fourier coefficients $f_G$ are given by,

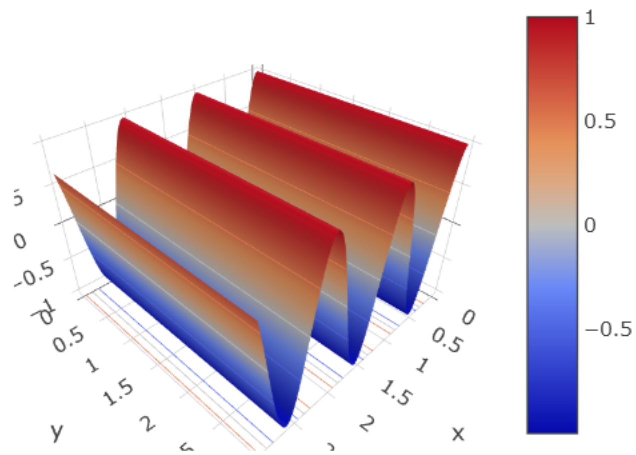
# Plane waves (Ebene Wellen)

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

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

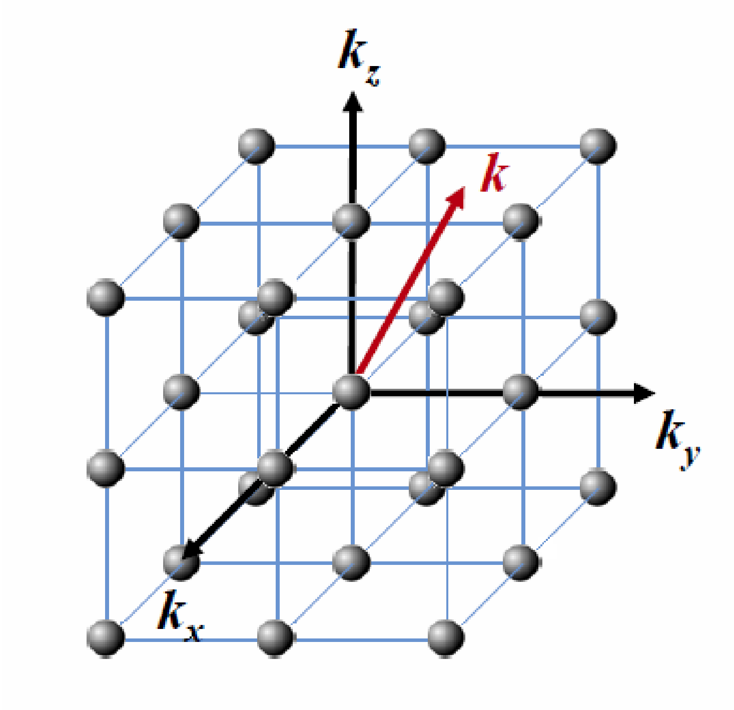



$$\exp\left(i\vec{k}\cdot\left(\vec{r}+\vec{r}_{\perp}\right)\right) = \exp\left(i\vec{k}\cdot\vec{r}\right)$$




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

# Reciprocal lattice (Reziprokes Gitter)




Most functions can be expressed in terms of plane waves

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

# Fourier Transforms

# 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

# Notations for Fourier Transforms

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

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

$d$ = 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

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

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

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.

# 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 $\alpha$ and $\beta$ are any constants.

**Similarity**

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

**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)

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

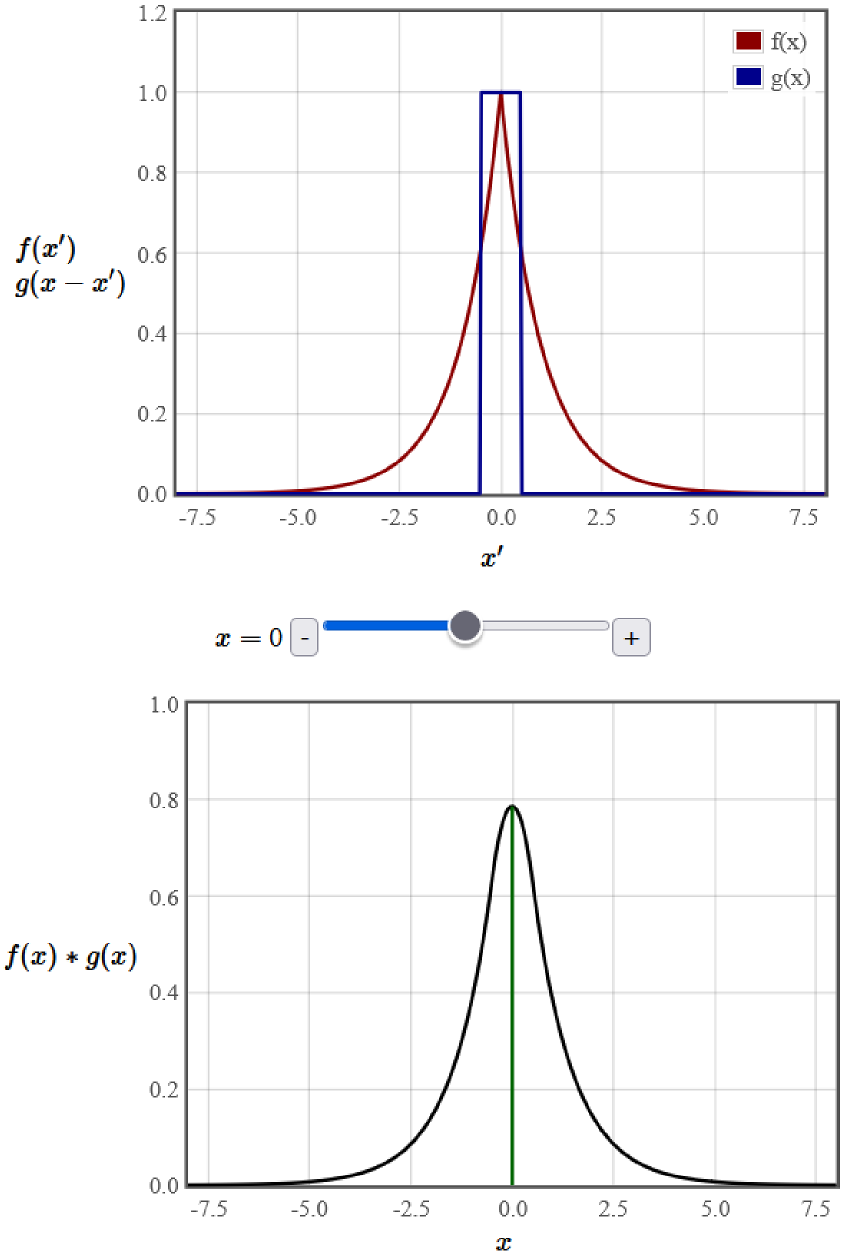
Notation [-1,-1]: $\mathcal{F}\{fg\} = \mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{2\pi}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}$.

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

# Convolution



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

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