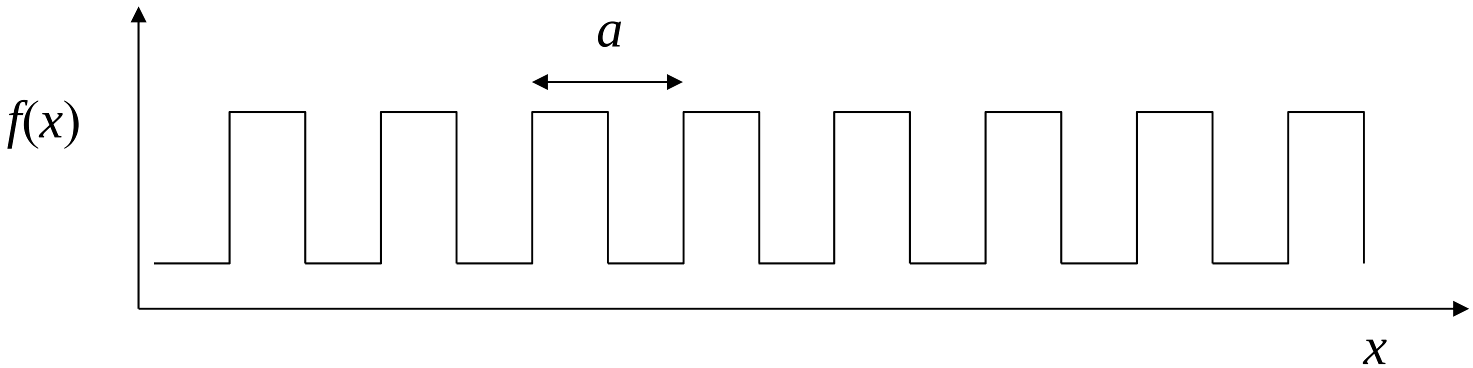
Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

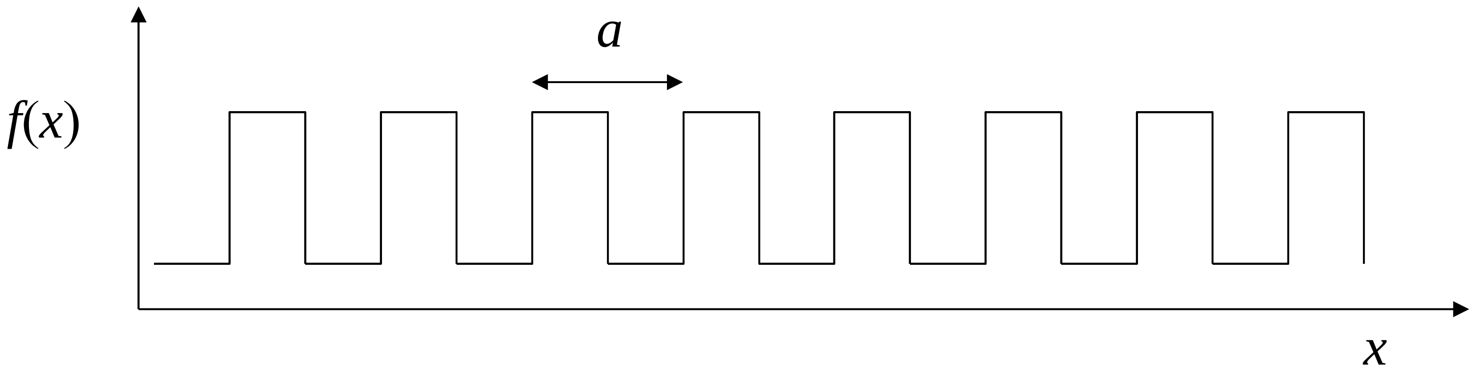
$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

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

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

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

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, 2-D, or 3-D

In two or three dimensions, a periodic function can be thought of as a pattern repeated on a Bravais lattice. It 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 vectors (depend on the Bravais lattice)

Structure factors (complex numbers)

In 1-D:

$$\vec{G} = \nu\vec{b} \qquad \nu = -\infty \ldots -1, 0, 1, \ldots \infty \qquad \left|\vec{b}\right| = \frac{2\pi}{a}$$

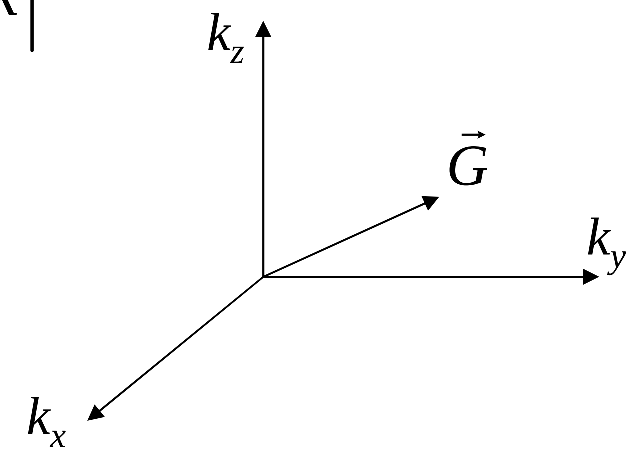
Reciprocal space (Reziproker Raum)
k-space (*k*-Raum)

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



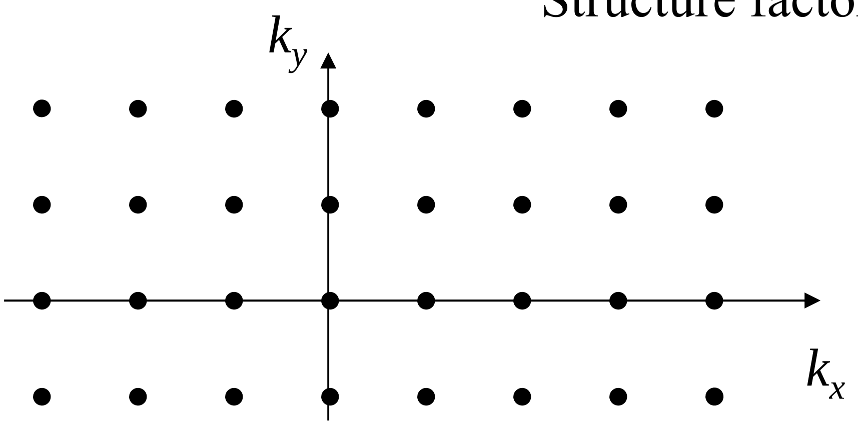
Reciprocal lattice (Reziprokes Gitter)

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

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

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

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

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

Only G = G' is non zero.

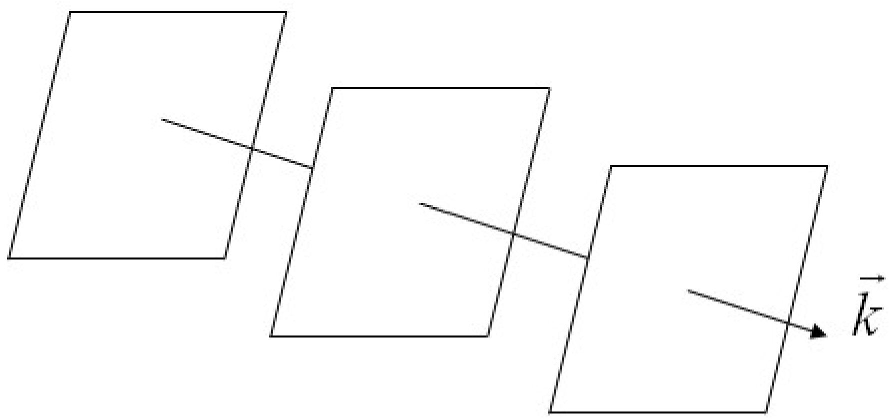
$$f_G = \frac{1}{a} \int_{-\infty}^{\infty} f_{cell}(x) e^{-iGx} dx$$

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

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

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

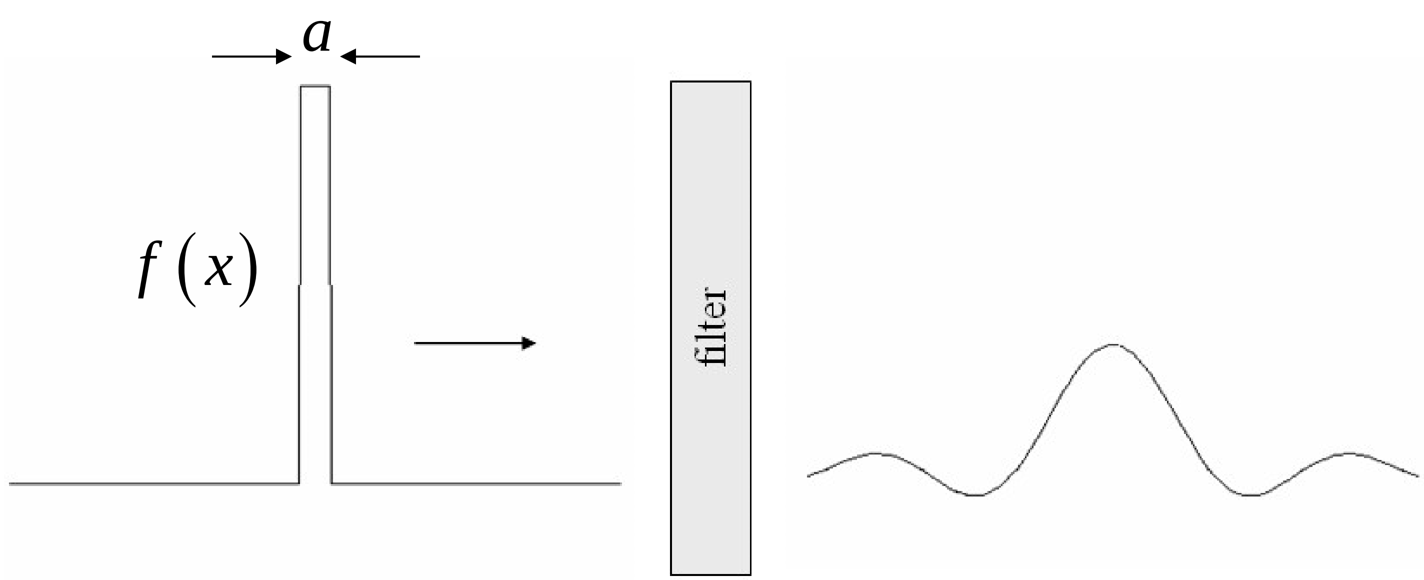
This can be inverted for $F(k)$

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

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

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

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

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

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

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

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

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

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

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]

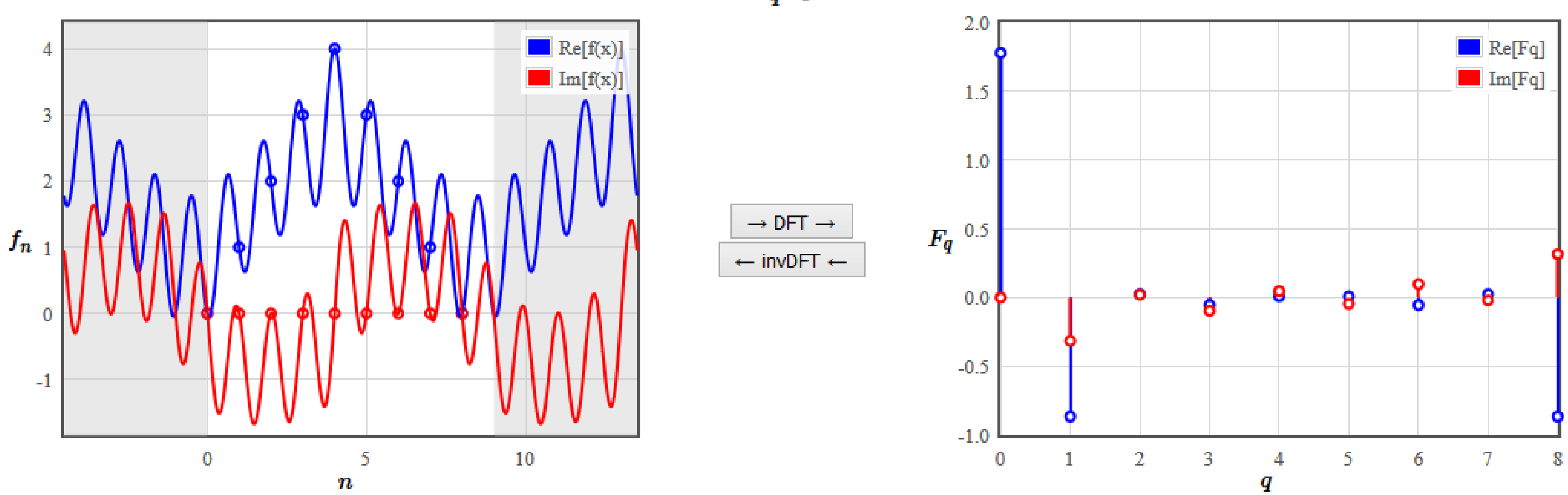
$$F_q = \frac{1}{N} \sum_{n=0}^{N-1} f_n e^{-i2\pi qn/N} \qquad q = 0, 1, \cdots, N-1.$$

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

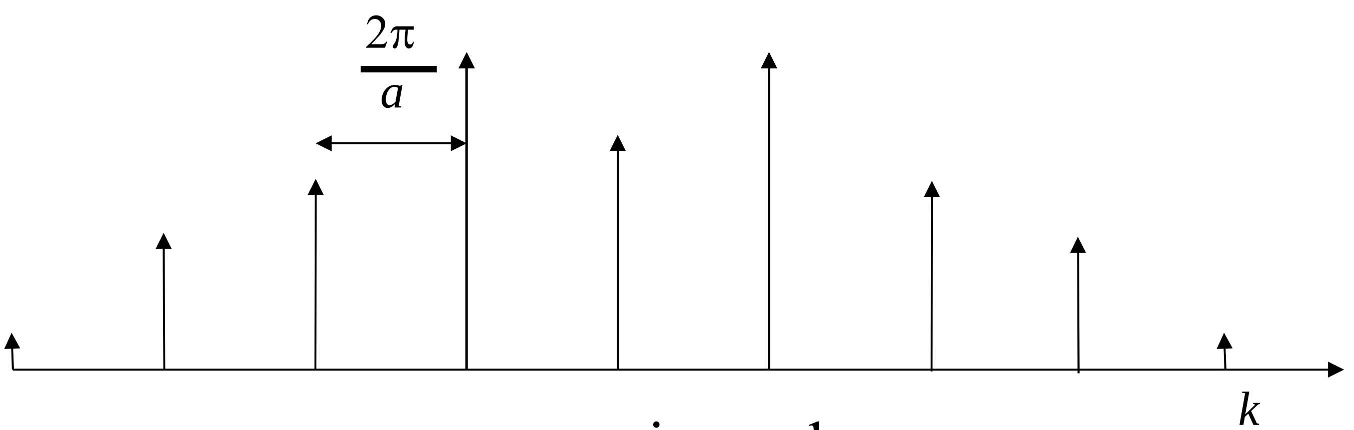
Notation [0,-1]: $\mathcal{F}\{fg\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

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

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

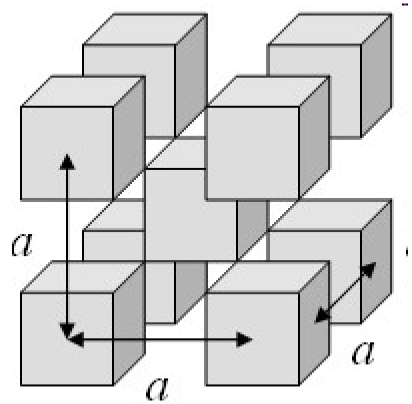
crystal = Bravais_lattice(r) * unit_cell(r)

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



reciprocal

Cubes on a bcc lattice



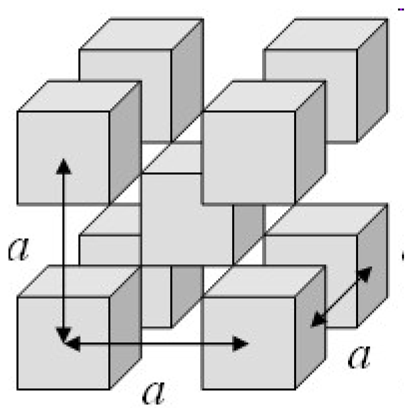
$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

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

$$\int\limits_{\text{unit cell}} f(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3r = f_{\vec{G}} V$$

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

Cubes on a bcc lattice



$$\int_{\text{unit cell}} f(\vec{r}) e^{-i\vec{G}\cdot\vec{r}} d^3 r = f_{\vec{G}} V$$

V is the volume of the primitive unit cell.

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

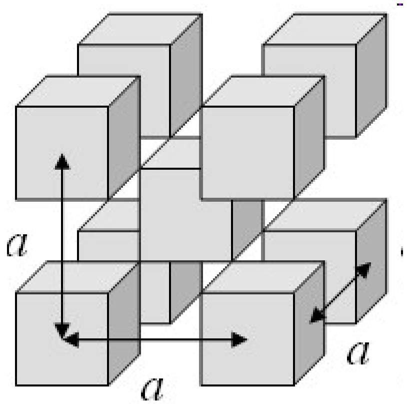
f_G is the Fourier transform of f_{cell} evaluated at G.
f_{cell} is zero outside the primitive unit cell.

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

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

Cubes on a bcc lattice

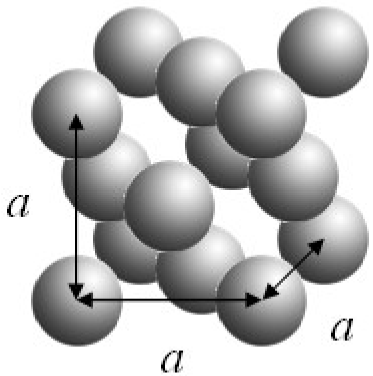
$$\int_{-\frac{a}{4}}^{\frac{a}{4}} \exp(-iG_x x)dx = \left.\frac{\exp(-iG_x x)}{-iG_x}\right|_{-\frac{a}{4}}^{\frac{a}{4}} = \left.\frac{\cos(-G_x x) + i\sin(-G_x x)}{-iG_x}\right|_{-\frac{a}{4}}^{\frac{a}{4}} = \frac{2\sin\left(\frac{G_x a}{4}\right)}{G_x}$$



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

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.

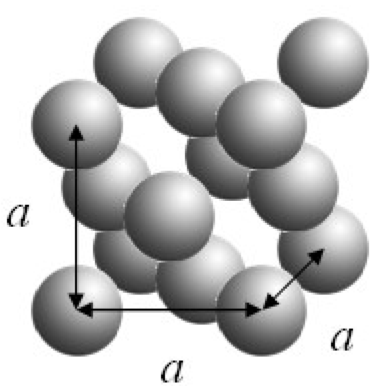
$$f_{\vec{G}} = \frac{1}{V}\int f_{cell}(\vec{r})\exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r = \frac{C}{V}\int_{\text{sphere}} \exp\left(-i\vec{G}\cdot\vec{r}\right)d^3r.$$

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

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

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

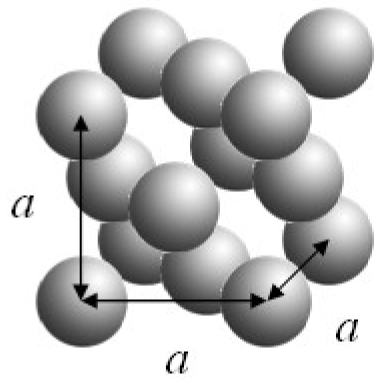
$$\frac{d}{d\theta}\cos\left(|G| r\cos\theta\right) = |G| r\sin\left(|G| r\cos\theta\right)\sin\theta \qquad \text{and}$$

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

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

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

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

Integrate over r

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

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

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

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

The quantization of the electromagnetic field

Wave nature and the particle nature of light

Unification of the laws for electricity and magnetism (described by Maxwell's equations) and light

Quantization of the harmonic oscillator

Planck's radiation law

Serves as a template for the quantization of phonons, magnons, plasmons, electrons, spinons, holons and other quantum particles that inhabit solids.

Maxwell's equations

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \mu_0 \vec{J} + \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t}$$

In vacuum the source terms J and ρ are zero.

The vector potential

$$\vec{B} = \nabla \times \vec{A}$$

$$\vec{E} = -\nabla V - \frac{\partial \vec{A}}{\partial t}$$

Maxwell's equations in terms of A Coulomb gauge $\nabla \cdot \vec{A} = 0$

$$\nabla \cdot \frac{\partial \vec{A}}{\partial t} = 0$$

$$\nabla \cdot \nabla \times \vec{A} = 0$$

$$\nabla \times \frac{\partial \vec{A}}{\partial t} = \frac{\partial}{\partial t} \nabla \times \vec{A}$$

$$\nabla \times \nabla \times \vec{A} = -\mu_0 \varepsilon_0 \frac{\partial^2 \vec{A}}{\partial t^2}$$

The wave equation

$$\nabla \times \nabla \times \vec{A} = -\mu_0 \varepsilon_0 \frac{\partial^2 \vec{A}}{\partial t^2}$$

Using the identity $\nabla \times \nabla \times \vec{A} = \nabla(\nabla \cdot \vec{A}) - \nabla^2 \vec{A}$

$$\boxed{c^2 \nabla^2 \vec{A} = \frac{\partial^2 \vec{A}}{\partial t^2}.}$$

normal mode solutions have the form: $\vec{A}(\vec{r}, t) = \vec{A}\cos(\vec{k} \cdot \vec{r} - \omega t)$

Normal mode solutions

wave equation: $$c^2\nabla^2\vec{A} = \frac{\partial^2\vec{A}}{\partial t^2}$$

normal mode solution: $$\vec{A}(\vec{r},t) = \vec{A}\cos(\vec{k}\cdot\vec{r} - \omega t)$$ ← Normalschwingungen oder Normalmoden

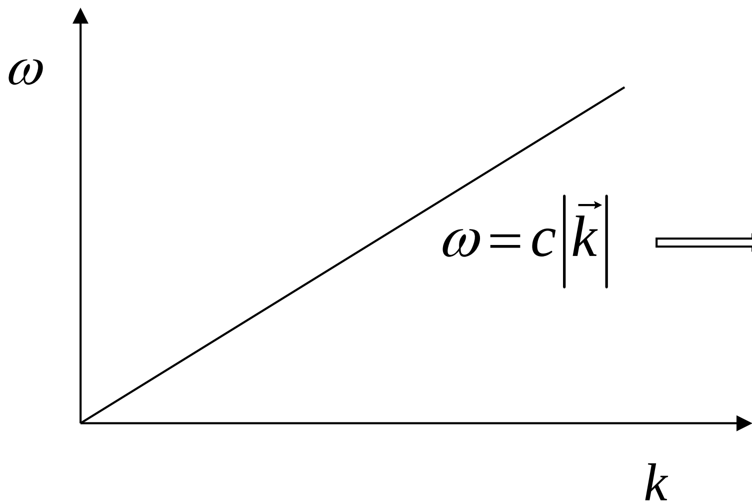
put the solution into the wave equation

$$c^2 k^2 \vec{A} = \omega^2 \vec{A}$$

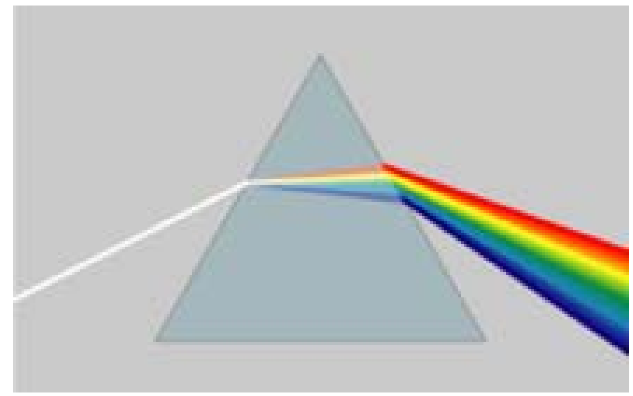
dispersion relation → $$\omega = c\left|\vec{k}\right|$$

$$f = \frac{c}{\lambda}$$

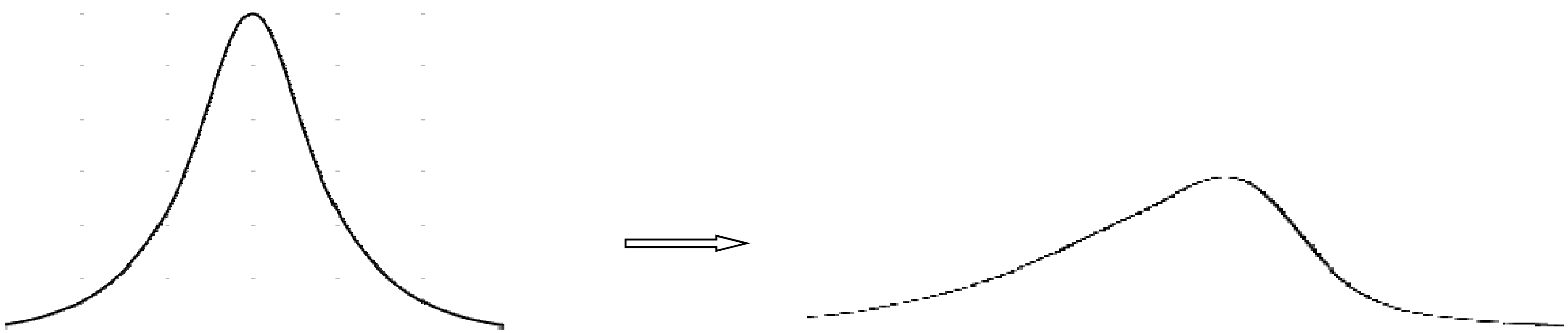
Dispersion relation



$$\omega = c\left|\vec{k}\right| \Longrightarrow f = \frac{c}{\lambda}$$



http://en.wikipedia.org/wiki/Dispersion_%28optics%29



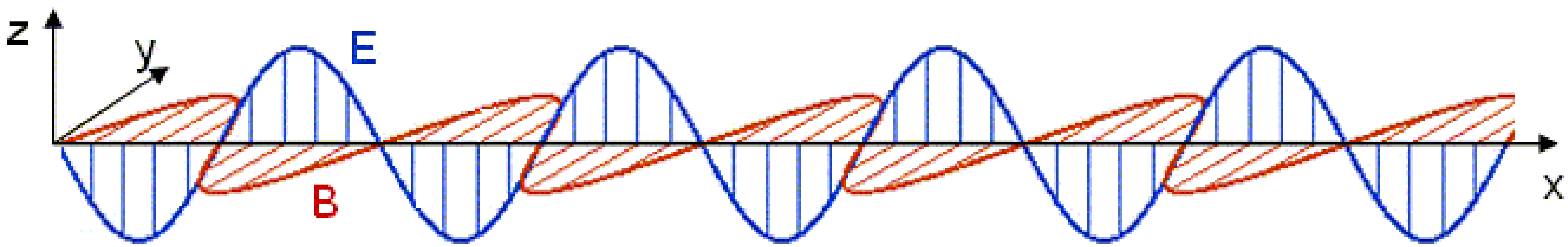
EM waves propagating in the *x* direction

$$\vec{A} = A_0 \cos(k_x x - \omega t)\hat{z}$$

The electric and magnetic fields are

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t} = -\omega A_0 \sin(k_x x - \omega t)\hat{z}$$

$$\vec{B} = \nabla \times \vec{A} = k_x A_0 \sin(k_x x - \omega t)\hat{y}$$



Quantization (using a trick)

The wave equation for a single mode.

$$-c^2\left(k_x^2+k_y^2+k_z^2\right)\vec{A}(\vec{k},t)=\frac{\partial^2\vec{A}(\vec{k},t)}{\partial t^2}$$

The equation for a single mode is mathematically equivalent to:

$$-\kappa x=m\frac{\partial^2 x}{\partial t^2}$$

$\kappa \leftrightarrow c^2k^2$, $m \leftrightarrow 1$

Quantization

Classical mathematical equivalence → quantum mathematical equivalence

$$E = \hbar\omega\left(j + \tfrac{1}{2}\right) \qquad j = 0, 1, 2\ldots$$

$$\omega = \sqrt{\frac{\kappa}{m}}$$

Rewriting this in terms of the electromagnetic field variables:

$\kappa \leftrightarrow c^2k^2$, $m \leftrightarrow 1$

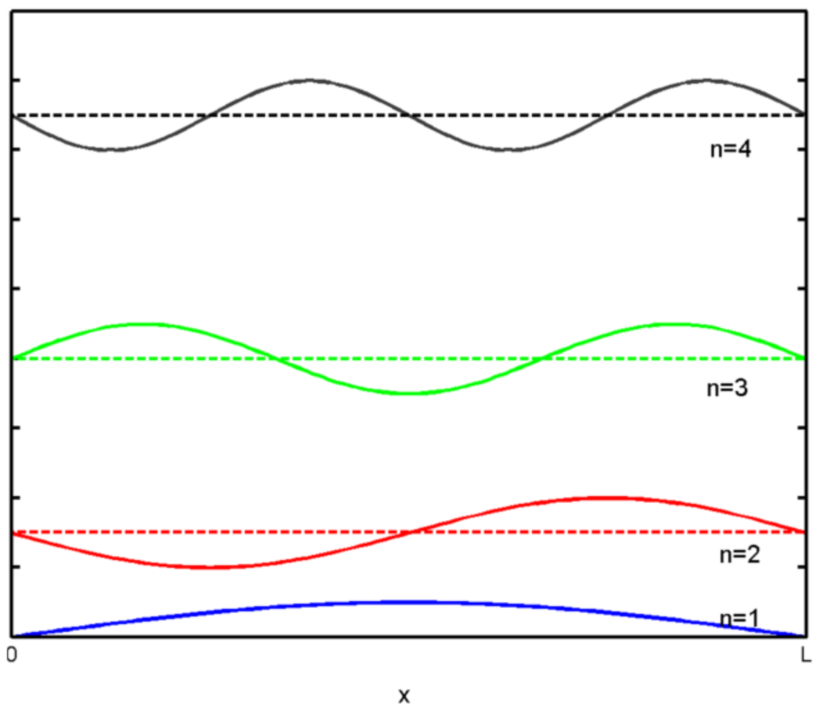
$$E = \hbar\omega\left(j + \tfrac{1}{2}\right) \qquad j = 0, 1, 2\ldots$$

Dispersion relation → $\omega = c\left|\vec{k}\right|$

j is the number of photons in that mode

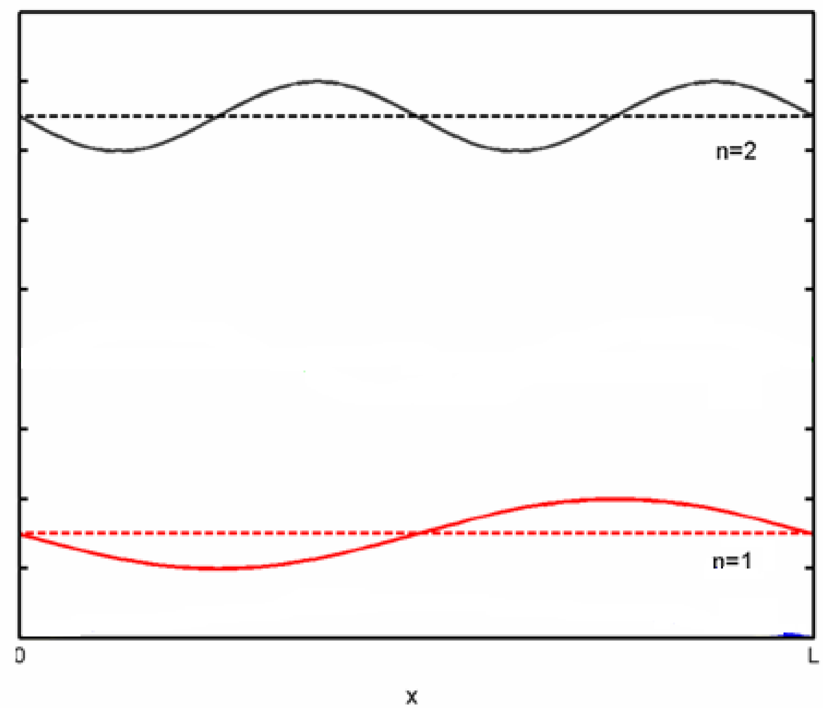
Boundary conditions

fixed boundary conditions



$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{L}$$

periodic boundary conditions



$$k = \pm\frac{2\pi}{\lambda} = \pm\frac{2n\pi}{L}$$