

An Introduction to
Fourier Transforms

D. S. Sivia

St. John's College
Oxford, England

August 12, 2015

Outline	2
Taylor Series	3
Taylor Series (0)	4
Taylor Series (1)	5
Taylor Series (2)	6
Taylor Series (3)	7
Taylor Series (4)	8
Fourier Series	9
Fourier Series (0)	10
Fourier Series (1)	11
Fourier Series (1)	12
Fourier Series (2)	13
Fourier Series (3)	14
Fourier Series (4)	15
Taylor Versus Fourier Series	16
Complex Fourier Series	17
Fourier Transform	18
Some Symmetry Properties	19
Convolution	20
Convolution Theorem	21
Auto-correlation Function	22
Auto-correlation Function (1)	23
Auto-correlation Function (2)	24
Fourier Optics	25
Young's Double Slits	26
Single Wide Slit	27
Two Wide Slits (0)	28
Two Wide Slits (1)	29
Two Wide Slits (2)	30
Two Wide Slits (3)	31
Finite Grating (0)	32
Finite Grating (1)	33
Finite Grating (2)	34

Finite Grating (3) 35
Write up of this Talk! 36
The phaseless Fourier problem 37
The phaseless Fourier problem 38

Outline

■ Approximating functions

- ◆ Taylor series
- ◆ Fourier series → transform

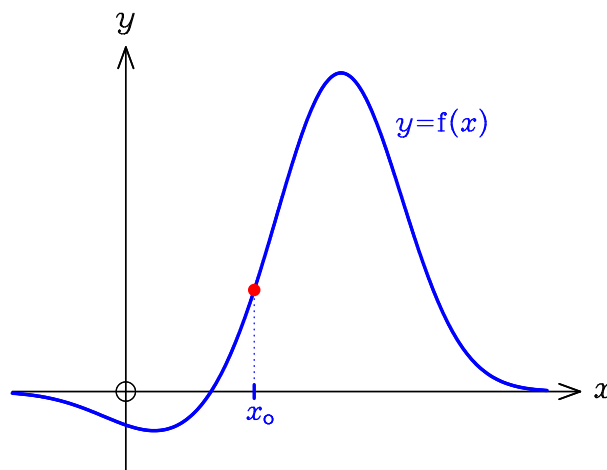
■ Some formal properties

- ◆ Symmetry
- ◆ Convolution theorem
- ◆ Auto-correlation function

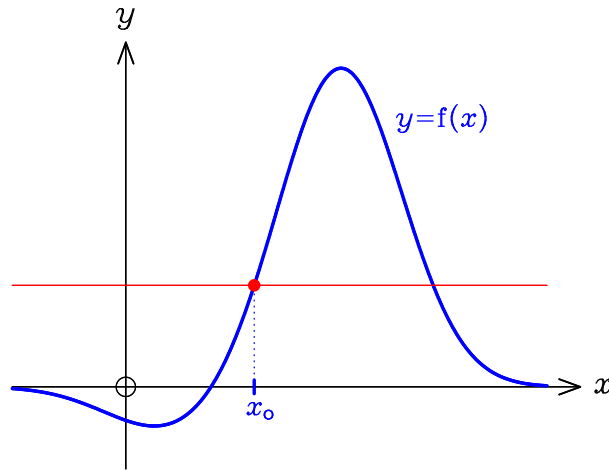
■ Physical insight

- ◆ Fourier optics

Taylor Series

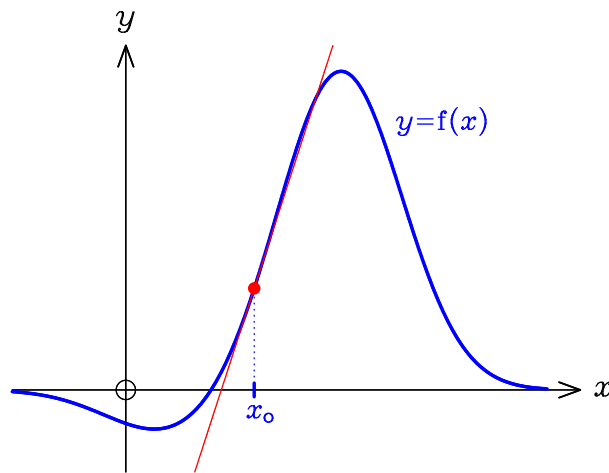


Taylor Series (0)



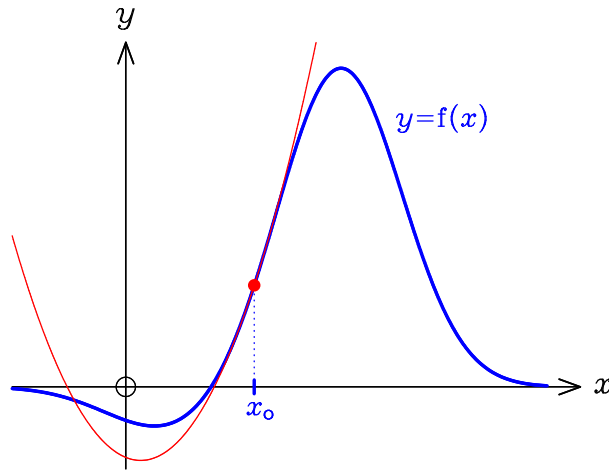
■ $f(x) \approx a_0$

Taylor Series (1)



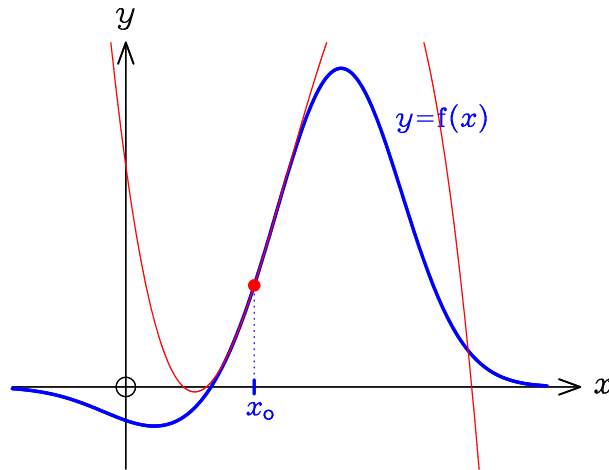
■ $f(x) \approx a_0 + a_1(x-x_0)$

Taylor Series (2)



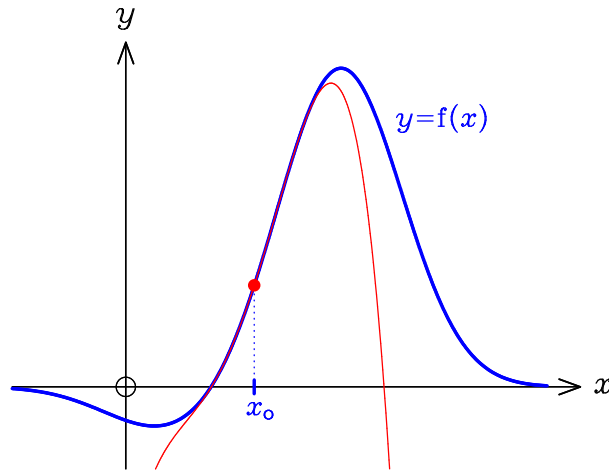
■ $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2$

Taylor Series (3)



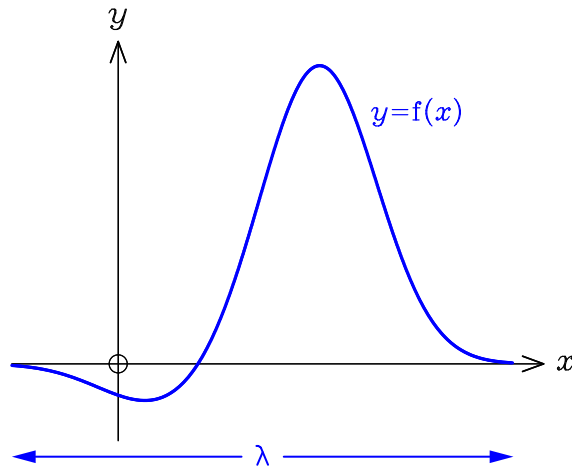
■ $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2 + a_3(x-x_0)^3$

Taylor Series (4)



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

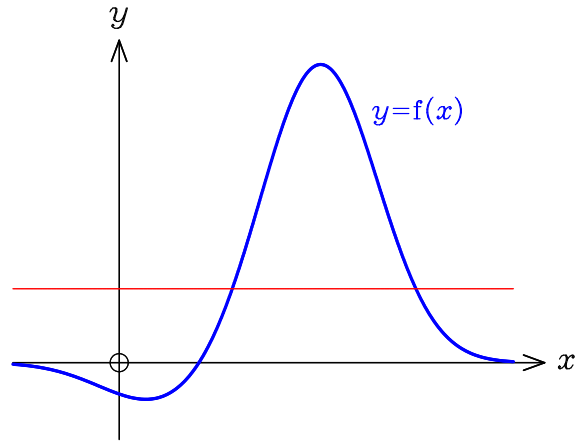
Fourier Series



■ Periodic: $f(x) = f(x+\lambda)$

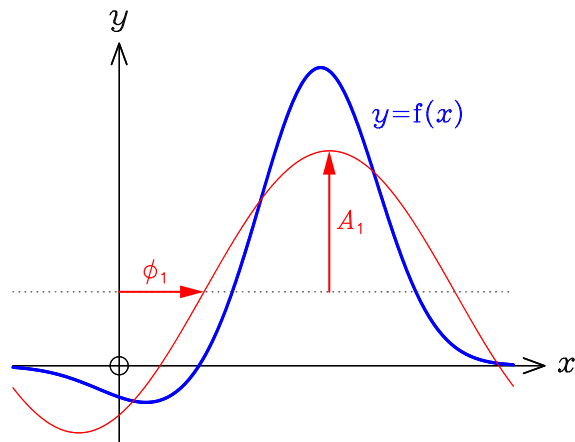
$k = \frac{2\pi}{\lambda}$ (wavenumber)

Fourier Series (0)



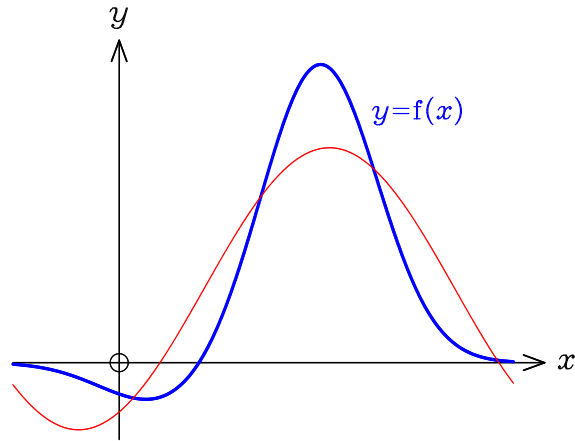
■ $f(x) \approx \frac{a_0}{2}$

Fourier Series (1)



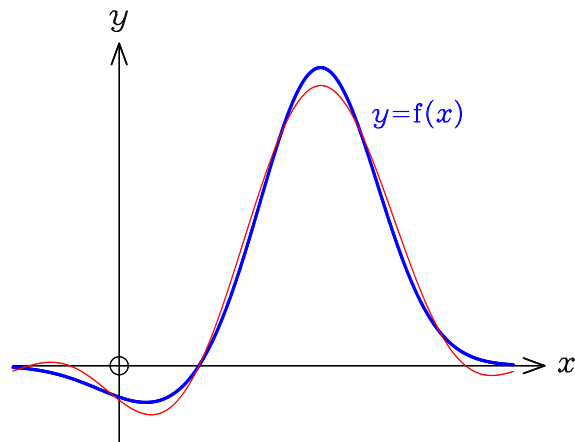
■ $f(x) \approx \frac{a_0}{2} + A_1 \sin(kx + \phi_1)$

Fourier Series (1)



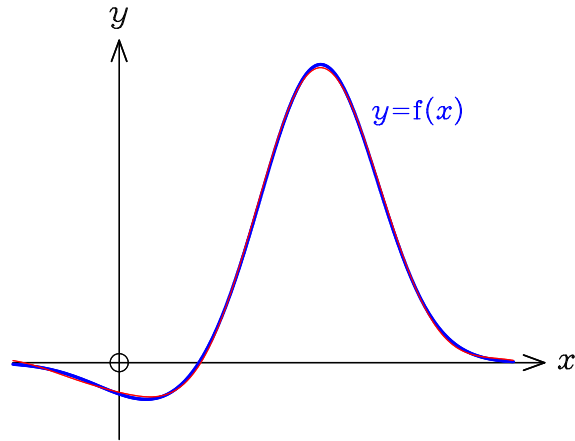
$$\blacksquare f(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + b_1 \sin(kx)$$

Fourier Series (2)



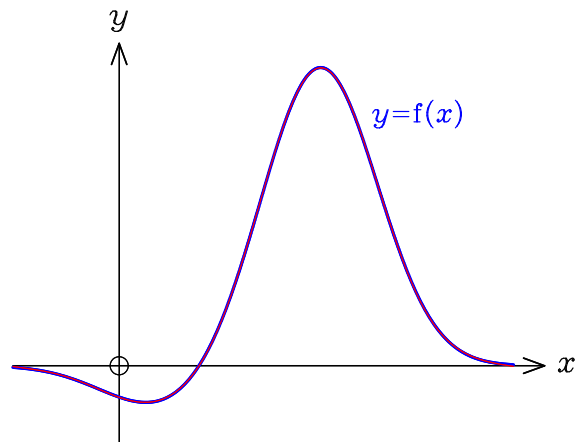
$$\blacksquare f(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + a_2 \cos(2kx) + b_1 \sin(kx) + b_2 \sin(2kx)$$

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)

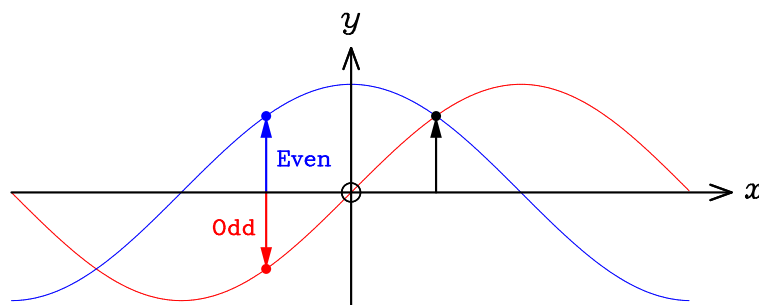
- ◆
$$f(x) = \int_{-\infty}^{\infty} F(q) e^{i q x} dq$$

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

Some Symmetry Properties

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

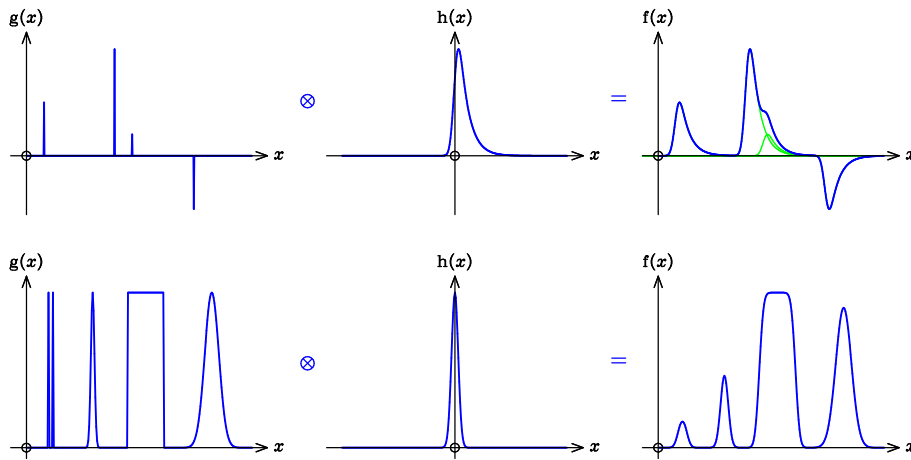
- Odd: $f(x) = -f(-x) \iff F(q) = -F(-q)$



- 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

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

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

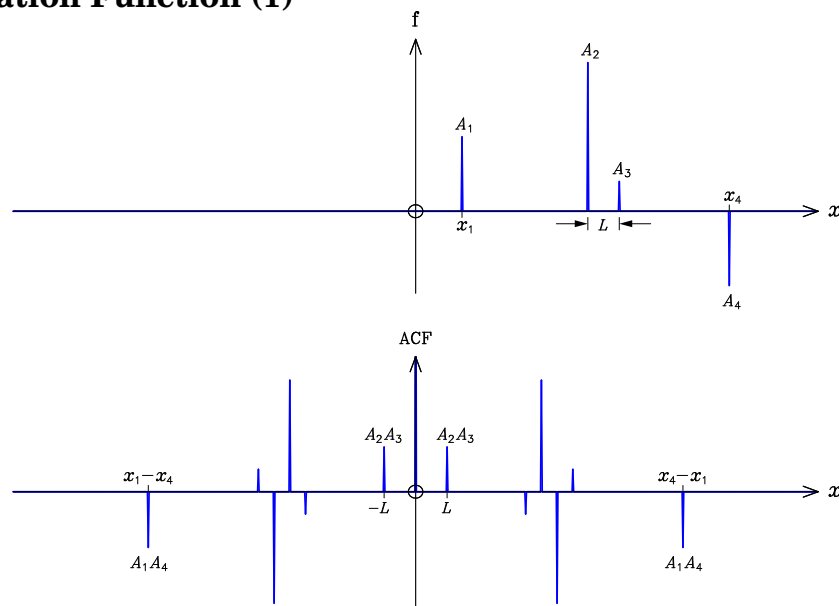
Auto-correlation Function

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

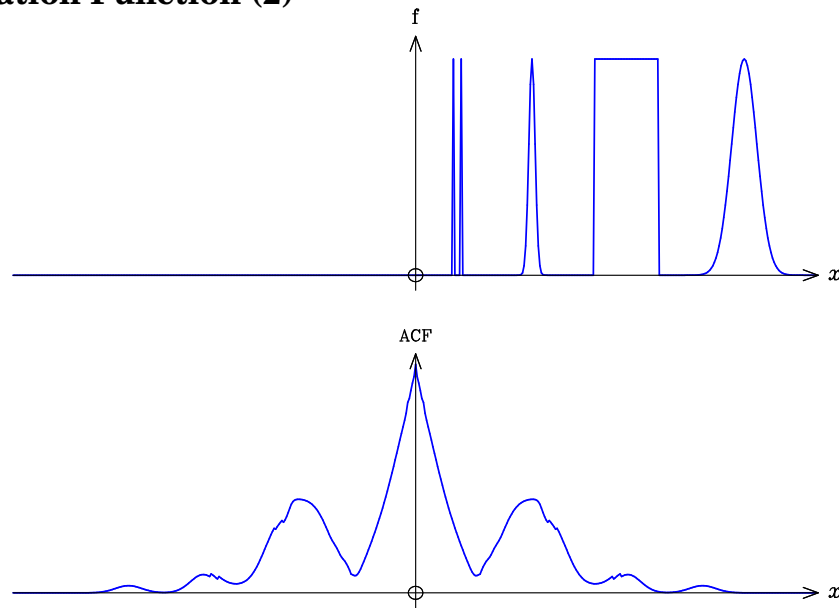
■ $\int_{-\infty}^{\infty} |F(q)|^2 e^{iqx} dq = \int_{-\infty}^{\infty} f(t)^* f(x+t) dt = \text{ACF}(x)$

◆ Patterson map

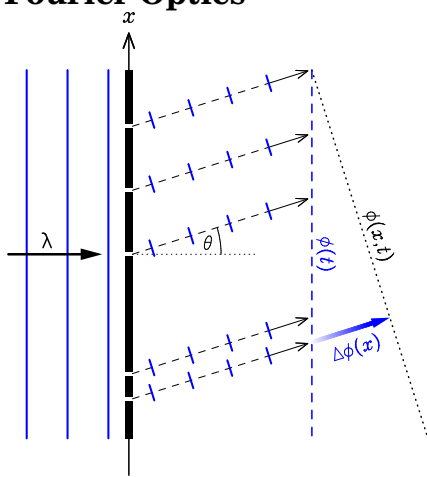
Auto-correlation Function (1)



Auto-correlation Function (2)



Fourier Optics

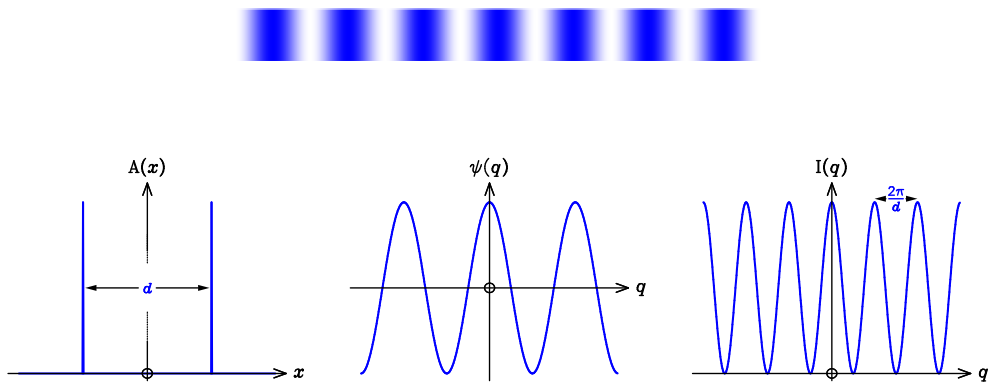


$$I(q) = |\psi(q)|^2$$

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

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

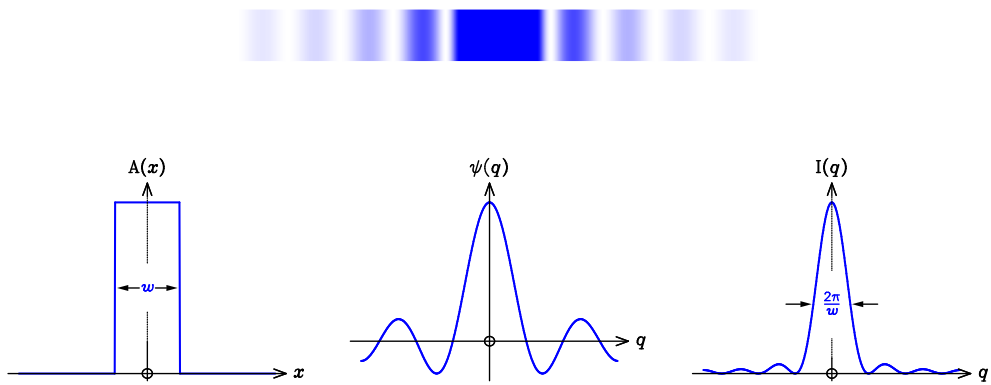
Young's Double Slits



Oxford School on Neutron Scattering

26 / 38

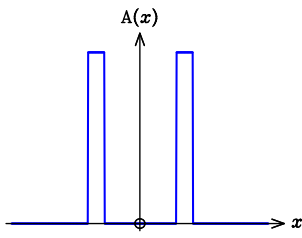
Single Wide Slit



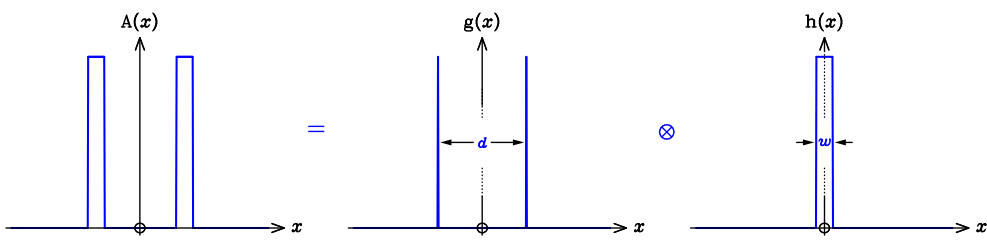
Oxford School on Neutron Scattering

27 / 38

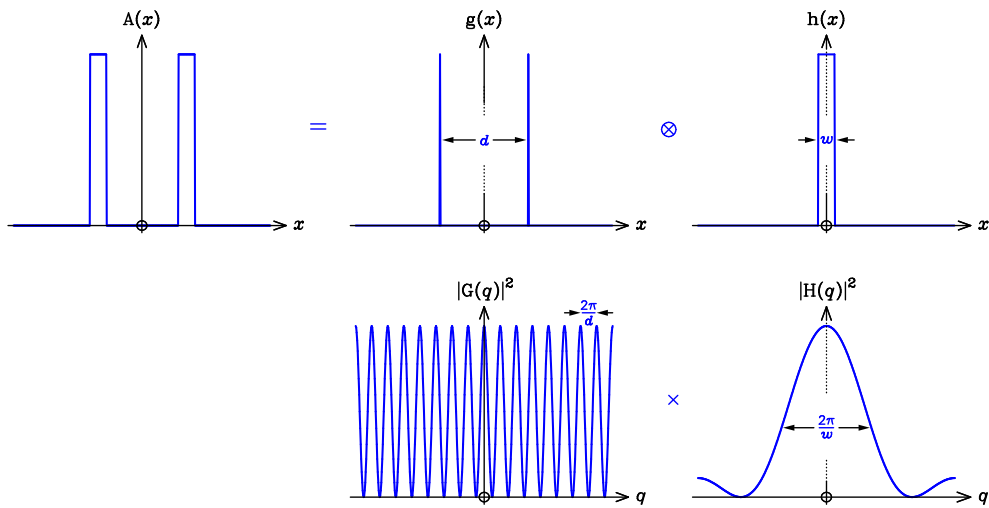
Two Wide Slits (0)



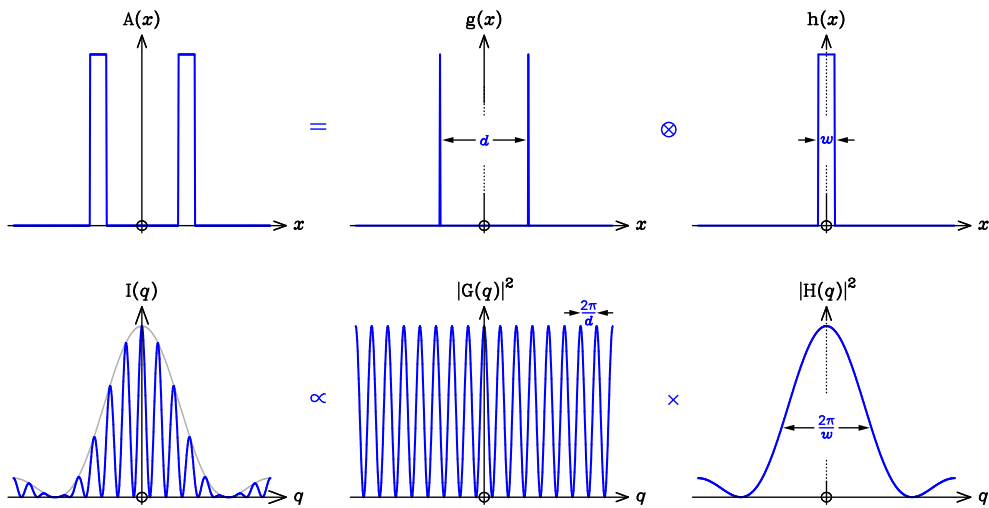
Two Wide Slits (1)



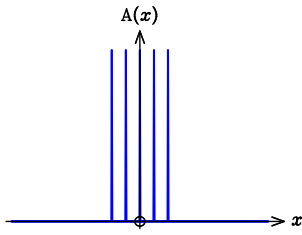
Two Wide Slits (2)



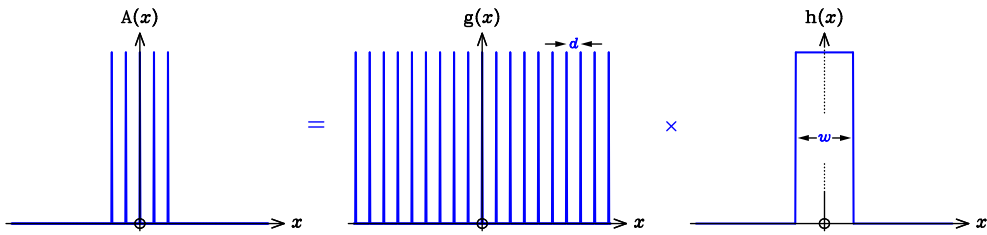
Two Wide Slits (3)



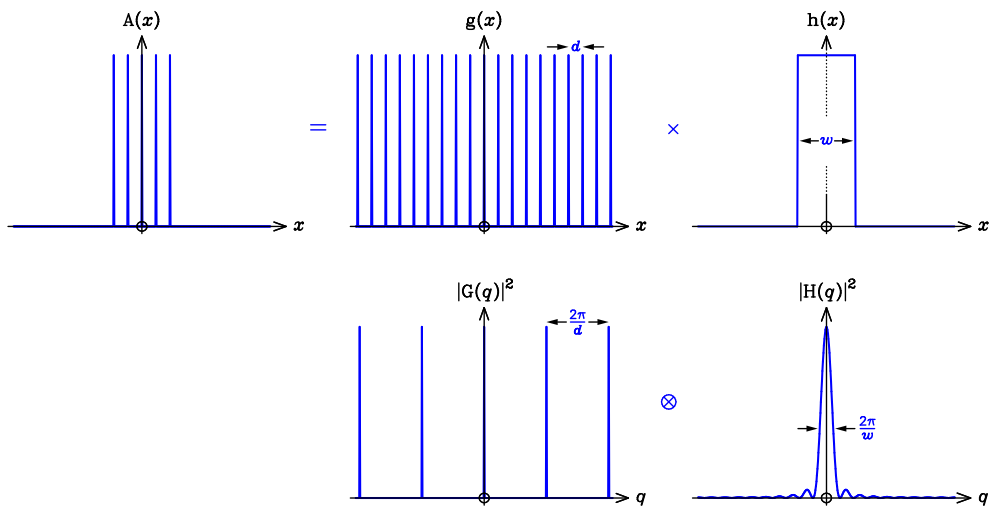
Finite Grating (0)



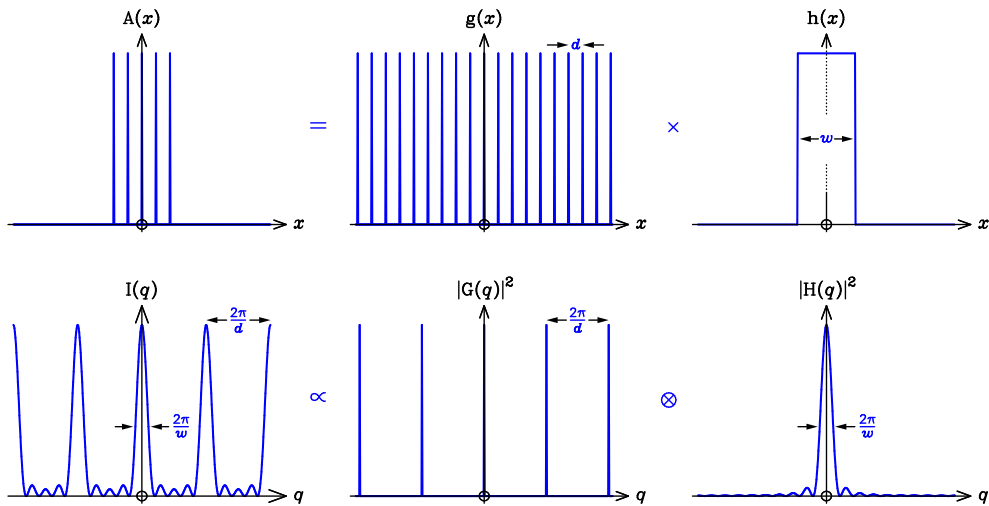
Finite Grating (1)



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

