An Introduction to

Fourier Transforms

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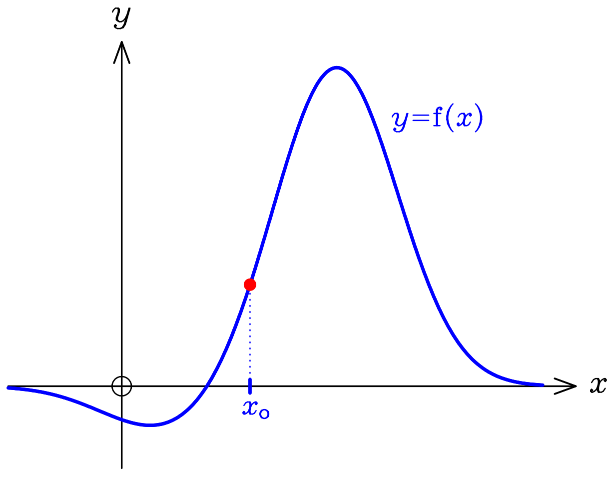
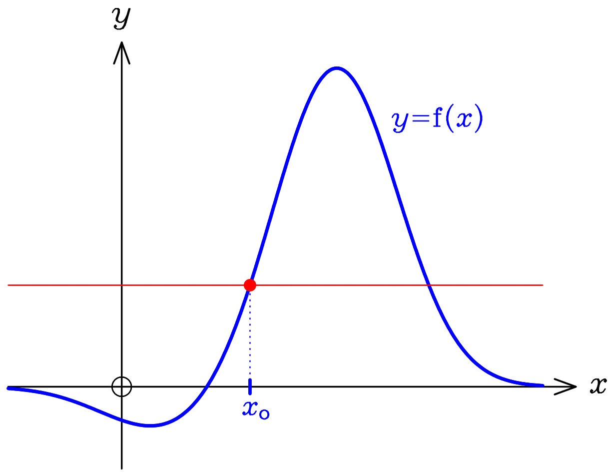
Outline

- Approximating functions
  - Taylor series
  - Fourier series → transform
- Some formal properties
  - Symmetry
  - Convolution theorem
  - Auto-correlation function
- Physical insight
  - Fourier optics

Taylor Series

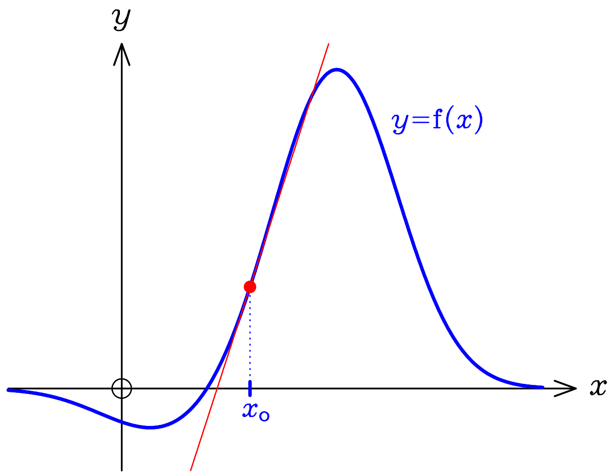


Taylor Series (0)



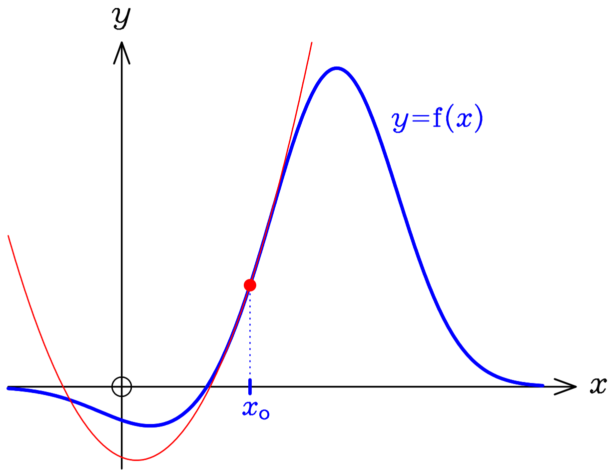
- $\mathrm{f}(x) \approx a_0$

Taylor Series (1)



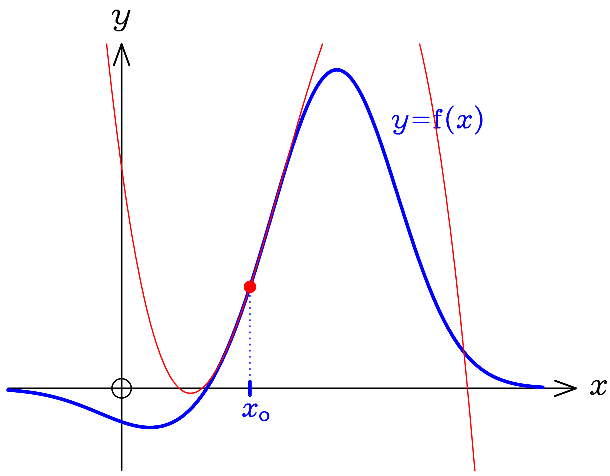
- $\mathrm{f}(x) \approx a_0 + a_1(x - x_o)$

Taylor Series (2)



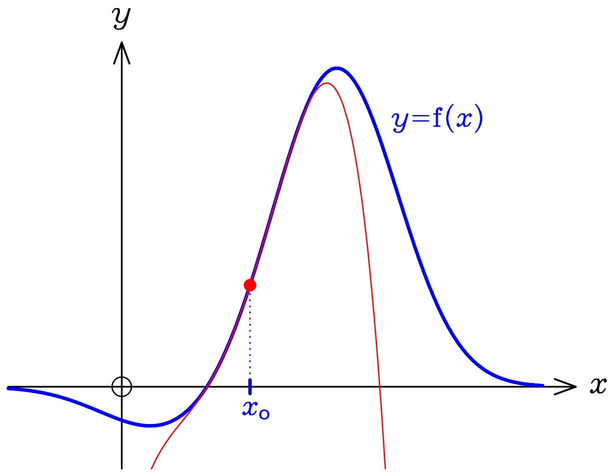
- $\mathrm{f}(x) \approx a_0 + a_1(x - x_o) + a_2(x - x_o)^2$

Taylor Series (3)



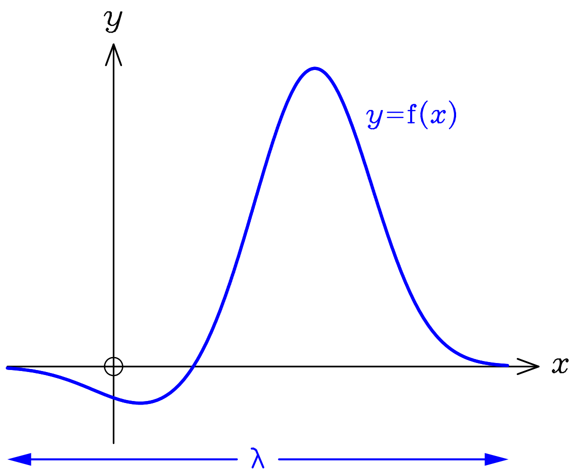
- $\mathrm{f}(x) \approx a_0 + a_1(x - x_o) + a_2(x - x_o)^2 + a_3(x - x_o)^3$

Taylor Series (4)



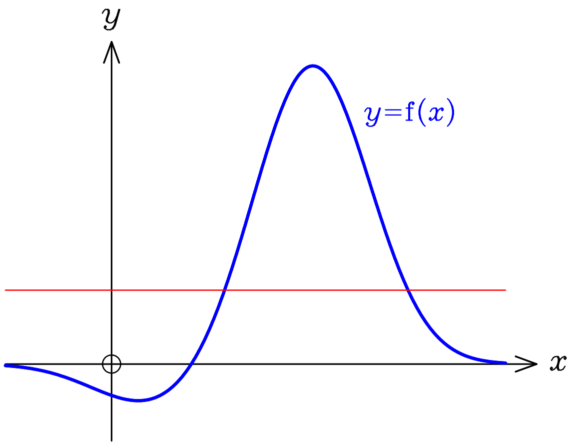
- $\mathrm{f}(x) \approx a_0 + a_1(x-x_o) + a_2(x-x_o)^2 + a_3(x-x_o)^3 + a_4(x-x_o)^4$

Fourier Series



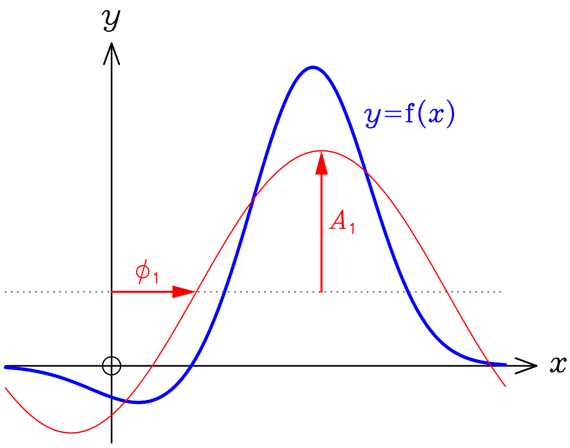
- Periodic: $\mathrm{f}(x) = \mathrm{f}(x+\lambda)$ $k = \dfrac{2\pi}{\lambda}$ (wavenumber)

Fourier Series (0)



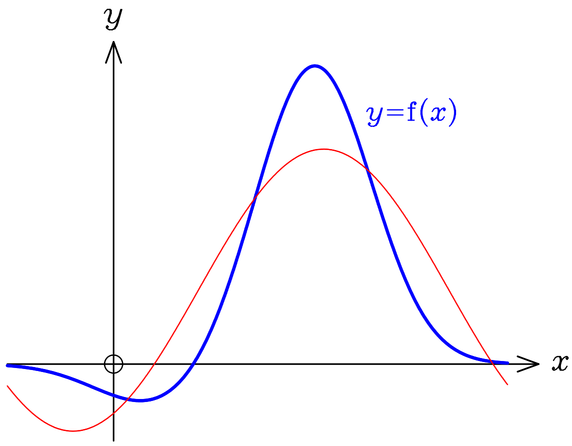
- $f(x) \approx \frac{a_0}{2}$

Fourier Series (1)



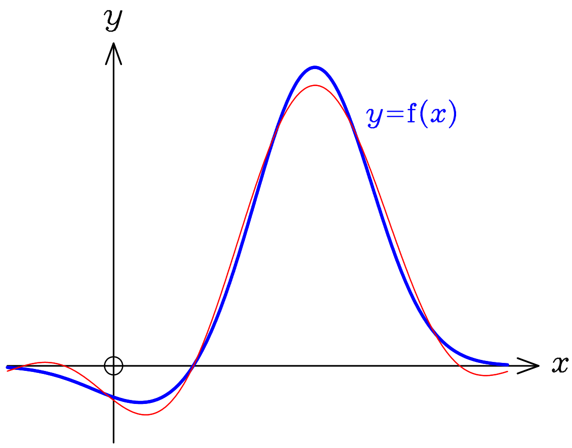
- $f(x) \approx \frac{a_0}{2} + A_1 \sin(kx+\phi_1)$

Fourier Series (1)



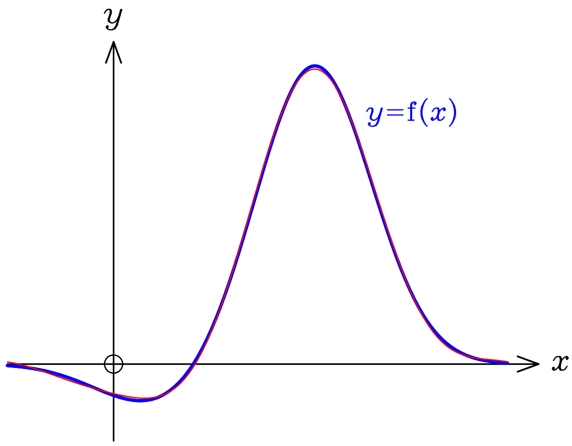
- $\mathrm{f}(x) \approx \frac{a_0}{2} + a_1\cos(kx) + b_1\sin(kx)$

Fourier Series (2)



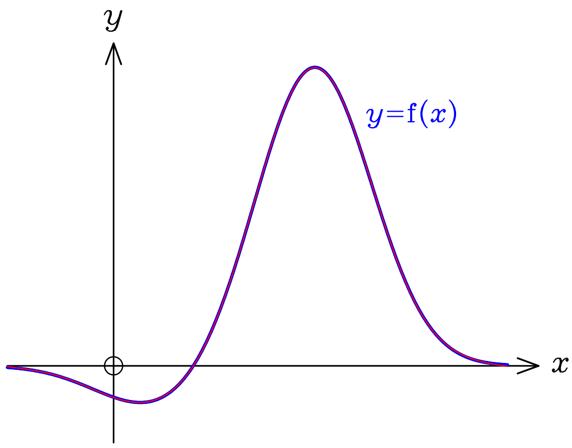
- $\mathrm{f}(x) \approx \frac{a_0}{2} + a_1\cos(kx) + a_2\cos(2kx) + b_1\sin(kx) + b_2\sin(2kx)$

Fourier Series (3)



- $\mathrm{f}(x) \approx \frac{a_0}{2} + a_1\cos(kx) + a_2\cos(2kx) + a_3\cos(3kx)$
  $+ b_1\sin(kx) + b_2\sin(2kx) + b_3\sin(3kx)$

Fourier Series (4)



- $\mathrm{f}(x) \approx \frac{a_0}{2} + a_1\cos(kx) + a_2\cos(2kx) + a_3\cos(3kx) + a_4\cos(4kx)$
  $+ b_1\sin(kx) + b_2\sin(2kx) + b_3\sin(3kx) + b_4\sin(4kx)$

Taylor Versus Fourier Series

- Taylor: $f(x) = \sum_{n=0}^{\infty} a_n (x-x_o)^n$ $\qquad |x-x_o|<R$
  - $a_n = \frac{1}{n!} \frac{d^n f}{dx^n}\Big|_{x_o}$

- Fourier: $f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(nkx) + b_n \sin(nkx)$ $\qquad k = \frac{2\pi}{\lambda}$
  - $a_n = \frac{2}{\lambda} \int_0^{\lambda} f(x) \cos(nkx)\, dx$ and $b_n = \frac{2}{\lambda} \int_0^{\lambda} f(x) \sin(nkx)\, dx$

Complex Fourier Series

$$\boxed{e^{i\theta} = \cos\theta + i\sin\theta} \quad , \quad \text{where } i^2 = -1$$

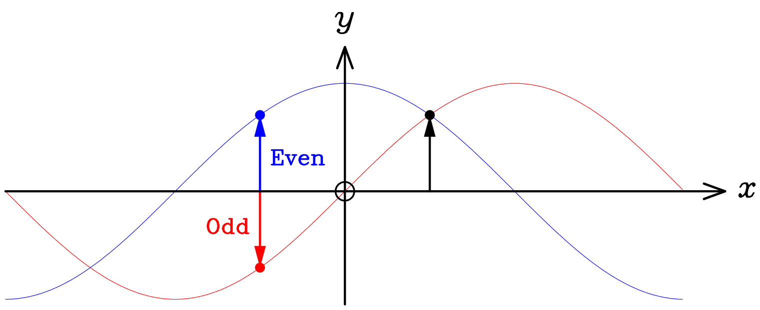
- Fourier: $f(x) = \sum_{n=-\infty}^{\infty} c_n e^{inkx}$
  - $c_n = \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} f(x)\, e^{-inkx}\, dx$
    - $c_{\pm n} = \frac{1}{2}(a_n \mp i b_n)$ for $n \geqslant 1$
    - $c_0 = a_0$

Fourier Transform

- As $\lambda \to \infty$, so that $k \to 0$ and $\mathrm{f}(x)$ is non-periodic,
  - $$\sum_{n=-\infty}^{\infty} c_n \, \mathrm{e}^{\mathrm{i}nkx} \longrightarrow \int_{-\infty}^{\infty} c(q) \, \mathrm{e}^{\mathrm{i}qx} \, \mathrm{d}q$$
- In the continuum limit,
  - Fourier sum (series) $\longrightarrow$ Fourier integral (transform)
  - $$\mathrm{f}(x) = \int_{-\infty}^{\infty} \mathrm{F}(q) \, \mathrm{e}^{\mathrm{i}qx} \, \mathrm{d}q$$
    - $$\mathrm{F}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{f}(x) \, \mathrm{e}^{-\mathrm{i}qx} \, \mathrm{d}x$$

Some Symmetry Properties

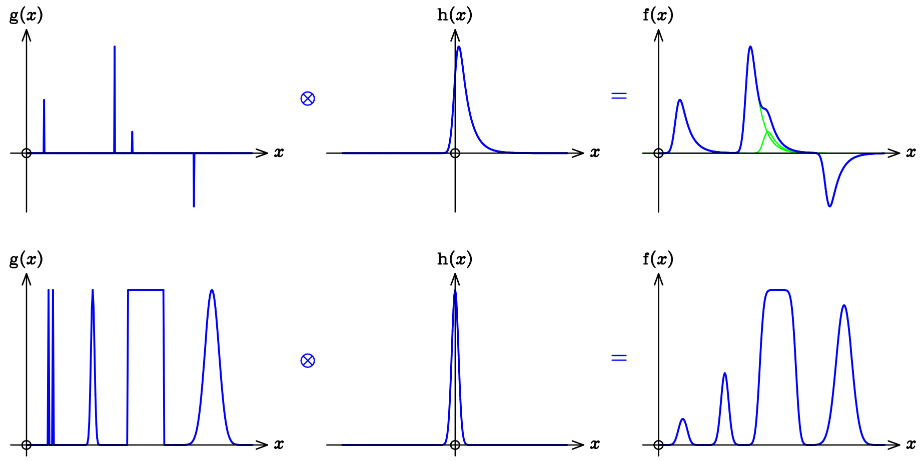
- Even: $\mathrm{f}(x) = \mathrm{f}(-x) \iff \mathrm{F}(q) = \mathrm{F}(-q)$
- Odd: $\mathrm{f}(x) = -\mathrm{f}(-x) \iff \mathrm{F}(q) = -\mathrm{F}(-q)$



- Real: $\boxed{\mathrm{f}(x) = \mathrm{f}(x)^* \iff \mathrm{F}(q) = \mathrm{F}(-q)^*}$ (Friedel pairs)

Convolution

$$f(x) = g(x) \otimes h(x) = \int_{-\infty}^{\infty} g(t)\, h(x-t)\, dt$$



Convolution Theorem

$$\boxed{f(x) = g(x) \otimes h(x) \iff F(q) = \sqrt{2\pi}\, G(q) \times H(q)}$$

$$f(x) = g(x) \times h(x) \iff F(q) = \frac{1}{\sqrt{2\pi}}\, G(q) \otimes H(q)$$

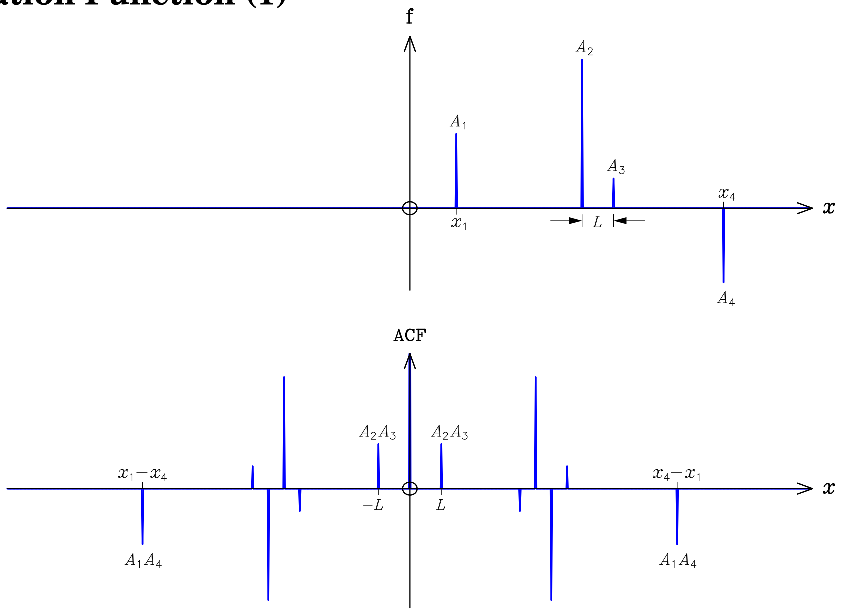
Auto-correlation Function

$$\int_{-\infty}^{\infty} \mathrm{F}(q)\, \mathrm{e}^{\mathrm{i}qx}\, \mathrm{d}q \;=\; \mathrm{f}(x)$$

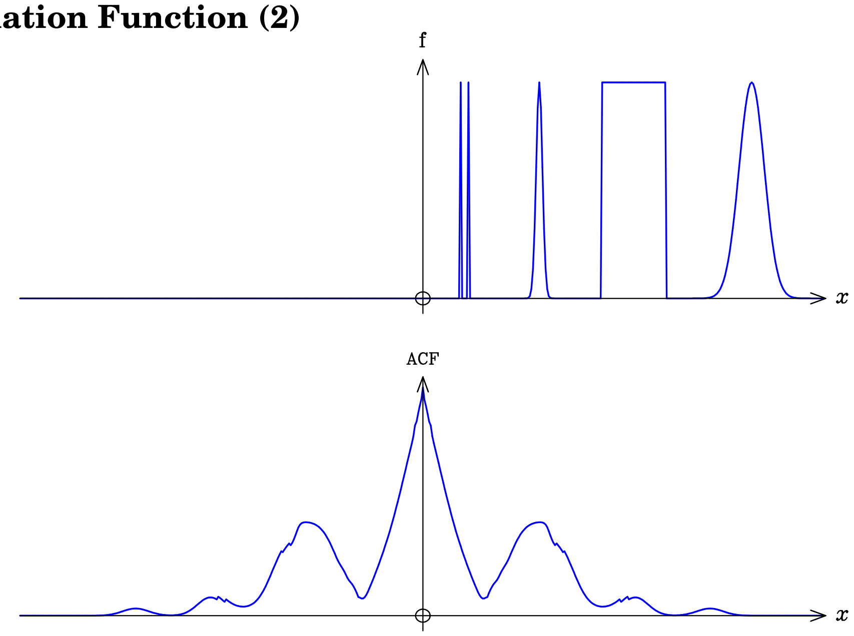
- $$\boxed{\int_{-\infty}^{\infty} \left|\mathrm{F}(q)\right|^2 \mathrm{e}^{\mathrm{i}qx}\, \mathrm{d}q \;=\; \int_{-\infty}^{\infty} \mathrm{f}(t)^*\, \mathrm{f}(x+t)\, \mathrm{d}t} \;=\; \mathrm{ACF}(x)$$

    - Patterson map

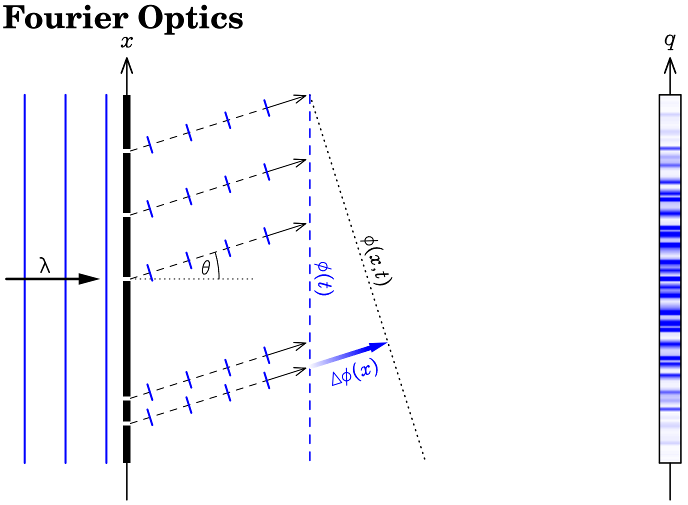
Auto-correlation Function (1)



Auto-correlation Function (2)



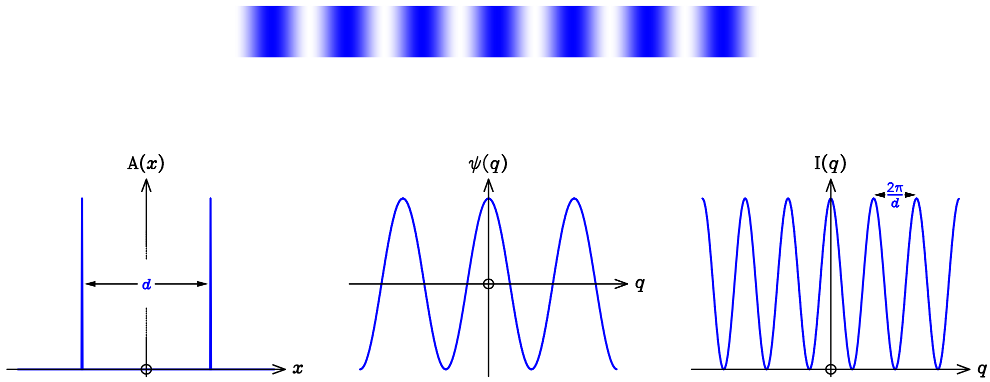
Fourier Optics



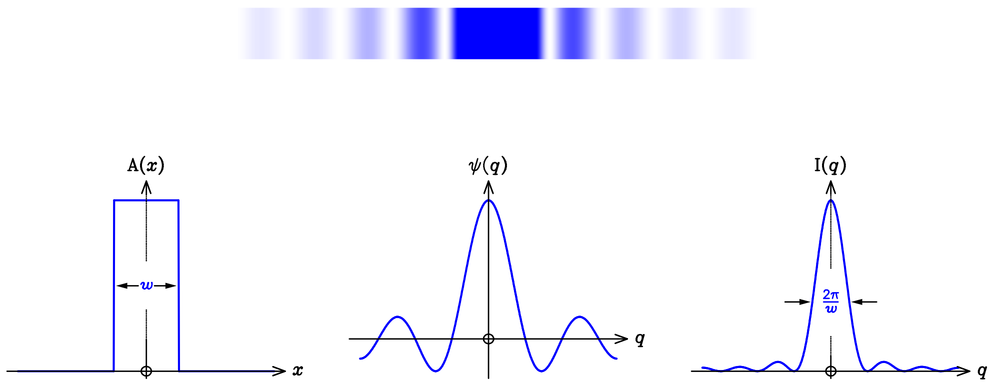
$$\mathrm{I}(q) = \left|\psi(q)\right|^2$$

- Fraunhofer: $\psi(q) = \psi_o \int_{-\infty}^{\infty} \mathrm{A}(x)\, \mathrm{e}^{\mathrm{i}\, qx}\, \mathrm{d}x$ where $q = \dfrac{2\pi \sin\theta}{\lambda}$

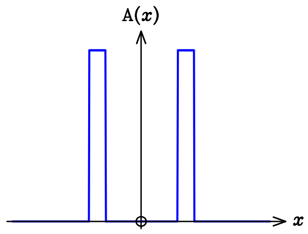
Young's Double Slits



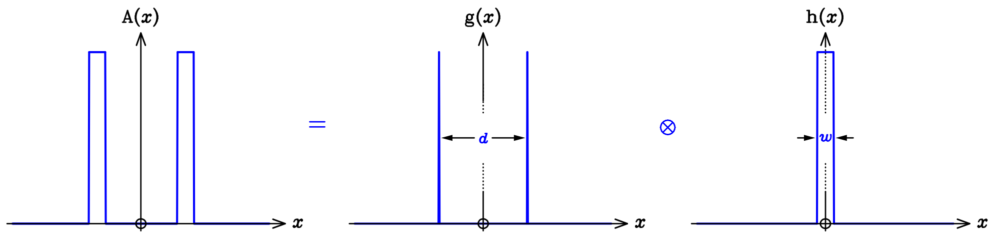
Single Wide Slit



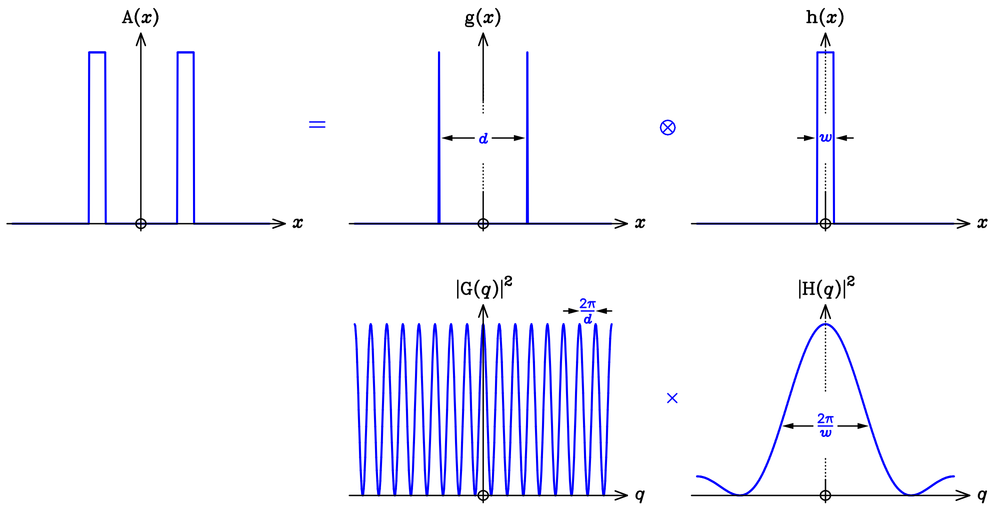
Two Wide Slits (0)



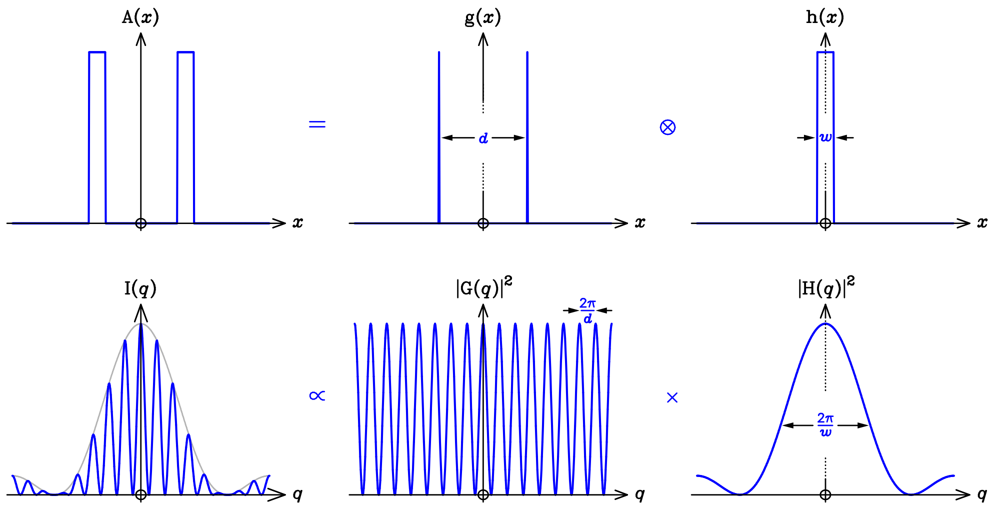
Two Wide Slits (1)



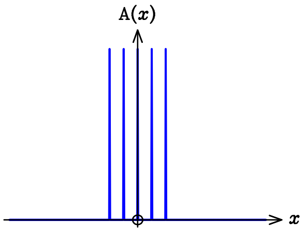
Two Wide Slits (2)



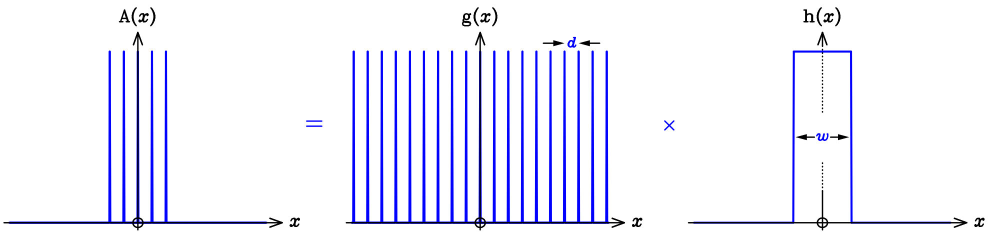
Two Wide Slits (3)



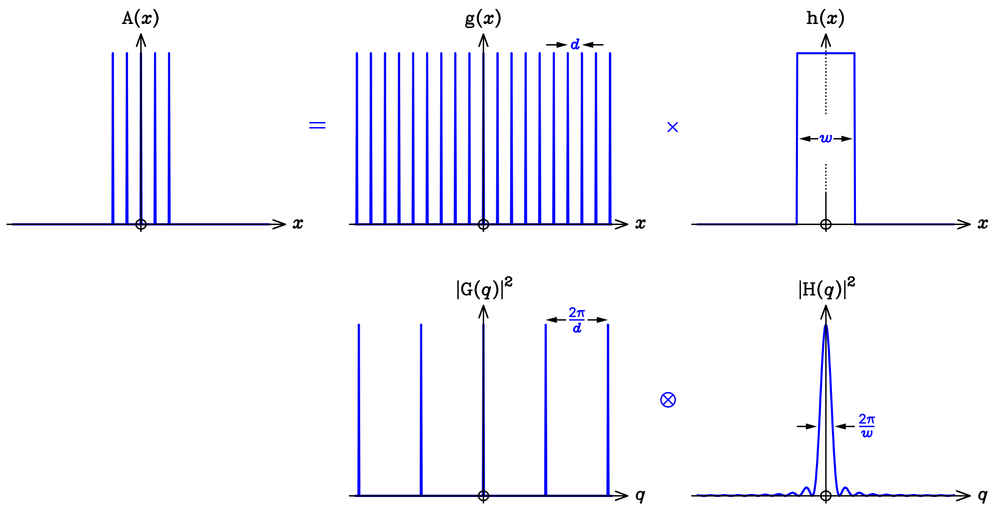
Finite Grating (0)



Finite Grating (1)



Finite Grating (2)



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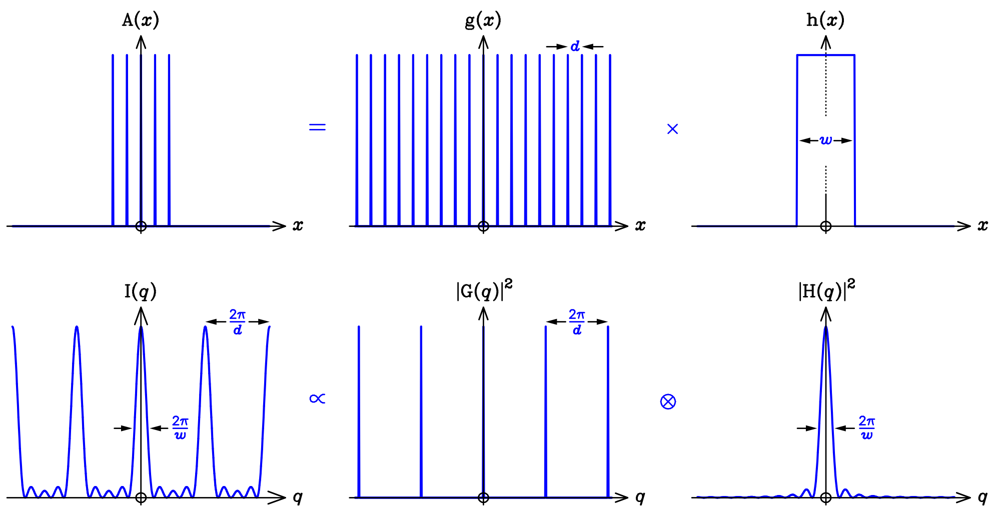

Write up of this Talk!

- Elementary Scattering Theory *for X-ray and Neutron Users* (Chapter 2)
  D. S. Sivia (2011), Oxford University Press

- Foundations of Science Mathematics (Chapter 15)
  Oxford Chemistry Primers Series, vol. **77** (and **82**)
  D. S. Sivia and *S. G. Rawlings* (1999), Oxford University Press

The phaseless Fourier problem

The phaseless Fourier problem