PHOT 222: Quantum Photonics
LECTURE 04

Michaël Barbier, Spring semester (2024-2025)

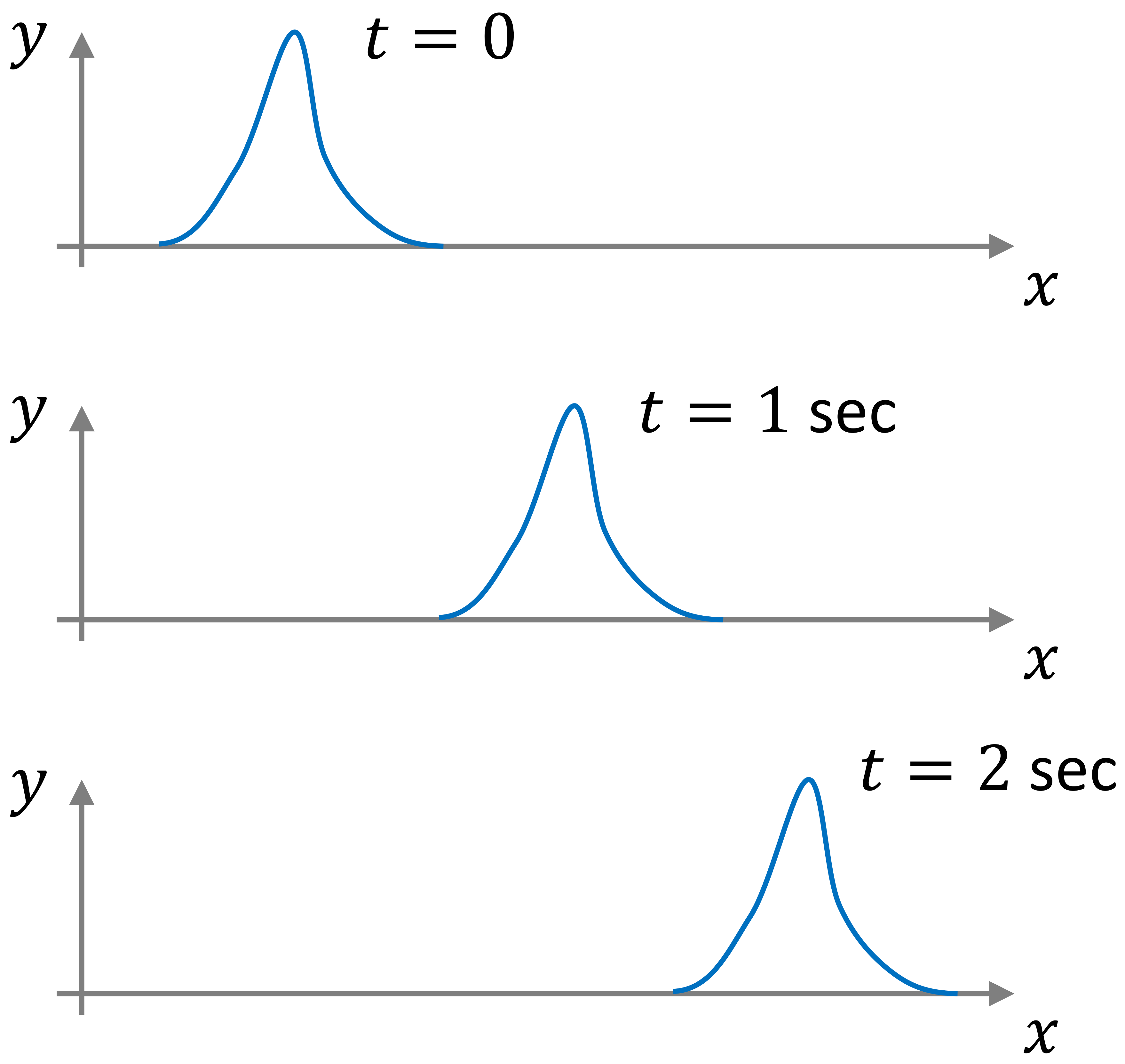
OVERVIEW OF THE COURSE

week	topic	Serway 9th	Young
Week 1	Relativity	Ch. 39	Ch. 37
Week 2	Waves and Particles	Ch. 40	Ch. 38-39
Week 3	Wave packets and Uncertainty	Ch. 40	Ch. 38-39
Week 4	**The Schrödinger equation and Probability**	**Ch. 41**	**Ch. 39**
Week 5	**Midterm exam 1**		
Week 6	Quantum particles in a potential		
Week 7	Harmonic oscillator		
Week 8	Tunneling through a potential barrier		
Week 9	The hydrogen atom, absorption/emission spectra		
Week 10	**Midterm exam 2**		
Week 11	Many-electron atoms		
Week 12	Pauli-exclusion principle		
Week 13	Atomic bonds and molecules		
Week 14	Crystalline materials and energy band structure		

Waves and the wave equation

TRAVELING WAVES AND PULSES

- Description 1D waves $y = \phi(x,t)$
- Traveling wave $\phi(x,t) \equiv f(x - vt)$
- For $x = vt$ the shape is constant
  - Right-traveling $\phi(x,t) \equiv f(x - vt)$
  - Left-traveling $\phi(x,t) \equiv f(x + vt)$



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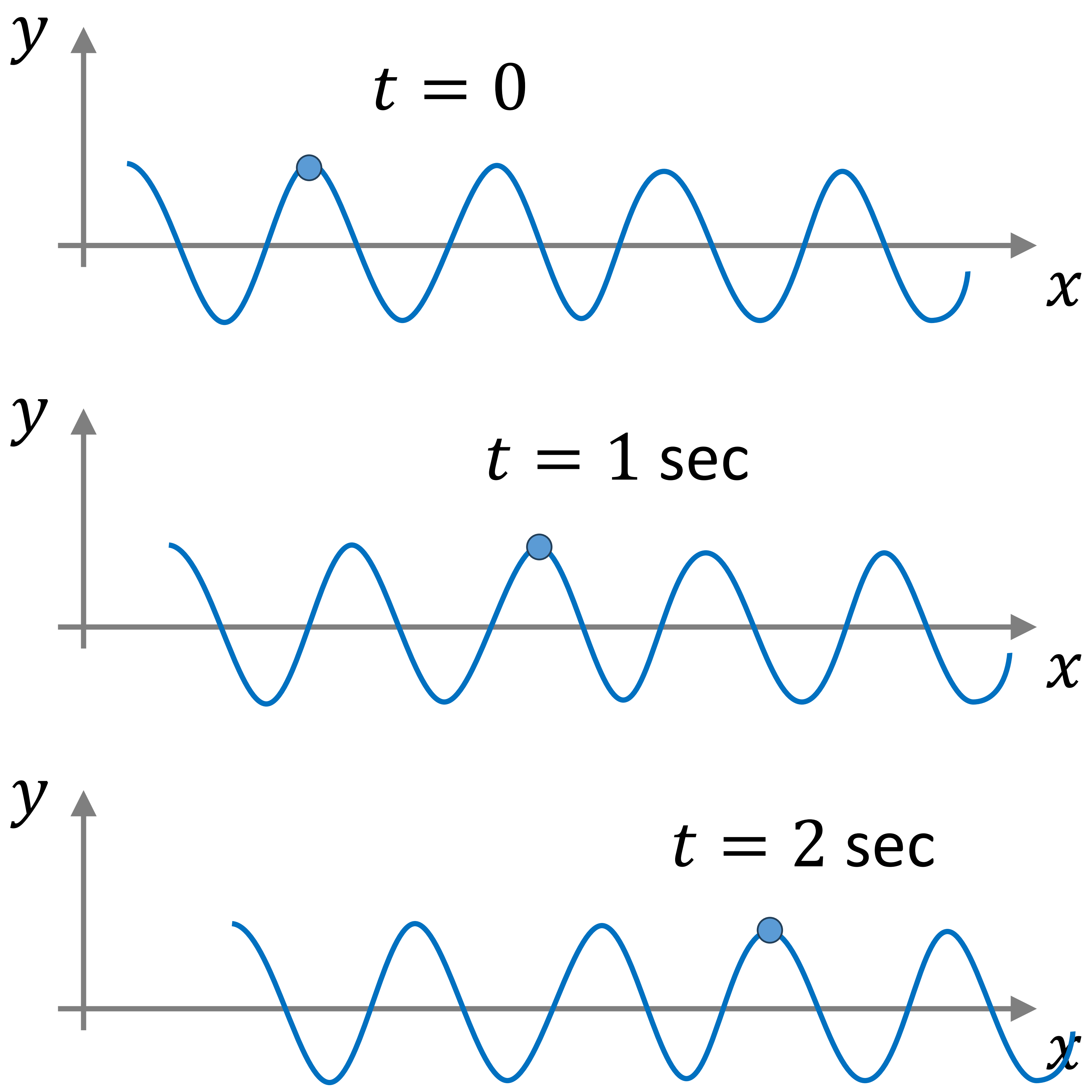


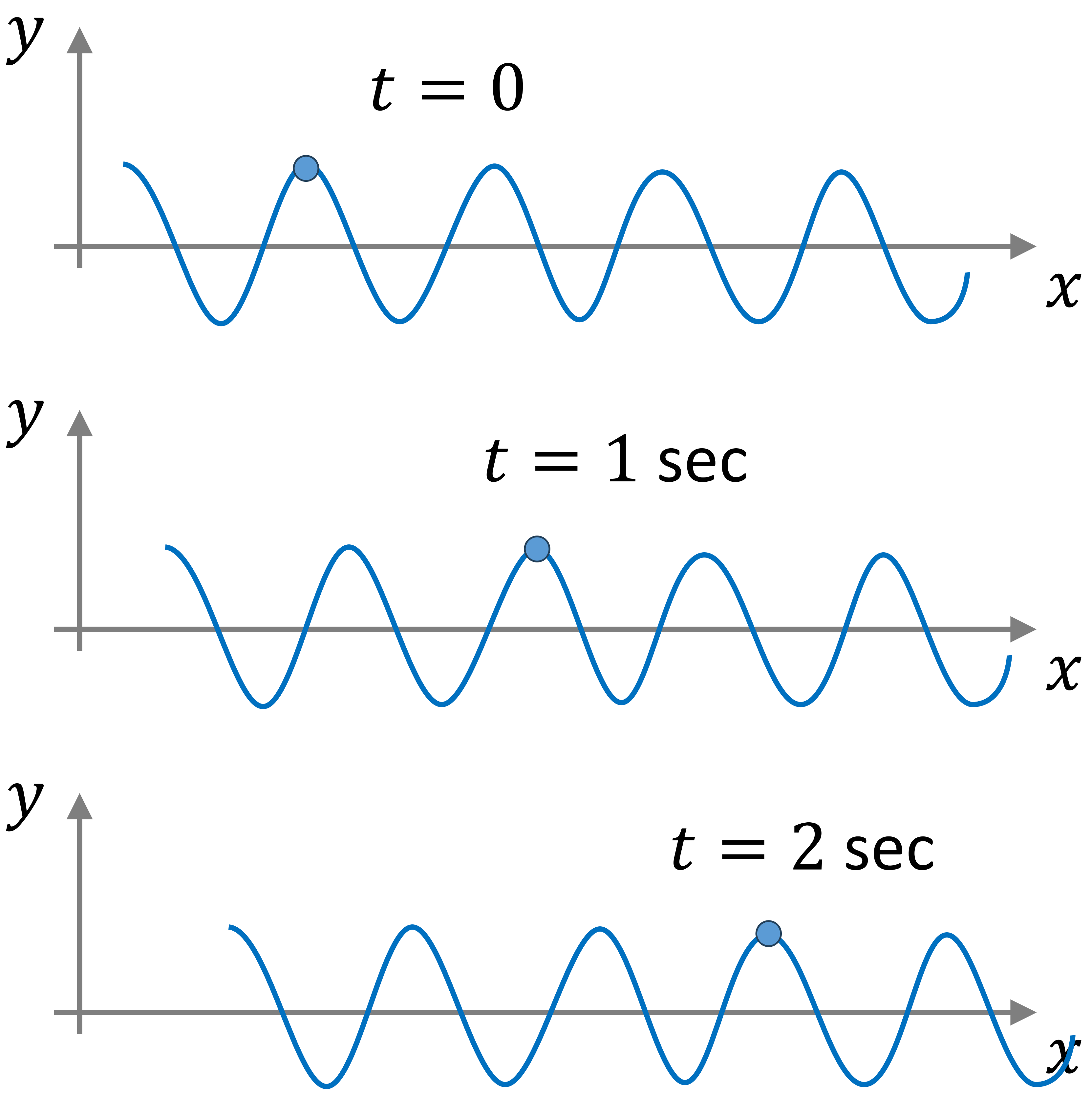
TRAVELING WAVES AND PULSES

- Standard form:

$$\phi(\mathrm{x},\mathrm{t}) = A\cos(kx - \omega t)$$

$f\,(x - vt)$?

$$= A\cos\left(\omega\left(\frac{k}{\omega}x - t\right)\right)$$



- Velocity $v = \dfrac{\omega}{k} = \lambda f$
- Wave number $k = \dfrac{2\pi}{\lambda}$
- Angular frequency $\omega = 2\pi f$

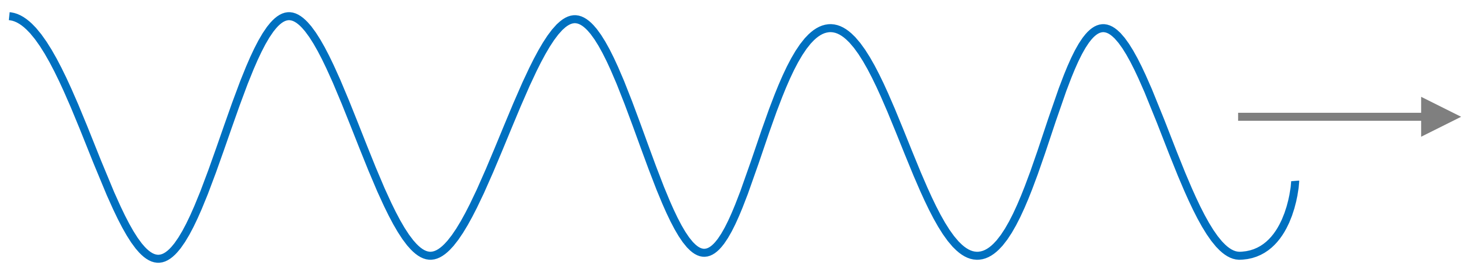
THE STANDARD WAVE EQUATION: SOUND, LIGHT

- Description of waves $\phi(x,t)$ by the wave equation :

$$\frac{\partial^2\phi}{\partial \mathrm{x}^2} = \frac{1}{v^2}\frac{\partial^2\phi}{\partial t^2}$$

Solution ?

$$\phi(\mathrm{x},\mathrm{t}) = A\cos(kx - \omega t)$$



- Are the solutions waves?

PARTIAL DERIVATIVES

- Description of waves $\phi(x,t)$ by the wave equation :

$$\frac{\partial^2 \phi}{\partial \mathrm{x}^2} = \frac{1}{v^2}\frac{\partial^2 \phi}{\partial t^2}$$

- Partial derivatives of function $f(x,y)$:

$$\frac{\partial f}{\partial x} = \frac{\partial f(x,y)}{\partial x} = \left(\frac{df(x,y)}{dx}\right)_{y\,=\,\mathrm{constant}}$$

- Possible difference: $\frac{df(x,y)}{dx} \neq \frac{\partial f(x,y)}{\partial x}$

PARTIAL DERIVATIVES

- Partial derivatives of function $f(x, y)$:

$$\frac{\partial f}{\partial x} = \frac{\partial f(x, y)}{\partial x} = \left(\frac{\mathrm{d}f(x, y)}{\mathrm{dx}}\right)_{y = \mathrm{constant}}$$

- Example 1: $f(x, y) = yx^2 + y$

$$\frac{\partial f}{\partial x} = \frac{\partial(yx^2 + y)}{\partial x} = 2xy, \qquad \frac{\partial f}{\partial y} = \frac{\partial(yx^2 + y)}{\partial y} = x^2 + 1$$

PARTIAL DERIVATIVES

- Partial derivatives of function $f(x, y)$:

$$\frac{\partial f}{\partial x} = \frac{\partial f(x, y)}{\partial x} = \left(\frac{\mathrm{d}f(x, y)}{\mathrm{dx}}\right)_{y = \text{constant}}$$

- Example 2: $f(x, y) = xy$

$$\frac{\partial f}{\partial x} = \frac{\partial (xy)}{\partial x} = y, \qquad \frac{\partial f}{\partial y} = \frac{\partial (xy)}{\partial y} = x$$

PARTIAL DERIVATIVES

- Partial derivatives of function $f(x, y)$:

$$\frac{\partial f}{\partial x} = \frac{\partial f(x, y)}{\partial \mathrm{x}} = \left(\frac{\mathrm{d} f(x, y)}{\mathrm{dx}}\right)_{y = \text{constant}}$$

- Example 3: $f(x, t) = \sin(t - ax)$

$$\frac{\partial f}{\partial x} = \frac{\partial \sin(t - ax)}{\partial x} = -a \cos(t - ax)$$

$$\frac{\partial f}{\partial t} = \frac{\partial \sin(t - ax)}{\partial t} = \cos(t - ax)$$

PARTIAL DERIVATIVES

- **Second (partial) derivative** of function $f(x, y)$:

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial \left(\frac{\partial f}{\partial x}\right)}{\partial x} = \left(\frac{\mathrm{d}^2 f(x, y)}{\mathrm{dx}^2}\right)_{y\,=\,\mathrm{constant}}$$

- Example 4: $f(x, t) = \cos(t - ax)$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 \cos(t - ax)}{\partial x^2} = \frac{\partial\, a \sin(t - ax)}{\partial x} = -a^2 \cos(t - ax)$$

PARTIAL DERIVATIVES

- **Second (partial) derivative** of function $f(x,y)$:

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial\left(\frac{\partial f}{\partial x}\right)}{\partial x} = \left(\frac{\mathrm{d}^2 f(x,y)}{\mathrm{d}x^2}\right)_{y\,=\,\mathrm{constant}}$$

- Example 4: $f(x,t) = \cos(t - ax)$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 \cos(t-ax)}{\partial x^2} = \frac{\partial\, a\sin(t-ax)}{\partial x} = -a^2\cos(t-ax)$$

$$\frac{\partial^2 f}{\partial t^2} = \frac{\partial^2 \cos(t-ax)}{\partial t^2} = \frac{\partial\ (-\sin(t-ax))}{\partial t} = -\cos(t-ax)$$

THE STANDARD WAVE EQUATION: SOUND, LIGHT

- Description of waves $\phi(x,t)$ by the wave equation :

$$\frac{\partial^2\phi}{\partial \mathrm{x}^2} = \frac{1}{v^2}\frac{\partial^2\phi}{\partial t^2}$$

- Partial differential equation, find solutions for $\phi(x,t)$

- Solution $f(x,t) = \cos(t - ax)$

$$\frac{\partial^2 f}{\partial x^2} = -a^2\cos(t - ax)$$

$$\frac{\partial^2 f}{\partial t^2} = -\cos(t - ax)$$

THE STANDARD WAVE EQUATION: SOUND, LIGHT

- Description of waves $\phi(x,t)$ by the wave equation :

$$\frac{\partial^2\phi}{\partial \mathrm{x}^2} = \frac{1}{v^2}\frac{\partial^2\phi}{\partial t^2}$$

- Partial differential equation, find solutions for $\phi(x,t)$

- Solution $\phi(x,t) = \cos\left(t - \frac{1}{v}x\right)$

$$\frac{\partial^2\phi}{\partial x^2} = -\frac{1}{v^2}\cos\left(t - \frac{1}{v}x\right)$$

$$\Rightarrow \qquad \frac{\partial^2\phi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\phi}{\partial t^2}$$

$$\frac{\partial^2\phi}{\partial t^2} = -\cos\left(t - \frac{1}{v}x\right)$$

THE STANDARD WAVE EQUATION: SOUND, LIGHT

- Description of waves $\phi(x,t)$ by the wave equation :

$$\frac{\partial^2\phi}{\partial \mathrm{x}^2} = \frac{1}{v^2}\frac{\partial^2\phi}{\partial t^2}$$

- Solutions for $\phi(x,t)$

$$\mathrm{A}\cos(kx - \omega t) \quad \text{and} \quad \mathrm{B}\sin(kx - \omega t)$$

- A linear combination is also a solution

$$\phi(x,t) = \mathrm{A}\cos(kx - \omega t) + \mathrm{B}\sin(kx - \omega t)$$

Particle waves

ENERGY OF PARTICLE WAVES

- Energy of a free particle

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

- de Broglie relations:

Energy: $E = hf = \hbar\omega$

Momentum: $p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k$

$$\Rightarrow E = hf = \hbar\omega$$

$$\Rightarrow \hbar\omega = \frac{\hbar^2 k^2}{2m}$$

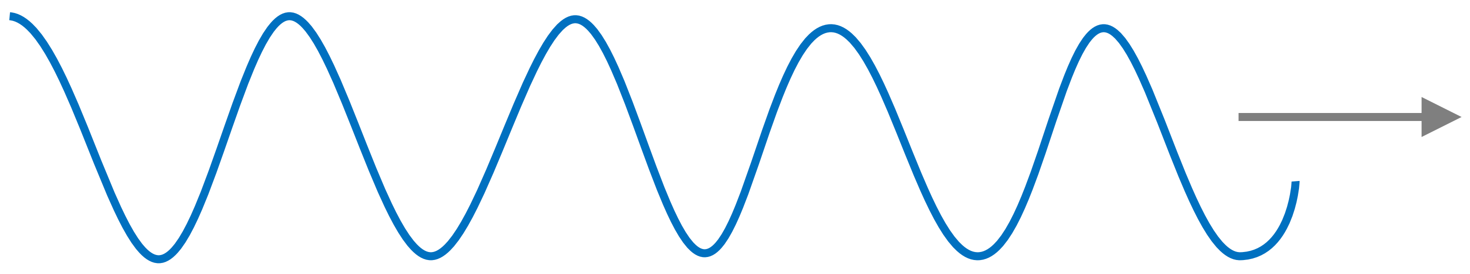
ENERGY OF PARTICLE WAVES

- Different relation than for standard waves

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}$$

Solution ?

$$\phi(\mathrm{x},\mathrm{t}) = A\cos(kx - \omega t)$$



- Schrodinger Wave equation of a free particle

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial \mathrm{x}^2} = i\hbar\frac{\partial\Psi}{\partial t}$$

The wave function & probability

THE WAVE FUNCTION OF A SINGLE PARTICLE

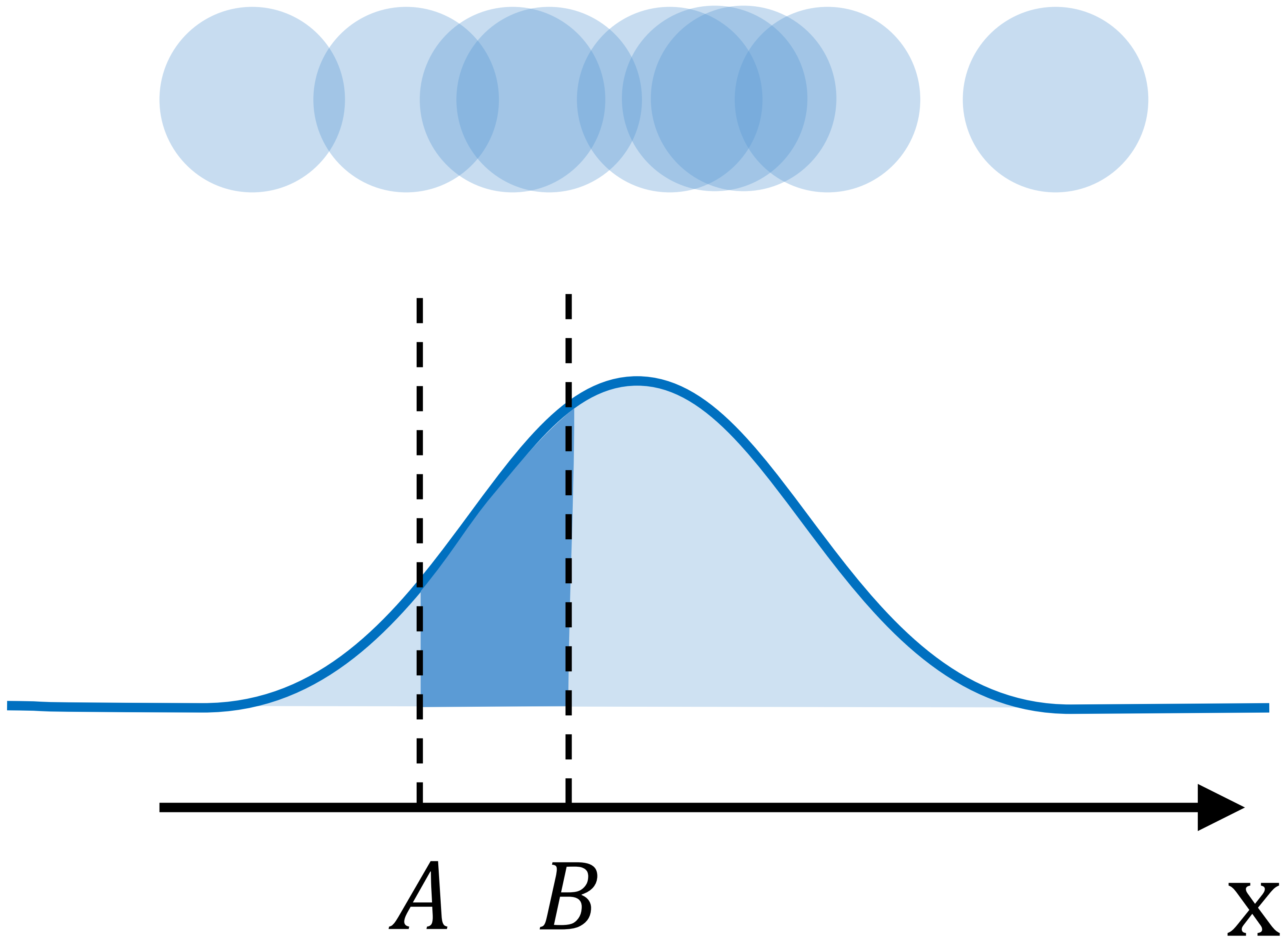
- When wave function Ψ represents a single particle then:

$$\Psi \;\rightarrow\; \Psi(\mathrm{x}, \mathrm{y}, \mathrm{z}, \mathrm{t})$$

- Probability (1D) to be found in interval

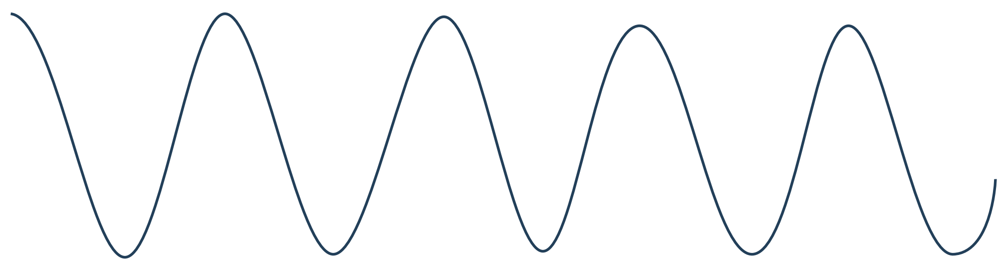
$$P(x \in [A, B]) = \int_A^B |\Psi(x,t)|^2 \, \mathrm{dx}$$

- If $[-\infty, \infty] \;\Rightarrow\; \int_{-\infty}^{+\infty} |\Psi(x,t)|^2 = 1$



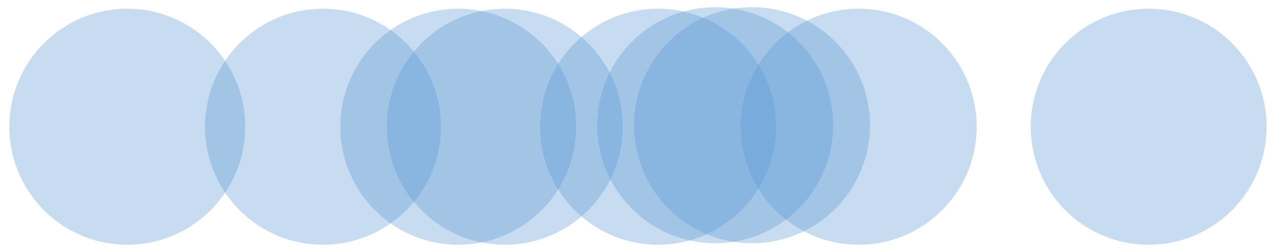
WAVE PACKET OF A FREE PARTICLE

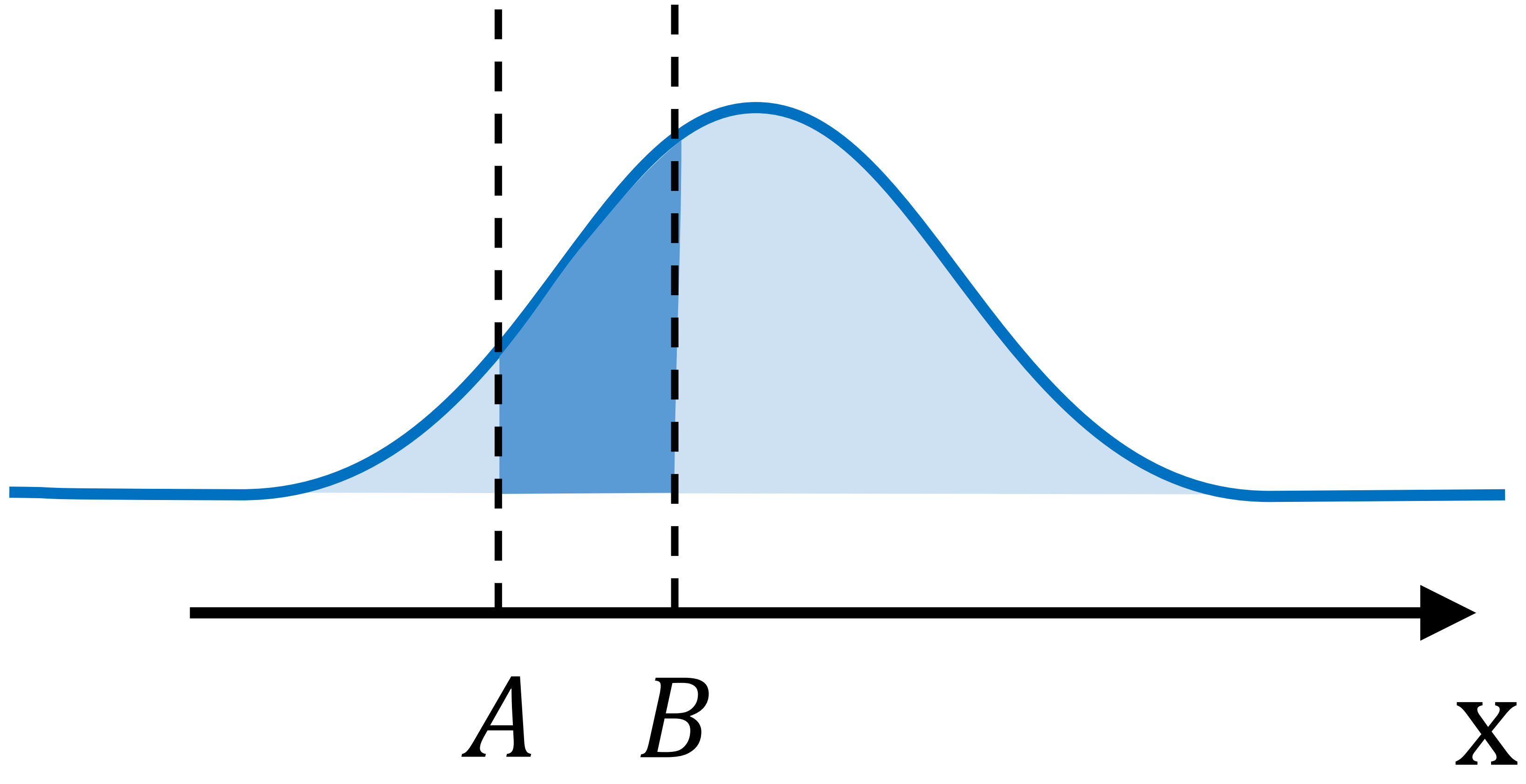
- Single wave is **not localized**



$$\Psi_{\text{wave}}(\mathrm{x},\mathrm{t}) = A\cos(kx - \omega t)$$

- Localized particles: a wave packet
- Ψ is a superposition of waves





$$\Psi(\mathrm{x},\mathrm{t}) = \sum_{k} A_k\cos(kx - \omega t)$$

THE WAVE FUNCTION REVISITED

- The wave function is a complex function:

$$\Psi = \mathrm{a} + i\,\mathrm{b}$$

- Probability density is the absolute value squared:

$$|\Psi|^2 = \Psi^*\,\Psi = (\mathrm{a} - i\,\mathrm{b})\,(\mathrm{a} + i\,\mathrm{b}) = \mathrm{a}^2 + \mathrm{b}^2$$

- By definition the probability density $|\Psi|^2 > 0$

THE WAVE FUNCTION

- Schrodinger’s equation of a free particle

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial \mathrm{x}^2} = i\hbar\frac{\partial\Psi}{\partial t}$$

- Time-dependency: rotating phase
- Complex wave packet

THE WAVE FUNCTION

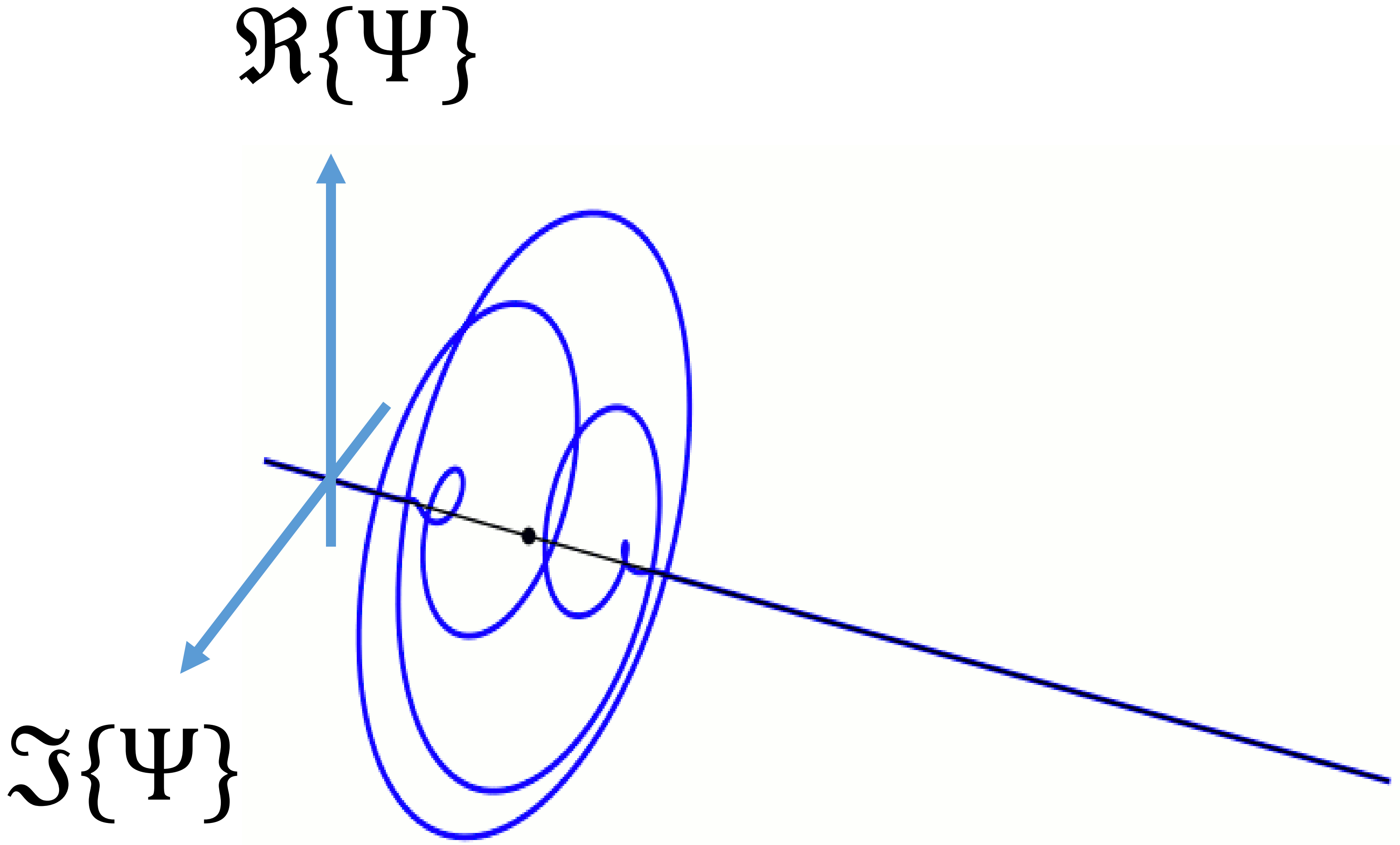
- Schrodinger's equation of a free particle

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial\Psi}{\partial t}$$

- Time-dependency: rotating phase
- Complex wave packet

Complex wave packet

$$\begin{aligned}\Psi &= a + i\,b \\ &= \Re\{\Psi\} + i\,\Im\{\Psi\}\end{aligned}$$



Adapted from Wikipedia: Gaussian wave packet with a=2, k=4

THE WAVE FUNCTION REVISITED

- The wave function is a complex function
- It describes a system, not always a single particle, examples:
    - A neutron traveling in a vacuum
    - An electron in trapped in a harmonic potential
    - A Helium atom with two interacting electrons orbiting the nucleus
    - The nuclei and electrons of the atoms in a semi-conductor

- The system can be a single particle in a potential
- Schrodinger's equation of a particle in a potential:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(x,t)\,\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

NORMALIZATION OF THE WAVE FUNCTION

- The wave function represents probability to find a particle

$$P(x \in [A, B]) = \int_A^B |\Psi(x, t)|^2 \ \mathrm{dx}$$

- Total probability must be one

$$P(x \in [-\infty, \infty]) = \int_{-\infty}^{\infty} |\Psi(x, t)|^2 \ \mathrm{dx} = 1$$

EXPECTATION VALUES

- The expectation value of the position of a particle

$$\langle x \rangle = \int_{-\infty}^{\infty} x \, |\Psi(x,t)|^2 \, \mathrm{dx}$$

- $\langle x \rangle$ can be still a function of time
- In general, the expectation value of a function $f(x)$ is given by:

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x) \, |\Psi(x,t)|^2 \, \mathrm{dx}$$

EXPECTATION VALUES

- The **variance** σ^2 or expectation value of the deviation from the mean squared: $(x - \langle x \rangle)^2$ is given by:

$$\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \int_{-\infty}^{\infty} (x - \langle x \rangle)^2 \, |\Psi(x,t)|^2 \; \mathrm{dx}$$

- We can simplify this as:

$$\begin{aligned} \sigma^2 = \langle (x - \langle x \rangle)^2 \rangle &= \langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \rangle \\ &= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 \\ &= \langle x^2 \rangle - \langle x \rangle^2 \end{aligned}$$

Resulting in the simplified definition: $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$

EXPECTATION VALUES

- We will see later on expectation values of operators $\hat{Q}$

$$\langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \hat{Q}\, \Psi(x,t)\, \mathrm{dx}$$

- Notice that for operators $\Psi^*(x,t)\hat{Q} \neq \hat{Q}\,\Psi^*(x,t)$ and therefore the integrand can (in general) not be reduced to:

$$\cancel{\langle \hat{Q} \rangle = \int_{-\infty}^{\infty} \hat{Q}\, |\Psi(x,t)|^2\, \mathrm{dx}}$$

SUMMARY PROBABILITY & WAVE FUNCTIONS

- Wave function $\Psi(x, y, z, t)$ interacts in a wave-like manner
- Schrodinger's equation allows complex wave functions
- Schrodinger's equation of a single particle:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial \mathrm{x}^2} + U(x,t)\,\Psi = -i\hbar\frac{\partial\Psi}{\partial t}$$

- The wave function should be normalized
- Expectation values link probability density and expected measurement outcomes