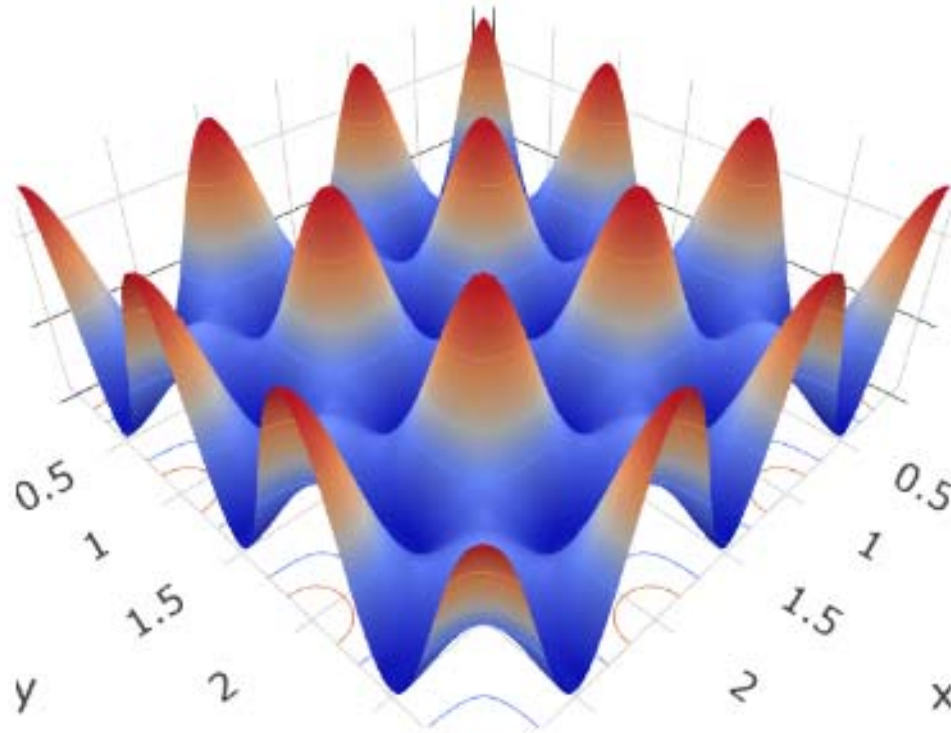


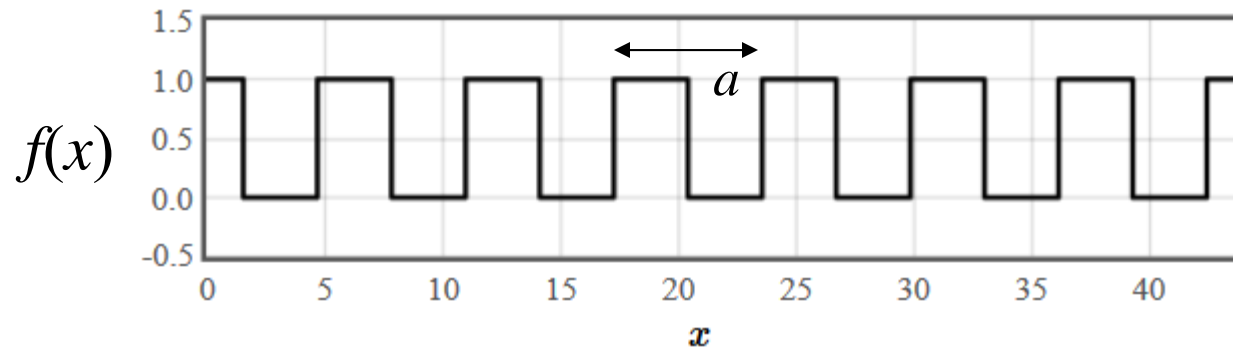
Fourier Series in one dimension

Periodic functions



Use a Fourier series to describe periodic functions

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

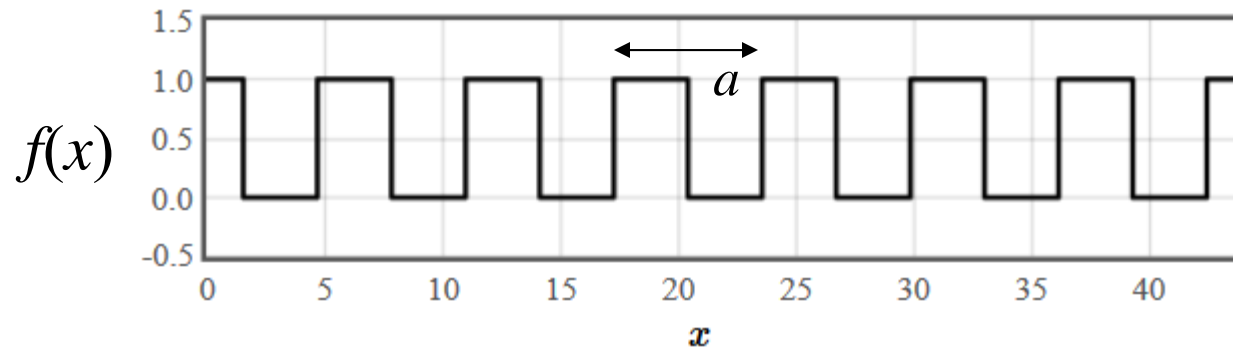
$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

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

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

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

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

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

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

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

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

reciprocal lattice vector

Determine the Fourier coefficients in 1-D

$$f(x) = \sum_G f_G e^{iGx}$$

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

$$\begin{aligned} \int_{\text{unit cell}} f(x) e^{-iG'x} dx &= \int_{\text{unit cell}} \sum_G e^{i(G-G')x} dx \\ &= \sum_G \int_{\text{unit cell}} \cos((G-G')x) + i \sin((G-G')x) dx = f_{G'} a \end{aligned}$$

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

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

Fourier series in 1-D, 2-D, or 3-D

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

Reciprocal lattice vectors G
(depend on the Bravais lattice)

Structure factors
(complex numbers)

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

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

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