

# 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

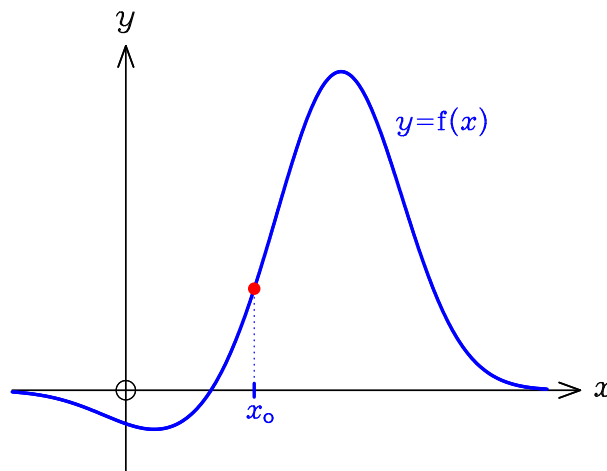
### ■ Physical insight

- ◆ Fourier optics

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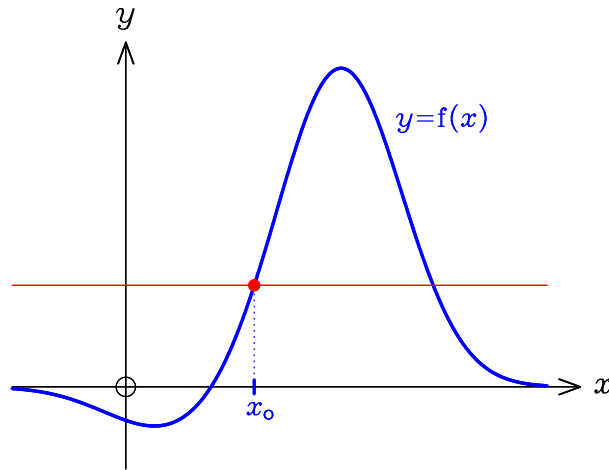
## Taylor Series



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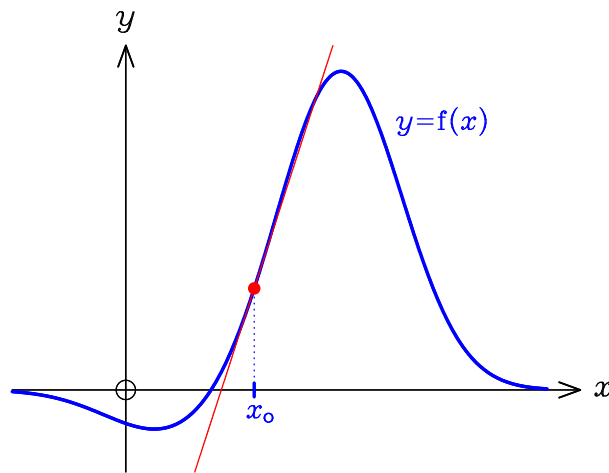
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### Taylor Series (0)



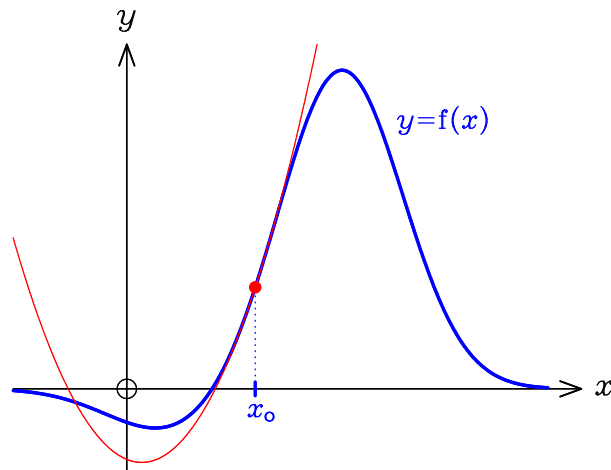
■  $f(x) \approx a_0$

### Taylor Series (1)



■  $f(x) \approx a_0 + a_1(x-x_0)$

## Taylor Series (2)

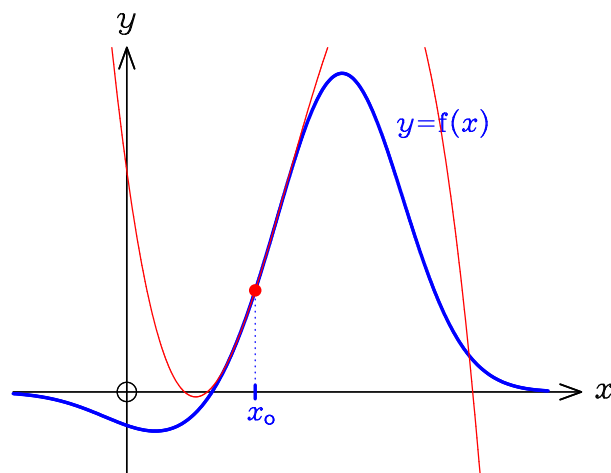


■  $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2$

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## Taylor Series (3)

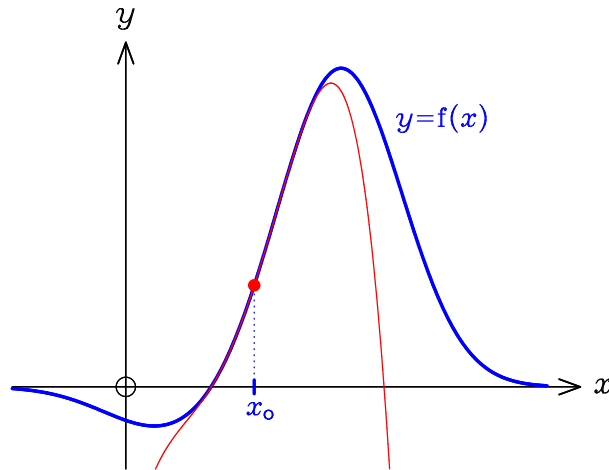


■  $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2 + a_3(x-x_0)^3$

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## Taylor Series (4)

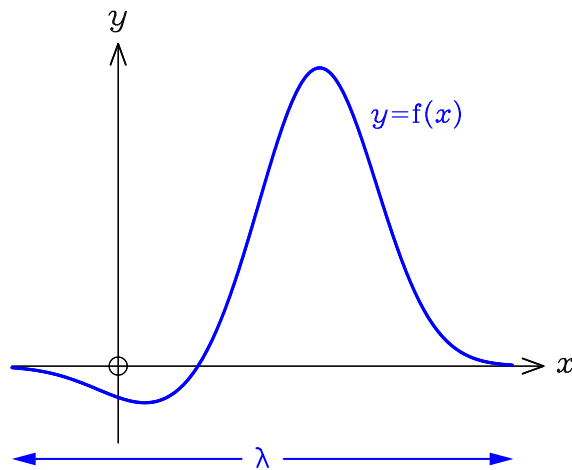


■  $f(x) \approx a_0 + a_1(x-x_0) + a_2(x-x_0)^2 + a_3(x-x_0)^3 + a_4(x-x_0)^4$

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## Fourier Series



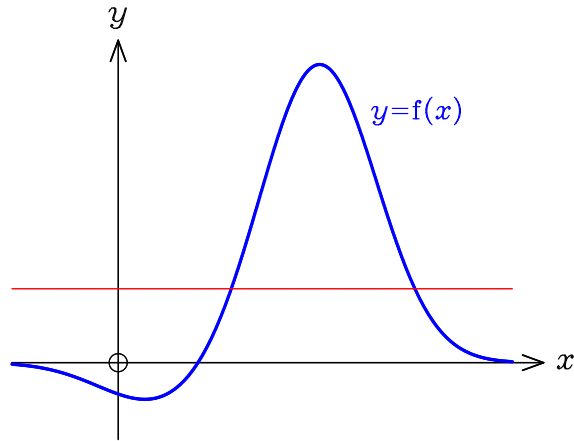
■ Periodic:  $f(x) = f(x+\lambda)$

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

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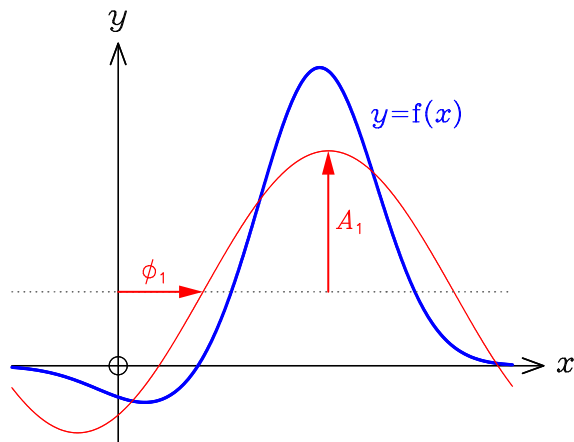
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### Fourier Series (0)



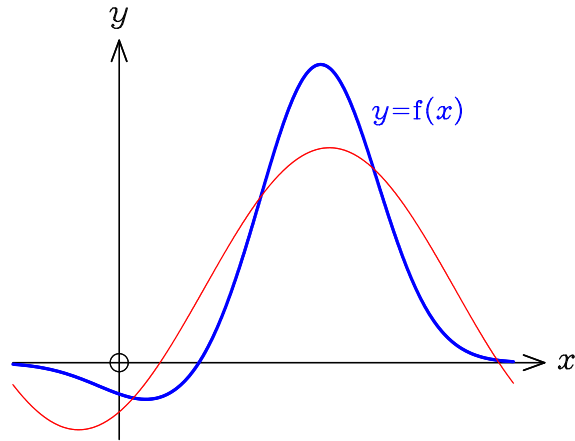
■  $f(x) \approx \frac{a_0}{2}$

### Fourier Series (1)



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

## Fourier Series (1)

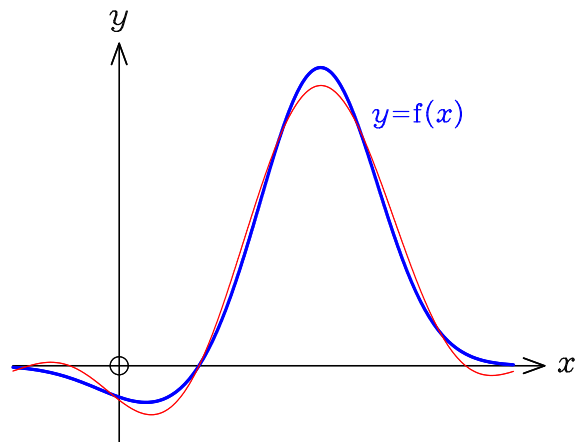


$$\blacksquare f(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + b_1 \sin(kx)$$

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## Fourier Series (2)



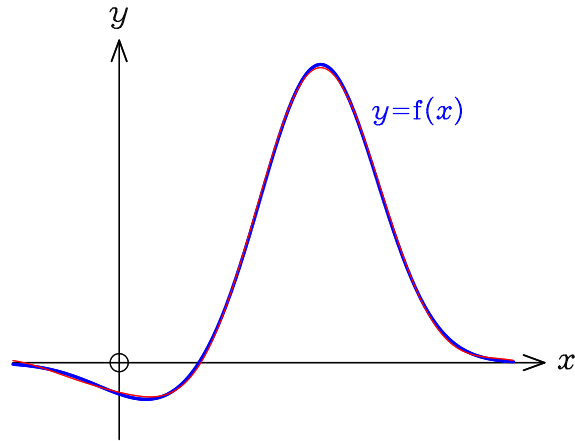
$$\blacksquare f(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + a_2 \cos(2kx) + b_1 \sin(kx) + b_2 \sin(2kx)$$

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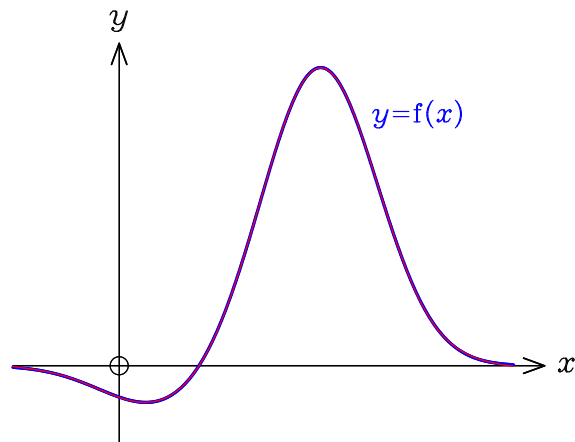


### Fourier Series (3)



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

### Fourier Series (4)



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

## 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     $b_n = \frac{2}{\lambda} \int_0^{\lambda} f(x) \sin(nkx) dx$

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## 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  $n \geq 1$

■  $c_0 = a_0$

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## Fourier Transform

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

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

- In the continuum limit,

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

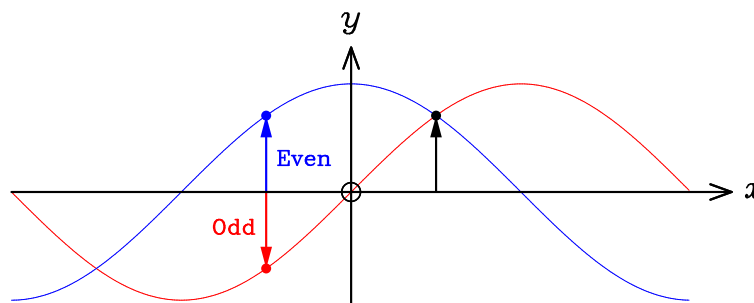
$$\blacklozenge f(x) = \int_{-\infty}^{\infty} F(q) e^{i q x} dq$$

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

## Some Symmetry Properties

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

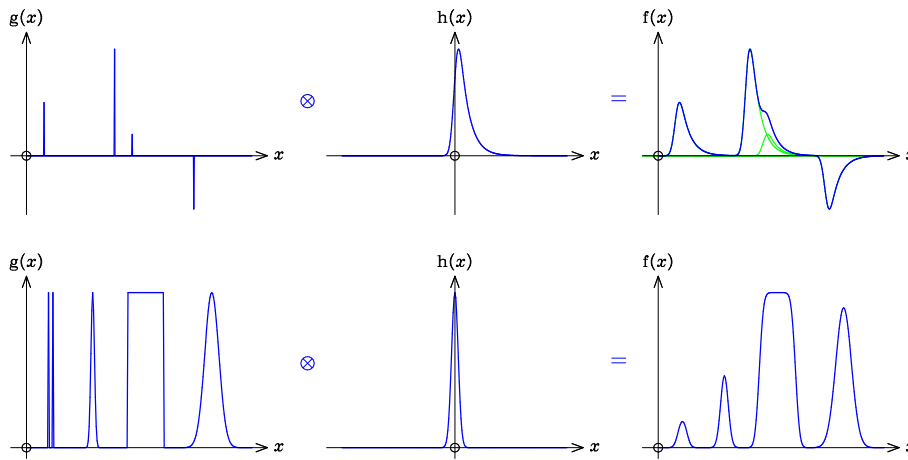
- Odd:  $f(x) = -f(-x) \iff F(q) = -F(-q)$



- 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

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

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

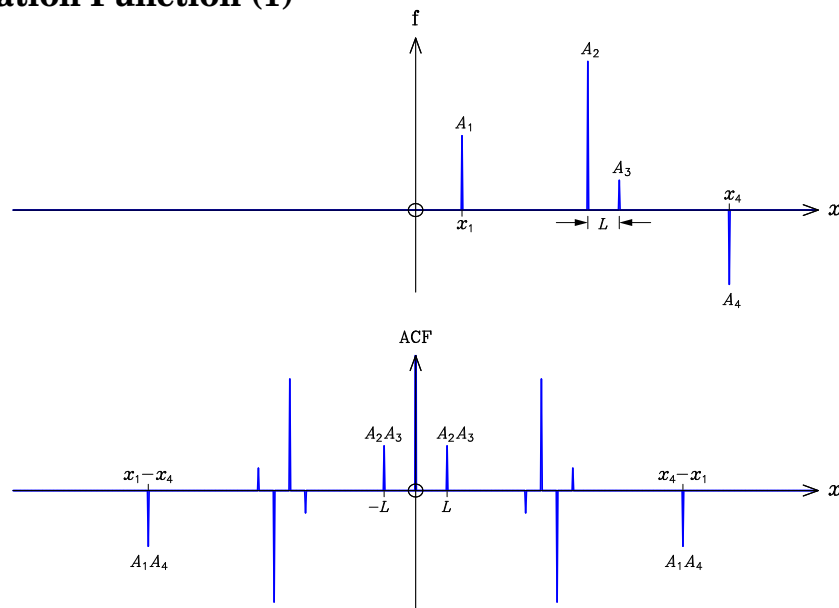
## Auto-correlation Function

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

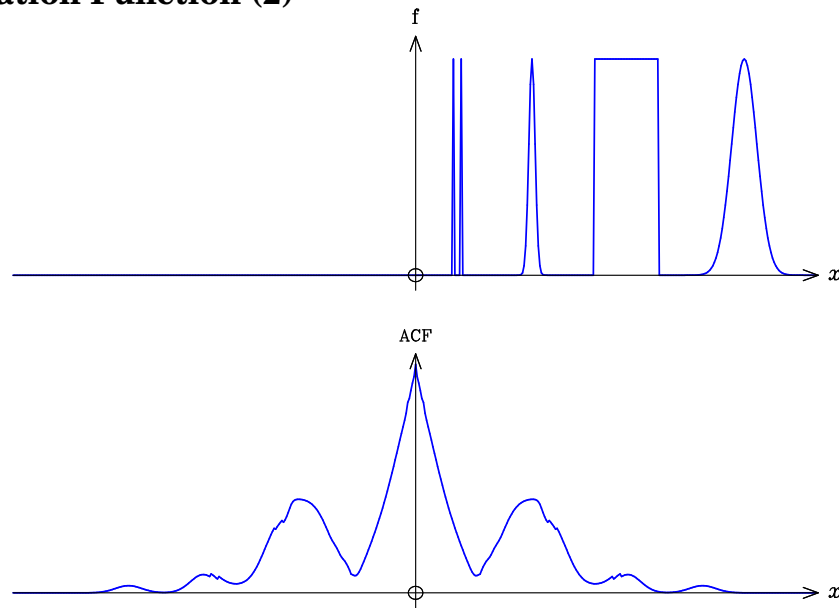
■  $\int_{-\infty}^{\infty} |F(q)|^2 e^{iqx} dq = \int_{-\infty}^{\infty} f(t)^* f(x+t) dt = \text{ACF}(x)$

◆ Patterson map

## Auto-correlation Function (1)



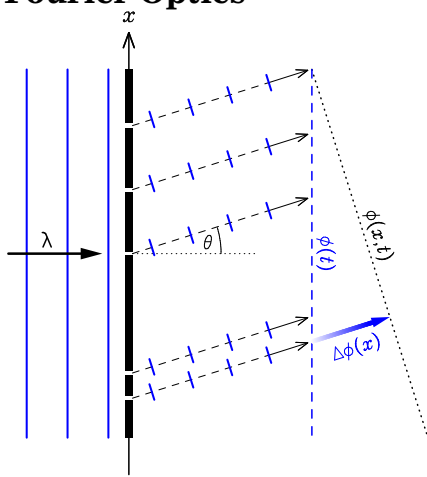
## Auto-correlation Function (2)



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## Fourier Optics



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

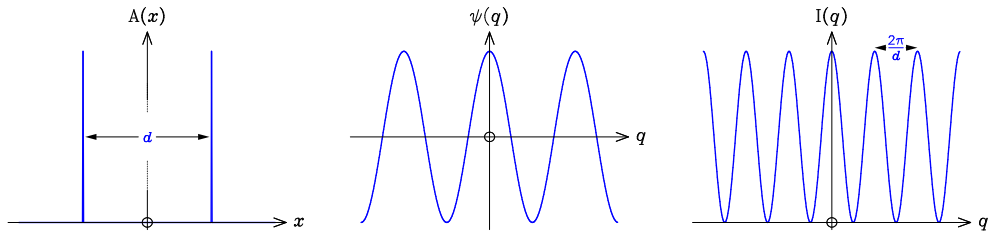
■ Fraunhofer:  $\psi(q) = \psi_0 \int_{-\infty}^{\infty} A(x) e^{iqx} dx$

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

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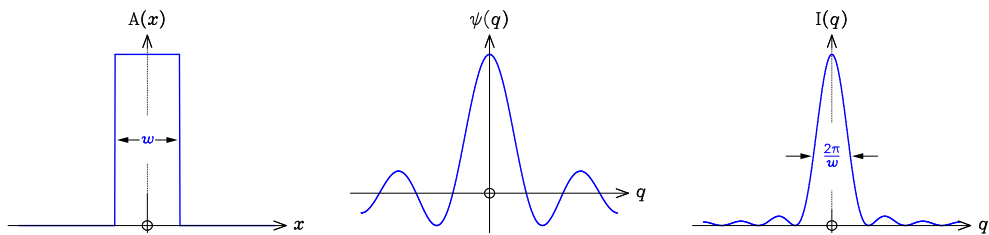
## Young's Double Slits



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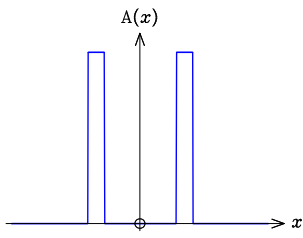
## Single Wide Slit



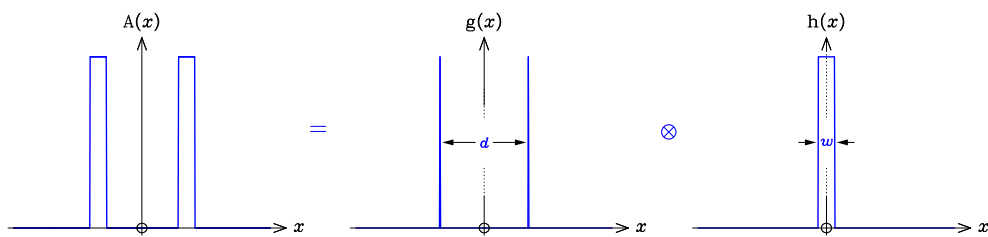
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## Two Wide Slits (0)

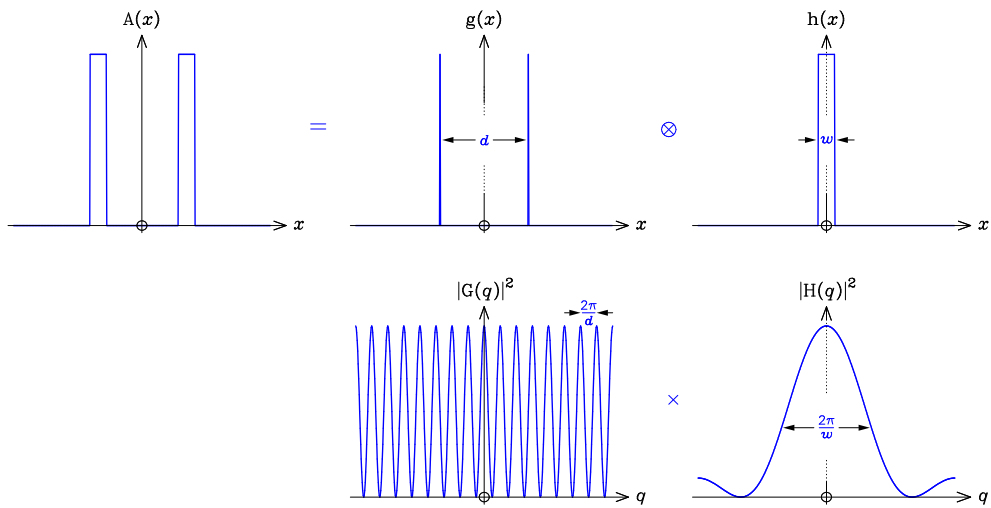


## Two Wide Slits (1)

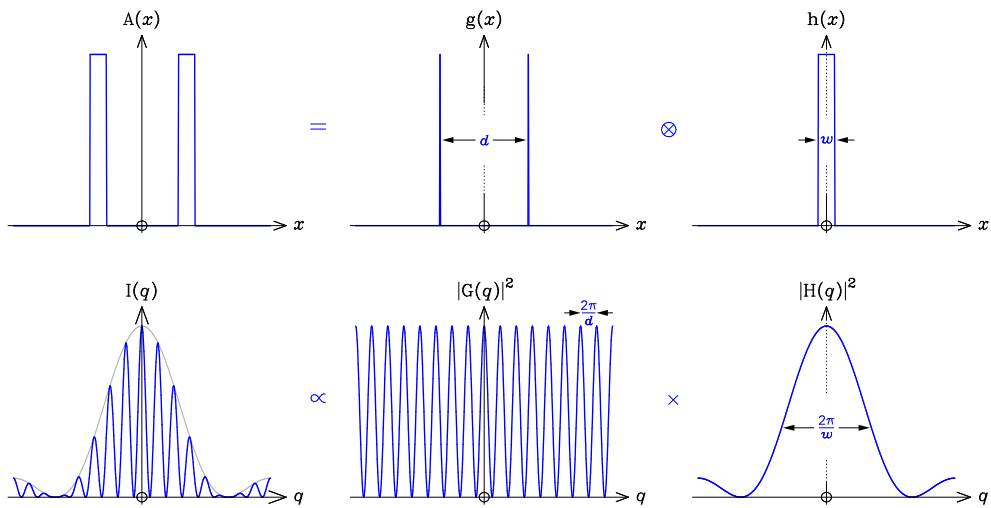




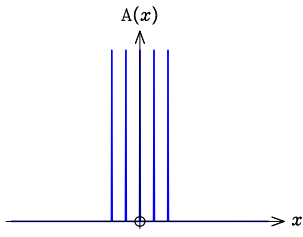
### Two Wide Slits (2)



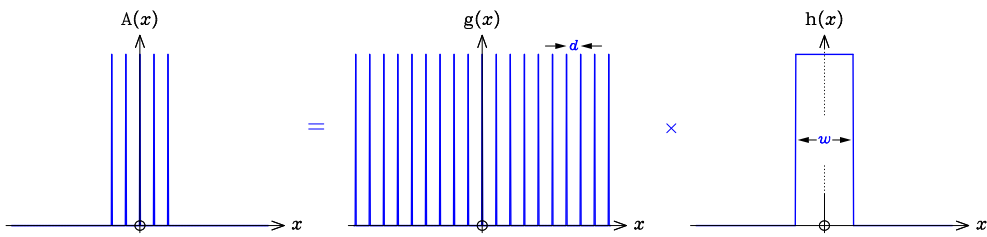
### Two Wide Slits (3)



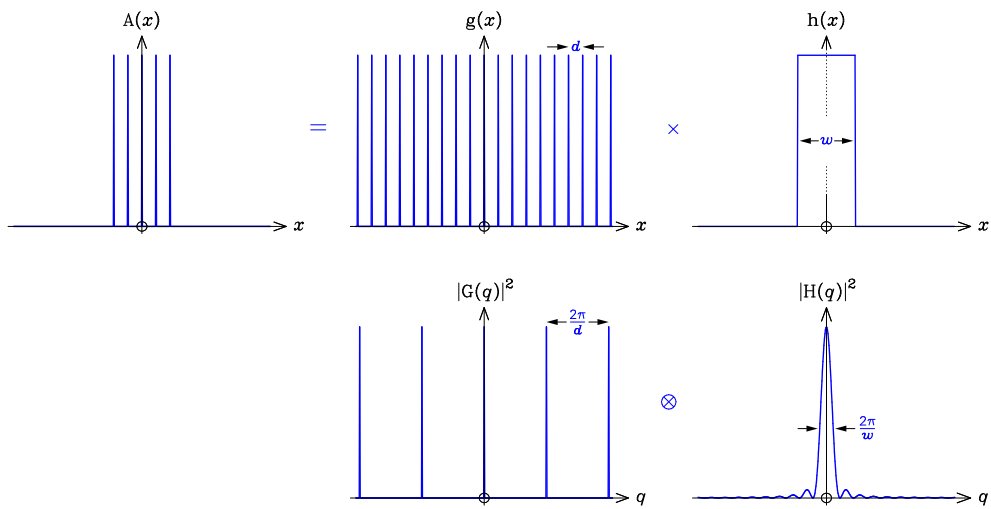
## Finite Grating (0)



## Finite Grating (1)



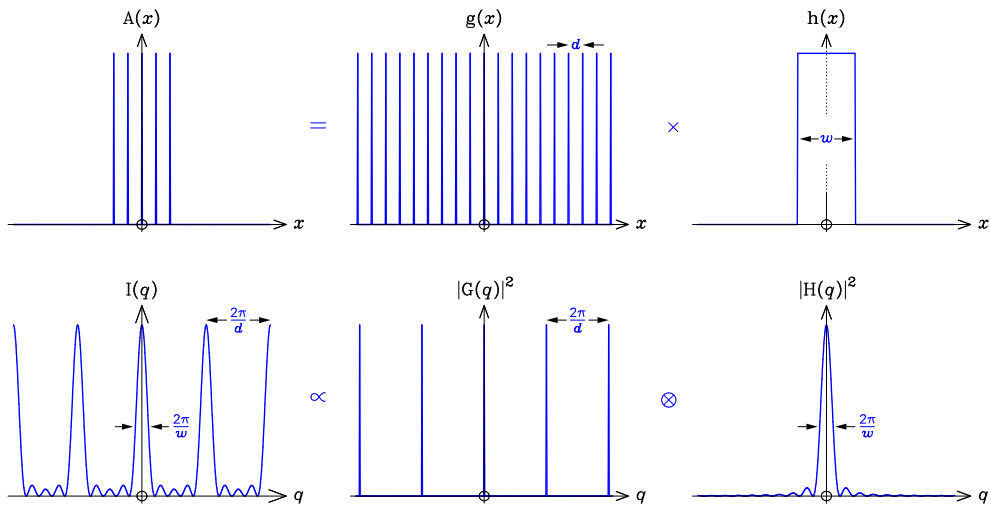
## Finite Grating (2)



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## Finite Grating (3)



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## Write up of this Talk!

- **Foundations of Science Mathematics** (Chapter 15)  
**Oxford Chemistry Primers Series, vol. 77**  
*D. S. Sivia and S. G. Rawlings* (1999), Oxford University Press
- **Elementary Scattering Theory for X-ray and Neutron Users** (Chapter 2)  
*D. S. Sivia* (October 2010), Oxford University Press