An Introduction to

Fourier Transforms

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Outline

- Approximating functions
  - Taylor series
  - Fourier series $\rightarrow$ transform

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- **Approximating functions**
  - Taylor series
  - Fourier series $\longrightarrow$ transform
- **Some formal properties**
  - Symmetry
  - Convolution theorem
  - Auto-correlation function

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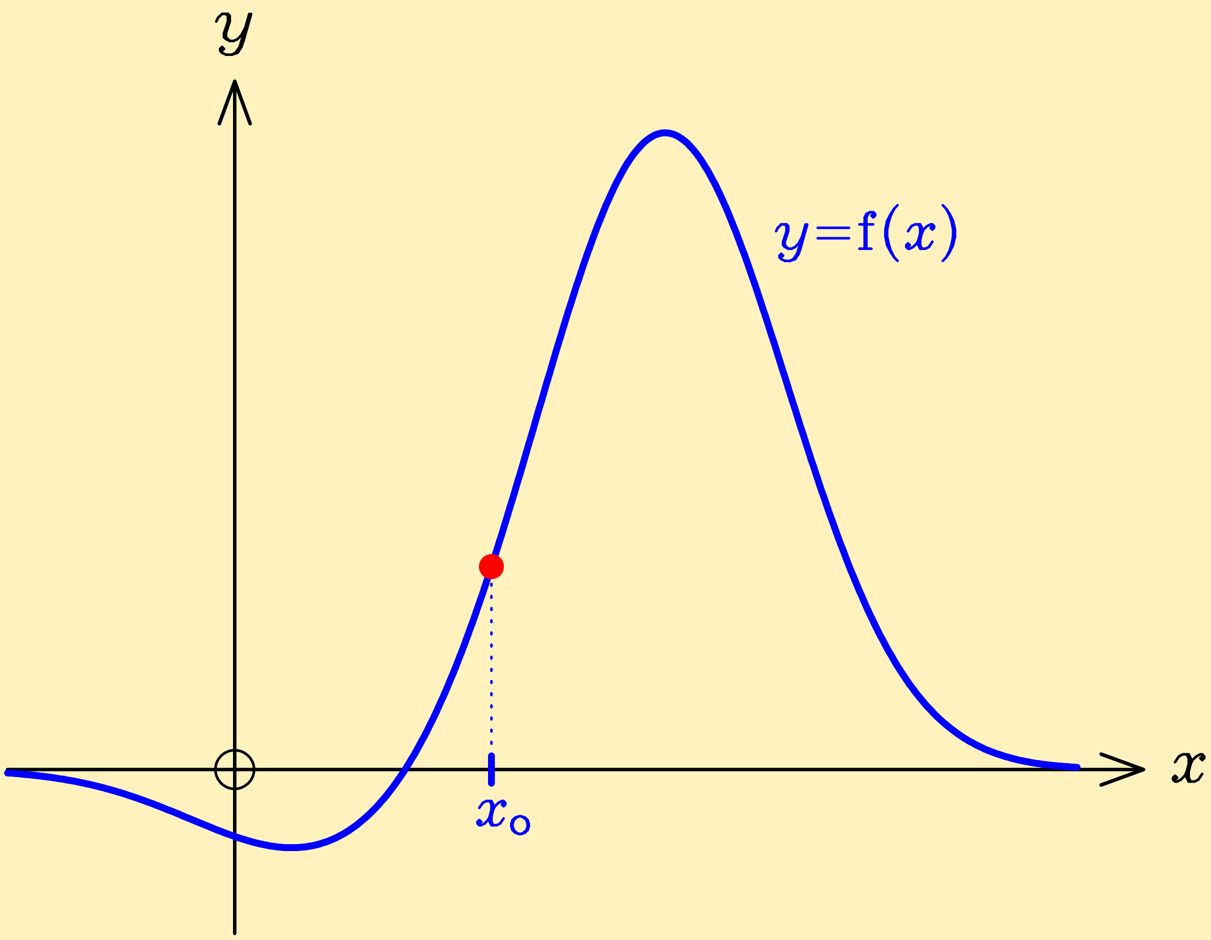
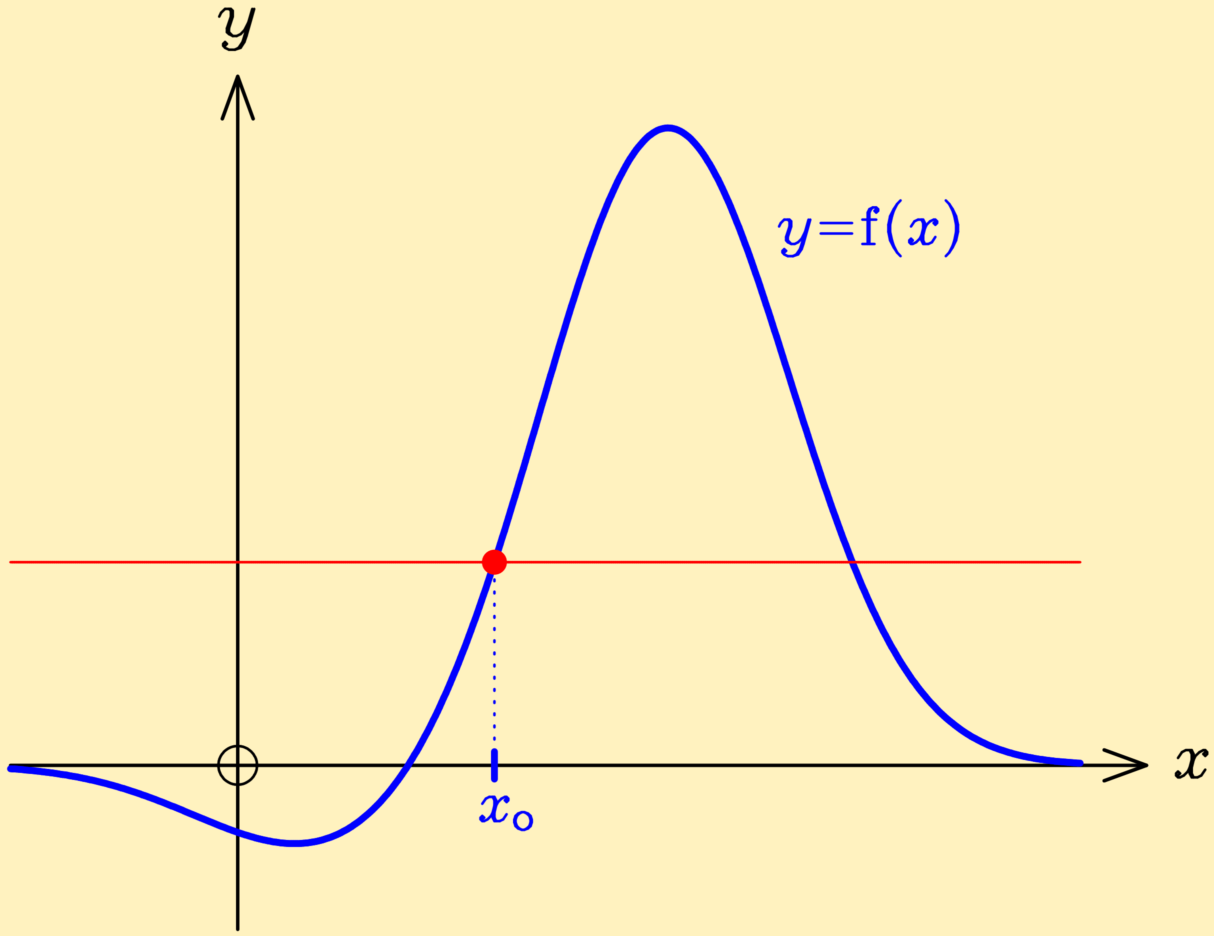
- **Approximating functions**
  - Taylor series
  - Fourier series $\rightarrow$ transform
- **Some formal properties**
  - Symmetry
  - Convolution theorem
  - Auto-correlation function
- **Physical insight**
  - Fourier optics

Taylor Series

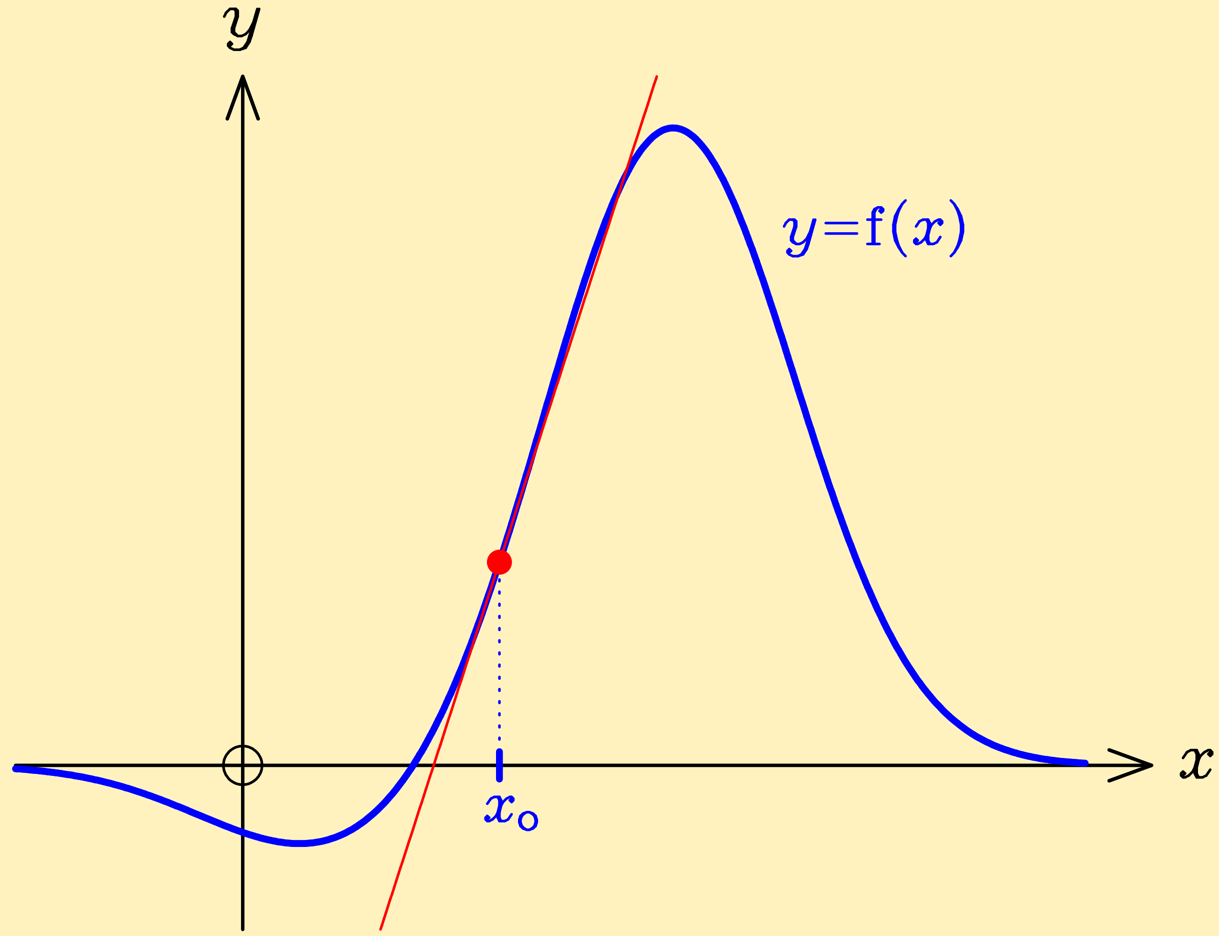


Taylor Series (0)



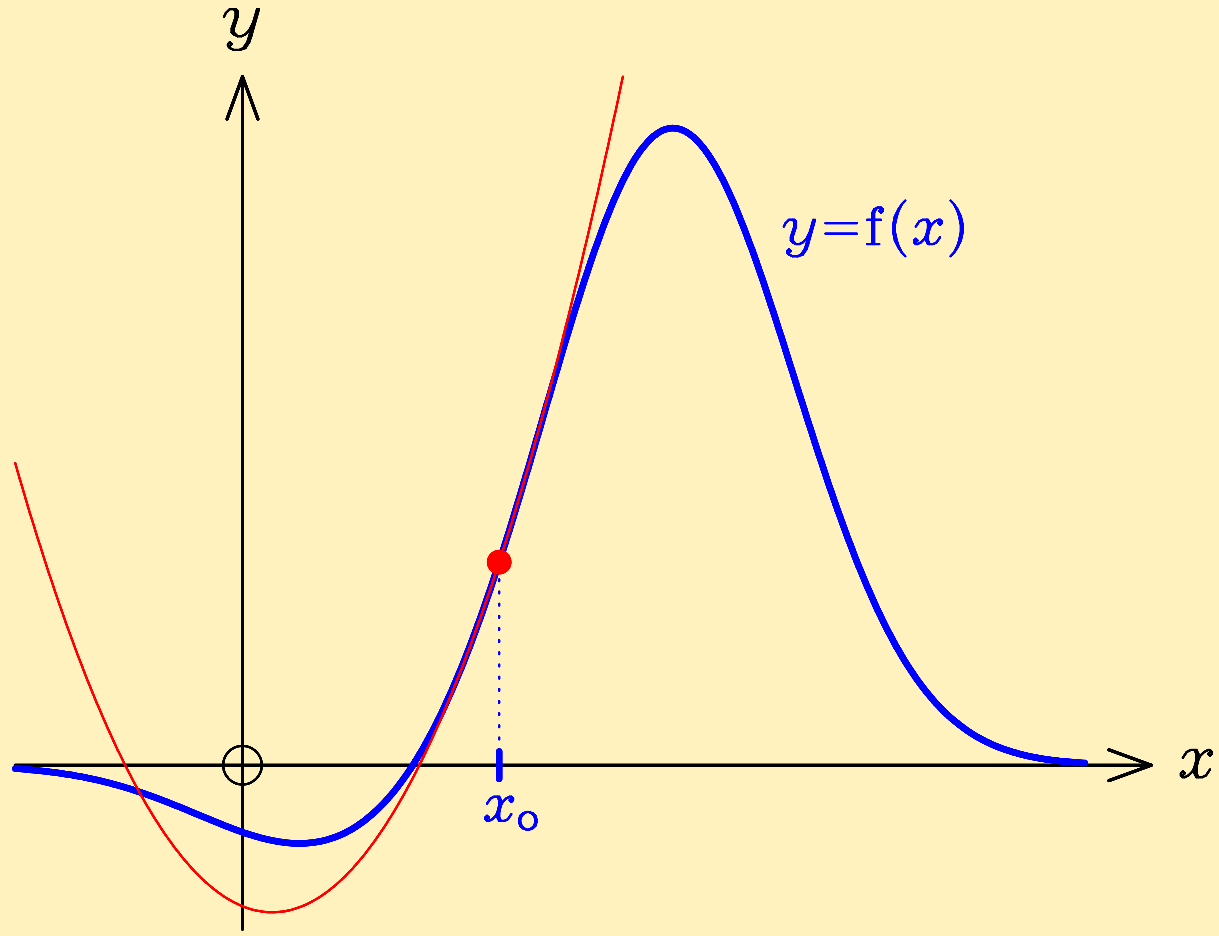
- $\mathrm{f}(x) \approx a_0$

Taylor Series (1)



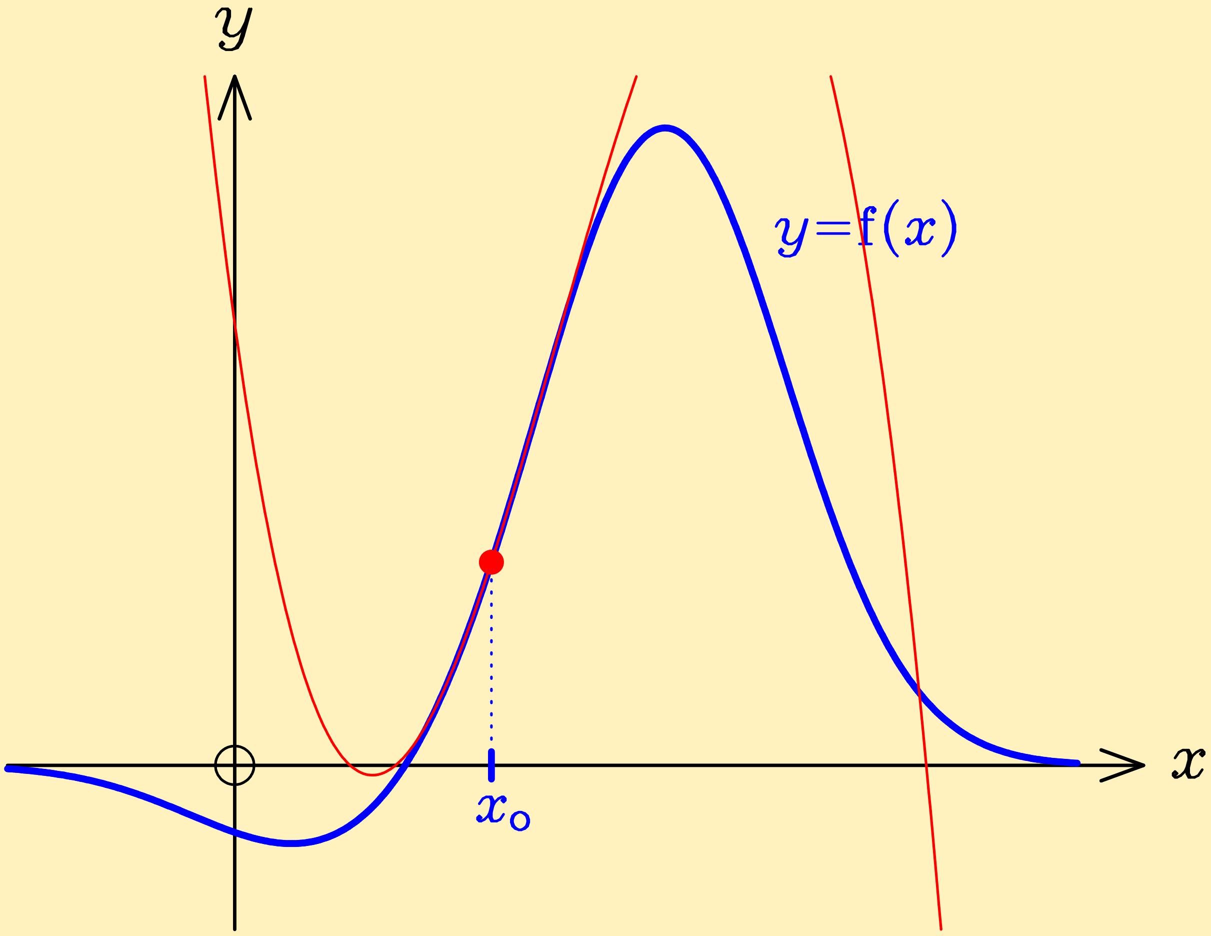
- $\mathrm{f}(x) \approx a_0 + a_1(x - x_o)$

Taylor Series (2)



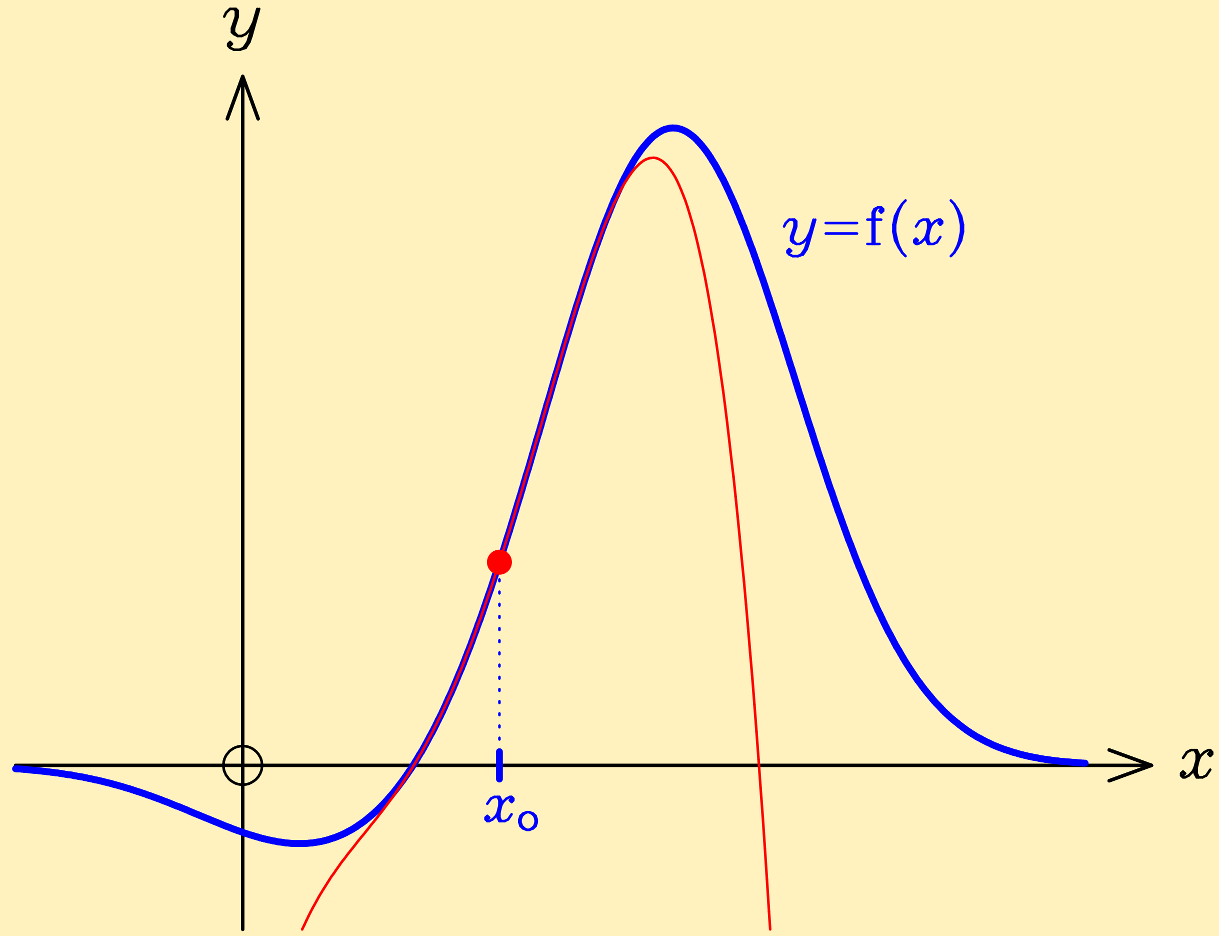
- $\mathrm{f}(x) \approx a_0 + a_1(x - x_\circ) + a_2(x - x_\circ)^2$

Taylor Series (3)



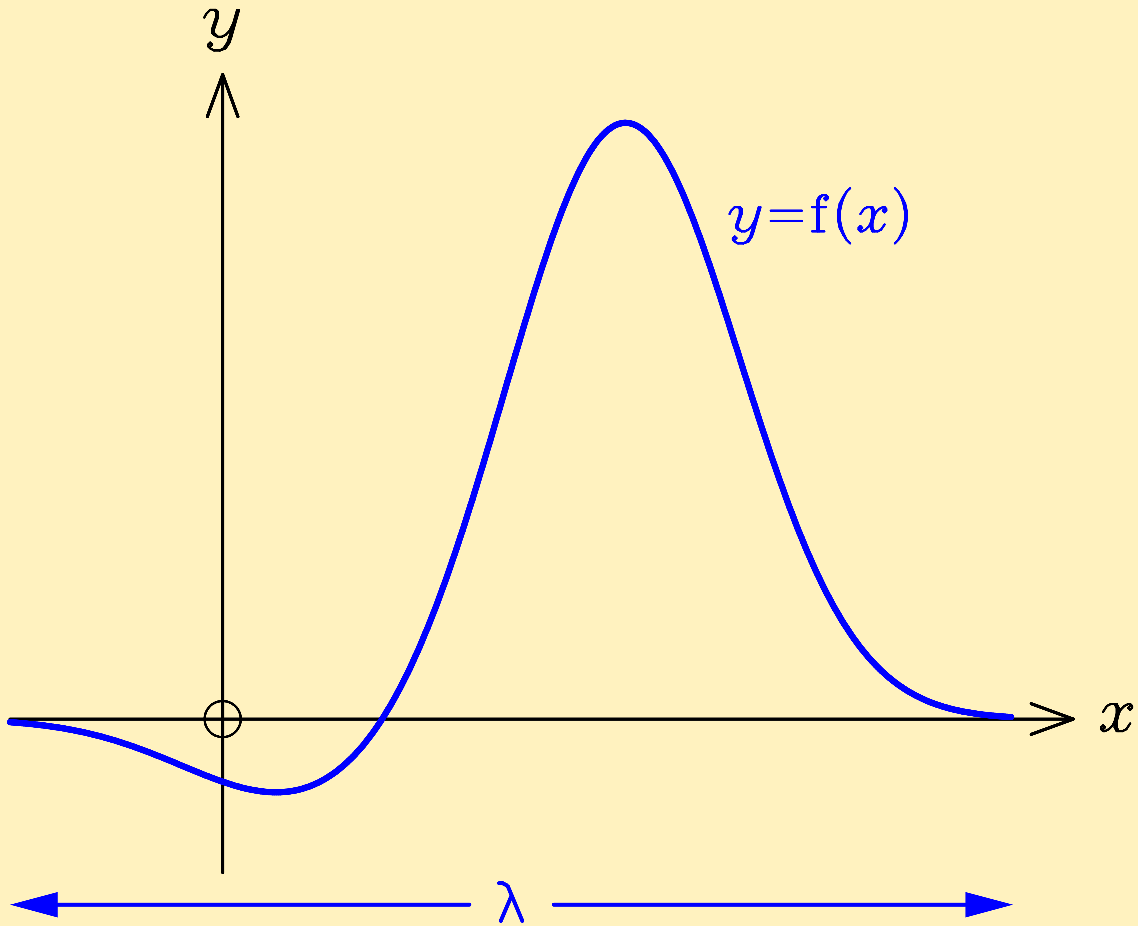
- $\mathrm{f}(x) \approx a_0 + a_1(x - x_o) + a_2(x - x_o)^2 + a_3(x - x_o)^3$

Taylor Series (4)



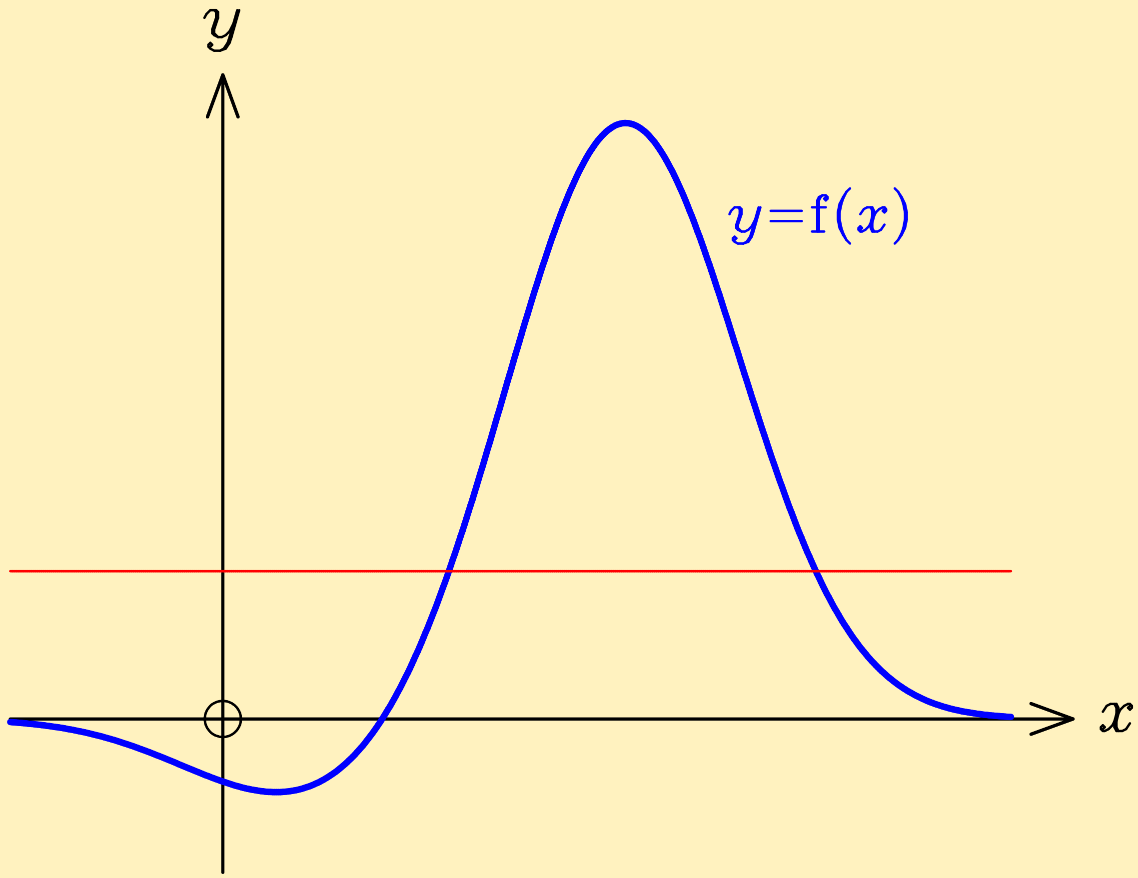
- $\mathrm{f}(x) \approx a_0 + a_1(x-x_o) + a_2(x-x_o)^2 + a_3(x-x_o)^3 + a_4(x-x_o)^4$

Fourier Series



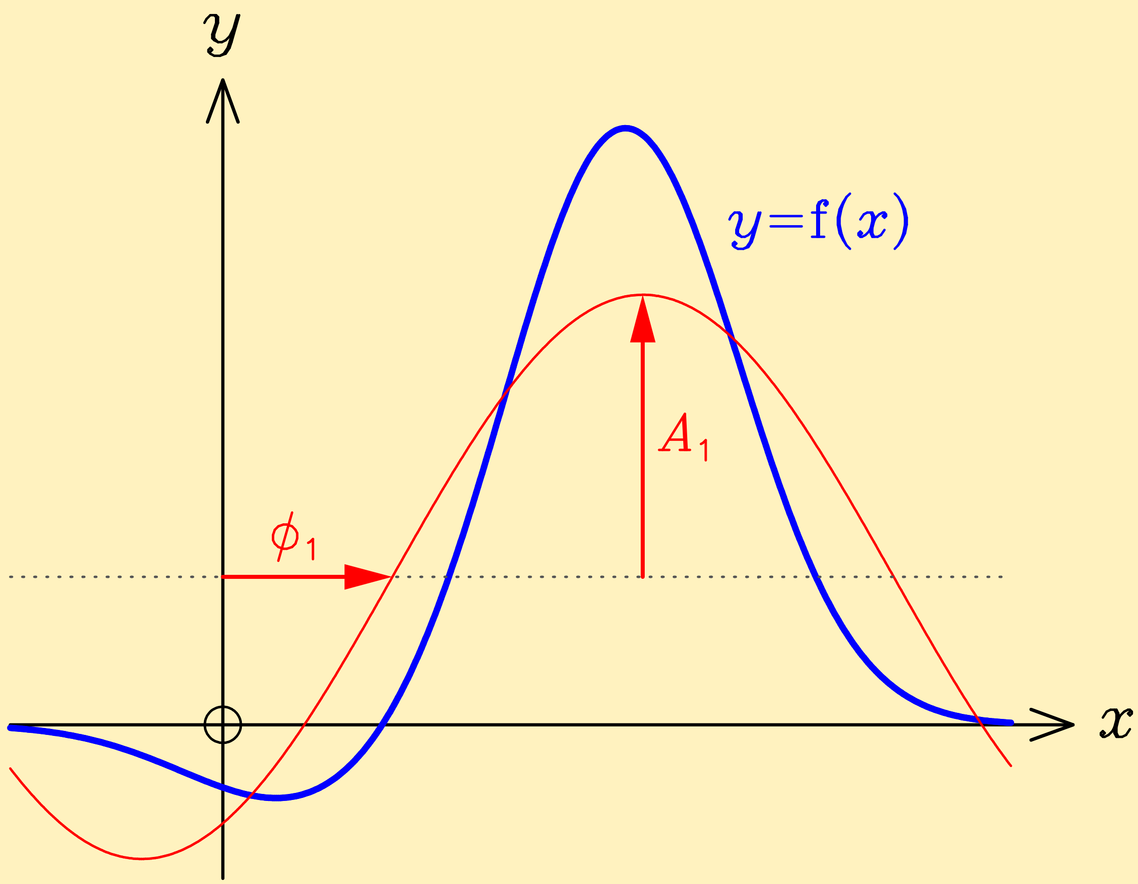
- Periodic: $\mathrm{f}(x) = \mathrm{f}(x+\lambda)$ $\qquad k = \dfrac{2\pi}{\lambda}$ (wavenumber)

Fourier Series (0)



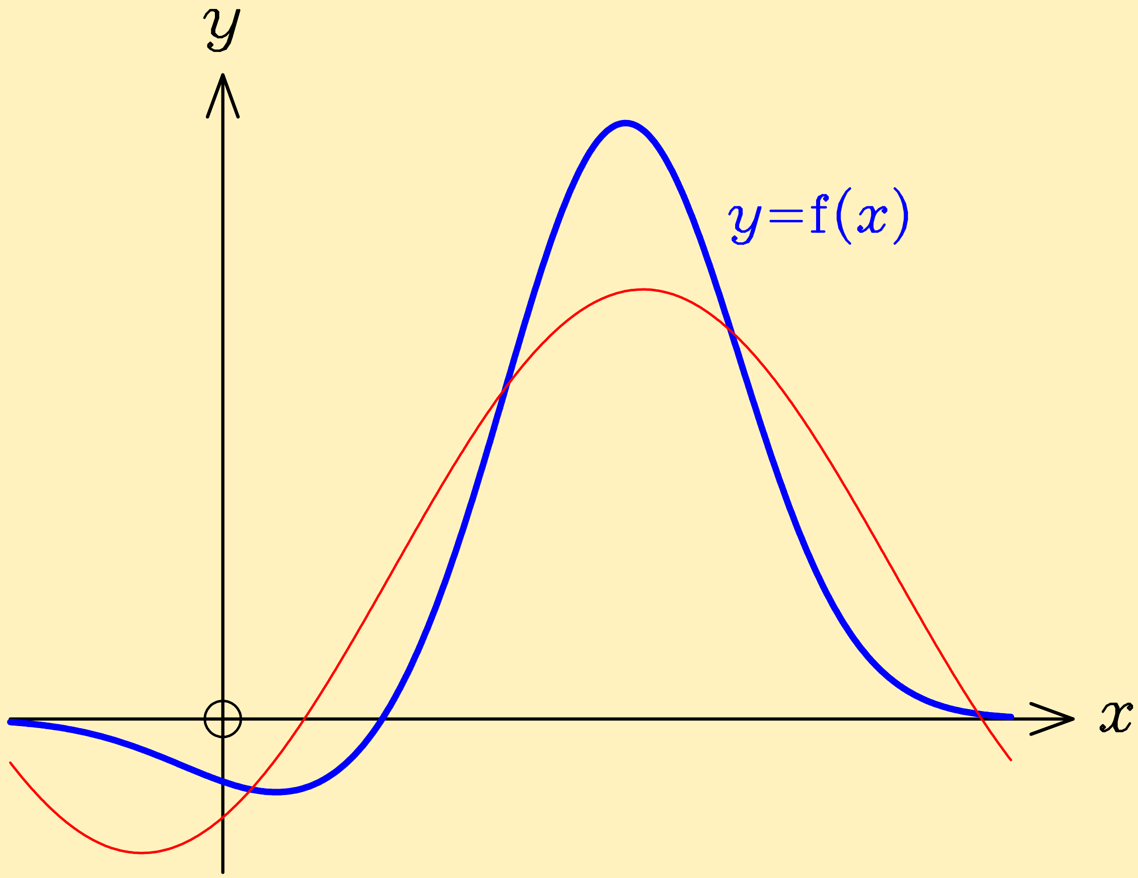
- $\mathrm{f}(x) \approx \frac{a_0}{2}$

Fourier Series (1)



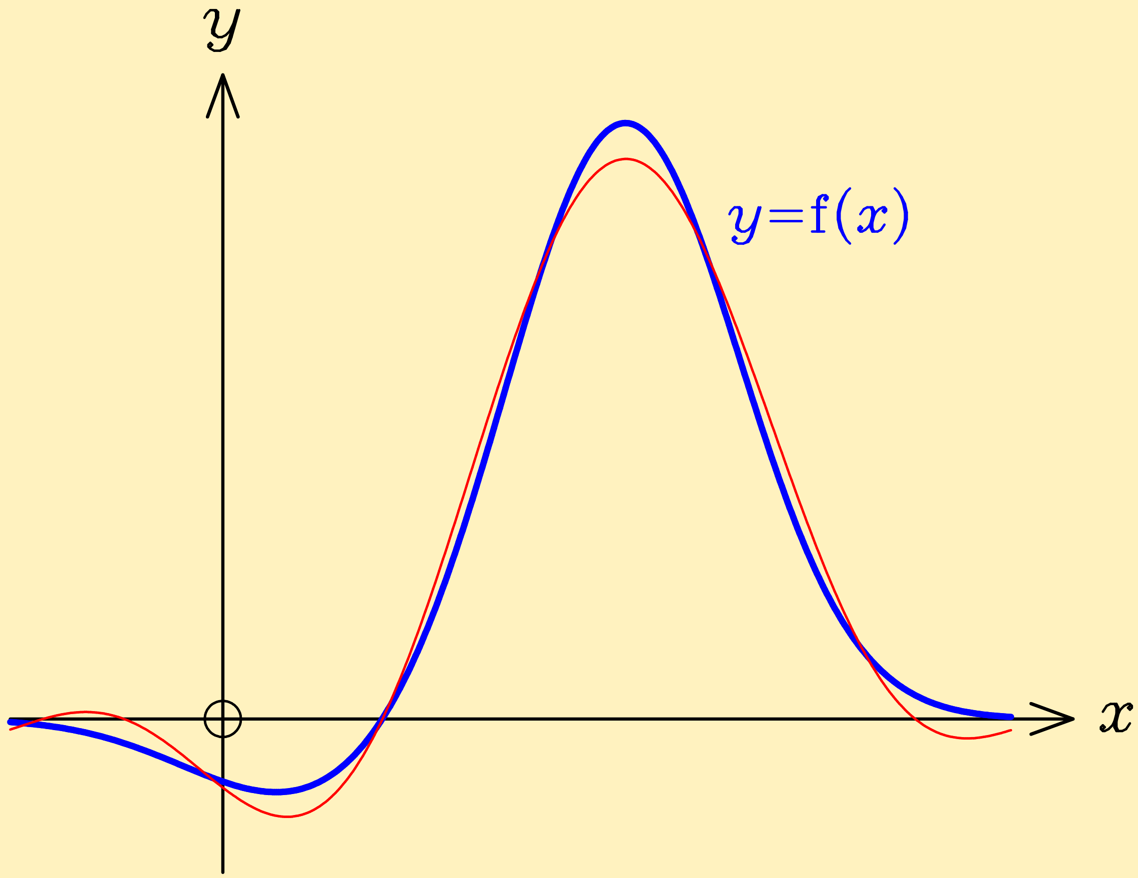
- $\mathrm{f}(x) \approx \frac{a_0}{2} + A_1 \sin(kx + \phi_1)$

Fourier Series (1)



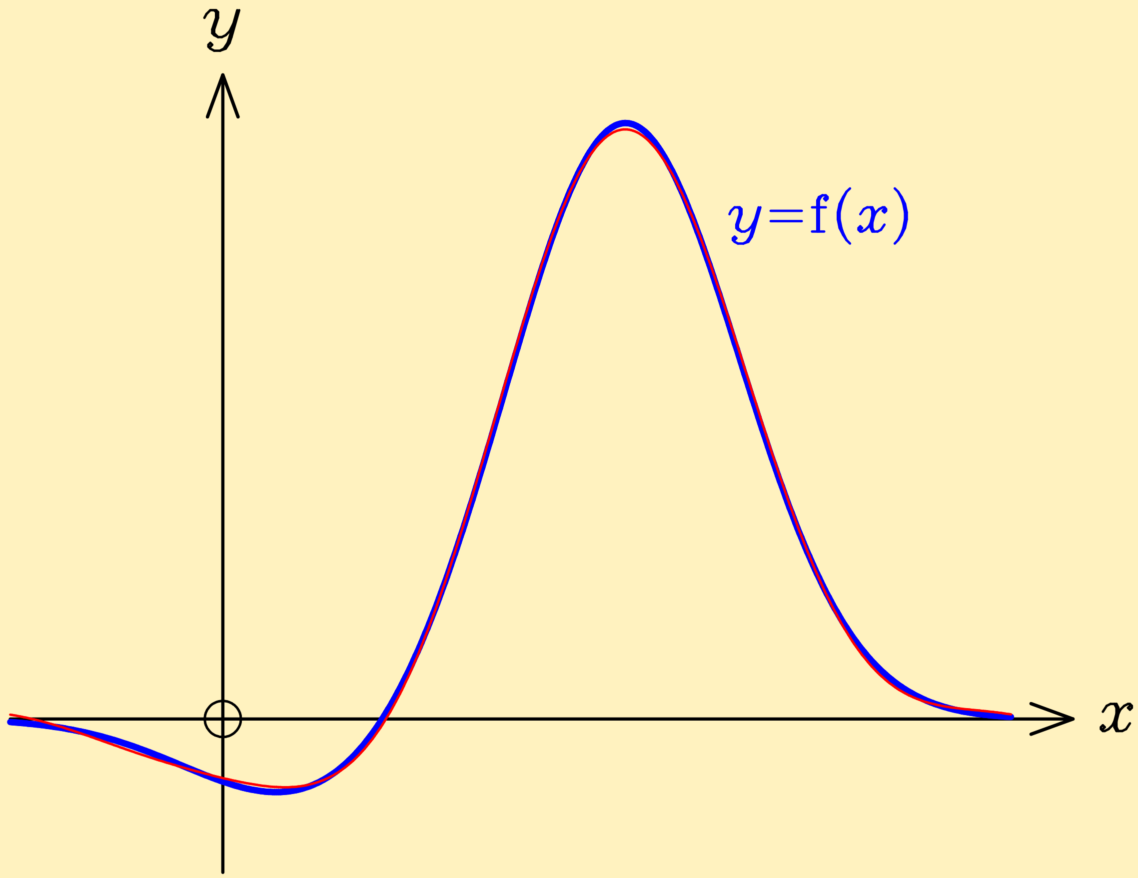
- $$\mathrm{f}(x) \approx \frac{a_0}{2} + a_1\cos(kx) + b_1\sin(kx)$$

Fourier Series (2)



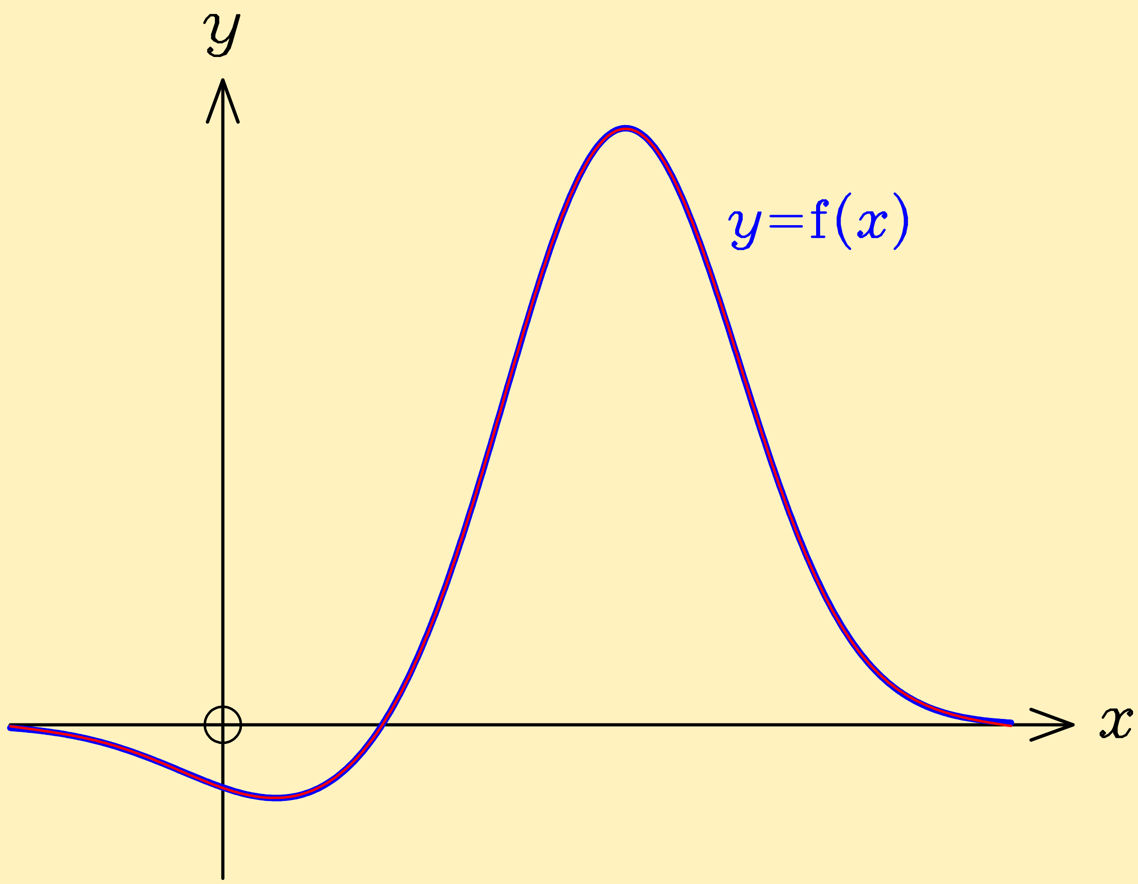
- $$\mathrm{f}(x) \approx \frac{a_0}{2} + a_1 \cos(kx) + a_2 \cos(2kx) + b_1 \sin(kx) + b_2 \sin(2kx)$$

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: $\mathrm{f}(x) = \sum_{n=0}^{\infty} a_n (x - x_\mathrm{o})^n$ $\qquad |x - x_\mathrm{o}| < R$
  - $a_n = \frac{1}{n!} \left. \frac{\mathrm{d}^n \mathrm{f}}{\mathrm{d}x^n} \right|_{x_\mathrm{o}}$

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

Complex Fourier Series

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

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- Fourier: $f(x) = \sum_{n=-\infty}^{\infty} c_n \, e^{inkx}$
  - $c_n = \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} f(x) \, e^{-inkx} \, dx$

Complex Fourier Series

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

Fourier Transform

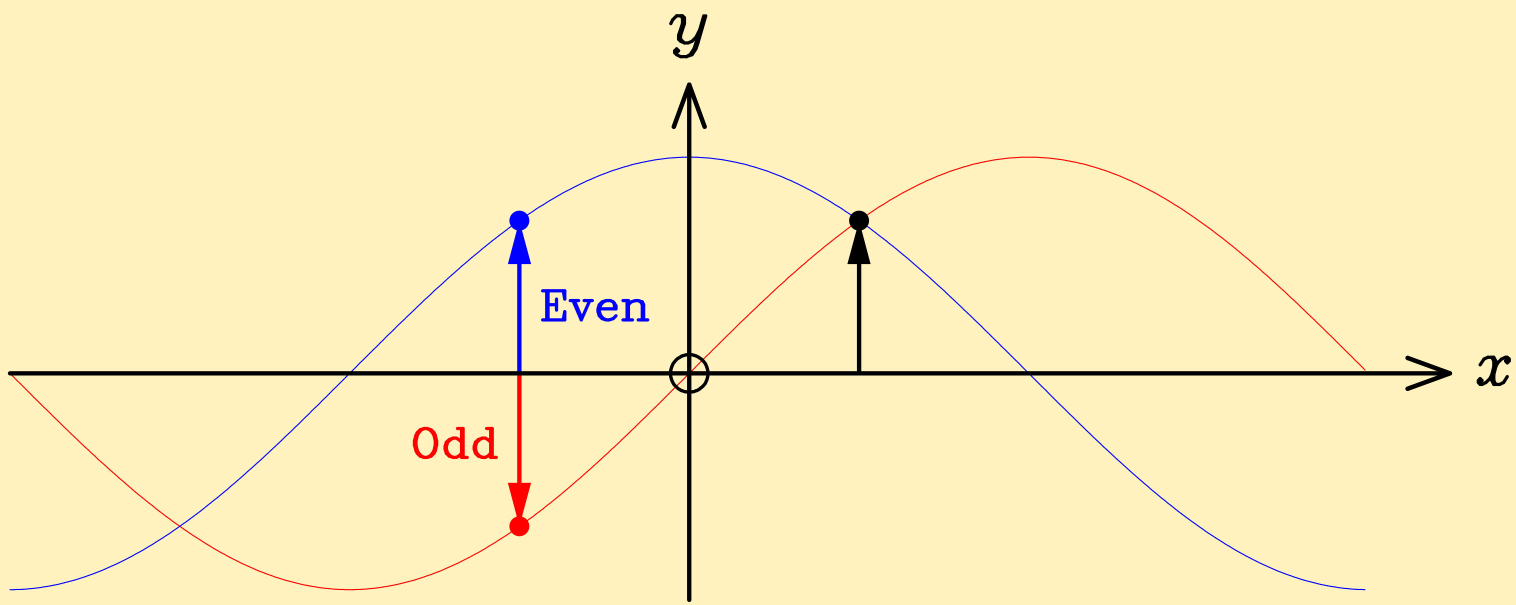
- **As** $\lambda \to \infty$, so that $k \to 0$ and $\mathrm{f}(x)$ is non-periodic,
  - $$\sum_{n=-\infty}^{\infty} c_n \, \mathrm{e}^{\mathrm{i}nkx} \longrightarrow \int_{-\infty}^{\infty} c(q) \, \mathrm{e}^{\mathrm{i}qx} \, \mathrm{d}q$$

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



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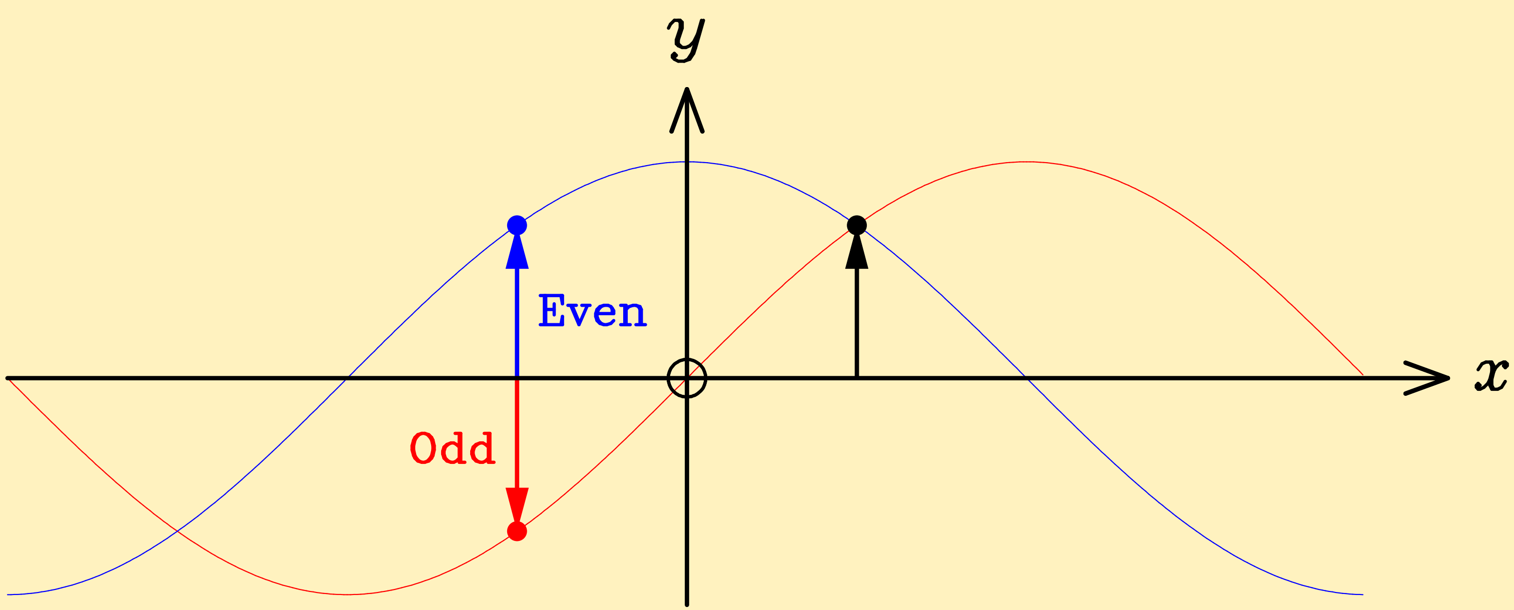
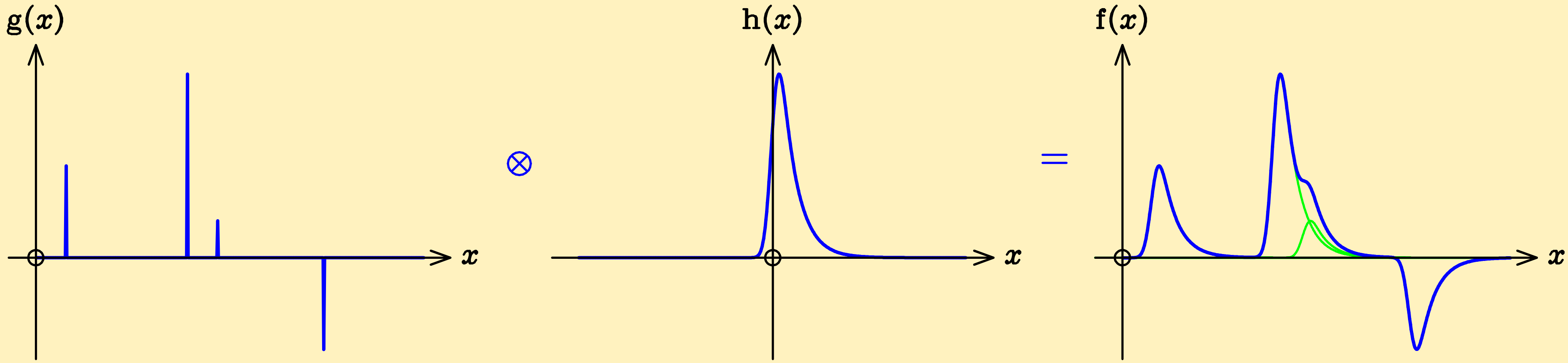


- Real: $\boxed{\mathrm{f}(x) = \mathrm{f}(x)^* \iff \mathrm{F}(q) = \mathrm{F}(-q)^*}$ **(Friedel pairs)**

Convolution

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



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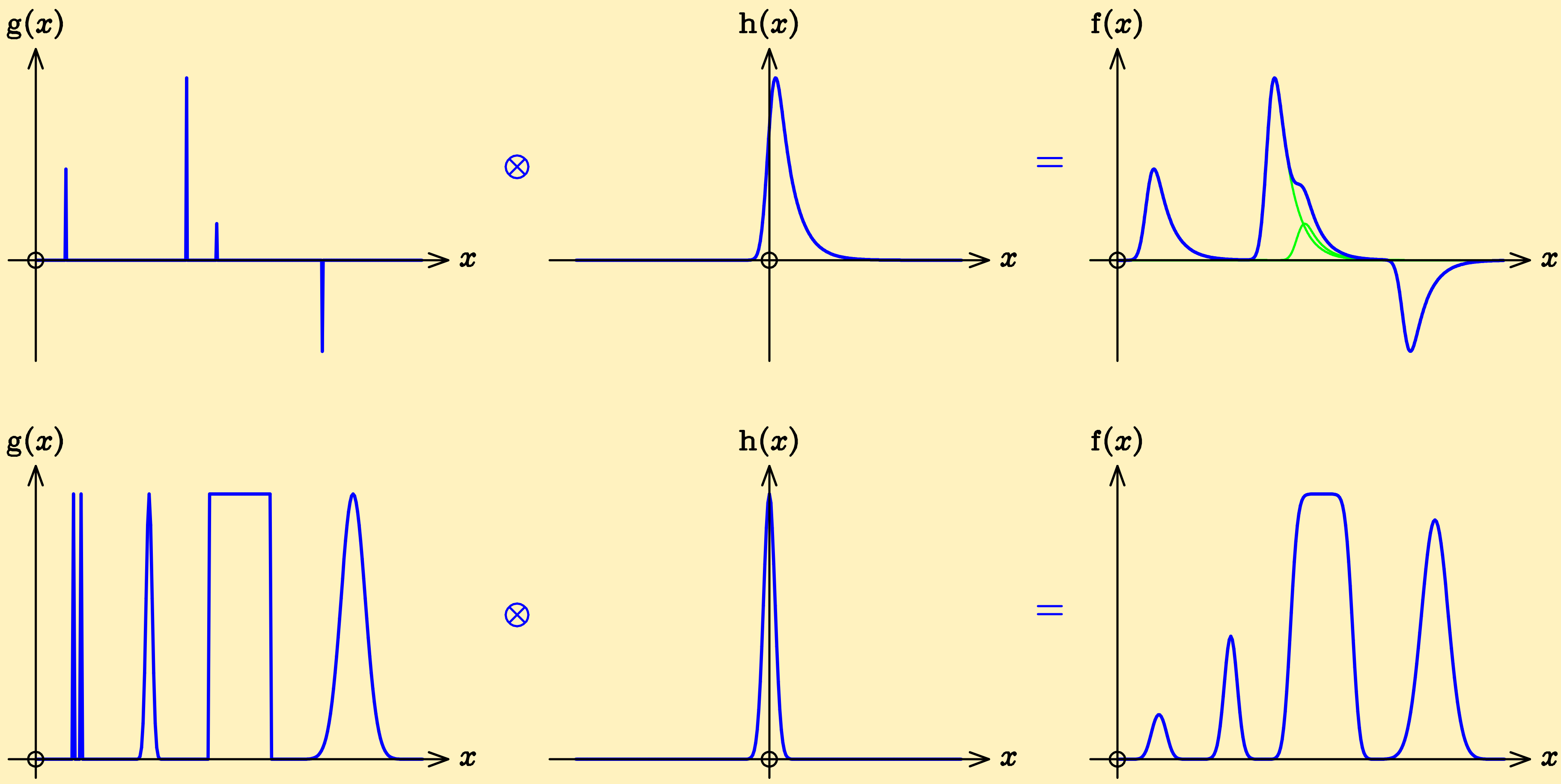

Convolution Theorem

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

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

Auto-correlation Function

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

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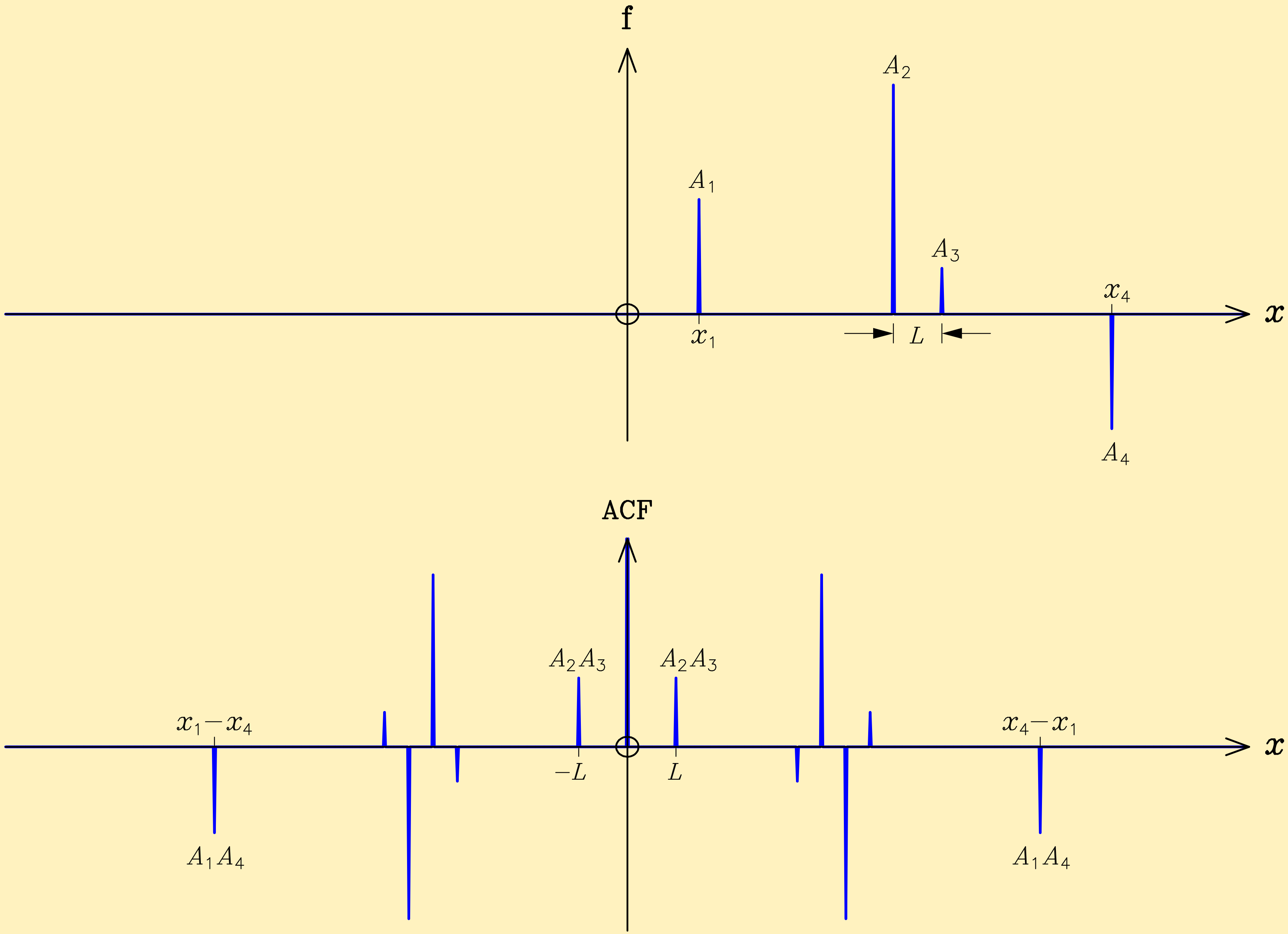
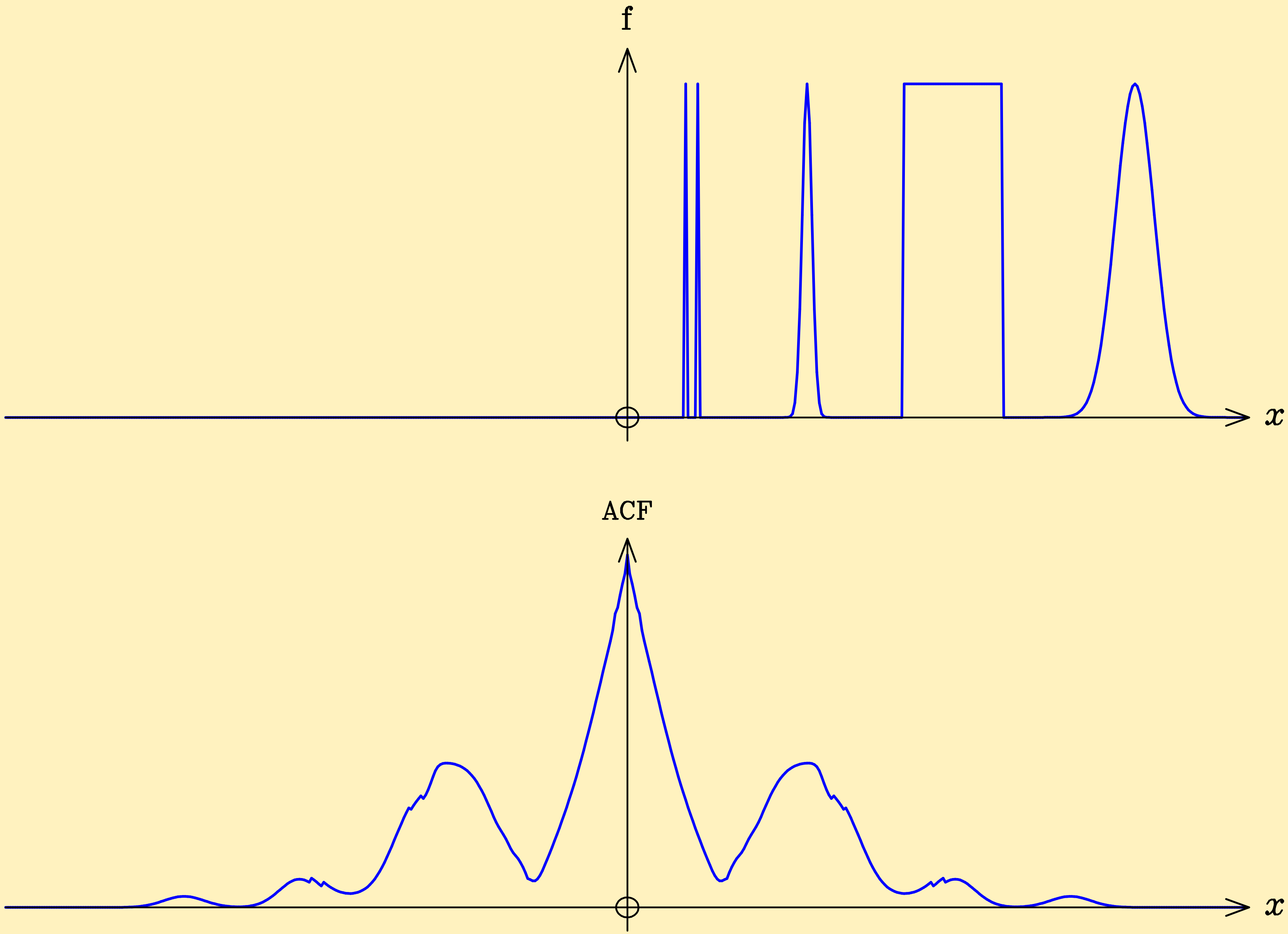
- $$\boxed{\int_{-\infty}^{\infty} \left|\mathrm{F}(q)\right|^2 \mathrm{e}^{\mathrm{i}qx}\, \mathrm{d}q = \int_{-\infty}^{\infty} \mathrm{f}(t)^*\, \mathrm{f}(x+t)\, \mathrm{d}t} = \mathrm{ACF}(x)$$

  - Patterson map

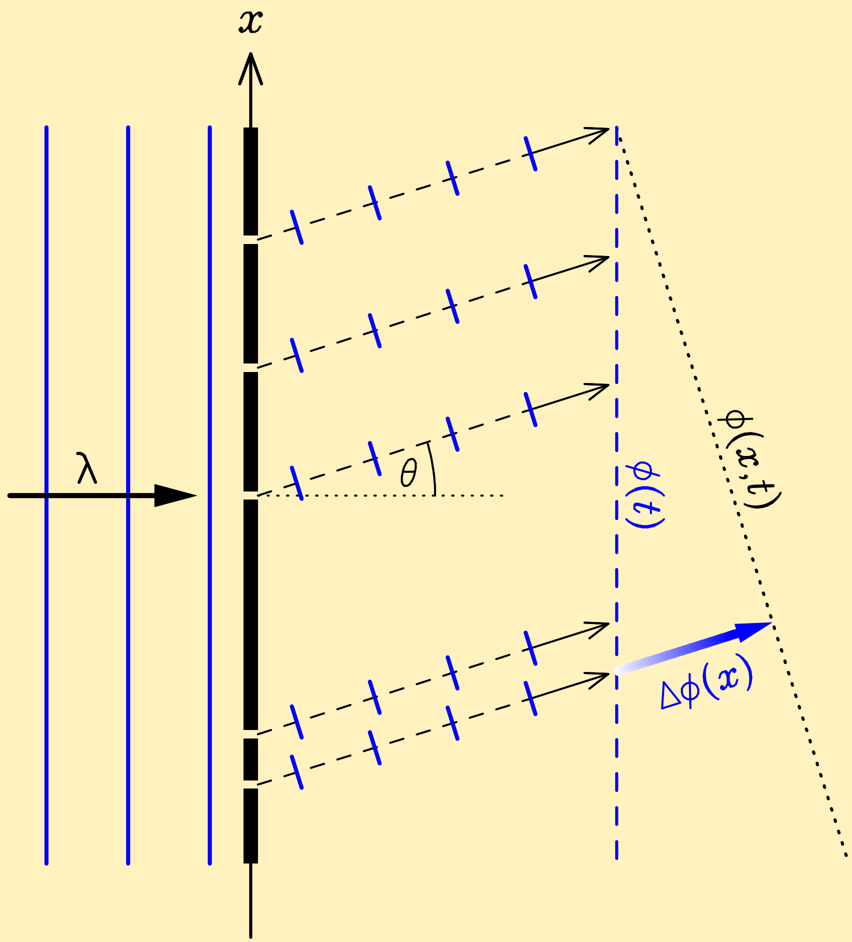
Auto-correlation Function (1)

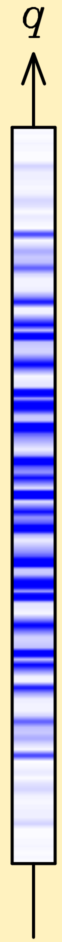


Auto-correlation Function (2)



Fourier Optics





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

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

Young's Double Slits

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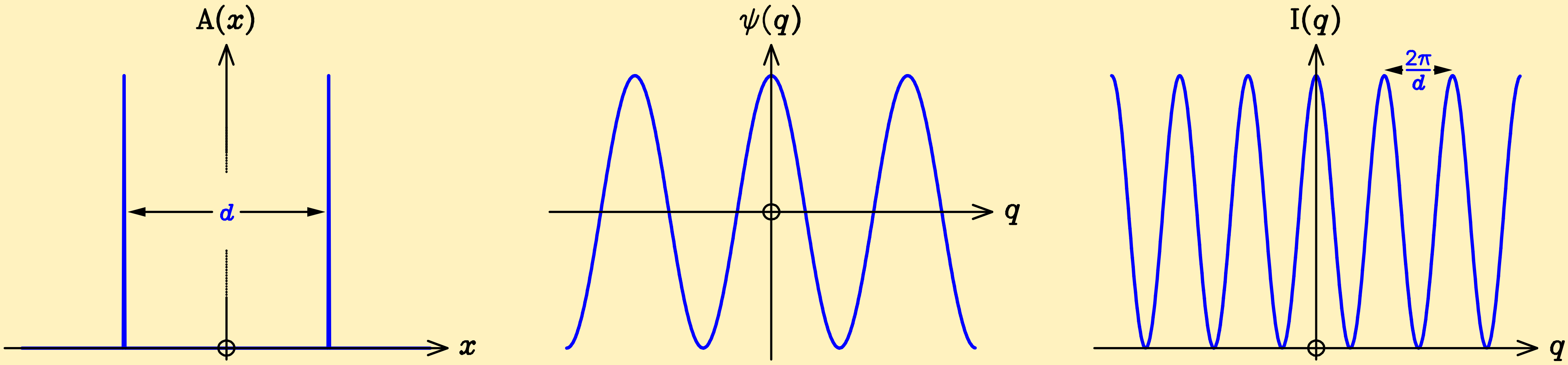

Single Wide Slit

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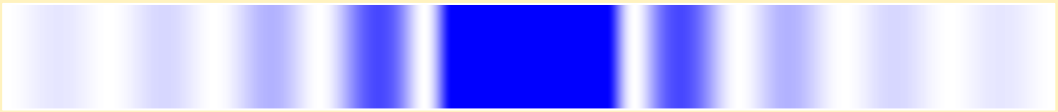

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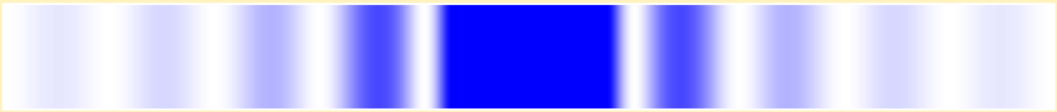
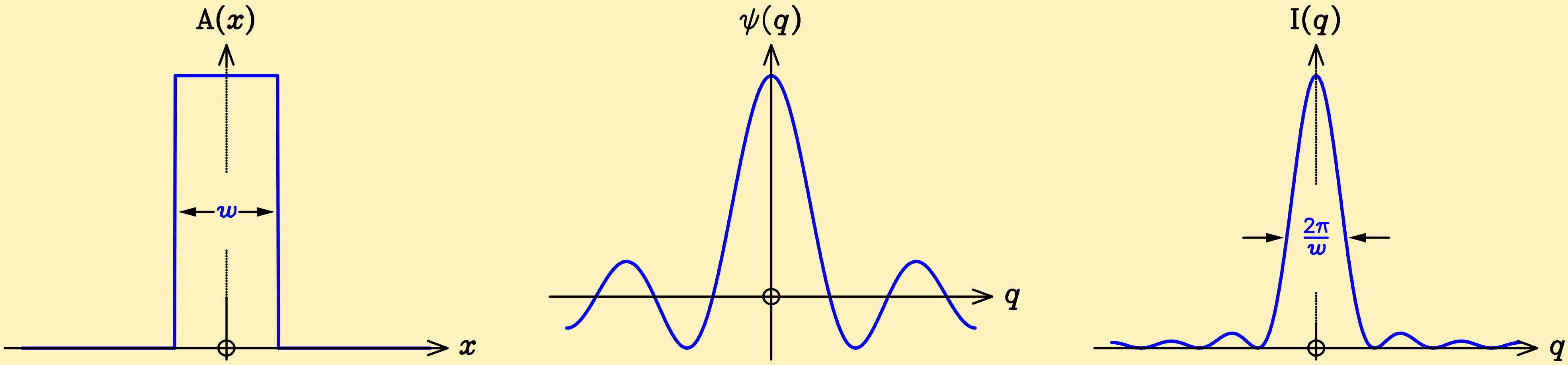
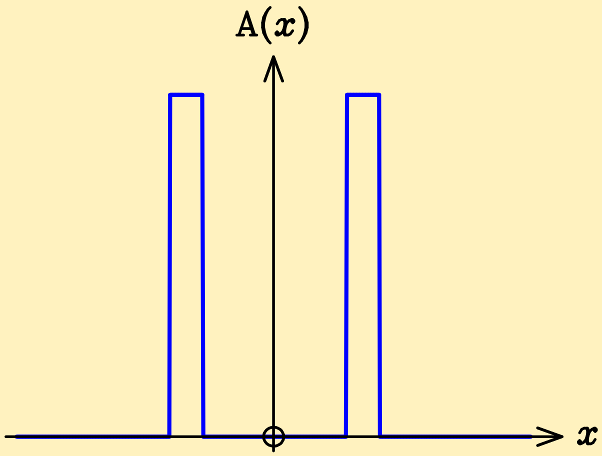
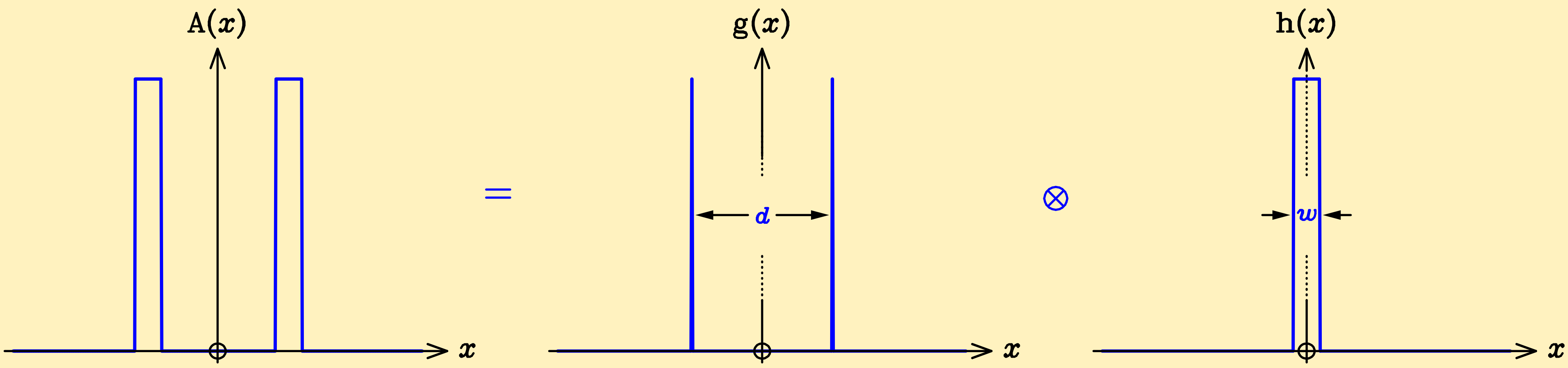




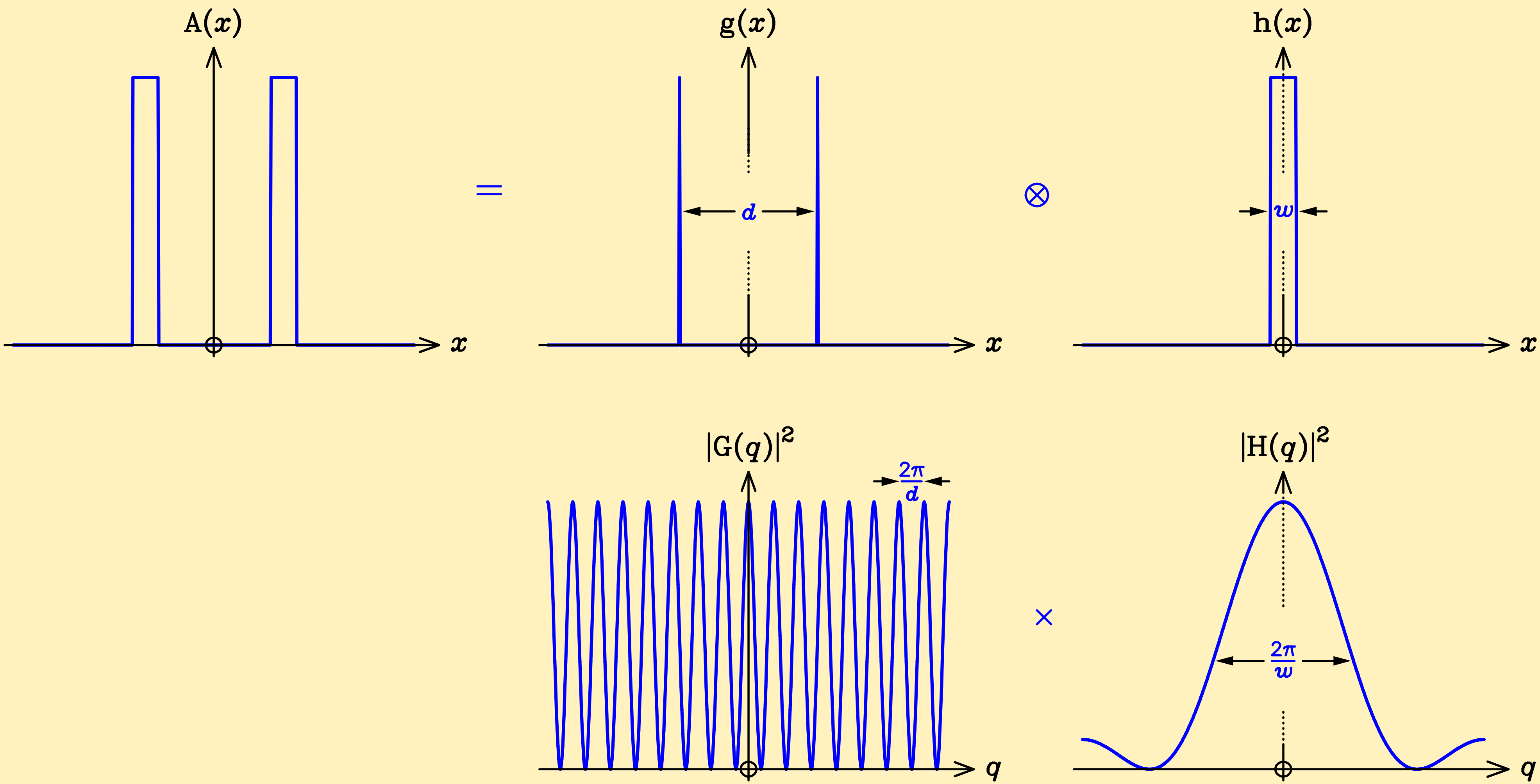
Two Wide Slits (0)



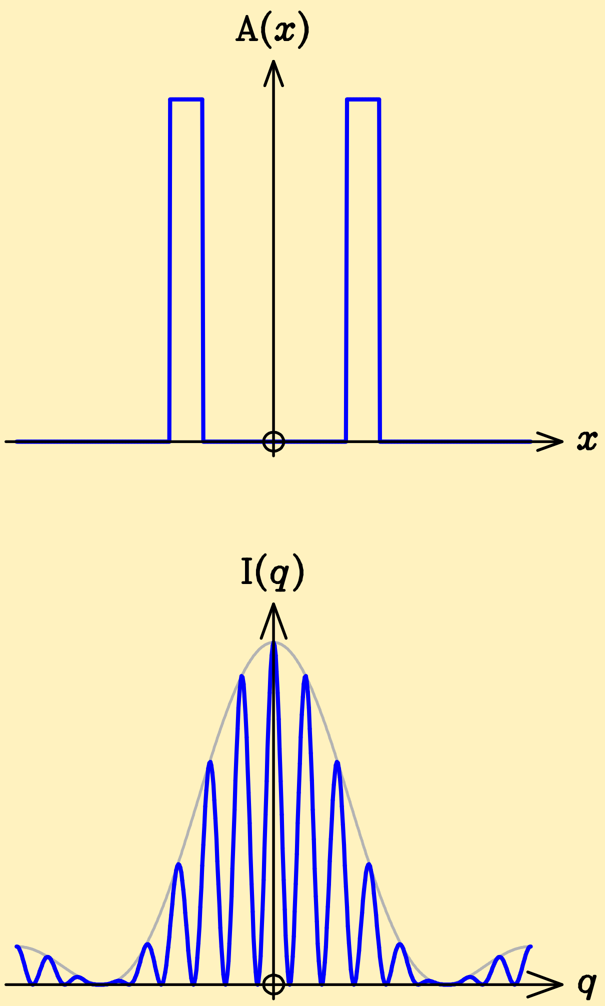
Two Wide Slits (1)



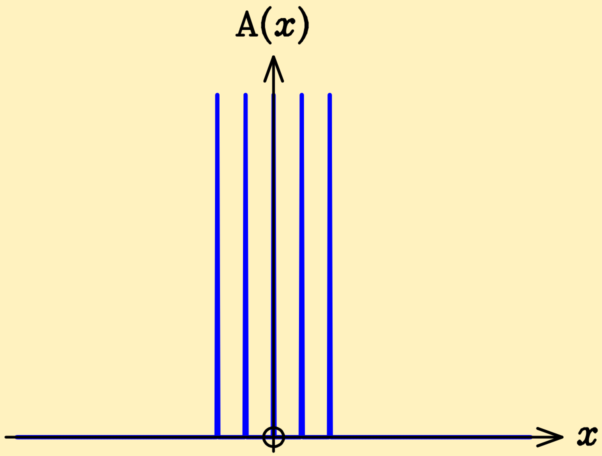
Two Wide Slits (2)



Two Wide Slits (3)



Finite Grating (0)



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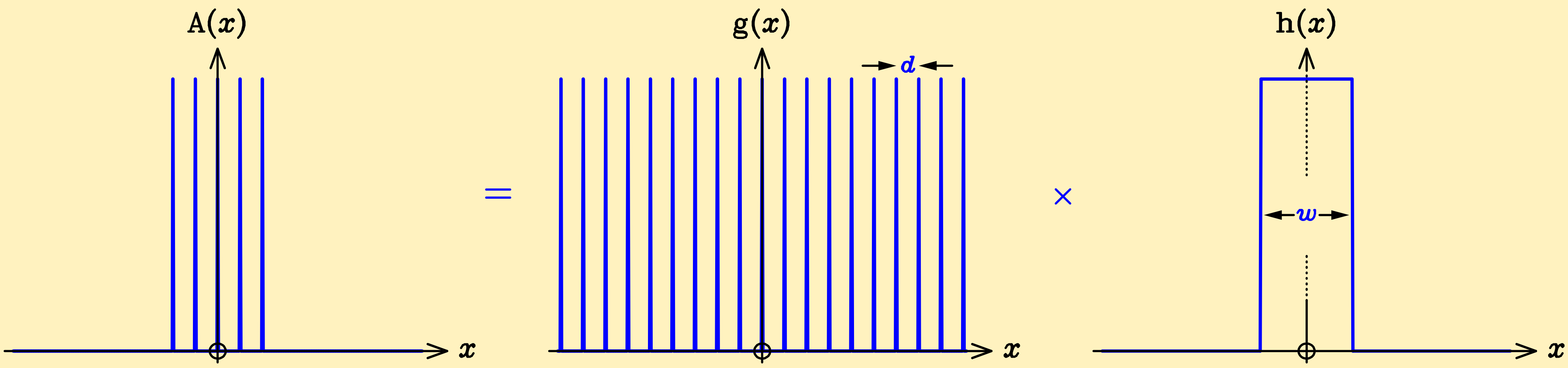

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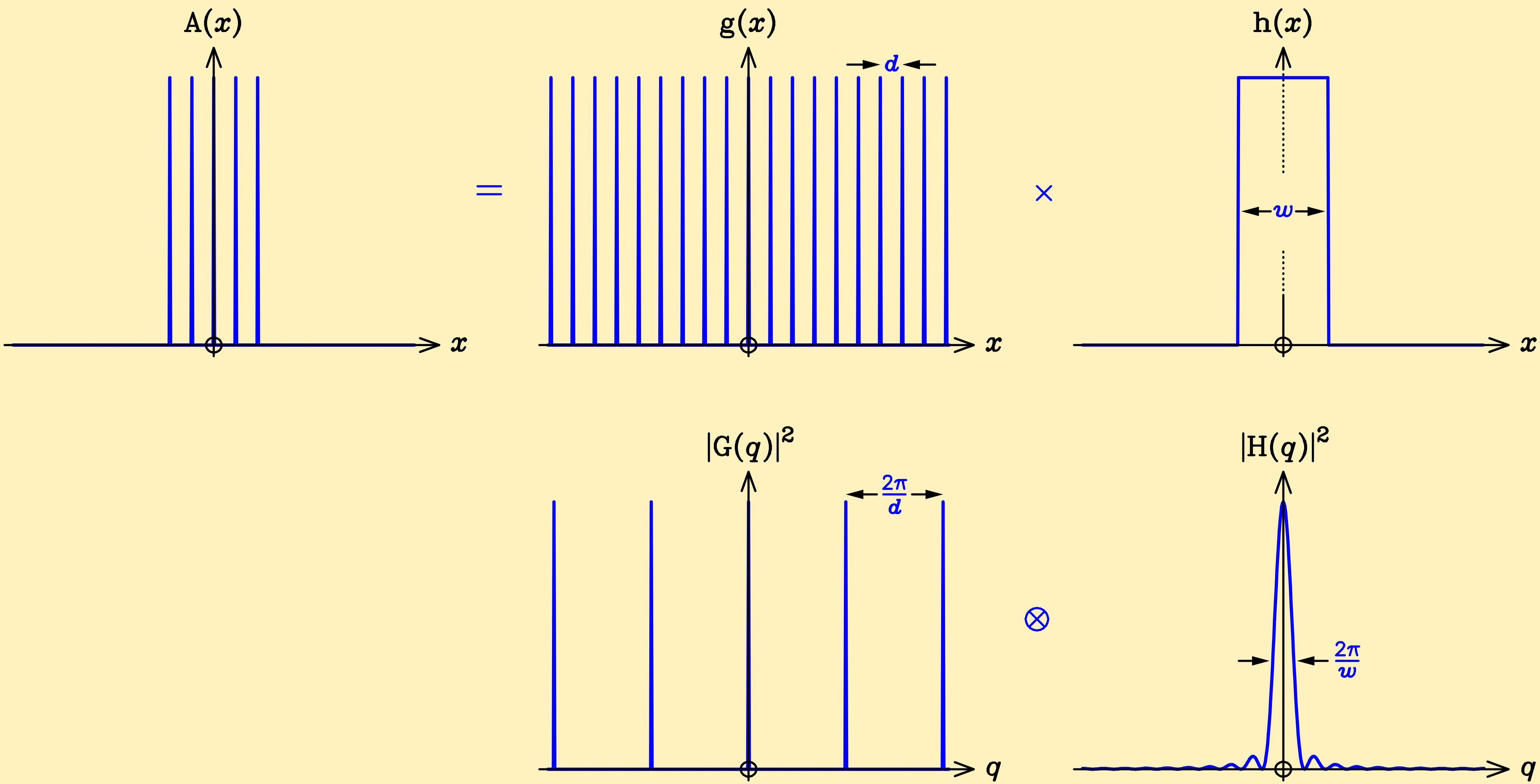

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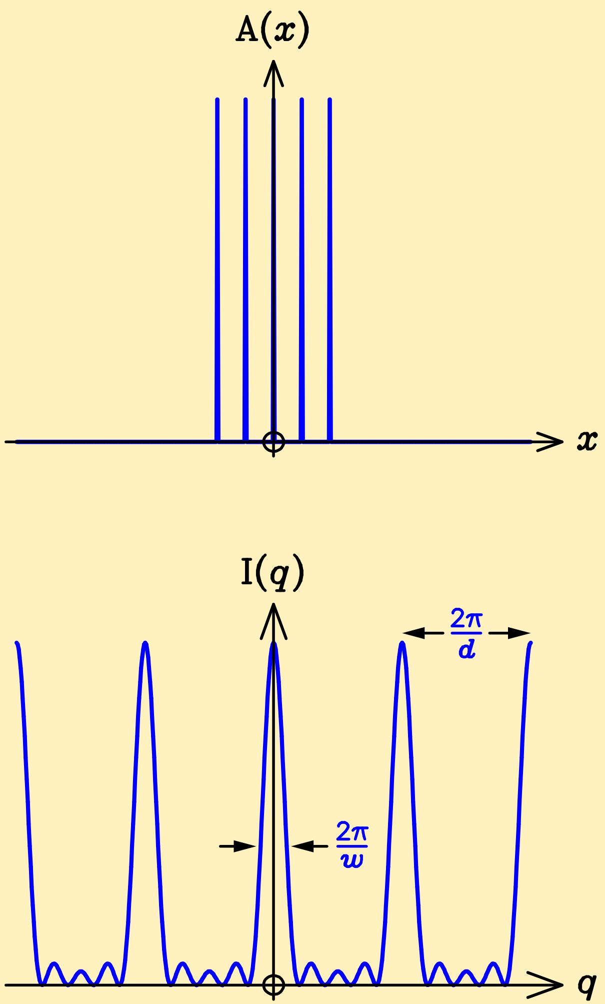

Write up of this Talk!

- 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 (January 2011), Oxford University Press

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

The phaseless Fourier problem

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