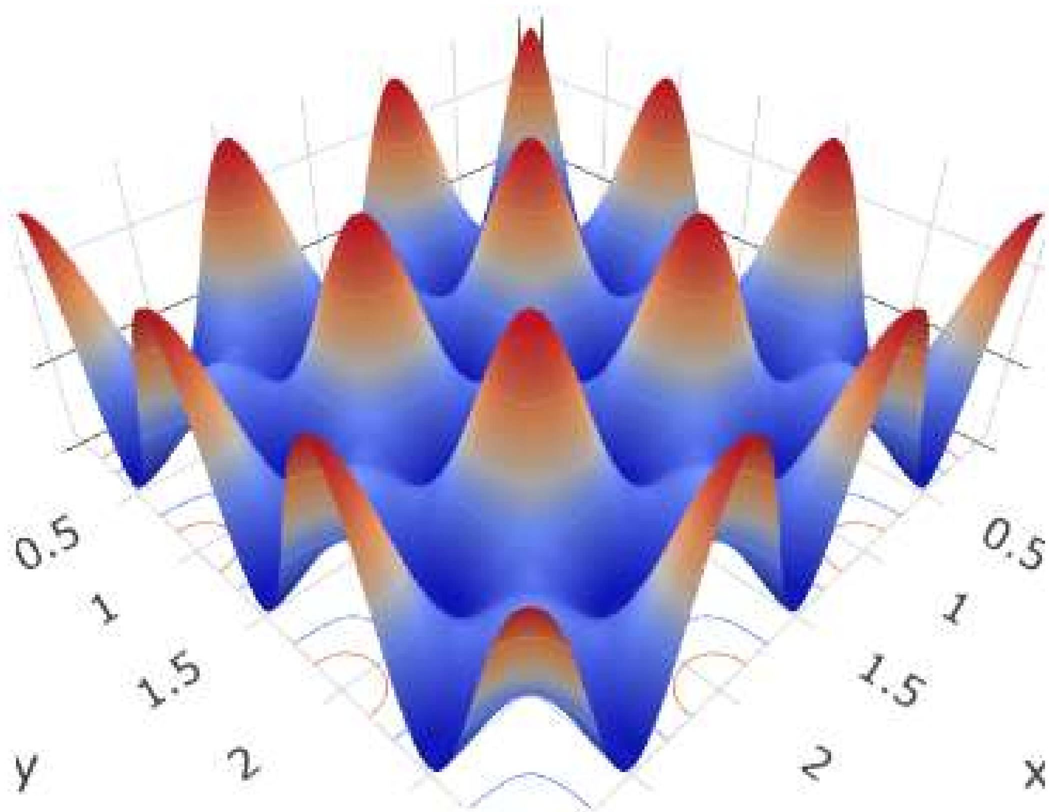
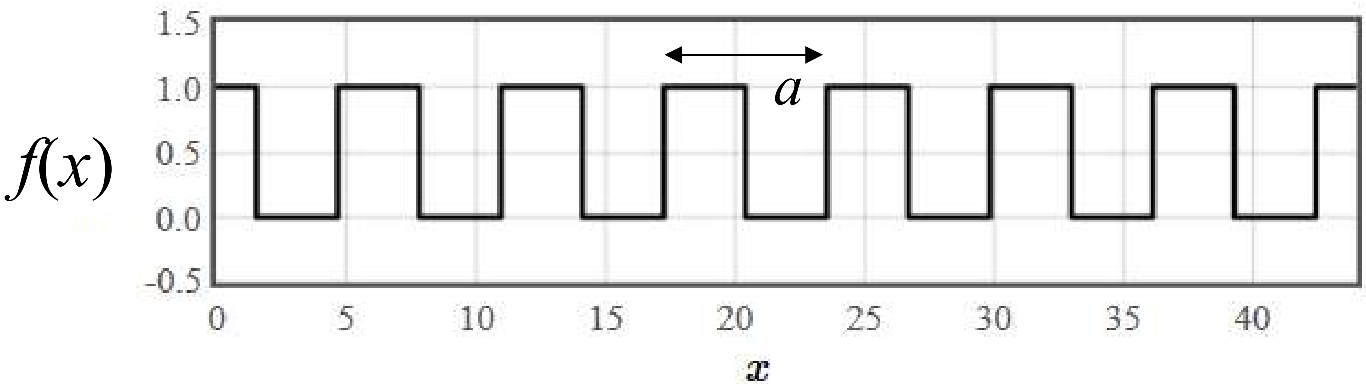
Periodic functions



Use a Fourier series to describe periodic functions

Expanding a 1-d function in a Fourier series



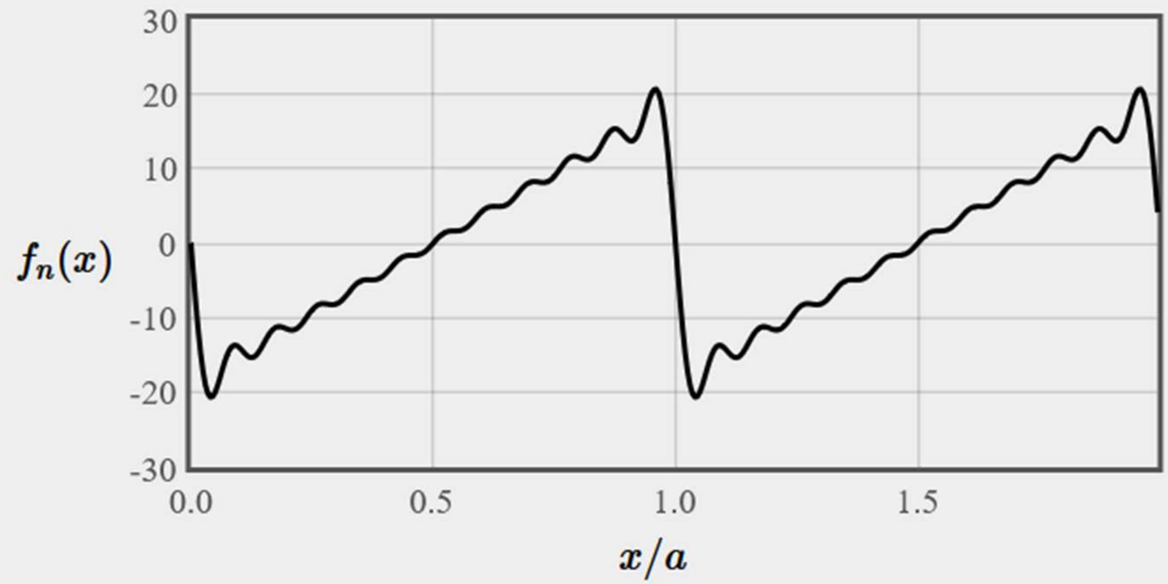
Any periodic function can be represented as a Fourier series.

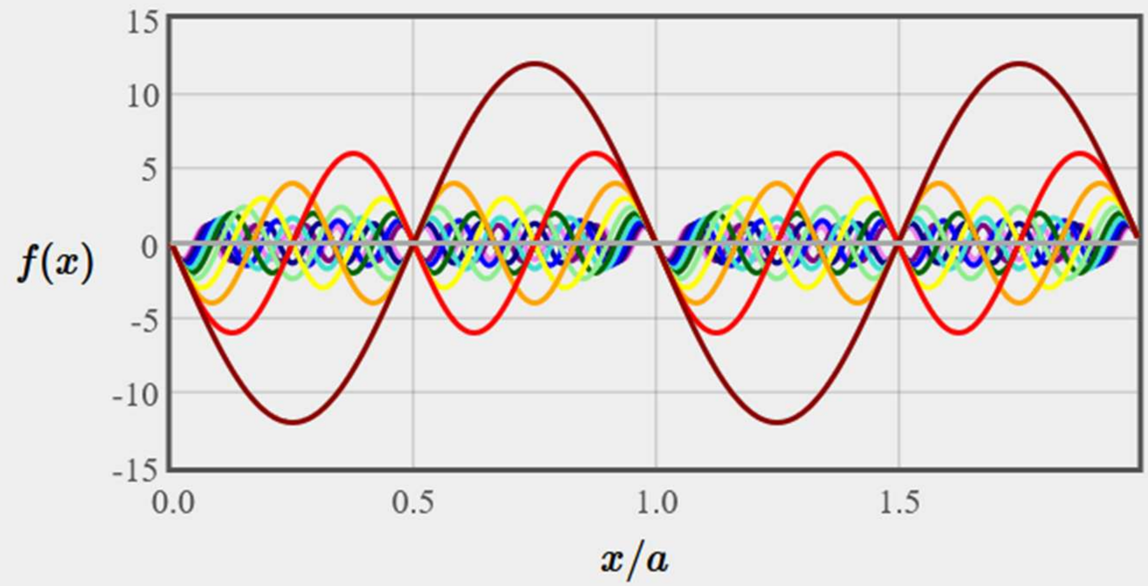
$$f(x) = f_0 + \sum_{n=1}^{\infty} c_n \cos(2\pi nx/a) + s_n \sin(2\pi nx/a)$$

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

$$\int_0^a f(x)\cos(2\pi n'x/a)\,dx = c_n \int_0^a \cos(2\pi n'x/a)\cos(2\pi n'x/a)\,dx = \frac{ac_n}{2}$$

$$c_n = \frac{2}{a}\int_0^a f(x)\cos(2\pi nx/a)\,dx$$



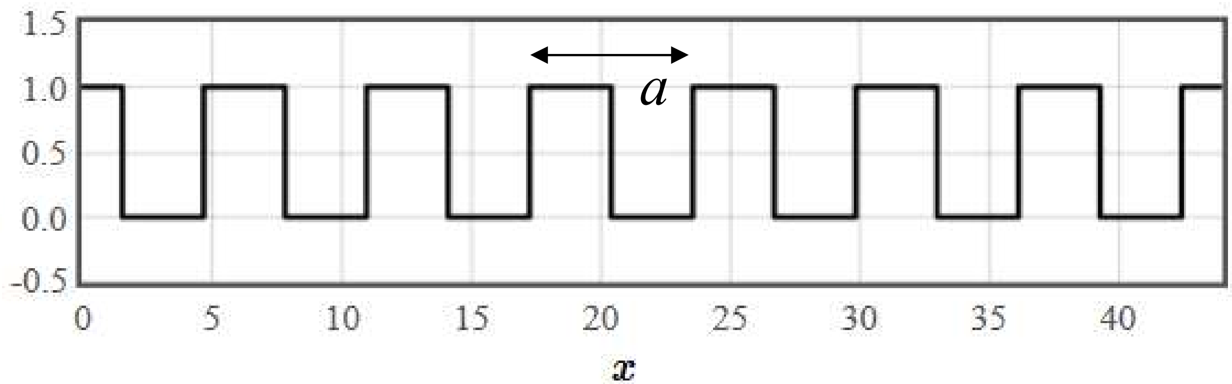


Number of periods displayed: 2

sine | cosine | odd square | even square | triangle

sawtooth | comb | pulse | beats | burst

Expanding a 1-d function in a Fourier series



$f(x)$

Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{n=1}^{\infty} c_n \cos(2\pi n x/a) + s_n \sin(2\pi n x/a)$$

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

$$f(x) = \sum_{n=-\infty}^{\infty} f_G e^{iG_n x} \qquad f_{G_n} = \frac{c_n}{2} - i\frac{s_n}{2} \qquad G_n = \frac{2\pi n}{a}$$

reciprocal lattice vector

Exponential functions

The derivative of an exponential function is an exponential function

$$\frac{d}{dx}e^x = e^x$$

$$e^{a+b} = e^a e^b$$

Euler's formula: $$e^{ix} = \cos x + i \sin x$$

$$e^{a+ib} = e^a \left(\cos b + i \sin b\right)$$

Exponential functions

The equation for a damped mass spring system is

$$m\frac{d^2x}{dt^2} = -b\frac{dx}{dt} - kx$$

For m=0.5, b=1, k=1,

$$0.5\frac{d^2x}{dt^2} + \frac{dx}{dt} + x = 0$$

Substitute $x = e^{\lambda t}$

$$0.5\lambda^2 \cancel{e^{\lambda t}} + \lambda \cancel{e^{\lambda t}} + \cancel{e^{\lambda t}} = 0.$$

$$0.5\lambda^2 + \lambda + 1 = 0$$

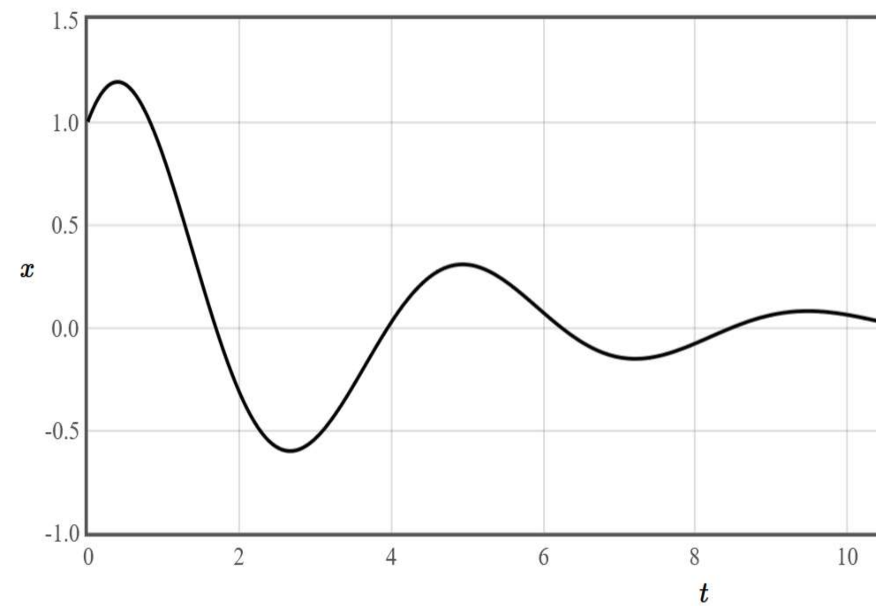
$$\lambda_\pm = -1 \pm i$$

Exponential functions

$$\lambda_{\pm} = -1 \pm i$$

The two solutions are

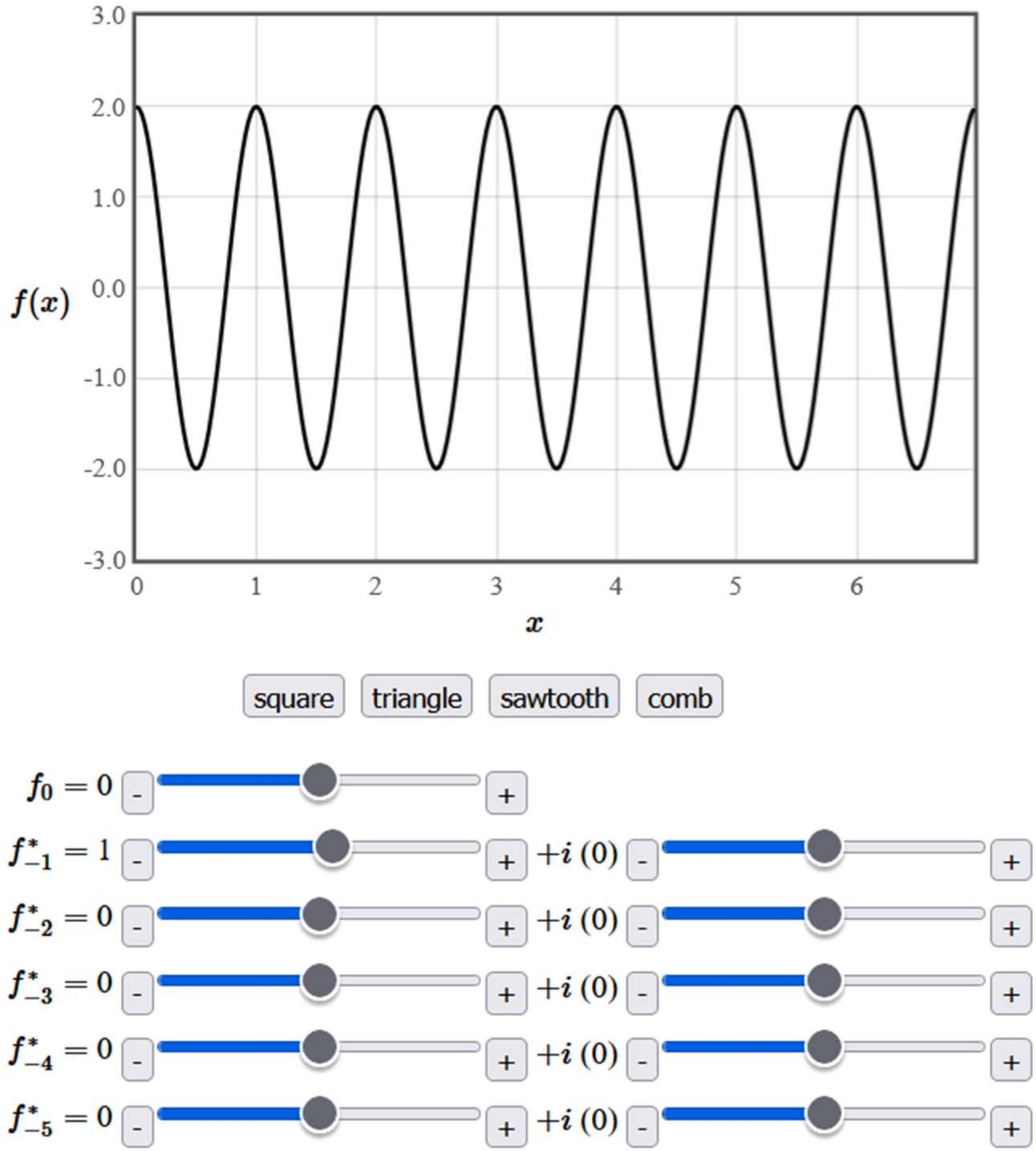
$$x_+(t) = e^{\lambda_+ t} = e^{-t}\left(\cos(t) + i\sin(t)\right)$$
$$x_-(t) = e^{\lambda_- t} = e^{-t}\left(\cos(t) - i\sin(t)\right)$$



The total solution, $x(t) = C_+ x_+ + C_- x_-$ will be real if

$$C_- = C_+^*$$

Fourier series in 1-D



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

Determine the Fourier coefficients in 1-D

$$f(x) = \sum_{n=-\infty}^{\infty} f_n e^{iG_n x}, \qquad G_n = \frac{2\pi n}{a}$$

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

$$\int_0^a f(x) e^{-iG'_n x} dx = \sum_{n=-\infty}^{\infty} \int_0^a f_n e^{iG_n x} e^{-iG'_n x} dx$$

Only the term where $G_n = G'_n$ is nonzero

$$f_n = \frac{1}{a} \int_0^a f(x) e^{-iG'_n x} dx$$

Fourier series in 3-D

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

$f(r)$ must be the same at $\vec{r} = 0, \vec{r} = \vec{a}_1, \vec{r} = \vec{a}_2$, and $\vec{r} = \vec{a}_3$

$$\exp\left(i\vec{G}\cdot\vec{a}_1\right) = 1,$$
$$\exp\left(i\vec{G}\cdot\vec{a}_2\right) = 1,$$
$$\exp\left(i\vec{G}\cdot\vec{a}_3\right) = 1.$$

$$\vec{G}\cdot\vec{a}_1 = 2\pi h,$$
$$\vec{G}\cdot\vec{a}_2 = 2\pi k,$$
$$\vec{G}\cdot\vec{a}_3 = 2\pi l,$$

h, k, and l are integers.

Fourier series in 3-D

$$\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

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

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0, & \text{for } i \neq j \end{cases}$$

Periodicity conditions

$$\vec{G}_{hkl} \cdot \vec{a}_1 = h\vec{b}_1 \cdot \vec{a}_1 = 2\pi h,$$
$$\vec{G}_{hkl} \cdot \vec{a}_2 = k\vec{b}_2 \cdot \vec{a}_2 = 2\pi k,$$
$$\vec{G}_{hkl} \cdot \vec{a}_3 = l\vec{b}_3 \cdot \vec{a}_3 = 2\pi l.$$

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

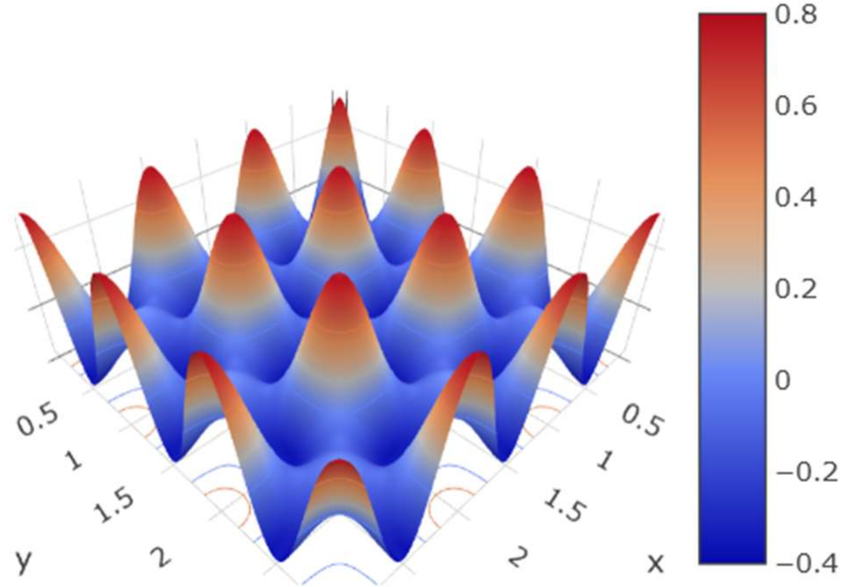
$$\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

h,k,l : integers

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

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

Two dimensional periodic functions



$f_{00} = 0$ - +

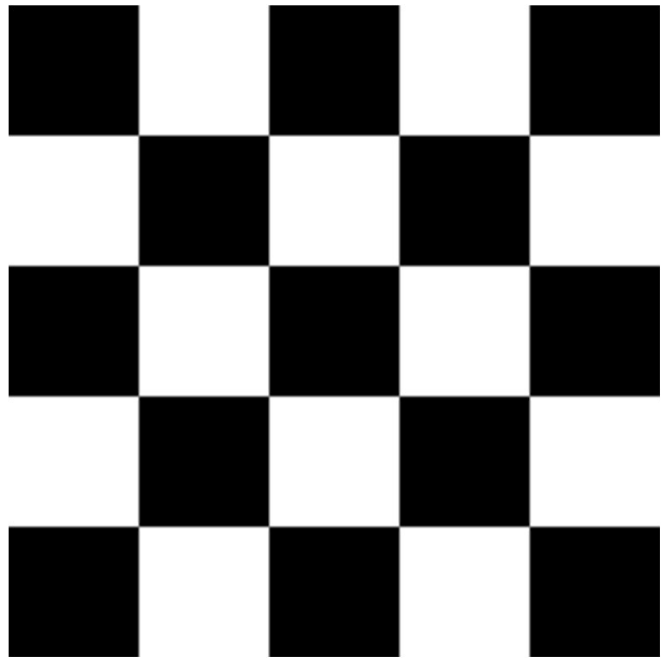
$f_{01} = f^*_{0-1} = 0.1$ - + $+i\ (0)$ - +

$f_{10} = f^*_{-10} = 0.1$ - + $+i\ (0)$ - +

$f_{11} = f^*_{-1-1} = 0.1$ - + $+i\ (0)$ - +

$f_{1-1} = f^*_{-11} = 0.1$ - + $+i\ (0)$ - +

Determine the Fourier coefficients



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

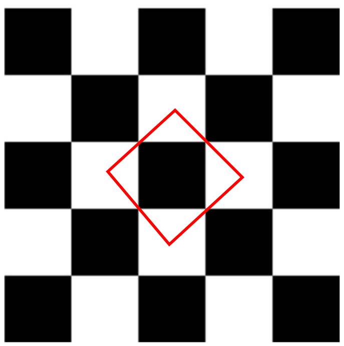
Determine the Fourier coefficients

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

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

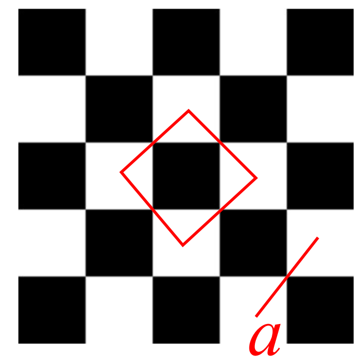
$$\int\limits_{\text{unit cell}} f(\vec{r})\exp(-i\vec{G}'\cdot\vec{r})d\vec{r} = \sum_{\vec{G}} \int\limits_{\text{unit cell}} f_{\vec{G}}\exp(-i\vec{G}'\cdot\vec{r})\exp(i\vec{G}\cdot\vec{r})d\vec{r}$$

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



Determine the Fourier coefficients

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



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

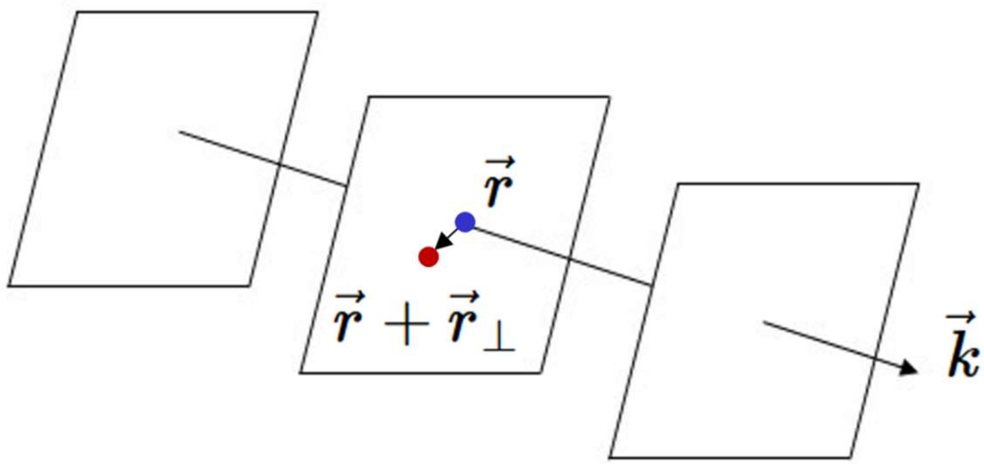
$$f_{\vec{G}} = \frac{C}{a^2} \frac{\left(\exp(-iG_x\sqrt{2}a/4) - \exp(iG_x\sqrt{2}a/4)\right)\left(\exp(-iG_y\sqrt{2}a/4) - \exp(iG_y\sqrt{2}a/4)\right)}{-G_xG_y}$$

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

Plane waves (Ebene Wellen)

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

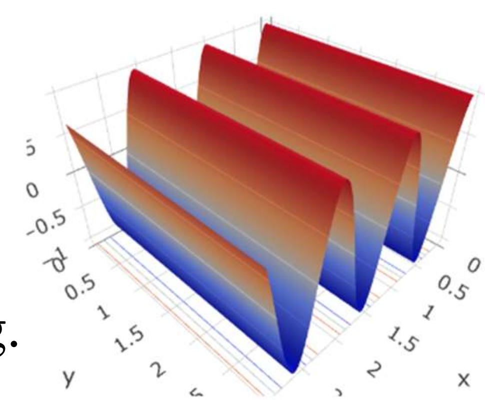
$$\lambda = \frac{2\pi}{\left|\vec{k}\right|}$$



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

Most functions can be expressed in terms of plane waves

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



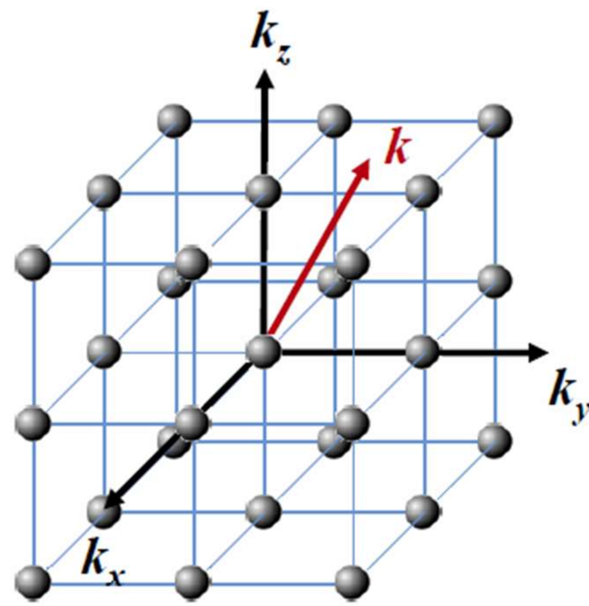
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

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

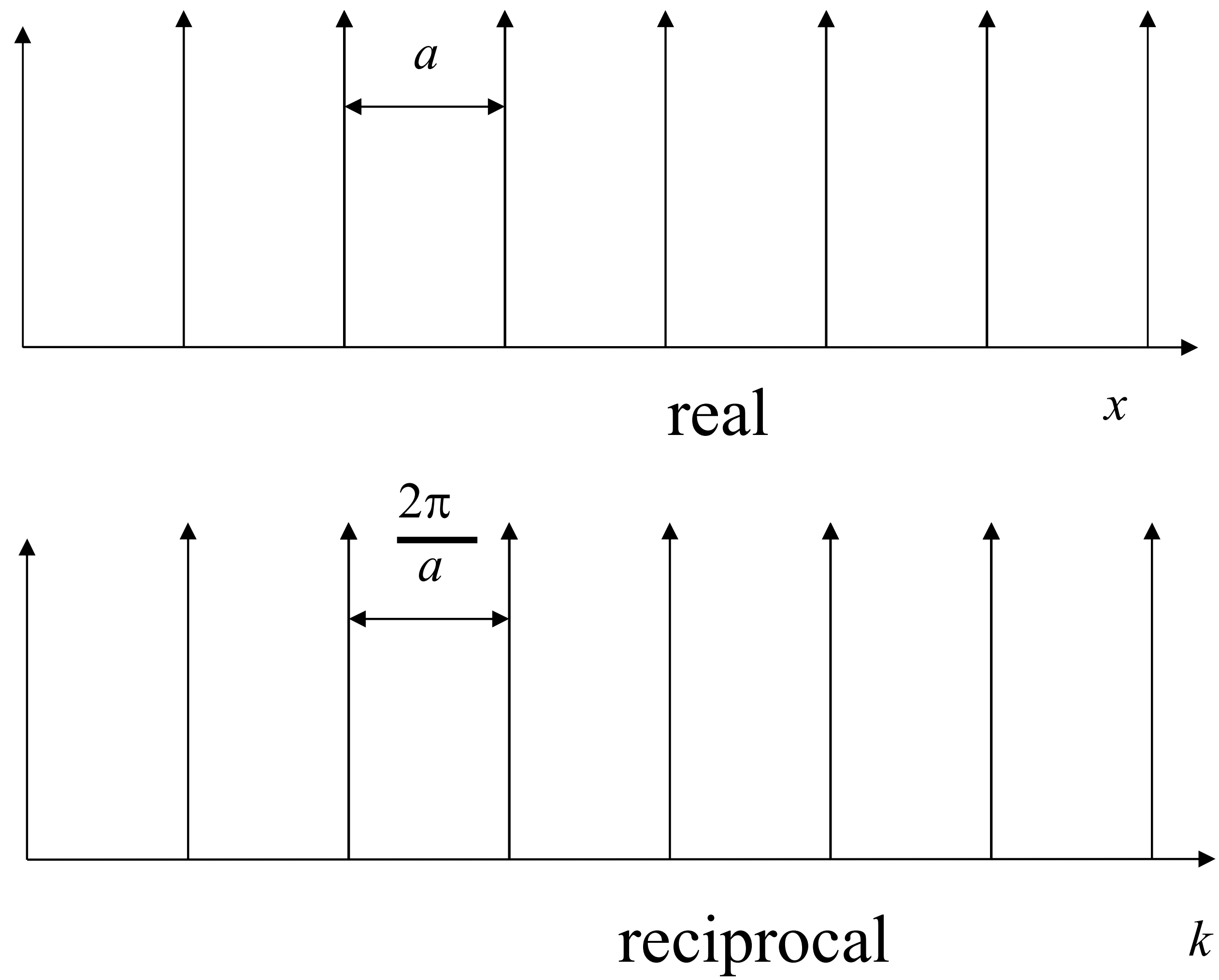
A *k*-vector points in the direction a wave is propagating.

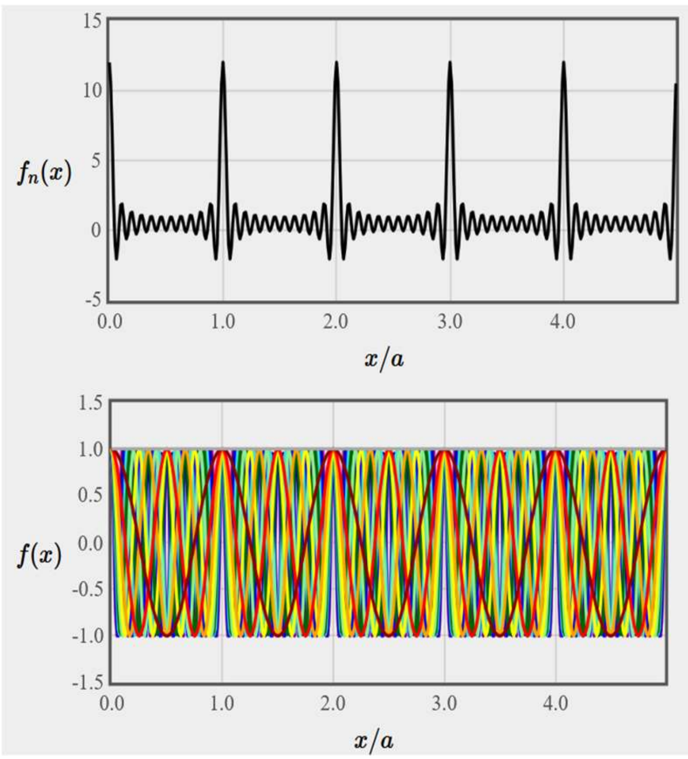
wavelength: $\lambda = \dfrac{2\pi}{|\vec{k}|}$ momentum: $\vec{p} = \hbar\vec{k}$

G-vectors form a lattice in *k*-space



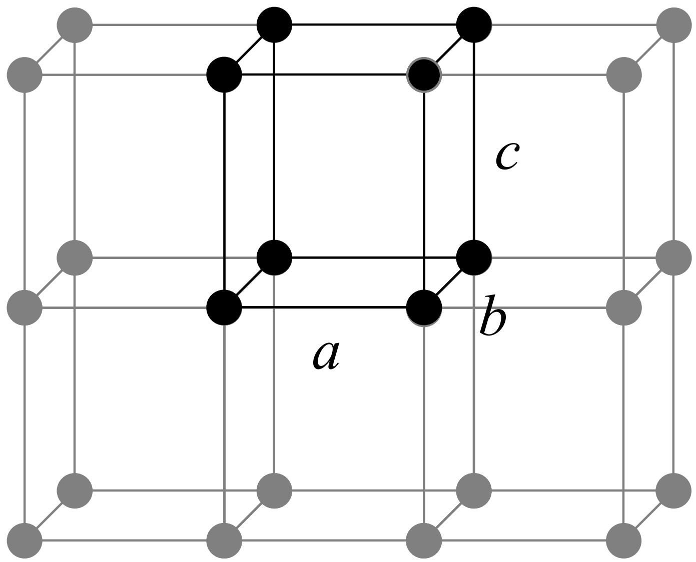
Bravais lattice and reciprocal lattice in 1-D

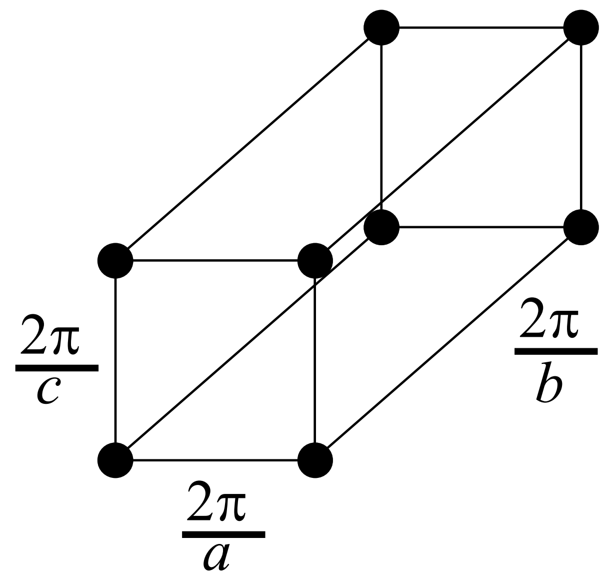




$$\cos\left(\frac{2\pi n x}{a}\right) \Rightarrow \cos(Gx) \qquad G = \frac{2\pi n}{a}$$

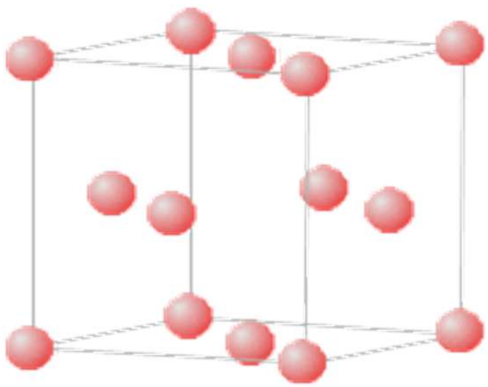
Reciprocal lattice of an orthorhombic lattice is an orthorhombic lattice



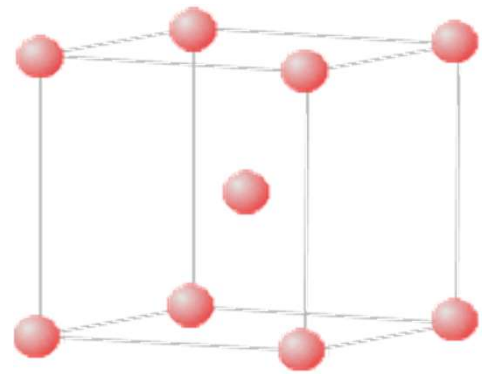


reciprocal lattice

The reciprocal lattice of an fcc lattice is a bcc lattice



a



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

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

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

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

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

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

Reciprocal lattice (Reziprokes Gitter)

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

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

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

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

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

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

$$\text{hex:} \qquad \vec{a}_1 = a\hat{x}, \qquad \vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}, \qquad \vec{a}_3 = c\hat{z},$$

$$\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}\left(\sqrt{3}\hat{k}_x - \hat{k}_y\right), \qquad \vec{b}_2 = \frac{4\pi}{\sqrt{3}a}\hat{k}_y, \qquad \vec{b}_3 = \frac{2\pi}{c}\hat{k}_z.$$

Reciprocal lattice (Reziprokes Gitter)

Primitive lattice vectors:

$\vec{a}_1 =$ 4.12E-10 $\hat{x}+$ 0 $\hat{y}+$ 0 $\hat{z}$ [m]

$\vec{a}_2 =$ 0 $\hat{x}+$ 4.12E-10 $\hat{y}+$ 0 $\hat{z}$ [m]

$\vec{a}_3 =$ 0 $\hat{x}+$ 0 $\hat{y}+$ 4.12E-10 $\hat{z}$ [m]

submit

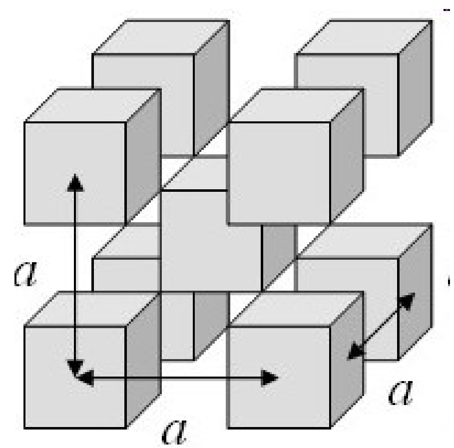
Primitive reciprocal lattice vectors

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = 1.525\mathrm{e}{+10}\ \hat{k}_x + 0.000\ \hat{k}_y + 0.000\ \hat{k}_z\ [\mathrm{m}^{-1}]$$

$$\vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = 0.000\ \hat{k}_x + 1.525\mathrm{e}{+10}\ \hat{k}_y + 0.000\ \hat{k}_z\ [\mathrm{m}^{-1}]$$

$$\vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = 0.000\ \hat{k}_x + 0.000\ \hat{k}_y + 1.525\mathrm{e}{+10}\ \hat{k}_z\ [\mathrm{m}^{-1}]$$

Cubes on a bcc lattice



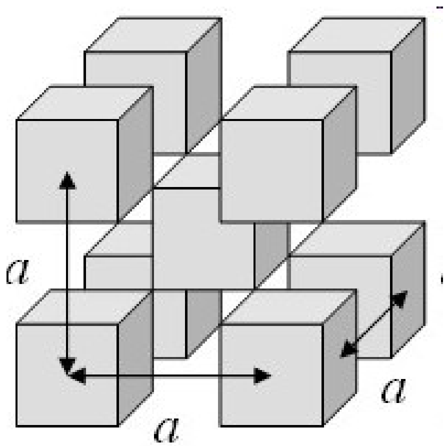
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

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.

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

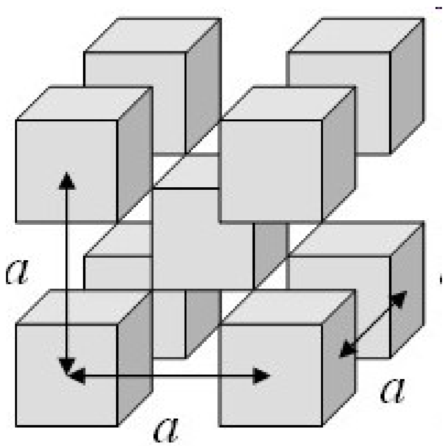
f_G is the Fourier transform of f_{cell} evaluated at G.
f_{cell} is zero outside the primitive unit cell.

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

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

Cubes on a bcc lattice

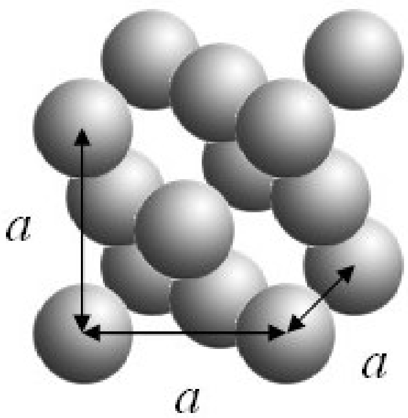
$$\int_{-\frac{a}{4}}^{\frac{a}{4}} \exp\left(-iG_x x\right)dx = \left.\frac{\exp\left(-iG_x x\right)}{-iG_x}\right|_{\frac{-a}{4}}^{\frac{a}{4}} = \left.\frac{\cos\left(-G_x x\right)+i\sin\left(-G_x x\right)}{-iG_x}\right|_{\frac{-a}{4}}^{\frac{a}{4}} = \frac{2\sin\left(\frac{G_x a}{4}\right)}{G_x}$$



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

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

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

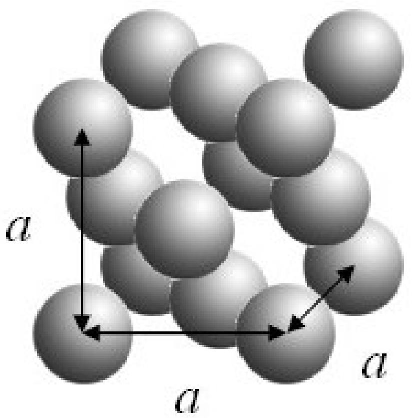
Multiply by $e^{-i\vec{G}'\cdot\vec{r}}$ and integrate over a primitive unit cell.

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

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

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

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.

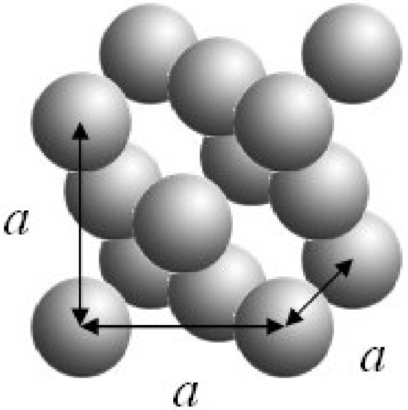
$$f_{\vec{G}} = \frac{1}{V}\int f_{cell}(\vec{r})\exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r = \frac{C}{V}\int_{\text{sphere}} \exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r.$$

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

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

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

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

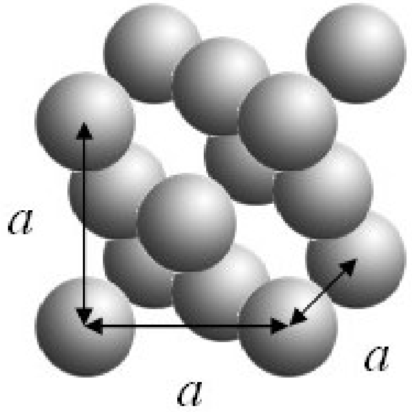
Both terms are perfect differentials

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

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

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

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



Spheres on any lattice

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

Integrate over r

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

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

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

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.

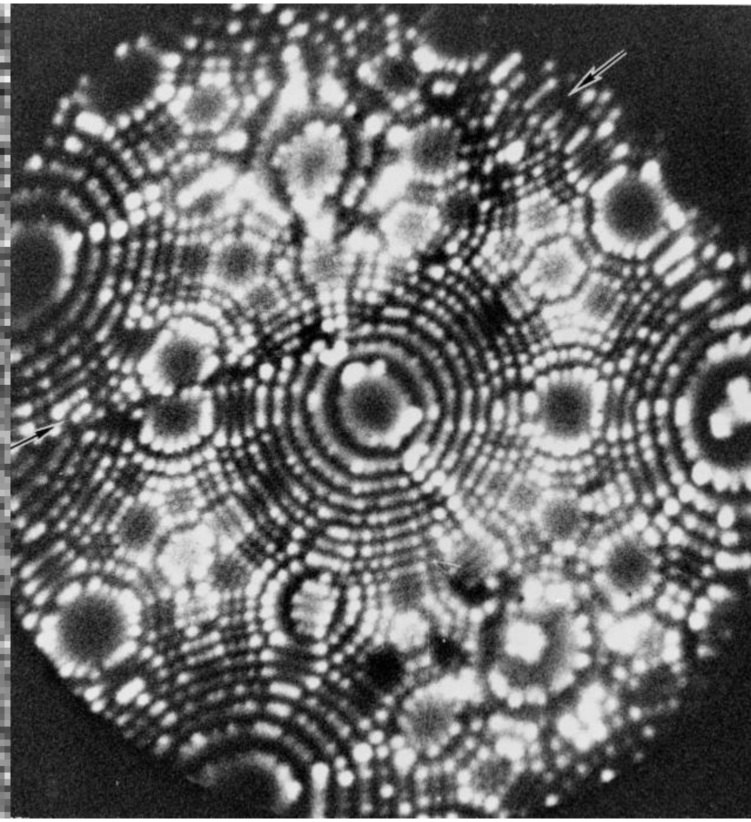
$$U(\vec{r}) = \frac{Ze^2}{V\epsilon_0}\sum_{\vec{G}}\left(\frac{\cos(|G|R)-1}{|G|^2} + \frac{\sin(|G|R) - |G|R\cos(|G|R)}{R|G|^3}\right)\exp\left(i\vec{G}\cdot\vec{r}\right).$$

For the exam

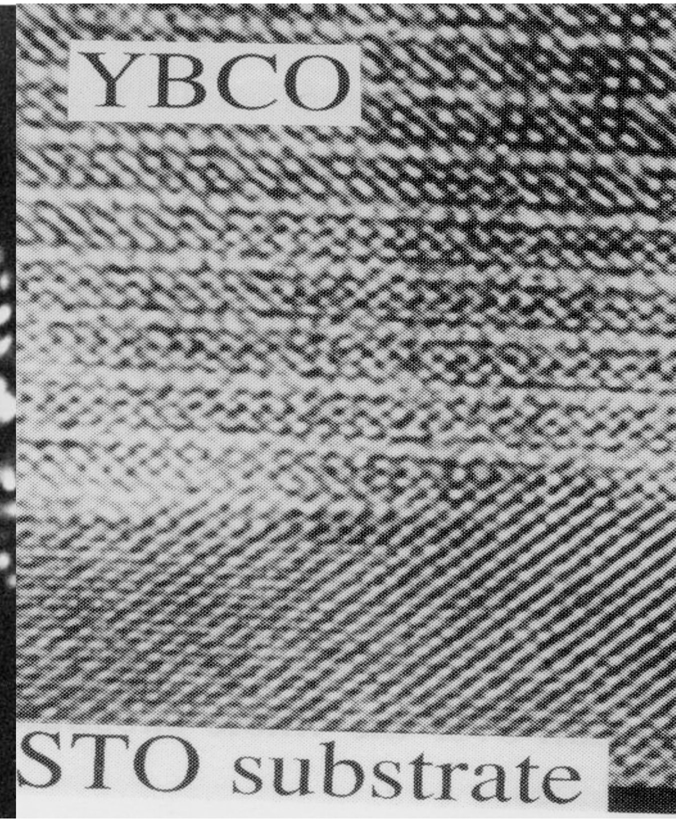
- You should know that every periodic function can be expressed as a Fourier series, $f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} \exp\left(i\vec{G} \cdot \vec{r}\right)$.
- You should be able to determine the primitive reciprocal lattice vectors of any Bravais lattice and construct the reciprocal lattice vectors $\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$.
- You should know that the reciprocal lattice of an orthorhombic lattice (a, b, c) is also an orthorhombic lattice $(2\pi/a, 2\pi/b, 2\pi/c)$ and that the reciprocal lattice of fcc is bcc and the reciprocal lattice of bcc is fcc.
- Given a periodic function in 1, 2, or 3 dimensions, you should be able to determine the coefficients $f_{\vec{G}}$ of the corresponding Fourier series.
- Know that the relation between the real space primitive lattice vectors and the reciprocal space lattice vectors is $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$.
- You should be able to describe what a plane wave is and give the formula for a plane wave.

Crystal structure determination

Scanning tunneling microscope



Field ion microscope



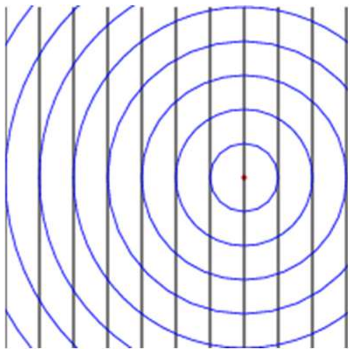
Transmission electron microscope

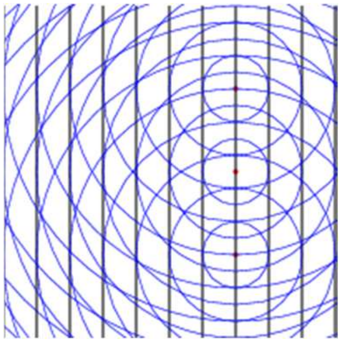
Usually x-ray diffraction is used to determine the crystal structure

Crystal diffraction (Beugung)

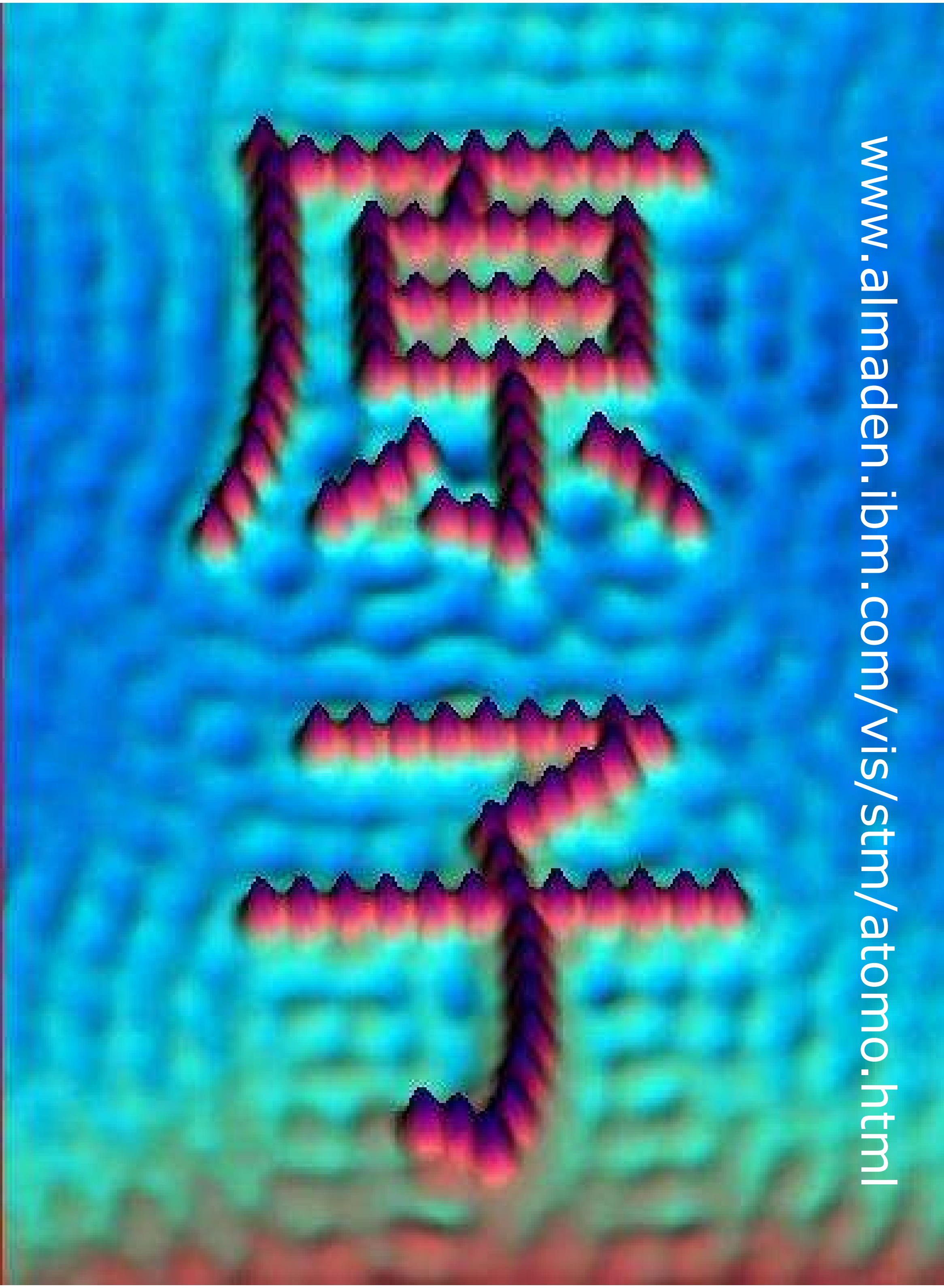
Everything moves like a wave but exchanges energy and momentum as a particle

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





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



Quantum Mechanics

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