

An Introduction to
Fourier Transforms

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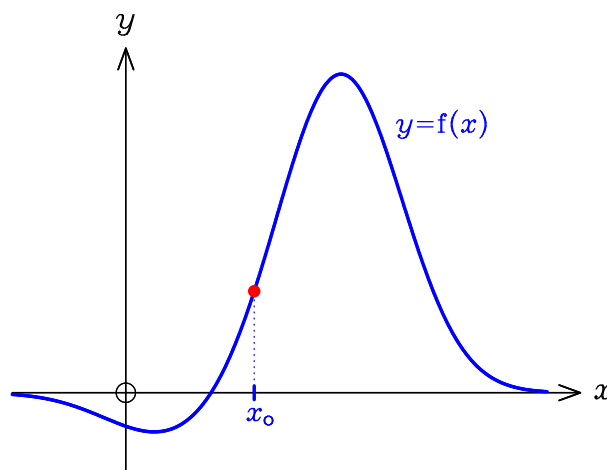
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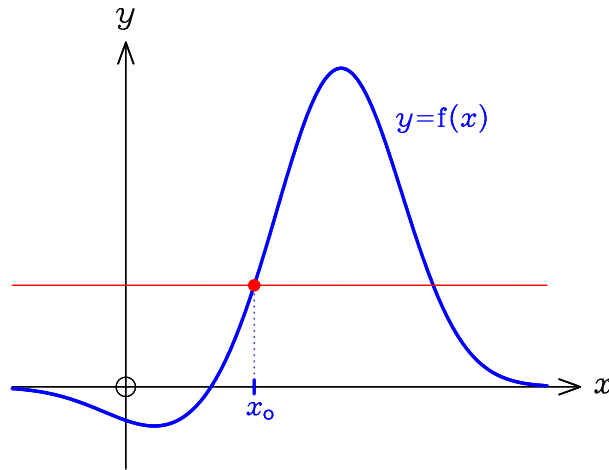
Outline

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

Taylor Series

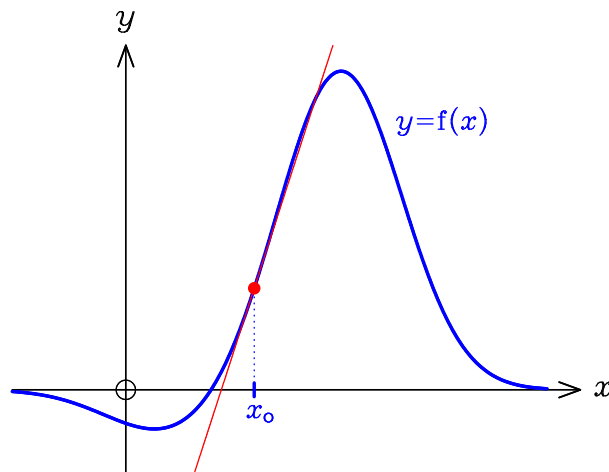


Taylor Series (0)



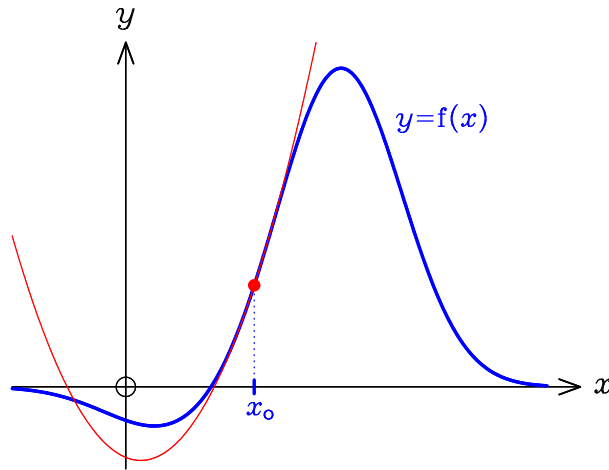
■ $f(x) \approx a_0$

Taylor Series (1)



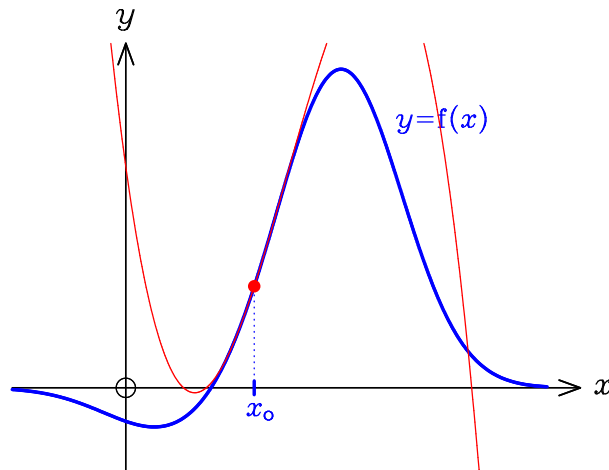
■ $f(x) \approx a_0 + a_1(x-x_0)$

Taylor Series (2)



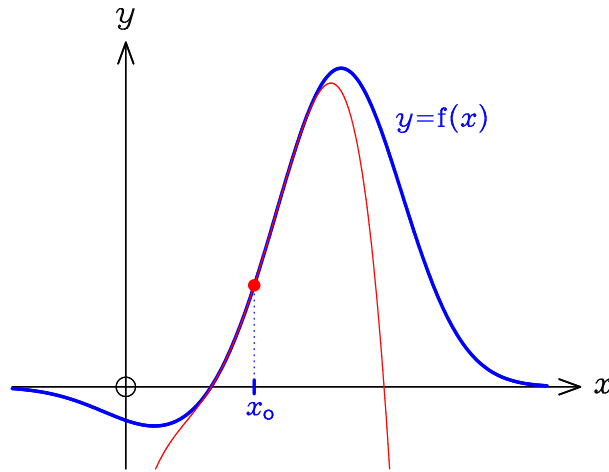
■ $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2$

Taylor Series (3)



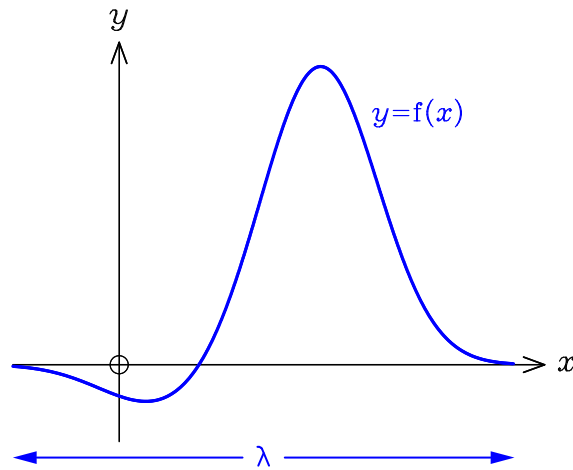
■ $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2 + a_3(x-x_0)^3$

Taylor Series (4)



■ $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2 + a_3(x-x_0)^3 + a_4(x-x_0)^4$

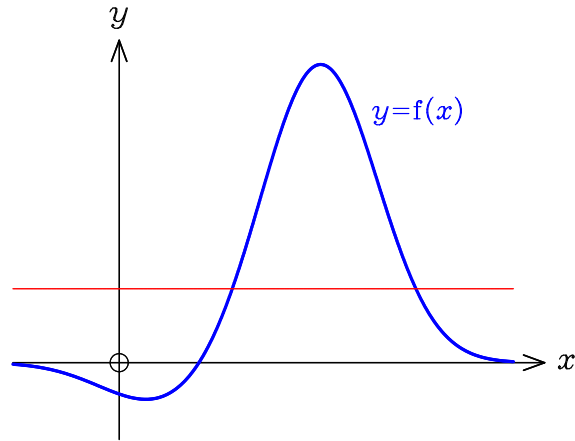
Fourier Series



■ Periodic: $f(x) = f(x+\lambda)$

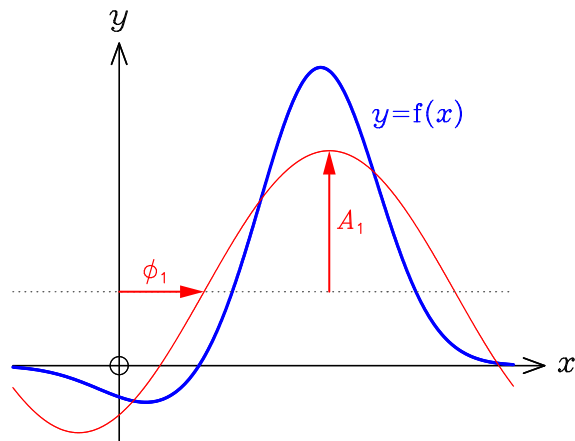
$k = \frac{2\pi}{\lambda}$ (wavenumber)

Fourier Series (0)



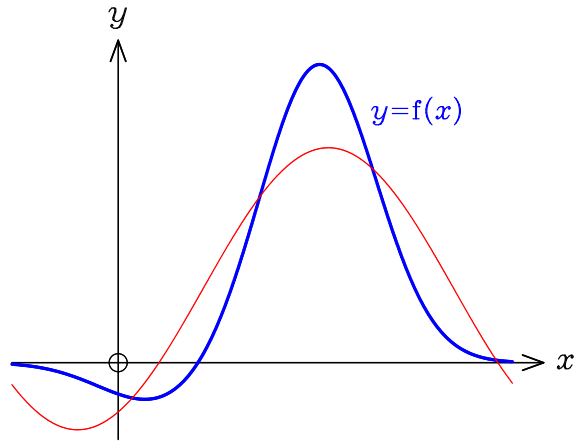
■ $f(x) \approx \frac{a_0}{2}$

Fourier Series (1)



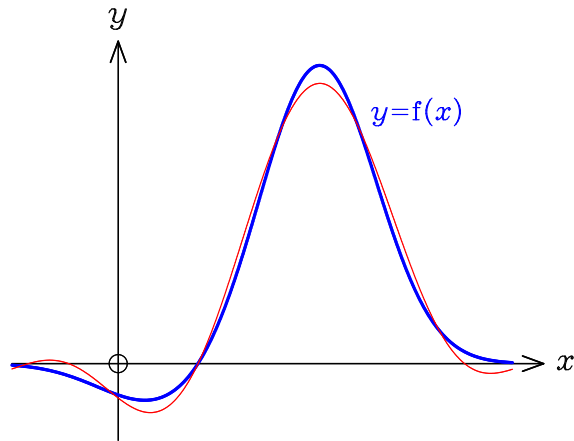
■ $f(x) \approx \frac{a_0}{2} + A_1 \sin(kx + \phi_1)$

Fourier Series (1)



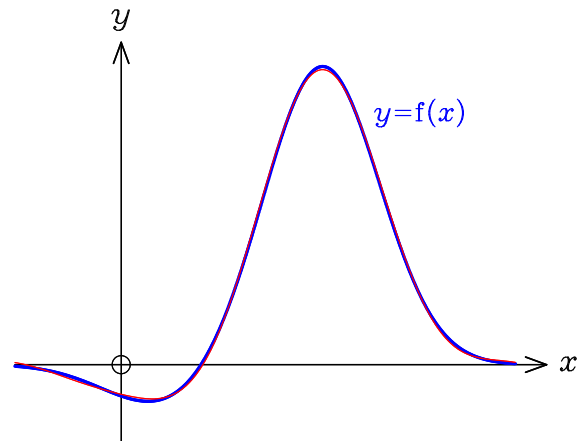
■ $f(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + b_1 \sin(kx)$

Fourier Series (2)



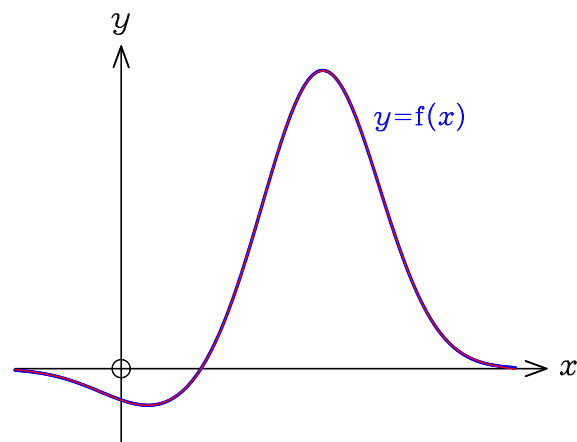
■ $f(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + a_2 \cos(2kx) + b_1 \sin(kx) + b_2 \sin(2kx)$

Fourier Series (3)



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

Fourier Series (4)



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

Taylor Versus Fourier Series

■ Taylor: $f(x) = \sum_{n=0}^{\infty} a_n (x-x_0)^n$ $|x-x_0| < R$

◆ $a_n = \frac{1}{n!} \left. \frac{d^n f}{dx^n} \right|_{x_0}$

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

◆ $a_n = \frac{2}{\lambda} \int_0^{\lambda} f(x) \cos(nkx) dx$ and $b_n = \frac{2}{\lambda} \int_0^{\lambda} f(x) \sin(nkx) dx$

Complex Fourier Series

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

■ 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 $n \geq 1$

■ $c_0 = a_0$

Fourier Transform

- As $\lambda \rightarrow \infty$, so that $k \rightarrow 0$ and $f(x)$ is non-periodic,

- ◆
$$\sum_{n=-\infty}^{\infty} c_n e^{in k x} \rightarrow \int_{-\infty}^{\infty} c(q) e^{i q x} dq$$

- In the continuum limit,

- ◆ Fourier sum (series) \rightarrow Fourier integral (transform)

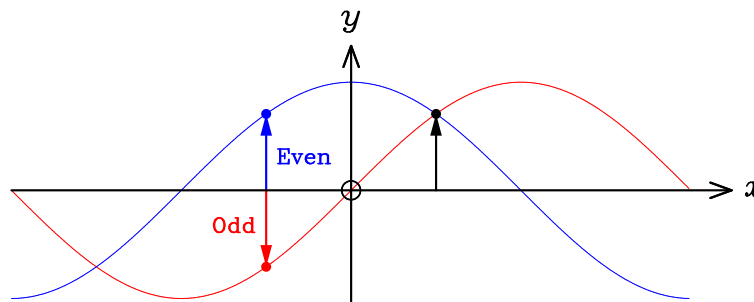
- ◆
$$f(x) = \int_{-\infty}^{\infty} F(q) e^{i q x} dq$$

- $$F(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-i q x} dx$$

Some Symmetry Properties

- Even: $f(x) = f(-x) \iff F(q) = F(-q)$

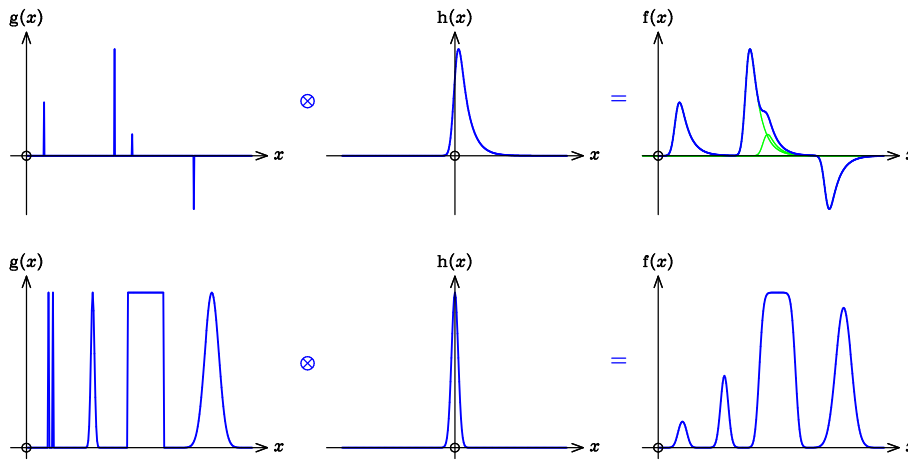
- Odd: $f(x) = -f(-x) \iff F(q) = -F(-q)$



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

Convolution

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



Convolution Theorem

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

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

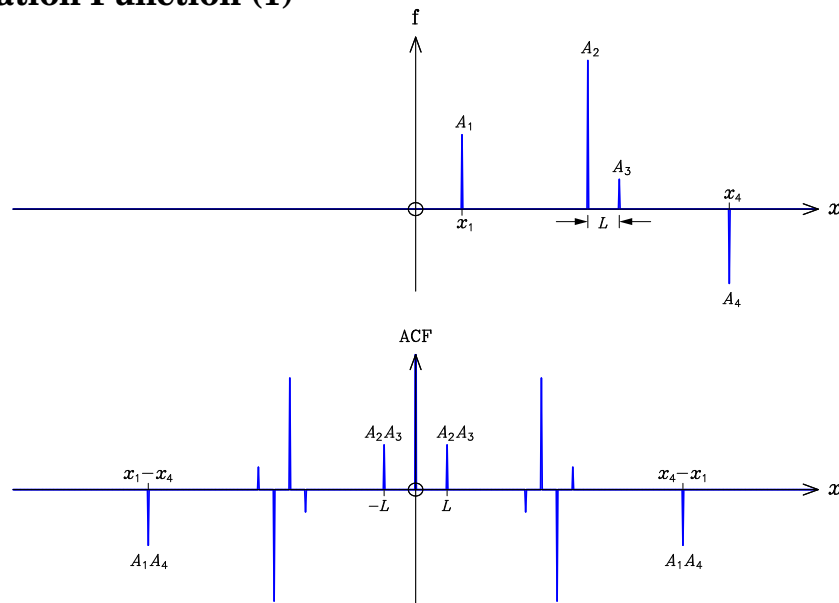
Auto-correlation Function

$$\int_{-\infty}^{\infty} F(q) e^{iqx} dq = f(x)$$

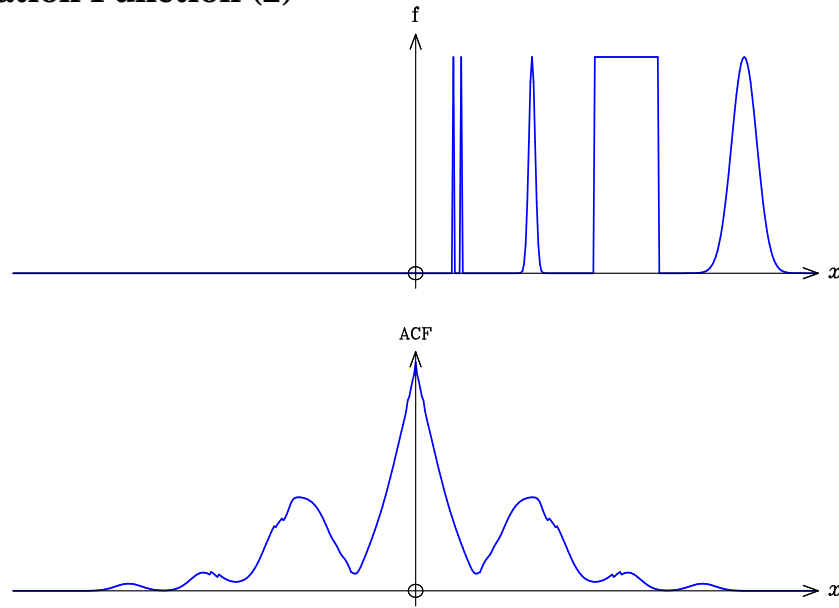
■ $\int_{-\infty}^{\infty} |F(q)|^2 e^{iqx} dq = \int_{-\infty}^{\infty} f(t)^* f(x+t) dt = \text{ACF}(x)$

◆ Patterson map

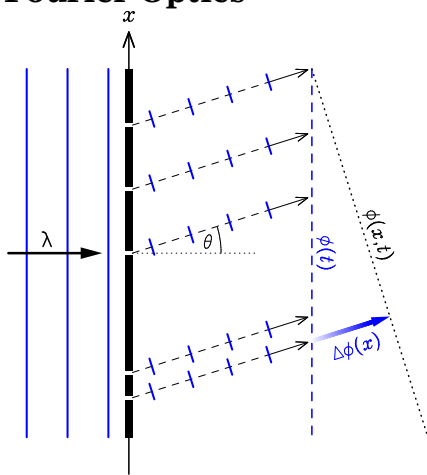
Auto-correlation Function (1)



Auto-correlation Function (2)



Fourier Optics

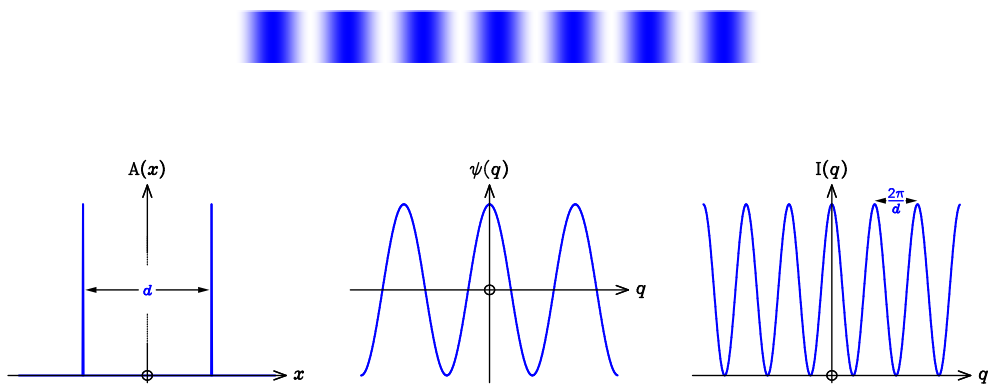


$$I(q) = |\psi(q)|^2$$

■ Fraunhofer: $\psi(q) = \psi_0 \int_{-\infty}^{\infty} A(x) e^{iqx} dx$

where $q = \frac{2\pi \sin \theta}{\lambda}$

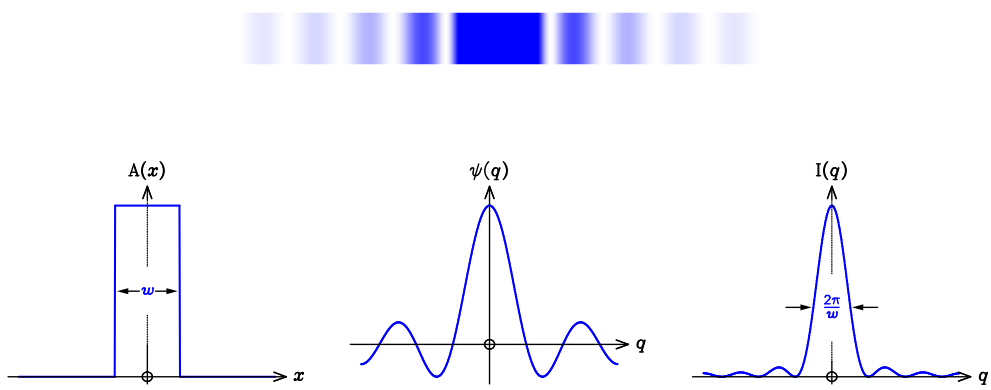
Young's Double Slits



Oxford School on Neutron Scattering

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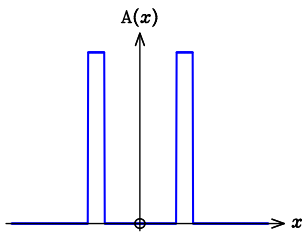
Single Wide Slit



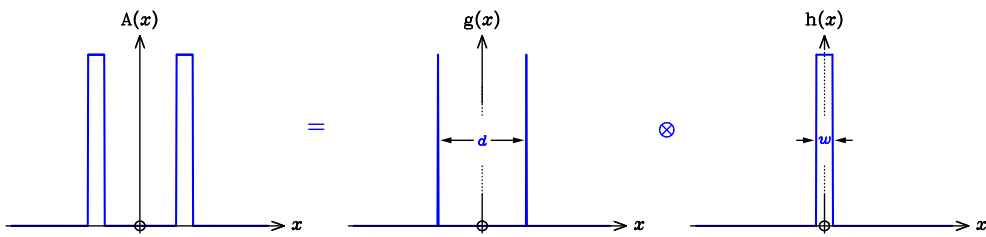
Oxford School on Neutron Scattering

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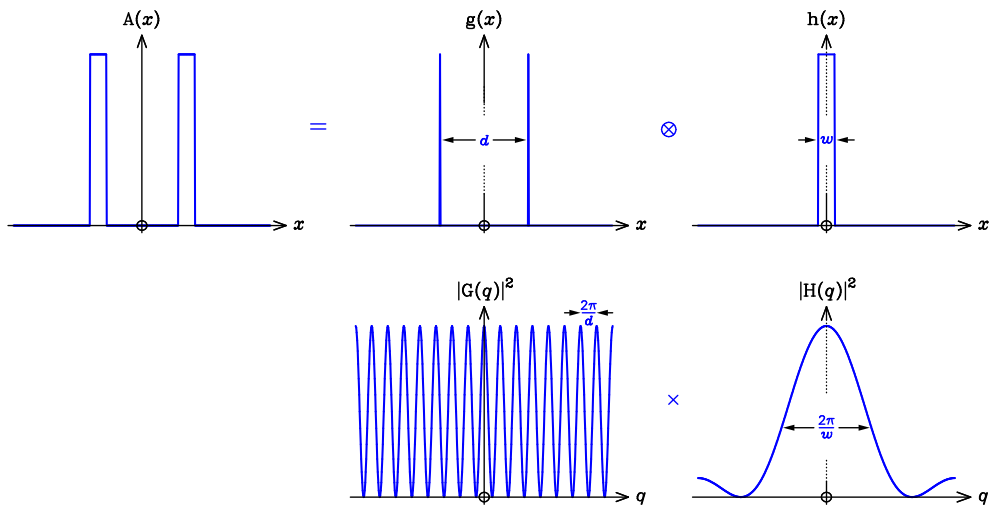
Two Wide Slits (0)



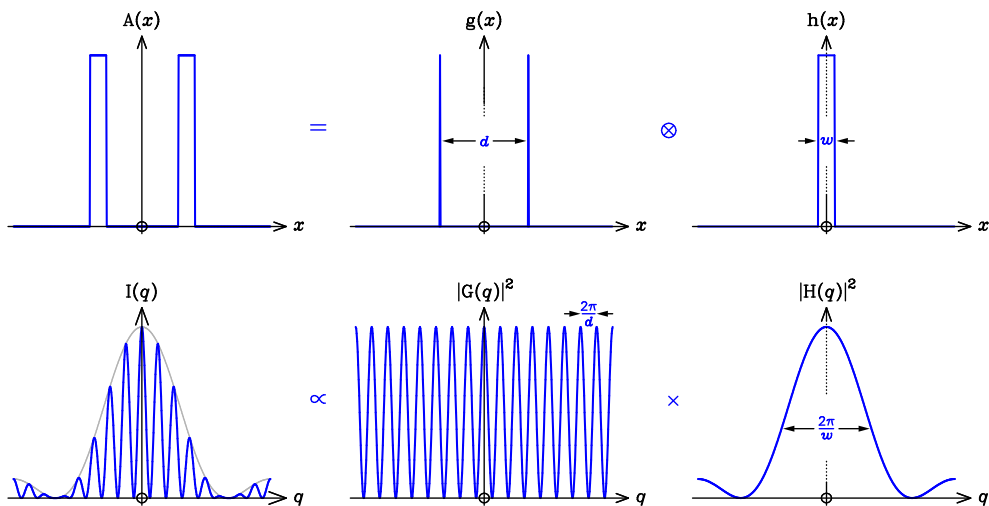
Two Wide Slits (1)



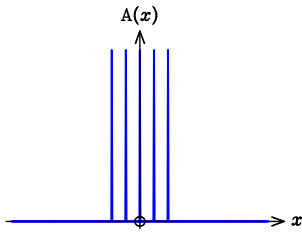
Two Wide Slits (2)



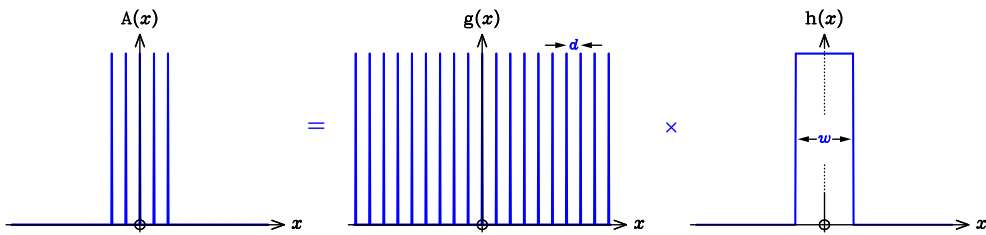
Two Wide Slits (3)



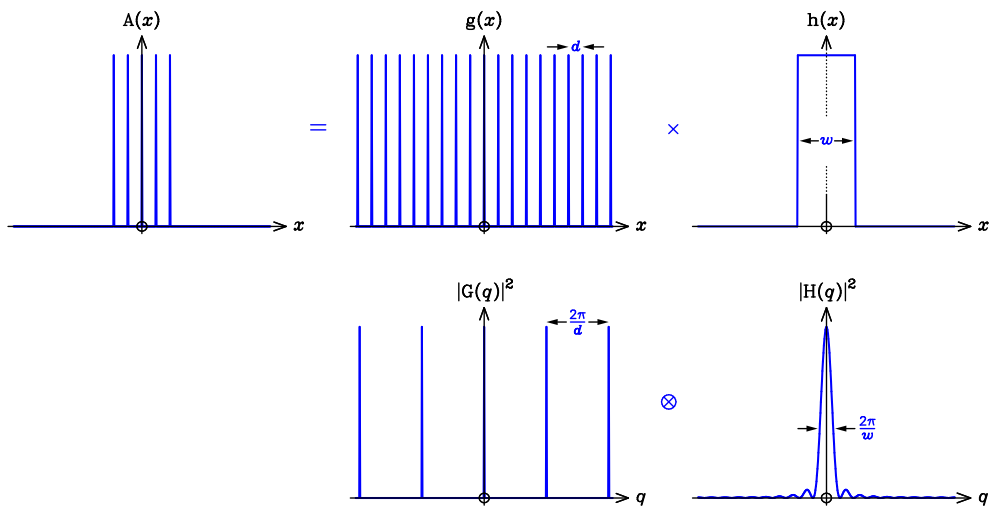
Finite Grating (0)



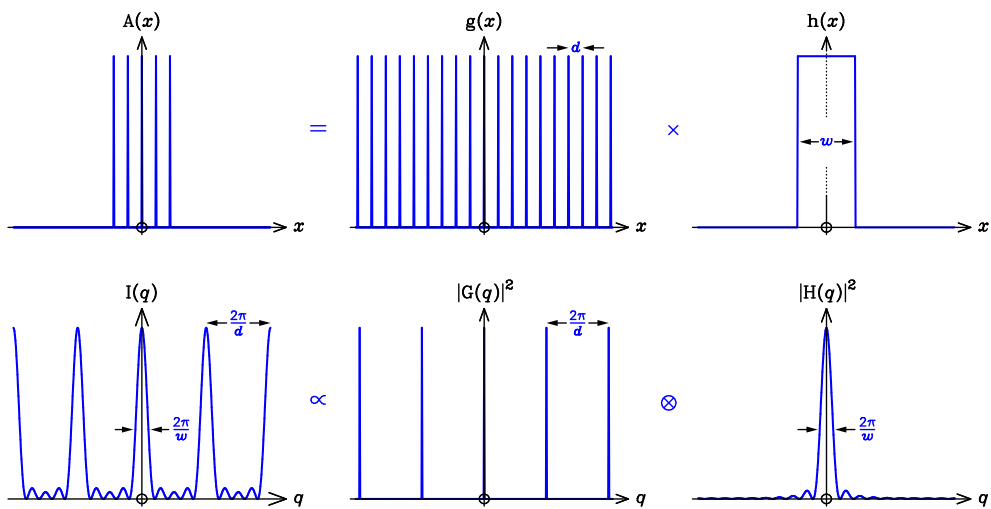
Finite Grating (1)



Finite Grating (2)



Finite Grating (3)



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

