Periodic functions, Fourier Series, and waves

Outline

1. Periodic functions, Harmonics
2. Trigonometric Fourier Series
3. Fourier Series in multiple dimensions and the reciprocal lattice
4. Waves

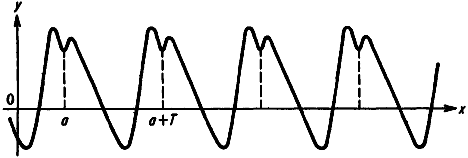
Periodic functions

Definition and properties

definition

A function $f(x)$ is periodic if there exists a constant $T > 0$ for which:

- $f(x+T) = f(x) \ \forall \ x$ in the domain of definition of the function
- it is understood that both x and $x+T$ belong to the domain
- familiar functions: $\cos x$, $\sin x$, $\tan x$, ...
- Entire graph obtained by repetition of the graph in $a \leq x \leq a+T$



Periodic functions

Definition and properties

- If two functions, $f(x)$ and $g(x)$ are periodic of period T:
  - $f(x) \pm g(x)$ are periodic of the same period, T
  - $f(x)g(x)$ is periodic of the same period, T
  - $f(x)/g(x)$ is periodic of the same period, T
- If $f(x)$ is periodic of period T, then the numbers $2T, 3T, \ldots$ and $-T, -2T, -3T \ldots$ are also periods (kT with $k \in \mathbb{Z}$ is also a period)
  - $f(x) = f(x+T) = f(x+2T) = f(x+3T) = \cdots$
  - $f(x) = f(x-T) = f(x-2T) = f(x-3T) = \cdots$
  - the period is not unique
- The periodic function defines a 1D lattice on the x axis
  - infinite points equally spaced by T

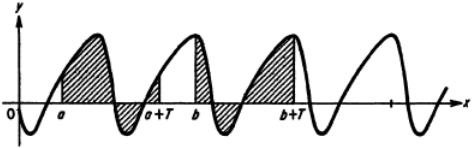
Periodic functions

Definition and properties

properties

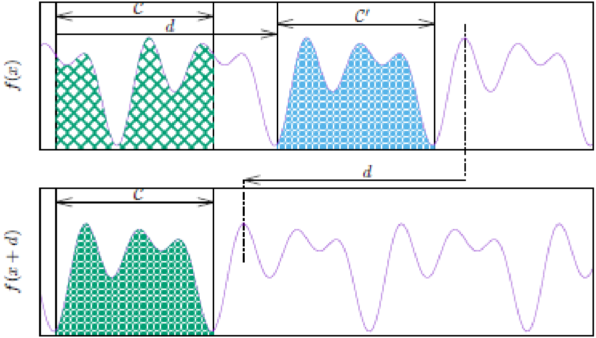
If $f(x)$ is integrable on an interval of length T then

1. $\int_a^{a+T} f(x)dx = \int_b^{b+T} f(x)dx, \forall a, b \in \mathbb{R}$
    - Define $H(z) = \int_z^{z+T} f(x)dx$, it is $\frac{dH(z)}{dz} = 0 \longrightarrow H(a) = H(b), \forall$ $a, b \in \mathbb{R}$
2. $\int_a^{a+T} f(x+d)dx = \int_a^{a+T} f(x)dx, \forall\ d \in \mathbb{R}$
    - the function can be arbitrarily translated on the real axis



Periodic functions

Definition and properties



$$\int_C f(x)\,dx = \int_{C'} f(x)\,dx = \int_C f(x+d)\,dx$$

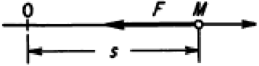
Harmonics

The simplest periodic function

The Harmonic oscillator

Consider a point mass M, of mass m, that moves along a straight line under the action of a restoring force $F = -ks$ ($k > 0$):

- $m\frac{d^2s}{dt^2} = -ks$ or $\frac{d^2s}{dt^2} + \omega^2 s = 0$
  - $\omega = \sqrt{\frac{k}{m}}$
- The solution can be written in the form $s(t) = A\sin(\omega t + \varphi)$
  - $|A|$: max. deviation from O
  - $T = \frac{2\pi}{\omega}$: period of oscillation
  - φ: initial phase, $s(t=0) = \sin\varphi$



Harmonics

The simplest periodic function

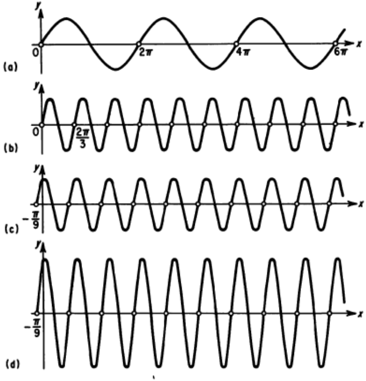
Appearance of the curve $y = A\sin(\omega x + \varphi)$

- Assume $\omega > 0$ ($\sin(-\omega x + \varphi) = -\sin(\omega x - \varphi)$)
- $y = \sin x$ for $A = 1$, $\omega = 1$, $\varphi = 0$
- $y = \cos x$ for $A = 1$, $\omega = 1$, $\varphi = \frac{\pi}{2}$
- $y = \sin(\omega x)$: set $z = \omega x$
    - uniform compression along the x-axis by a factor ω (if $\omega > 1$) or expansion (if $\omega < 1$)
- $y = \sin(\omega x + \varphi)$: set $z = \omega x + \varphi$
    - shift of the graph of $\sin(\omega x)$ along the x-axis by $-\frac{\varphi}{\omega}$
- $y = A\sin(\omega x + \varphi)$ is obtained from that of $y = \sin(\omega x + \varphi)$ by multiplying all ordinates by the constant A

Harmonics

The simplest periodic function

Appearance of the curve $y = A \sin(\omega x + \varphi)$



(a) $y = \sin x$; (b) $y = \sin 3x$; (c) $y = \sin(3x + \frac{\pi}{3})$; (d) $y = 2\sin(3x + \frac{\pi}{3})$

Harmonics

The simplest periodic function

General representation

- Every harmonics can be written as: $y = a\cos\omega x + b\sin\omega x$
  - $a = A\sin\varphi$
  - $b = A\cos\varphi$
- Conversely:
  - $A = \sqrt{a^2 + b^2}$
  - $\sin\varphi = \frac{a}{A} = \frac{a}{\sqrt{a^2+b^2}}$
  - $\cos\varphi = \frac{b}{A} = \frac{b}{\sqrt{a^2+b^2}}$
- The harmonic with period $T = 2l$ can be written as:

$$a\cos\left(\frac{\pi x}{l}\right) + b\sin\left(\frac{\pi x}{l}\right)$$

1. Periodic functions, Harmonics
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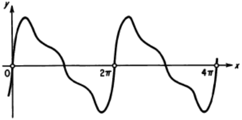
Trigonometric Fourier series

Trigonometric polinomials and series

Trigonometric polynomials

- Let's consider the harmonic:
    - $a_k \cos\left(\frac{\pi k x}{l}\right) + b_k \sin\left(\frac{\pi k x}{l}\right)$ $(k = 1, 2, \dots)$
- Each member is:
    - periodic of period $T_k = \frac{2l}{k}$ and frequency $\omega_k = \frac{\pi k}{l}$
    - has a common period $T = 2l = kT_k$
- $s_n(x) = A + \sum_{k=1}^{n} \left(a_k \cos\left(\frac{\pi k x}{l}\right) + b_k \sin\left(\frac{\pi k x}{l}\right)\right)$
    - is periodic of period $2l$
    - can represent quite general functions



graph of $y = \sin x + \frac{1}{2}\sin(2x) + \frac{1}{4}\sin(3x)$

Trigonometric Fourier series

Trigonometric polinomials and series

Trigonometric series

- If convergent, the infinite trigonometric series:
  - $A + \sum_{k=1}^{\infty} \left(a_k \cos\left(\frac{\pi kx}{l}\right) + b_k \sin\left(\frac{\pi kx}{l}\right)\right)$
- Represents a function of period $T = 2l$
- Can represent a wide class of functions
  - complicated oscillatory motion represented as superposition of individual simple oscillations
- If a function $f(x)$ of period $2l$ is represented by such a series:
  - $f(x) = A + \sum_{k=1}^{\infty} \left(a_k \cos\left(\frac{\pi kx}{l}\right) + b_k \sin\left(\frac{\pi kx}{l}\right)\right)$
- Then setting $t = \frac{\pi x}{l}$
  - $\varphi(t) = f\left(\frac{tl}{\pi}\right) = A + \sum_{k=1}^{\infty} (a_k \cos(kt) + b_k \sin(kt))$
  - $\varphi(t)$ is periodic of period $T = 2\pi$
  - we can focus on functions of period 2π

Trigonometric Fourier series

The orthogonality of sines and cosines

The basic trigonometric system

- The functions in the set:
  - $1, \cos(x), \sin(x), \cos(2x), \sin(2x) \ldots, \cos(nx), \sin(nx) \ldots$
- Have the common period of 2π
- Are pairwise orthogonal on the interval $[-\pi, \pi]$:
  - $\int_{-\pi}^{\pi} \cos(nx) dx = 0 \ (n = 1, 2, \ldots)$
  - $\int_{-\pi}^{\pi} \sin(nx) dx = 0 \ (n = 1, 2, \ldots)$
  - $\int_{-\pi}^{\pi} \cos(nx) \sin(mx) dx = 0 \ \forall n, m$
  - $\int_{-\pi}^{\pi} \sin(nx) \sin(mx) dx = \pi\delta_{mn}$
  - $\int_{-\pi}^{\pi} \cos(nx) \cos(mx) dx = \pi\delta_{mn}$

Trigonometric Fourier series

The orthogonality of sines and cosines

Orthogonal systems

- Two functions $\psi(x)$ and $\varphi(x)$ are orthogonal on the interval $[a, b]$ if:

$$\int_a^b \psi(x)\varphi(x)dx = 0$$

- The basic trigonometric system is orthogonal in any interval of the type $[a, a+2\pi]$
- Hint: to verify it use the well-known formulae:
    - $\cos\alpha\cos\beta = \frac{1}{2}[\cos(\alpha+\beta) + \cos(\alpha-\beta)]$
    - $\sin\alpha\sin\beta = \frac{1}{2}[\cos(\alpha-\beta) - \cos(\alpha+\beta)]$
    - $\sin\alpha\cos\beta = \frac{1}{2}[\sin(\alpha+\beta) + \sin(\alpha-\beta)]$

Trigonometric Fourier series

Fourier series for functions of period 2π

- Suppose a (integrable) function $f(x)$ of period 2π is given the following expansion:

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left(a_k \cos(kx) + b_k \sin(kx)\right)$$

- How are the coefficients (Fourier coefficients) determined from a knowledge of $f(x)$?
- The task is easy if we assume that the series above and those to be written (i.e. $f(x)\cos(nx)$,$f(x)\sin(nx)$) can be:
  - integrated term by term
  - the integral of the sum is the sum of the integrals
- This is the case if the series is uniformly convergent on a given interval and its terms are continuous on the interval

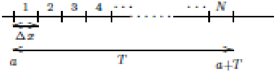
Trigonometric Fourier series

Fourier series for functions of period 2π

Fourier series of a function

- $a_0 = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)dx$
- $\frac{a_0}{2}$ is the average value of $f(x)$ in the interval $[-\pi, \pi]$:

$$\begin{aligned}\frac{1}{T}\int_a^{a+T} f(x)dx &= \lim_{N\to\infty}\frac{1}{N\Delta x}\sum_{i=1}^{N} f(x_i)\Delta x \\ &= \lim_{N\to\infty}\frac{\sum_{i=1}^{N} f(x_i)}{N} = < f(x) >\end{aligned}$$



Trigonometric Fourier series

Fourier series for functions of period 2π

Fourier series of a function

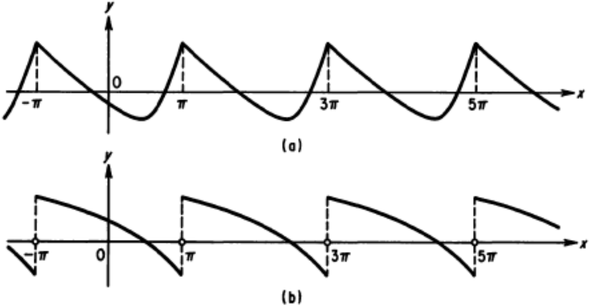
- $a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)dx$
- $b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(nx)dx$
- the same coefficients are obtained with $\int_{-\pi}^{\pi} \longrightarrow \int_{a}^{a+2\pi}$
- $f(x) \sim \frac{a_0}{2} + \sum_{k=1}^{\infty}(a_k\cos(kx) + b_k\sin(kx))$
    - if we do not know in advance its convergence and if it sums to $f(x)$
- If $f(x)$ is defined only on $[-\pi,\pi]$, its Fourier series is its periodic extension on the real axis

Trigonometric Fourier series

Fourier series for functions of period 2π

Periodic extensions of a function defined on $[-\pi, \pi]$

- For $f(x)$ continuous on $[-\pi, \pi]$, the extension has discontinuities (jump discontinuities):
  - at points $x = (2k+1)\pi$, $k = 0, \pm 1, \pm 2 \ldots$ when $f(\pi) \neq f(-\pi)$
  - at $x = a + 2k\pi$, $k = 0, \pm 1, \pm 2 \ldots$ when $f(a) \neq f(a+2\pi)$



Trigonometric Fourier series

Fourier series for functions of period 2π

Right-hand and left-hand limits: jump discontinuities

- Let $\lim_{\substack{x\to x_0\\ x<x_0}} f(x) = f(x_0-0)$ and $\lim_{\substack{x\to x_0\\ x>x_0}} f(x) = f(x_0+0)$ if both exist and are finite
    - $f(x_0-0)$: left-hand limit of $f(x)$ at x_0
    - $f(x_0+0)$: right-hand limit of $f(x)$ at x_0
- If f is continuous in x_0: $f(x_0+0) = f(x_0) = f(x_0-0)$
- If $f(x_0-0) \neq f(x_0+0)$:
    - x_0 is a point of jump discontinuity if both exist
        - $\delta = f(x_0+0) - f(x_0-0)$: jump of the function
    - x_0 is a point of discontinuity of the second kind if at least one of them does not exist

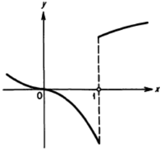
Trigonometric Fourier series

Fourier series for functions of period 2π

Right-hand and left-hand limits: jump discontinuities

$$f(x) = \begin{cases} -x^3 & x < 1 \\ 0 & x = 1 \\ \sqrt{x} & x > 1 \end{cases}$$

- In the graph of the function, at $x = 1$:
  - $f(1-0) = -1$, $f(1+0) = 1 \longrightarrow \delta = f(1+0) - f(1-0) = 2$



Trigonometric Fourier series

Fourier series for functions of period 2π

Smooth and piecewise smooth functions

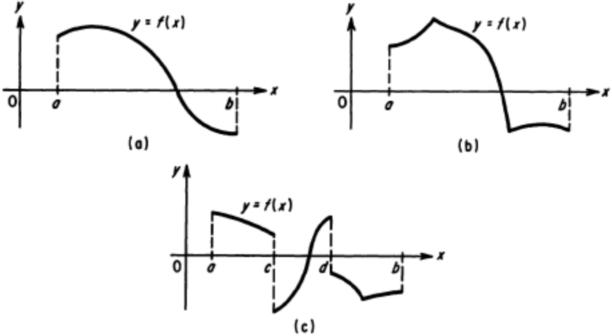
- $f(x)$ is said to be smooth on the interval $[a, b]$ if is has a continuous derivative on $[a, b]$:
    - the graph is a smooth curve without any ”corners”
- $f(x)$ is said to be piecewise smooth on the interval $[a, b]$ if:
    - either $f(x)$ and its derivative are both continuous on $[a, b]$
    - they have only a finite number of jump discontinuities on $[a, b]$
- A continuous or discontinuous function $f(x)$ defined on the whole real axis is piecewise smooth if it is piecewise smooth on every interval of finite length

Trigonometric Fourier series

Fourier series for functions of period 2π

Smooth and piecewise smooth functions

- Graph (a): smooth function
- Graph (b): continuous piecewise smooth function
- Graph (c): discontinuous piecewise smooth function



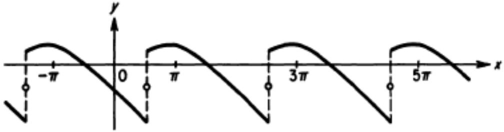
Trigonometric Fourier series

Fourier series for functions of period 2π

A criterion for the convergence of Fourier series

The Fourier series of a piecewise smooth (continuous or discontinuous) function $f(x)$ of period 2π converges for all values of x. The sum of the series equals $f(x)$ at every point of continuity and equals the number $\frac{1}{2}[f(x+0)+f(x-0)]$ at every point of discontinuity. If $f(x)$ is continuous everywhere, then the series converges absolutely and uniformly.

- Convergence at the endpoints:
  - to $f(x)$ if $f(-\pi)=f(\pi)$
  - to $\frac{f(-\pi)+f(\pi)}{2}$ if $f(-\pi)\neq f(\pi)$

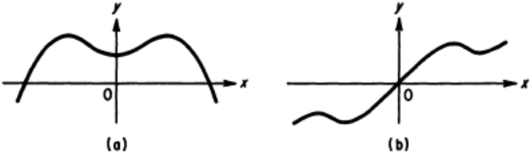


Trigonometric Fourier series

Fourier series for functions of period 2π

Even and odd functions

- $f(x)$ is an even function if $f(x) = f(-x)\ \forall x$
    - symmetric with respect to the y axis
    - $\int_{-l}^{l} f(x)dx = 2\int_{0}^{l} f(x)dx$
    - provided $f(x)$ is defined and integrable in $[-l, l]$
- $f(x)$ is a odd function if $f(-x) = -f(x)\ \forall x$
    - symmetric with respect to the origin $(f(0) = 0)$
    - $\int_{-l}^{l} f(x)dx = 0$



(a) even function; (b) odd function

Trigonometric Fourier series

Fourier series for functions of period 2π

Even and odd functions: properties

- The product $f(x) = \psi(x)\varphi(x)$ of two even or odd functions is an even function
  - $f(-x) = \psi(-x)\varphi(-x) = \psi(x)\varphi(x) = f(x)$
  - $f(-x) = \psi(-x)\varphi(-x) = [-\psi(x)][-\varphi(x)] = f(x)$
- The product $f(x) = \psi(x)\varphi(x)$ of a even and a odd function is an odd function
  - $f(-x) = \psi(-x)\varphi(-x) = -\psi(x)\varphi(x) = -f(x)$
- $\cos nx$ $(n = 0, 1, 2 \ldots)$ and $\sin nx$ $(n = 1, 2 \ldots)$ are respectively even and odd

Trigonometric Fourier series

Fourier series for functions of period 2π

Cosine series

- If $f(x)$ is an even function defined on $[-\pi, \pi]$ (or even periodic) then:
  - $f(x)\cos(nx)$ is even
  - $f(x)\sin(nx)$ is odd
- Its Fourier series contains only cosines:

$$f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(nx)$$

- $a_n = \frac{2}{\pi}\int_0^{\pi} f(x)\cos(nx)dx$ $(n = 0, 1, 2 \ldots)$
- $b_n = 0$ $(n = 1, 2 \ldots)$
- An even extension onto $[-\pi, 0]$ if $f(x)$ is defined on $[0, \pi]$

Trigonometric Fourier series

Fourier series for functions of period 2π

Sine series

- If $f(x)$ is an odd function defined on $[-\pi, \pi]$ (or odd periodic) then:
    - $f(x)\cos(nx)$ is odd
    - $f(x)\sin(nx)$ is even
- Its Fourier series contains only sines:

$$f(x) \sim \sum_{n=1}^{\infty} b_n \sin(nx)$$

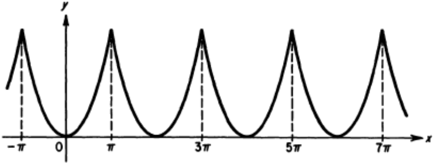
- $a_n = 0$ $(n = 0, 1, 2 \ldots)$
- $b_n = \frac{2}{\pi} \int_0^{\pi} f(x) \sin(nx) dx$ $(n = 1, 2 \ldots)$
- the series vanishes for $x = k\pi$
- An odd extension onto $[-\pi, 0]$ if $f(x)$ is defined on $[0, \pi]$ (necessarily $f(0) = 0$)

Trigonometric Fourier series

Examples of expansions in Fourier series

Expansion of $f(x) = x^2$ $(-\pi \leq x \leq \pi)$

- $f(x)$ is even, the extended function is continuous and piecewise smooth; its Fourier series converges absolutely and uniformly to $f(x)$:
  - $\forall x \in [-\pi, \pi]$
  - to its periodic extension outside $[-\pi, \pi]$
- $x^2 = \frac{\pi^2}{3} - 4\left(\cos x - \frac{\cos(2x)}{2^2} + \frac{\cos(3x)}{3^2} + \dots\right)$
  - $a_0 = \frac{2}{\pi}\int_0^\pi x^2 dx = \frac{2\pi^2}{3}$
  - $a_n = \frac{2}{\pi}\int_0^\pi x^2 \cos(nx) dx = \frac{4}{n^2}\cos(n\pi) = (-1)^n \frac{4}{n^2}$
  - $b_n = 0$ $(n = 1, 2, \dots)$

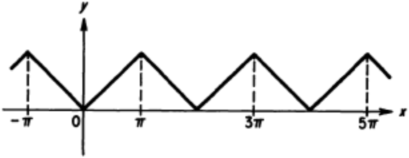


Trigonometric Fourier series

Examples of expansions in Fourier series

Expansion of $f(x) = |x|$ $(-\pi \le x \le \pi)$

- $f(x)$ is even, the extended function is continuous and piecewise smooth; its Fourier series converges absolutely and uniformly to $f(x)$:
  - $\forall x \in [-\pi, \pi]$
  - to its periodic extension outside $[-\pi, \pi]$
- $|x| = \frac{\pi}{2} - \frac{4}{\pi}\left(\cos x + \frac{\cos(3x)}{3^2} + \frac{\cos(5x)}{5^2} + \dots\right)$
  - $a_0 = \frac{2}{\pi}\int_0^\pi x dx = \pi$
  - $a_n = \frac{2}{\pi}\int_0^\pi x\cos(nx)dx = \frac{2}{\pi n^2}[\cos(n\pi) - 1] = \frac{2}{\pi n^2}[(-1)^n - 1]$
  - $b_n = 0$ $(n = 1, 2, \dots)$

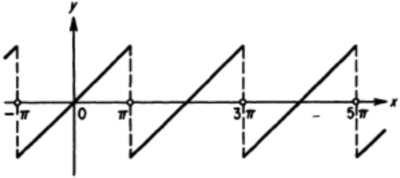


Trigonometric Fourier series

Examples of expansions in Fourier series

Expansion of $f(x) = x \ (-\pi \leq x \leq \pi)$

- $f(x)$ is odd, the extended function is piecewise smooth and discontinuous at the point $x = (2k+1)\pi \ (k = 0, \pm 1, \pm 2 \ldots)$; its Fourier series converges to zero at the points of discontinuity.
- $x = 2\left(\sin x - \frac{\sin(2x)}{2} + \frac{\sin(3x)}{3} - \ldots\right)$
  - $a_n = 0 \ (n = 0, 1, 2, \ldots)$
  - $b_n = \frac{2}{\pi}\int_0^{\pi} x \sin(nx) dx = -\frac{2}{n}[\cos(n\pi)] = \frac{2}{n}[(-1)^{n+1}]$



Trigonometric Fourier series

Fourier series for functions of period 2π

The complex form of Fourier series

- Given $f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos(nx) + b_n \sin(nx))$
  - $a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(nx) dx \ (n = 0, 1, 2, \dots)$
  - $b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(nx) dx \ (n = 1, 2, \dots)$
- It can be put in the equivalent complex form: $f(x) \sim \sum_{n=-\infty}^{\infty} c_n e^{inx}$
  - $c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-inx} dx$, $(n = 0, \pm 1, \pm 2, \dots)$
  - $c_0 = \frac{a_0}{2}$
  - $c_n = \frac{1}{2}(a_n - ib_n)$ for $n > 0$
  - $c_{-n} = \frac{1}{2}(a_n + ib_n) = c_n^*$ for $n > 0$ (if $f(x)$ is real)

Trigonometric Fourier series

Fourier series for functions of period 2π

The Euler's identity: $e^{i\alpha} = \cos\alpha + i\sin\alpha$

- Expand $e^{i\alpha}$, $\alpha \in \mathbb{R}$ in Taylor's series around $\alpha = 0$:

$$\begin{aligned} e^{i\alpha} &= \sum_{n=0}^{\infty} \frac{(i\alpha)^n}{n!} = 1 + i\alpha + \frac{(i)^2}{2!}\alpha^2 + \frac{(i)^3}{3!}\alpha^3 + \frac{(i)^4}{4!}\alpha^4 + \frac{(i)^5}{5!}\alpha^5 + \dots \\ &= \left(1 - \frac{\alpha^2}{2!} + \frac{\alpha^4}{4!} + \dots\right) + i\left(\alpha - \frac{\alpha^3}{3!} + \frac{\alpha^5}{5!} + \dots\right) \\ &= \cos\alpha + i\sin\alpha \end{aligned}$$

  - $\cos x = \sum_{n=0}^{\infty}(-)^n \frac{x^{2n}}{(2n)!} = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \dots$
  - $\sin x = \sum_{n=0}^{\infty}(-)^n \frac{x^{2n+1}}{(2n+1)!} = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \dots$
- It follows that $e^{-i\alpha} = \cos\alpha - i\sin\alpha$

Trigonometric Fourier series

Fourier series for functions of period 2π

The complex form of Fourier series

- $\cos x = \frac{e^{ix}+e^{-ix}}{2} \longrightarrow \cos(nx) = \frac{e^{inx}+e^{-inx}}{2}$
- $\sin x = \frac{e^{ix}-e^{-ix}}{2i} \longrightarrow \sin(nx) = \frac{e^{inx}-e^{-inx}}{2i}$

$$\begin{aligned} f(x) &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos(nx) + b_n \sin(nx)\right] \\ &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \left(\frac{e^{inx} + e^{-inx}}{2}\right) + b_n \left(\frac{e^{inx} - e^{-inx}}{2i}\right)\right] \\ &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[c_n e^{inx} + c_{-n} e^{-inx}\right] = \sum_{n=-\infty}^{\infty} c_n e^{inx} \end{aligned}$$

Trigonometric Fourier series

Fourier series for functions of period 2π

The complex form of Fourier series

- $c_0 = \frac{a_0}{2} = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)dx$
- $c_n = \frac{a_n - ib_n}{2} = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)e^{-inx}dx$
- $c_{-n} = \frac{a_n + ib_n}{2} = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)e^{inx}dx$
- Can be obtained directly from $f(x) \sim \sum_{n=-\infty}^{\infty} c_n e^{inx}$ by using the result:
$$\int_{-\pi}^{\pi} e^{i(n-m)x}dx = 2\pi\delta_{nm}$$

Trigonometric Fourier series

Fourier series for functions of period $2l$

- The results can be readily applied to functions periodic of period $2l$ instead of 2π.
- If $f(x)$ has period $2l$, then set $x = \frac{lt}{\pi}$, $\varphi(t) = f(\frac{lt}{\pi})$ is periodic with period 2π:
    - $\varphi(t + 2k\pi) = f\left(\frac{l(t+2k\pi)}{\pi}\right) = f\left(\frac{lt}{\pi} + 2kl\right) = f(x) = f(\frac{lt}{\pi}) = \varphi(t)$
- $\varphi(t) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos(nx) + b_n \sin(nx)\right)$
    - $a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(nx)dx \; (n = 0, 1, 2, \ldots)$
    - $b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(nx)dx \; (n = 1, 2, \ldots)$
- Changing variable $x = \frac{lt}{\pi}$:
  $f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{n\pi x}{l}\right) + b_n \sin\left(\frac{n\pi x}{l}\right)\right)$
    - $a_n = \frac{1}{l}\int_{-l}^{l} f(x)\cos\left(\frac{n\pi x}{l}\right)dx \; (n = 0, 1, 2, \ldots)$
    - $b_n = \frac{1}{l}\int_{-l}^{l} f(x)\sin\left(\frac{n\pi x}{l}\right)dx \; (n = 1, 2, \ldots)$

Trigonometric Fourier series

Fourier series for functions of period $2l$

- The system: $1, \cos\left(\frac{\pi x}{l}\right), \sin\left(\frac{\pi x}{l}\right), \cos\left(\frac{2\pi x}{l}\right), \sin\left(\frac{2\pi x}{l}\right) \dots$
  - is composed of functions of the common period $2l$
  - is pairwise orthogonal on any interval of length $2l$
- The same considerations about the convergence of the Fourier series apply.
- $f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{n\pi x}{l}\right) + b_n \sin\left(\frac{n\pi x}{l}\right)\right)$
  - $a_n = \frac{1}{l} \int_{-l}^{l} f(x) \cos\left(\frac{n\pi x}{l}\right) dx \; (n = 0, 1, 2, \dots)$
  - $b_n = \frac{1}{l} \int_{-l}^{l} f(x) \sin\left(\frac{n\pi x}{l}\right) dx \; (n = 1, 2, \dots)$

Trigonometric Fourier series

Fourier series for functions of period 2*l*

- The complex form reads: $f(x) \sim \sum_{N=-\infty}^{\infty} c_n e^{\frac{in\pi x}{l}}$
    - $c_n = \frac{1}{2l}\int_{-l}^{l} f(x) e^{-\frac{in\pi x}{l}}$
    - $c_0 = \frac{a_0}{2}$, $c_n = \frac{1}{2}(a_n - ib_n)$, $c_{-n} = \frac{1}{2}(a_n + ib_n)$ $(n = 1, 2, \ldots)$
- If $f(x)$ is an even function: $f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{l}\right)$
    - $a_n = \frac{2}{l}\int_0^l f(x)\cos\left(\frac{n\pi x}{l}\right)dx$ $(n = 0, 1, 2, \ldots)$
- If $f(x)$ is an odd function: $f(x) \sim \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{l}\right)$
    - $b_n = \frac{2}{l}\int_0^l f(x)\sin\left(\frac{n\pi x}{l}\right)dx$ $(n = 1, 2, \ldots)$

Trigonometric Fourier series

Fourier series for functions of period T

- The system: $1, \cos\left(\frac{2\pi x}{T}\right), \sin\left(\frac{2\pi x}{T}\right), \cos\left(\frac{4\pi x}{T}\right), \sin\left(\frac{4\pi x}{T}\right) \dots$
  - is composed of functions of the common period T
  - is pairwise orthogonal on any interval of length T
- The same considerations about the convergence of the Fourier series apply.
- $f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{2\pi nx}{T}\right) + b_n \sin\left(\frac{2\pi nx}{T}\right)\right)$
  - $a_n = \frac{2}{T} \int_0^T f(x) \cos\left(\frac{2\pi nx}{T}\right) dx \; (n = 0, 1, 2, \dots)$
  - $b_n = \frac{2}{T} \int_0^T f(x) \sin\left(\frac{2\pi nx}{T}\right) dx \; (n = 1, 2, \dots)$

Trigonometric Fourier series

Fourier series for functions of period T

- The complex form reads: $f(x) \sim \sum_{N=-\infty}^{\infty} c_n e^{\frac{i2\pi nx}{T}}$
    - $c_n = \frac{1}{T}\int_0^T f(x) e^{-\frac{i2\pi nx}{T}}$
    - $c_0 = \frac{a_0}{2}$, $c_n = \frac{1}{2}(a_n - ib_n)$, $c_{-n} = \frac{1}{2}(a_n + ib_n)$ $(n = 1, 2, \ldots)$
- If $f(x)$ is an even function: $f(x) \sim \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{2\pi nx}{T}\right)$
    - $a_n = \frac{4}{T}\int_0^T f(x) \cos\left(\frac{2\pi nx}{T}\right) dx$ $(n = 0, 1, 2, \ldots)$
- If $f(x)$ is an odd function: $f(x) \sim \sum_{n=1}^{\infty} b_n \sin\left(\frac{2\pi nx}{T}\right)$
    - $b_n = \frac{2}{l}\int_0^T f(x) \sin\left(\frac{2\pi nx}{T}\right) dx$ $(n = 1, 2, \ldots)$

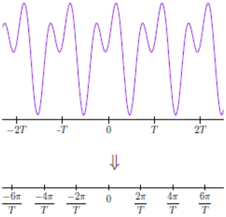
1. Periodic functions, Harmonics
2. Trigonometric Fourier Series
3. Fourier Series in multiple dimensions and the reciprocal lattice
4. Waves

Fourier series in multiple dimensions

The reciprocal lattice in one dimension

summary

- For a T-periodic function: $f(x) = \sum_n B_n e^{i\frac{2\pi nx}{T}}$
  - $B_n = \frac{1}{T}\int_a^{a+T} f(x) e^{-i\frac{2\pi nx}{T}} dx$
  - defines a 1D lattice of equally spaced points $x_n = nT$, $n \in \mathbb{Z}$
- The Fourier expansion is uniquely determined by the set of (angular) frequencies $k_n = \frac{2\pi n}{T}$, $n \in \mathbb{Z}$: the reciprocal lattice, $\mathcal{R}^*$



direct and reciprocal lattices generated by a T-periodic function

Fourier series in multiple dimensions

The reciprocal lattice in one dimension

summary

- Therefore:

$$f(x) = \sum_{k \in \mathcal{R}^*} B_k e^{ikx}$$

- with coefficients:

$$B_k = \frac{1}{T} \int_a^{a+T} f(x) e^{-ikx} dx$$

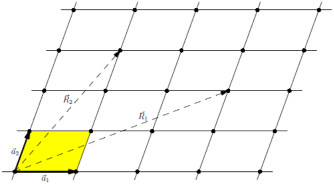
  - f defines both a direct lattice and a reciprocal lattice (Fourier space)

Fourier series in multiple dimensions

Periodicity in 2D and 3D

Periodic functions in 2D

- A 2D periodic function induces a 2D Bravais lattice:
  - generated by two primitive vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$.
  - each lattice point can be written as $\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$, $n_1, n_2 \in \mathbb{Z}$
- A 2D function is periodic on the 2D Bravais lattice if:
  - $f(\boldsymbol{r}+\boldsymbol{R}) = f(\boldsymbol{r})$, $\forall \boldsymbol{R} \in \mathcal{R}$, $\forall \boldsymbol{r} \in \mathbb{R}^2$



A 2D Bravais lattice, defined by the primitive vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$

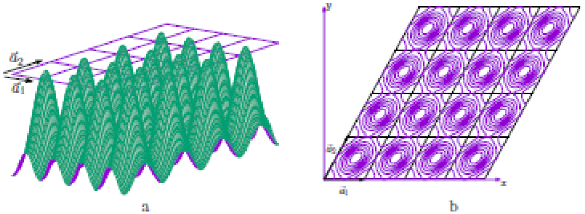
Fourier series in multiple dimensions

Periodicity in 2D and 3D

Periodic functions in 2D

- Example:

$$f(x,y) = 2g_0\left(\cos\left(\frac{2\pi}{\lambda_x}x\right) + \cos\left(\frac{2\pi}{\lambda_y}y\right)\right) + 2g_1\left(\cos\left(\frac{2\pi}{\lambda_x}x\right) + \cos\left(\frac{2\pi}{\lambda_y}y\right)\right)$$



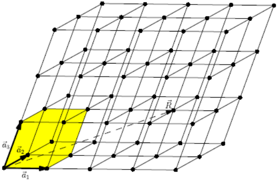
A 2D periodic function and the associated Bravais lattice

Fourier series in multiple dimensions

Periodicity in 2D and 3D

Periodic functions in 3D

- A 3D periodic function induces a 3D Bravais lattice:
  - generated by three primitive vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$
  - Each lattice point can be written as $\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$, $n_1, n_2, n_3 \in \mathbb{Z}$
- A 3D function is periodic on the 3D Bravais lattice if:
  - $f(\boldsymbol{r} + \boldsymbol{R}) = f(\boldsymbol{r})$, $\forall \boldsymbol{R} \in \mathcal{R}$, $\forall \boldsymbol{r} \in \mathbb{R}^3$



A 3D Bravais lattice, defined by the primitive vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$

Fourier series in multiple dimensions

The Fourier expansion of a function of 2 or 3 variables

General formula

Let's propose the following expansion for a periodic function f:

$$f(\boldsymbol{r}) = \sum_{\boldsymbol{k}} B_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

- We assume $B_{\boldsymbol{k}}$ independent of $\boldsymbol{r}$
- We need to:
  - find the set of allowed $\boldsymbol{k}$
  - find the coefficients $B_{\boldsymbol{k}}$
- The above formula reduces to the 1D case considered before

Fourier series in multiple dimensions

The Fourier expansion of a function of 2 or 3 variables

The $\boldsymbol{k}$ vectors (first part)

- Enforce the periodicity condition $f(\boldsymbol{r} + \boldsymbol{R}) = f(\boldsymbol{r})$:

$$e^{i\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{R})} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

  - each $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ must have the periodicity of the Bravais lattice
- Factoring the exponential:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

- fundamental constraint:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = 1$$

  - $\boldsymbol{k} \cdot \boldsymbol{R} = 2\pi n$, $n \in \mathbb{Z}$

Fourier series in multiple dimensions

The reciprocal lattice

The $\boldsymbol{k}$ vectors (first part)

- Vectors $\boldsymbol{k}$ can we written as a linear combination of a basis of $\mathbb{R}^D$ ($D = 2, 3$): $\boldsymbol{k} = \sum_{j=1}^{D} m_j \boldsymbol{b}_j,\ m_j \in \mathbb{R}$
- $\boldsymbol{R} \in \mathcal{R} \longrightarrow \boldsymbol{R} = \sum_l n_l \boldsymbol{a}_l,\ n_l \in \mathbb{Z}$, so that $\boldsymbol{k} \cdot \boldsymbol{R} = \sum_{jl} m_j n_l \boldsymbol{b}_j \cdot \boldsymbol{a}_l = 2\pi n$
- A sufficient (and necessary) condition is:

$$\begin{cases} \boldsymbol{b}_j \cdot \boldsymbol{a}_l = 2\pi\delta_{jl} \\ m_j \in \mathbb{Z} \end{cases}$$

- So that:

$$\forall \boldsymbol{R} \in \mathcal{R} \quad \boldsymbol{k} \cdot \boldsymbol{R} = \sum_{j,l} m_j n_l \boldsymbol{b}_j \cdot \boldsymbol{a}_l = 2\pi \overbrace{\sum_j m_j n_j}^{=n} = 2\pi n \quad n \in \mathbb{Z}$$

Fourier series in multiple dimensions

The reciprocal lattice

The $\boldsymbol{k}$ vectors (first part)

- $\boldsymbol{k} = \sum_{j=1}^{D} m_j \boldsymbol{b}_j$, $m_j \in \mathbb{Z}$
- Vectors $\boldsymbol{k}$ span a D-dimensional $(D = 2, 3)$ Bravais lattice: $\boldsymbol{k} \in \mathcal{R}^*$
- $\mathcal{R}^*$: reciprocal lattice associated with $\mathcal{R}$
- $\boldsymbol{b}_j$, $j = 1, \ldots, D$: primitive vectors of $\mathcal{R}^*$ (to be found later)

Fourier series in multiple dimensions

The Fourier coefficients

The $B_{\boldsymbol{k}}$ coefficients

- $f(\boldsymbol{r}) = \sum_{\boldsymbol{k}\in\mathcal{R}^*} B_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
- Multiply both sides by $e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}}$ and integrate over the volume V of the primitive cell:

$$\int_V f(\boldsymbol{r}) e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}} d\boldsymbol{r} = \sum_{\boldsymbol{k}\in\mathcal{R}^*} B_{\boldsymbol{k}} \int_V e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} d\boldsymbol{r}$$

- Using the relation $\int_V e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} d\boldsymbol{r} = V\delta_{\boldsymbol{k},\boldsymbol{k}'}$:

$$B_{\boldsymbol{k}} = \frac{1}{V}\int_V f(\boldsymbol{r}) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} d\boldsymbol{r}$$

Fourier series in multiple dimensions

The Fourier coefficients

Proof of the orthogonality condition: $\int_V e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} d\boldsymbol{r} = V\delta_{\boldsymbol{k},\boldsymbol{k}'}$

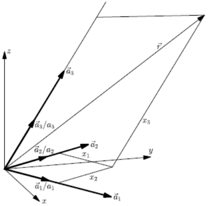
- If $\boldsymbol{k} = \boldsymbol{k}' \longrightarrow \int_V e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} d\boldsymbol{r} = \int_V d\boldsymbol{r} = V$
- If $\boldsymbol{k} - \boldsymbol{k}' = \boldsymbol{K} \neq \boldsymbol{0} \longrightarrow \int_V e^{i\boldsymbol{K}\cdot\boldsymbol{r}} d\boldsymbol{r} = \int_V e^{i\boldsymbol{K}\cdot(\boldsymbol{r}+\boldsymbol{d})} d\boldsymbol{r}, \forall \boldsymbol{d} \in \mathbb{R}^D$
    - $e^{i\boldsymbol{K}\cdot\boldsymbol{r}}$ has the periodicity of the Bravais lattice
- $\left(1 - e^{i\boldsymbol{K}\cdot\boldsymbol{d}}\right) \int_V e^{i\boldsymbol{K}\cdot\boldsymbol{r}} d\boldsymbol{r} = 0 \ \forall \boldsymbol{d} \in \mathbb{R}^D$
    - $\longrightarrow \int_V e^{i\boldsymbol{K}\cdot\boldsymbol{r}} d\boldsymbol{r} = 0$

Fourier series in multiple dimensions

The Fourier coefficients

A more rigorous proof for $\boldsymbol{k} \neq \boldsymbol{k}'$

- Let $\boldsymbol{k} = \sum_{j=1}^{D} m_j \boldsymbol{b}_j$; $\boldsymbol{k}' = \sum_{j=1}^{D} m'_j \boldsymbol{b}_j$; $\{m_j, m'_j\} \in \mathbb{Z}$; $D = 2, 3$
- Let $\boldsymbol{r} = \sum_{j=1}^{D} x_j \hat{\boldsymbol{a}}_j = \sum_{j=1}^{D} x_j \frac{\boldsymbol{a}_j}{a_j}$, $x_j \in \mathbb{R}$
  - x_j: vector's components on the $\hat{\boldsymbol{a}}_j$ axes
- $(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{r} = \boldsymbol{K} \cdot \boldsymbol{r} = 2\pi \sum_{j=1}^{D} (m_j - m'_j) \frac{x_j}{a_j}$
- Generally the reference system of $\{\hat{\boldsymbol{a}}_j\}_{j=1 \dots D}$ is not orthogonal.



The three primitive vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$ are generally non orthogonal

Fourier series in multiple dimensions

The Fourier coefficients

A more rigorous proof for $\boldsymbol{k} \neq \boldsymbol{k}'$

- Therefore:

$$\int_V e^{i\boldsymbol{K}\cdot\boldsymbol{r}} d\boldsymbol{r} = \prod_{j=1}^{D} \int_0^{a_j} e^{i2\pi(m_j - m_j')\frac{x_j}{a_j}} dx_j$$

- Since $\boldsymbol{K} \neq 0$ for at least one index n, $(m_n - m_n') \neq 0$:

$$\int_0^{a_n} e^{i2\pi(m_n - m_n')\frac{x_n}{a_n}} dx_n = 0 \longrightarrow \int_V e^{i\boldsymbol{K}\cdot\boldsymbol{r}} d\boldsymbol{r} = 0$$

Fourier series in multiple dimensions

The reciprocal lattice vectors

The $\boldsymbol{k}$ vectors (second part)

- The defining condition $\boldsymbol{b}_j \cdot \boldsymbol{a}_i = 2\pi\delta_{ij}$ gives us geometric rules.
- 2D case:
  - $\boldsymbol{b}_1 \perp \boldsymbol{a}_2$
  - $\boldsymbol{b}_2 \perp \boldsymbol{a}_1$
- 3D case:
  - $\boldsymbol{b}_1 \perp \boldsymbol{a}_2, \boldsymbol{a}_3$
  - $\boldsymbol{b}_2 \perp \boldsymbol{a}_3, \boldsymbol{a}_1$
  - $\boldsymbol{b}_3 \perp \boldsymbol{a}_1, \boldsymbol{a}_2$
- Linear systems that can be solved analytically (not instructive)
- We will use vector algebra (elegant and instructive)

Fourier series in multiple dimensions

The reciprocal lattice vectors

The 3D case

- Let's use the properties of the vector cross product $\boldsymbol{b}_i = \xi_i(\boldsymbol{a}_j \times \boldsymbol{a}_k)$:
    - a vector ⊥ to the plane spanned by $\{\boldsymbol{a}_j, \boldsymbol{a}_k\}$
- Enforcing the condition $\boldsymbol{b}_i \cdot \boldsymbol{a}_i = 2\pi \longrightarrow \xi_i = \frac{2\pi}{\boldsymbol{a}_i \cdot (\boldsymbol{a}_j \times \boldsymbol{a}_k)}$
- Therefore:

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

Fourier series in multiple dimensions

The reciprocal lattice vectors

The triple product $\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$

- Geometrically is the volume of the primitive cell.
- Can be written as the determinant of the 3×3 matrix:

$$\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

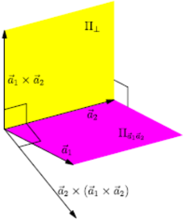
- changes sign by exchange of two rows or columns
- invariant by cyclic permutations of its rows or columns
- $\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3) = \boldsymbol{a}_2 \cdot (\boldsymbol{a}_3 \times \boldsymbol{a}_1) = \boldsymbol{a}_3 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2)$

Fourier series in multiple dimensions

The reciprocal lattice vectors

The 2D case

- Let's write 2D vectors as 3D vectors in the x–y plane:
  - $\boldsymbol{a}_1 \equiv (a_{1x}, a_{1y}, 0)$; $\boldsymbol{a}_2 \equiv (a_{2x}, a_{2y}, 0)$
  - $\boldsymbol{b}_1 \equiv (b_{1x}, b_{1y}, 0)$; $\boldsymbol{b}_2 \equiv (b_{2x}, b_{2y}, 0)$
- Define:
  - $\boldsymbol{a}_3 = \boldsymbol{a}_1 \times \boldsymbol{a}_2$
  - $\Pi_{\boldsymbol{a}_1,\boldsymbol{a}_2}$: plane spanned by $\{\boldsymbol{a}_1, \boldsymbol{a}_2\}$
  - $\Pi_\perp$ containing $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$ ($\perp \Pi_{\boldsymbol{a}_1,\boldsymbol{a}_2}$)



Fourier series in multiple dimensions

The reciprocal lattice vectors

The 2D case

- The vector $\boldsymbol{a}_2 \times (\boldsymbol{a}_1 \times \boldsymbol{a}_2) \equiv \boldsymbol{a}_2 \times \boldsymbol{a}_3$ is:
  - $\perp \boldsymbol{a}_2, \perp \Pi_\perp$
  - contanied in $\Pi_{\boldsymbol{a}_1, \boldsymbol{a}_2}$
  - cannot be $\perp \boldsymbol{a}_1$
- The condition $\boldsymbol{b}_1 \perp \boldsymbol{a}_2$ is satisfied if:
  - $\boldsymbol{b}_1 = \xi_1 \boldsymbol{a}_2 \times \boldsymbol{a}_3$
  - $\boldsymbol{b}_1 \cdot \boldsymbol{a}_1 = 2\pi \longrightarrow \xi_1 = \frac{2\pi}{\boldsymbol{a}_2 \times (\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_1}$
- Similarly $\boldsymbol{b}_2 \perp \boldsymbol{a}_1$ is satisfied if:
  - $\boldsymbol{b}_2 = \xi_2 \boldsymbol{a}_1 \times \boldsymbol{a}_3$
  - from $\boldsymbol{b}_2 \cdot \boldsymbol{a}_2 = 2\pi \longrightarrow \xi_2 = \frac{2\pi}{\boldsymbol{a}_1 \times (\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_2}$

Fourier series in multiple dimensions

The reciprocal lattice vectors

The 2D case

- We formally obtain the same results of the 3D case:

$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3}$$
$$\boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3}$$

Fourier series in multiple dimensions

The reciprocal lattice vectors

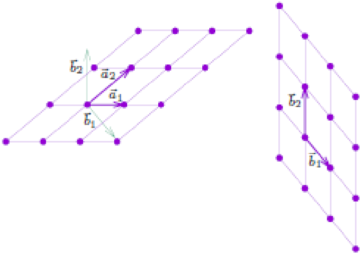
Geometrical interpretation: 2D case

- $\boldsymbol{a}_2 \times \boldsymbol{a}_3$ has the following properties:
  - $|\boldsymbol{a}_2 \times \boldsymbol{a}_3| = a_2 a_3$
  - $\perp \boldsymbol{a}_2$
  - is contained in $\Pi_{\boldsymbol{a}_1, \boldsymbol{a}_2}$
- $|\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)| = A a_3$
  - A: area of the 2D direct primitive cell
- $b_1 = |\boldsymbol{b}_1| = 2\pi \frac{a_2}{A}$
- Analogously: $b_2 = |\boldsymbol{b}_2| = 2\pi \frac{a_1}{A}$

Fourier series in multiple dimensions

The reciprocal lattice vectors

Geometrical interpretation: 2D case

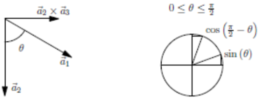


how to build $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ primitive vectors of the reciprocal space

Fourier series in multiple dimensions

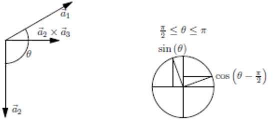
The reciprocal lattice vectors

Geometrical interpretation: 2D case



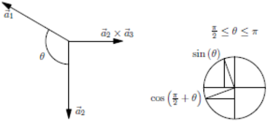
$$|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\, a_1 \overbrace{a_2 a_3}^{|\vec{a}_2 \times \vec{a}_3|} \overbrace{\cos\left(\frac{\pi}{2} - \theta\right)}^{\sin(\theta)} \,|$$

$$= |\, \overbrace{a_1 a_2 \sin(\theta)}^{A} a_3 \,| = A a_3$$



$$|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\, a_1 \overbrace{a_2 a_3}^{|\vec{a}_2 \times \vec{a}_3|} \overbrace{\cos\left(\theta - \frac{\pi}{2}\right)}^{\sin(\theta)} \,|$$

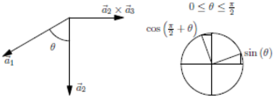
$$= |\, \overbrace{a_1 a_2 \sin(\theta)}^{A} a_3 \,| = A a_3$$



$$|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\, a_1 \overbrace{a_2 a_3}^{|\vec{a}_2 \times \vec{a}_3|} \cos\left(2\pi - \frac{\pi}{2} - \theta\right) \,|$$

$$= |\, a_1 a_2 a_3 \cos\left(-\frac{\pi}{2} - \theta\right) \,| = |\, a_1 a_2 a_3 \overbrace{\cos\left(\frac{\pi}{2} + \theta\right)}^{-\sin(\theta)} \,|$$

$$= |\, \overbrace{a_1 a_2 (-\sin(\theta))}^{-A} a_3 \,| = A a_3$$



$$|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\, a_1 \overbrace{a_2 a_3}^{|\vec{a}_2 \times \vec{a}_3|} \overbrace{\cos\left(\frac{\pi}{2} + \theta\right)}^{-\sin(\theta)} \,|$$

$$= |\, \overbrace{a_1 a_2 (-\sin(\theta))}^{-A} a_3 \,| = A a_3$$

Fourier series in multiple dimensions

The reciprocal lattice vectors

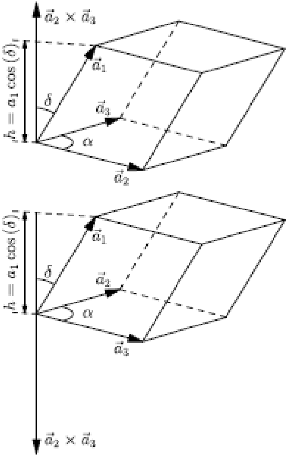
Geometrical interpretation: 3D case

- $\boldsymbol{b}_1$ is $\perp$ to the face of the direct primitive cell spanned by $\{\boldsymbol{a}_1, \boldsymbol{a}_2\}$
- $b_1 = |\boldsymbol{b}_1| = 2\pi \frac{A_{23}}{V}$
    - A_{23}: area of the face
    - V: volume of the direct primitive cell
- $b_2 = |\boldsymbol{b}_2| = 2\pi \frac{A_{13}}{V}$
- $b_3 = |\boldsymbol{b}_3| = 2\pi \frac{A_{12}}{V}$

Fourier series in multiple dimensions

The reciprocal lattice vectors

Geometrical interpretation: 3D case



$$|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\ a_1\,(a_2 a_3 \sin(\alpha)) \cos(\delta)\ |$$

$$= |\ \overbrace{a_1 \cos(\delta)}^{h}\overbrace{a_2 a_3 \sin(\alpha)}^{A_{23}}\ | = |h A_{23}| = V$$

$$|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = |\ a_1\,(a_2 a_3 \sin(\alpha)) \cos(\pi - \delta)\ |$$

$$= |\ \overbrace{-a_1 \cos(\delta)}^{-h}\overbrace{a_2 a_3 \sin(\alpha)}^{A_{23}}\ | = |-h A_{23}| = V$$

Fourier series in multiple dimensions

Summary

- The Fourier series expansion for a periodic function $f(\boldsymbol{r})$, defining a Bravais lattice $\mathcal{R}$, reads:

$$f(\boldsymbol{r}) = \sum_{\boldsymbol{k} \in \mathcal{R}^*} B_{\boldsymbol{k}} e^{i \boldsymbol{k} \cdot \boldsymbol{r}}$$

  - $\boldsymbol{k}$'s define the reciprocal lattice $\mathcal{R}^*$
- With coefficients:

$$B_{\boldsymbol{k}} = \frac{1}{V} \int_V f(\boldsymbol{r}) e^{-i \boldsymbol{k} \cdot \boldsymbol{r}} d\boldsymbol{r}$$

  - V: volume of the primitive cell of the direct lattice $\mathcal{R}$

Fourier series in multiple dimensions

Summary

- $\mathcal{R}^*$, is spanned by primitive vectors $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$:

$$\boldsymbol{k} = \sum_j m_j \boldsymbol{b}_j \qquad m_j \in \mathbb{Z}$$

- defined with respect to the direct lattice primitive vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ $(\boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij})$:

$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3}$$
$$\boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3}$$
$$\boldsymbol{b}_3 = 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3}$$

  - $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{a}_3 = \boldsymbol{a}_1 \times \boldsymbol{a}_2$ in 2D

Fourier series in multiple dimensions

An equivalent definition of the reciprocal lattice

the reciprocal lattice

Given a direct Bravais lattice $\mathcal{R}$, whose points are the set of vectors $\boldsymbol{R}$, the reciprocal lattice $\mathcal{R}^*$ associated with it is composed of all vectors $\boldsymbol{k}$ such that $\boldsymbol{k} \cdot \boldsymbol{R} = 2\pi n,\ n \in \mathbb{Z},\ \forall \boldsymbol{R} \in \mathcal{R}$:

- $\boldsymbol{k} \in \mathcal{R}^* \iff \boldsymbol{k} \cdot \boldsymbol{R} = 2\pi n,\ n \in \mathbb{Z},\ \forall \boldsymbol{R} \in \mathcal{R}$
- $\Rightarrow$ seen before
- $\Leftarrow$: prove that $\boldsymbol{d} \notin \mathcal{R}^* \Rightarrow \exists \boldsymbol{R} \in \mathcal{R} : \boldsymbol{d} \cdot \boldsymbol{R} = 2\pi x\ x \notin \mathbb{Z}$
    - $\boldsymbol{d} = x_j \boldsymbol{b}_j + \sum_{\substack{i=1 \\ i \neq j}} x_i \boldsymbol{b}_i$ with $x_j \notin \mathbb{Z}$
    - for $\boldsymbol{a}_j \in \mathcal{R}$, $\boldsymbol{d} \cdot \boldsymbol{a}_j = 2\pi x_j$

Fourier series in multiple dimensions

Symmetry properties

real, even and odd functions

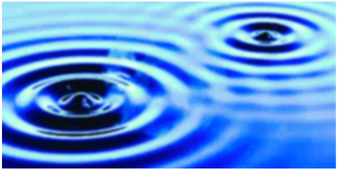
- $f(\boldsymbol{r})$ is real: $f(\boldsymbol{r})^* = f(\boldsymbol{r}) \iff B_{-\boldsymbol{k}} = B^*_{\boldsymbol{k}}$
- $f(\boldsymbol{r})$ is even: $f(-\boldsymbol{r}) = f(\boldsymbol{r}) \Rightarrow B_{-\boldsymbol{k}} = B_{\boldsymbol{k}}$
  - if $f(\boldsymbol{r})$ is real, $B_{\boldsymbol{k}}$ are real
- $f(\boldsymbol{r})$ is odd: $f(-\boldsymbol{r}) = -f(\boldsymbol{r}) \Rightarrow B_{-\boldsymbol{k}} = -B_{\boldsymbol{k}}$
  - if $f(\boldsymbol{r})$ is real, $B_{\boldsymbol{k}}$ are imaginary

Waves

Generalities

Definition and examples

- A wave is a perturbation of a physical quantity (field) which propagates with a given velocity
    - region: can be mono-,bi-,tridimensional
    - physical quantity: can be a scalar or a vector
    - perturbation: change from a reference value
- Examples: water waves (travelling waves)
    - perturbation: height of the surface w.r.t. an average value
    - region: sea, lake, . . .



example of waves: water waves

Waves

Generalities

Definition and examples

- Example of stationary waves: guitar string in motion
  - perturbation: displacement of the string from its rest position
  - region: the string
  - its ends are fixed

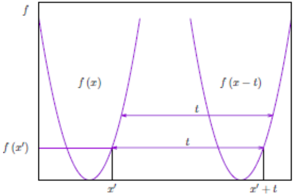
example of waves: water waves

Waves

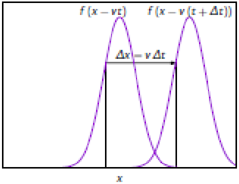
Traveling waves

Traveling waves in one dimension

- A function of two variables, space and time, $u(x,t)$
  - Maps (x,t) to a field (scalar or vector)
- Generic form: $u(x,t) = f(x \pm vt)$
  - v: velocity with which the perturbation propagates
  - to the positive x-axis (-) or negative (+)



graph of $f(x-t)$ compared to $f(x)$



v is the velocity of the wave

Waves

Traveling waves

Sinusoidal Traveling waves in one dimension

- The simplest form for a sinusoidal periodic wave moving right is:

$$u(x,t) = A\cos\left(\frac{2\pi}{\lambda}(x - vt) + \Phi_0\right)$$

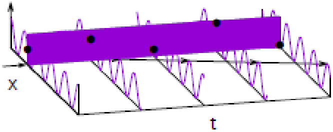
  - argument of the cos function: phase
  - the wave propagates with a constant velocity v, periodic in both x and t
  - A: amplitude (maximum variation).
  - the motion is restricted in the interval $[-A, A]$
  - Φ_0: initial phase ($u(x=0,t=0) = A\cos\Phi_0$).

Waves

Sinusoidal Traveling waves in one dimension

space and time periods

- Since the wave is periodic in both x and t, there are two periods
- Spatial period: λ (wavelength)
  - wave number: $k = \frac{2\pi}{\lambda}$: phase change (in rad.) per unit change of x at fixed time
- Time period: $T = \frac{\lambda}{v} = \frac{1}{\nu}$
  - ν: frequency
  - $\omega = 2\pi\nu = \frac{2\pi\lambda}{v}$: angular frequency
- More compactly: $u(x,t) = A\cos\left(kx - \omega t\right)$



$u(x,t) = A\cos\frac{2\pi}{\lambda}(x - vt)$

Waves

Stationary waves in one dimension

properties

- The simplest form for a stationary sinusoidal periodic wave is:

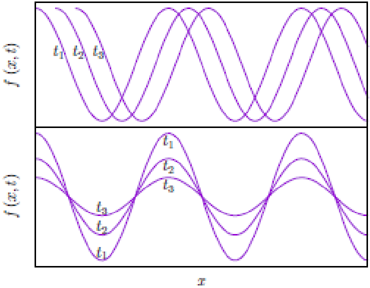
$$u(x,t) = A\cos(kx)\cos(\omega t)$$

- its graph does not translate in time
- spatial and temporal parts are separated
- nodes do not change in time
  - $x_n = \frac{1}{k}(2n+1)\frac{\pi}{2}$
- at $x_0 \neq x_n \longrightarrow u(x_0,t) = A'(x_0)\cos(\omega t)$
  - periodic motion restricted on $[-A'(x_0), A'(x_0)]$

Waves

Waves in one dimension

Travelling vs stationary waves



traveling (up) vs stationary (down) wave, for $t_1 < t_2 < t_3$

Waves

Plane waves

Sinusoidal traveling waves 2D and 3D

- We will consider sinusoidal periodic traveling waves of the form:

$$u(\boldsymbol{r}, t) = A\cos(k\boldsymbol{r} \cdot \hat{\boldsymbol{n}} - \omega t)$$

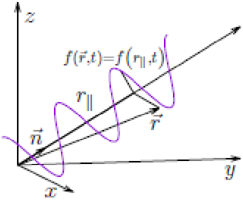
- $\boldsymbol{r}$: Position vector, (x, y, z).
- $\hat{\boldsymbol{n}}$: Unit vector in the direction of propagation of the wave.
- At fixed $\boldsymbol{r}_0$: periodic motion of frequency ω
- plane waves: points of constant phase are planes $\perp$ $\hat{\boldsymbol{n}}$
  - set $\boldsymbol{r} = \boldsymbol{r}_\parallel + \boldsymbol{r}_\perp$
  - $u(\boldsymbol{r}, t) = u(r_\parallel, t) = A\cos\left(kr_\parallel - \omega t\right)$

Waves

Plane waves

Sinusoidal traveling waves 2D and 3D

- Effectively a 1D wave moving along the direction $\hat{\boldsymbol{n}}$.
- Wavenumber depends on the direction: $kr_{\parallel}$
- Defines a corresponding wavelength in the direction of $\hat{\boldsymbol{n}}$: $k = \frac{2\pi}{\lambda}$

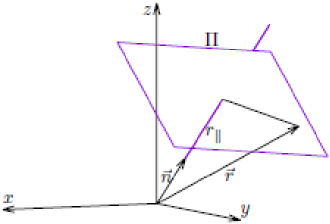


Waves

Plane waves

Wave fronts

- A wave front is the locus of space points with constant phase at a given time.
- For plane waves, these are planes Π orthogonal to $\hat{\boldsymbol{n}}$
- $\forall \boldsymbol{r} \in \Pi : \quad k\boldsymbol{r} \cdot \hat{\boldsymbol{n}} - \omega t = k\boldsymbol{r}_{\|} - \omega t = \text{const}$
- All points on Π share the same distance $r_{\|}$ from the origin.



plane Π is a wave front

Waves

Plane waves

Wave fronts spacing

- An infinite family of wave fronts exists, spaced by λ:

$$|(kr_{\parallel,1} - \omega t) - (kr_{\parallel,2} - \omega t)| = 2\pi$$

- Solving for the distance between consecutive fronts:

$$\Delta r_{\parallel} = r_{\parallel,1} - r_{\parallel,2} = \frac{2\pi}{k} = \lambda$$

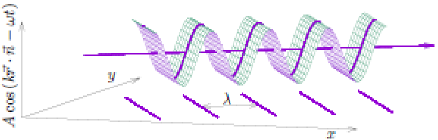
- The spacing equals the wavelength λ along $\hat{\boldsymbol{n}}$.

Waves

Plane waves

Propagation direction

- If Π is a wave front, $\forall \boldsymbol{r} \in \Pi$, $kr_{\|} - \omega t = Q$ (constant)
- It follows that $r_{\|} = \frac{Q}{k} + \frac{\omega}{k} t$
    - the palen moves aways from the origin at a constant $v = \frac{dr_{\|}}{dt} = \frac{\omega}{k} = \frac{\lambda}{T}$
- For a bidimensional plane wave, wavefronts are straight lines
- From now on, define $\boldsymbol{k} = k\hat{\boldsymbol{n}}$



a bidimensional plane wave at a fixed t

Waves

Plane waves

Bravais lattice for the spatial part of a plane wave

- The spatial part is a 2D or 3D periodic function: it defines a Bravais lattice
- Put $u(\boldsymbol{r}, 0) = A\cos(\boldsymbol{k}\cdot\boldsymbol{r})$, $\hat{\boldsymbol{n}} = (n_x, n_y, n_z)$, $\boldsymbol{r} = (x, y, z)$:

$$u(\boldsymbol{r}, 0) = A\cos\left[2\pi\left(\frac{1}{\lambda_x}, \frac{1}{\lambda_y}, \frac{1}{\lambda_z}\right)\cdot(x, y, z)\right]$$

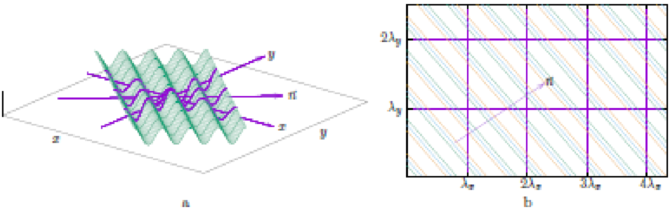
  - $\lambda_x = \frac{\lambda}{n_x}, \ldots$ wavelengths in the directions of the coordinate axes

Waves

Plane waves

Bravais lattice for the spatial part of a plane wave

- $u(\boldsymbol{r}, 0)$ is periodic on a Bravais lattice defined by the primitive vectors $\boldsymbol{a}_x = \lambda_x(1,0,0)$, $\boldsymbol{a}_y = \lambda_y(0,1,0)$,$\boldsymbol{a}_z = \lambda_z(0,0,1)$



a bidimensional plane wave at a fixed t and its Bravais lattice

Waves

Stationary plane waves

2D or 3D stationary plane wave

- Similarly to the 1D case, for 2D and 3D stationary plane waves spatial and temporal parts are separated:

$$u(\boldsymbol{r}, t) = A\cos(\boldsymbol{k}\cdot\boldsymbol{r})\cos(\omega t)$$

- Nodes are straight lines (2D) or planes (3D):
  - 2D: $y = \frac{2n+1}{k_y}\frac{\pi}{2} - \frac{k_x}{k_y}x$
  - 3D: $\boldsymbol{k}\cdot\boldsymbol{r} = (2n+1)\frac{\pi}{2}$, plane $\perp$ $\boldsymbol{k}$
- At fixed $\boldsymbol{r}_0$: $-A\cos(\boldsymbol{k}\cdot\boldsymbol{r}_0) < u(\boldsymbol{r}_0, t) < A\cos(\boldsymbol{k}\cdot\boldsymbol{r}_0)$

Waves

Traveling plane waves

The complex exponential form

- A traveling plane wave can be written as the real part of a complex exponential:

$$u(\boldsymbol{r}, t) = \mathfrak{Re}\left[Ae^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)}\right]$$

- Algebraic manipulations are significantly easier: perform calculations with complex exponentials, then extract the real part.
- The term plane wave is used also to refer to the spatial part of a plane wave.
    - the Fourier expansion is also sometimes termed plane waves expansion

Waves

Traveling plane waves

Example

- Turn the sum of two plane waves of the same frequency and wavelength, but different amplitudes and initial phases, into a single plane wave with the same frequency and wavelength of the two original waves:

$$\begin{aligned} & A_1 \cos\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_1\right) \pm A_2 \cos\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_2\right) \\ = \; & \sqrt{\left(A_1\cos\phi_1 \pm A_2\cos\phi_2\right)^2+\left(A_1\sin\phi_1 \pm A_2\sin\phi_2\right)^2} \\ & \cos\left(x+\tan^{-1}\left(\frac{A_1\sin\phi_1 \pm A_2\sin\phi_2}{A_1\cos\phi_1 \pm A_2\cos\phi_2}\right)\right) \end{aligned}$$

- $x=\boldsymbol{k}\cdot\boldsymbol{r}-\omega t$
- This covers also the cases:
  - $A_1 \sin\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_1\right) \pm A_2 \sin\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_2\right)$
  - $A_1 \cos\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_1\right) \pm A_2 \sin\left(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t+\phi_2\right)$

Waves

Stationary plane waves

The complex exponential form

- Since space and time parts are separated, the spatial part is purely real or purely imaginary and the temporal part is a complex exponential:

$$u(\boldsymbol{r}, t) = \mathfrak{Re}\left[A\cos(\boldsymbol{k}\cdot\boldsymbol{r})\exp(-i\omega t)\right]$$

$$u(\boldsymbol{r}, t) = \mathfrak{Re}\left[iA\sin(\boldsymbol{k}\cdot\boldsymbol{r})\exp(-i\omega t)\right]$$