PHOT 222: Quantum Photonics
LECTURE 06

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**	**Ch. 41**	**Ch. 39**
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		

Quantum mechanical rules so far

WAVE FUNCTION: SCHRODINGER'S EQUATION

- Wave function determines system

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

- **1925: Schrodinger's equation**

- Schrodinger's equation for particle :

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

Erwin Schrodinger
Picture from Wikipedia

WAVE FUNCTION: PROBABILITY DENSITY

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$$\Psi \rightarrow \Psi(x, y, z, t)$$

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

- **1925 - … Probability interpretation of the wave function:**

$$\mathrm{P} \propto |\Psi(\mathrm{x}, \mathrm{y}, \mathrm{z}, \mathrm{t})|^2$$

Max Born
Picture from Wikipedia

1D PARTICLE: PROBABILITY DENSITY FUNCTION

- Wave function determines system

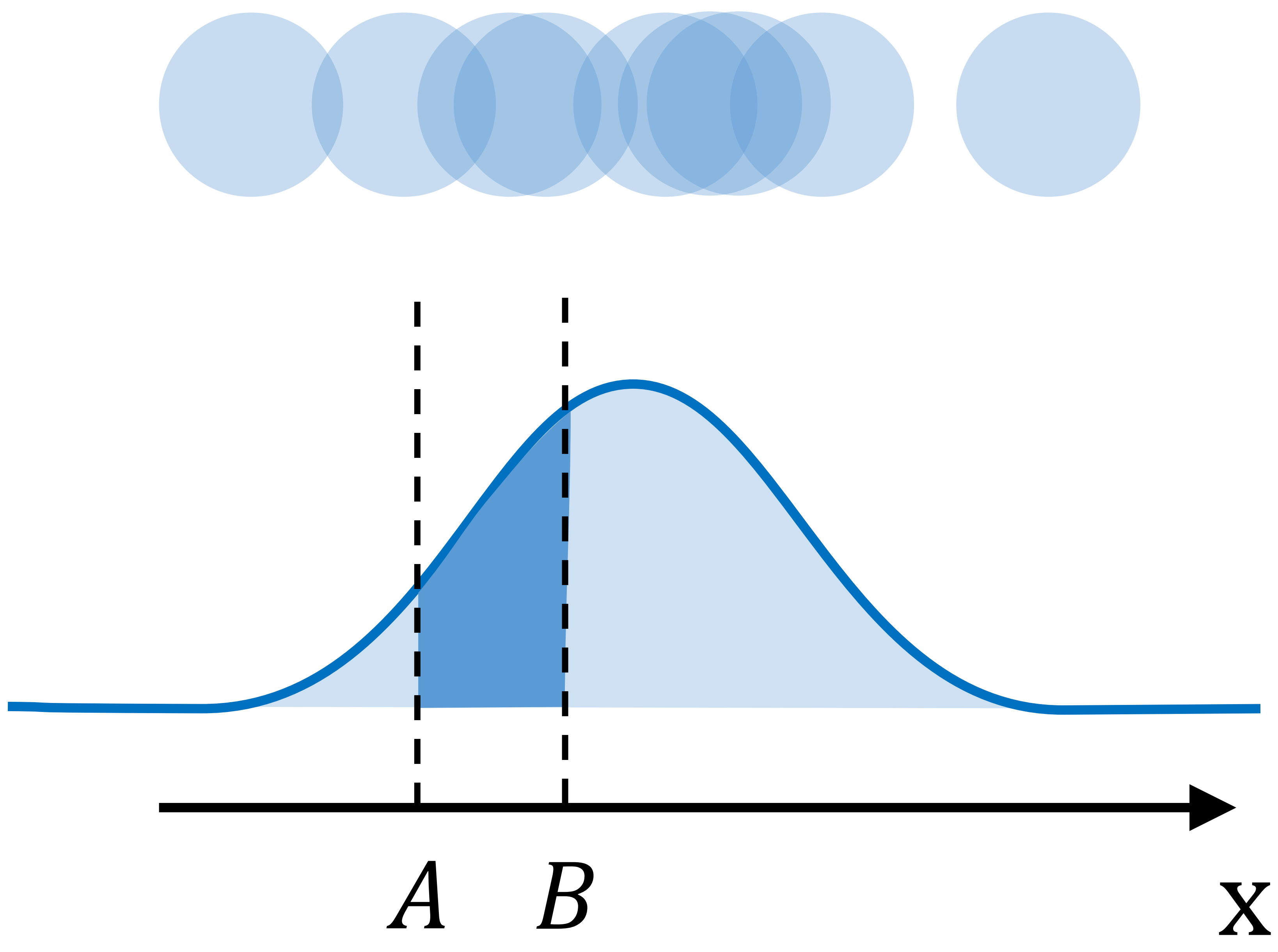
$$\Psi \;\rightarrow\; \Psi(x,t)$$

- Schrodinger's equation for particle :

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

- **Probability (1D) to be found in interval**

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



1D PARTICLE WAVE FUNCTION

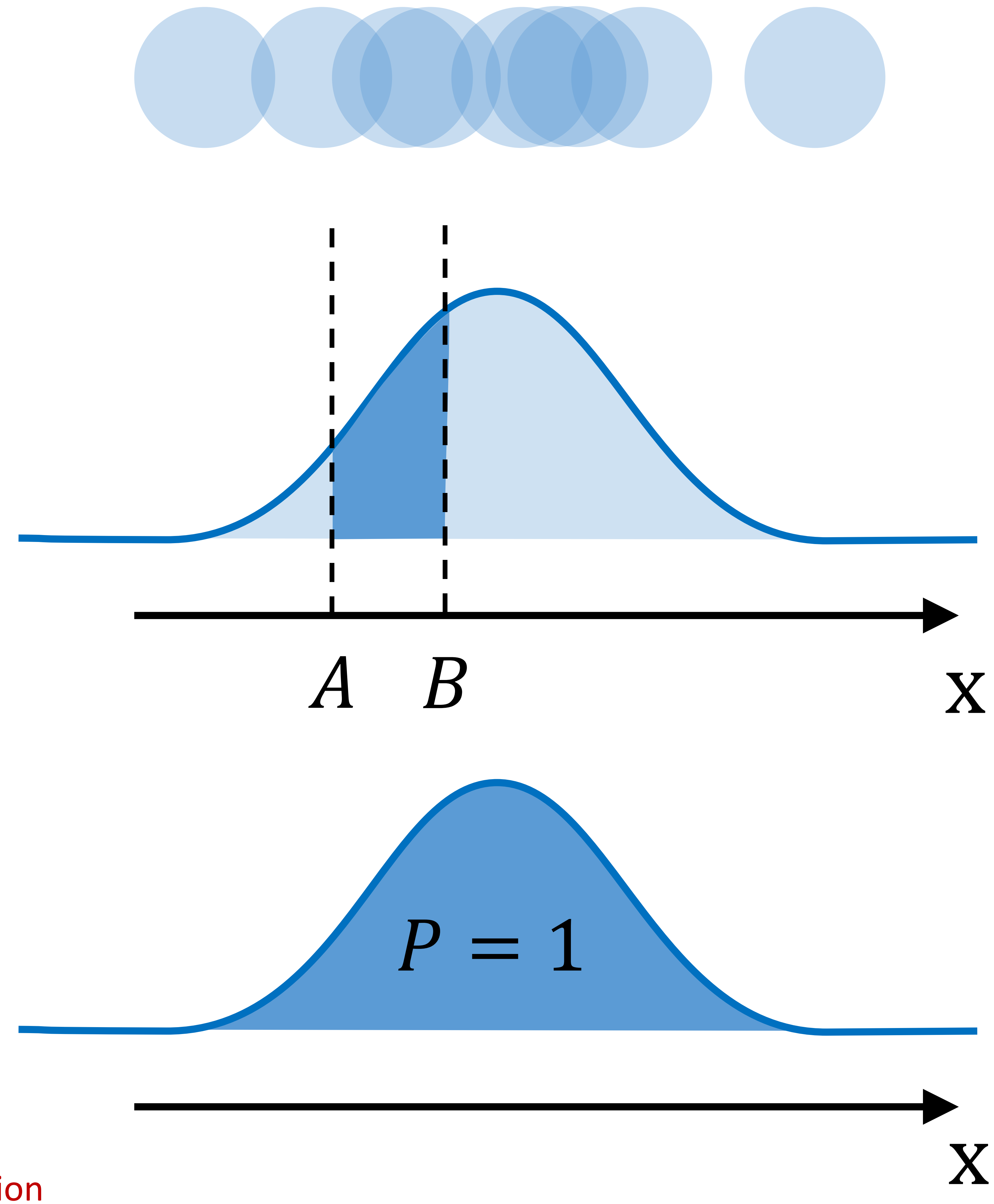
- **Probability (1D) to be found in interval**

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

- **Total probability is normalized**

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

- Particle to be found somewhere with probability equal to 1

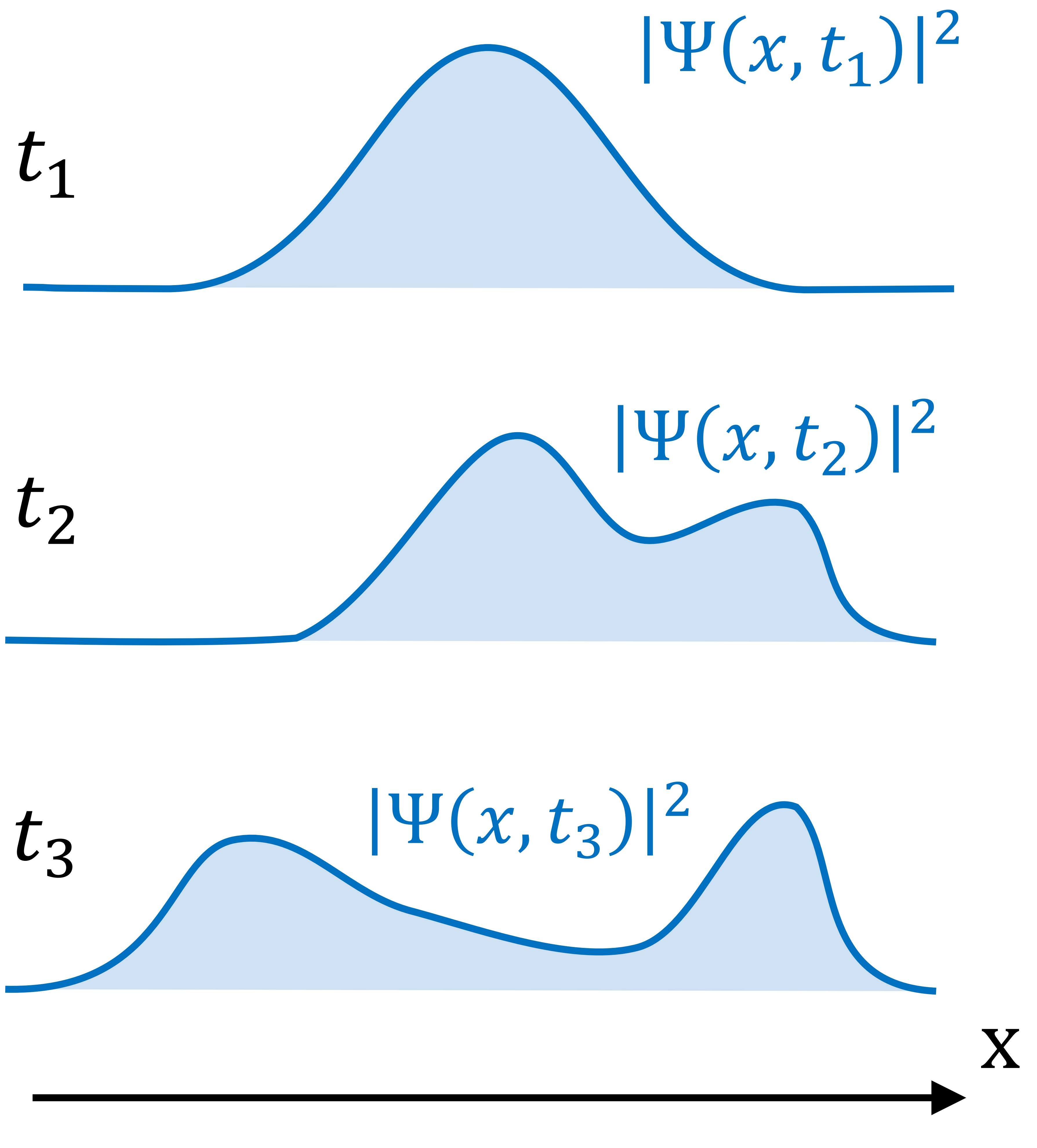


1D PARTICLE EQUATIONS OF MOTION

- Schrodinger's equation :

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

- Wave function defines **probability**
- Probability density ➡ the particle **position** and evolves with time



1D PARTICLE EQUATIONS OF MOTION

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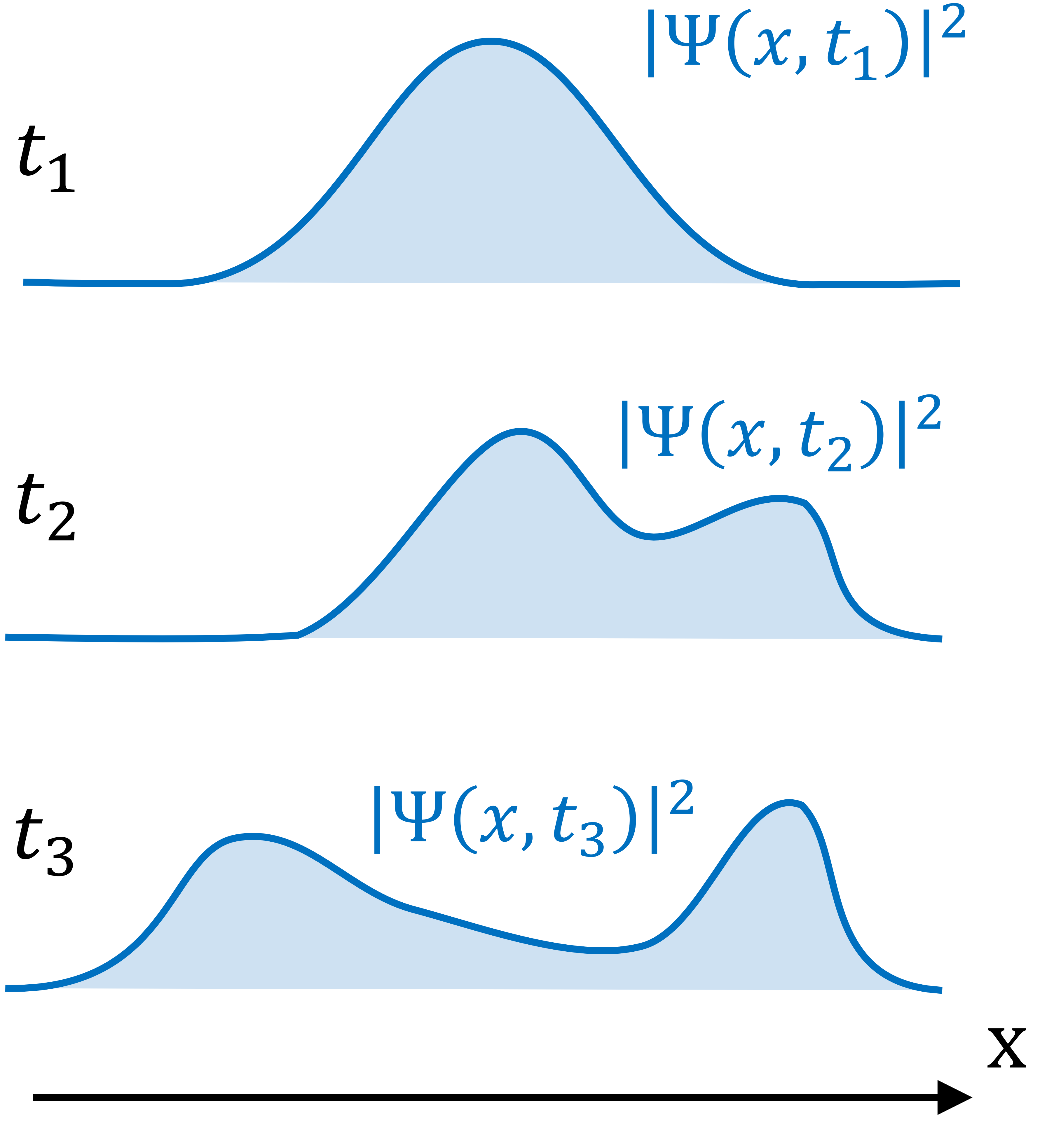
- Wave function defines **probability**
- Probability density ⇨ the particle **position** and evolves with time

How to calculate the wave function ?



Time-independent schrodinger's equation

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

Schrodinger's equation of a particle in a potential:

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

1st Assumption: $U(x,t) = U(x)$

2nd Assumption: Separation of variables:

$$\Psi(x,t) = \psi(x)\,\Theta(\mathrm{t})$$

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

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

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

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

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

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

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Divide by $\Psi(x,t)=\psi(x)\,\Theta(\mathrm{t})$:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\,\psi(x)}{\partial \mathrm{x}^2}+U(x)=i\hbar\frac{1}{\Theta(\mathrm{t})}\frac{\partial\,\Theta(\mathrm{t})}{\partial t}$$

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

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

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1D PARTICLE WAVE FUNCTION IN A POTENTIAL

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

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

Divide by $\Psi(x,t) = \psi(x)\,\Theta(t)$:

x and t independent needs to be constant

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\, \psi(x)}{\partial x^2} + U(x) = E = i\hbar\frac{1}{\Theta(t)}\frac{\partial\,\Theta(t)}{\partial t}$$

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

System of two differential equations:

$$\begin{cases} -\dfrac{\hbar^2}{2m}\dfrac{1}{\psi(x)}\dfrac{\partial^2 \psi(x)}{\partial \mathrm{x}^2} + U(x) = E \\ i\hbar \dfrac{1}{\Theta(\mathrm{t})}\dfrac{\partial\, \Theta(\mathrm{t})}{\partial t} = E \end{cases}$$

- Can we solve these equations for $\psi(x)$ and $\Theta(\mathrm{t})$?
- If we can solve these equations: $\Psi(x,t) = \psi(x)\,\Theta(\mathrm{t})$

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

System of two differential equations:

$$\begin{cases} -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\,\psi(x)}{\partial \mathrm{x}^2} + U(x)\,\psi(x) = E\,\psi(x) \\[2ex] i\hbar\dfrac{\partial\,\Theta(\mathrm{t})}{\partial t} = E\,\Theta(\mathrm{t}) \end{cases}$$

- Can we solve these equations for $\psi(x)$ and $\Theta(\mathrm{t})$?
- If we can solve these equations: $\Psi(x,t) = \psi(x)\,\Theta(\mathrm{t})$

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

Solving the time-dependent part:

$$i\hbar \frac{\partial\, \Theta(\mathrm{t})}{\partial t} = E\, \Theta(\mathrm{t})$$

$$\Longrightarrow \quad \frac{\partial\, \Theta(\mathrm{t})}{\partial t} = -i\,\frac{E}{\hbar}\, \Theta(\mathrm{t})$$

This is a first order differential equation:

$$\Theta(\mathrm{t}) = A\, \mathrm{e}^{-iE\,t/\hbar} = \mathrm{e}^{-iE\,t/\hbar}$$

With A some constant which we can put equal to one

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

This is a first order differential equation:

$$\Theta(\mathrm{t}) = A\,\mathrm{e}^{-iE\,t/\hbar} = \mathrm{e}^{-iE\,t/\hbar}$$

The time-dependent part is very simple: phase rotating in time !

$$\Longrightarrow \quad \Psi(x,t) = \psi(x)\,\Theta(\mathrm{t}) = \psi(x)\,\mathrm{e}^{-iEt/\hbar}$$

Requirement: potential independent of time: $U(x,t) = U(x)$

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

What about the time-independent equation?

$$-\frac{\hbar^2}{2m}\frac{\partial^2\,\psi(x)}{\partial \mathrm{x}^2}+U(x)\,\psi(x)=E\,\psi(x)$$

This is the famous **time-independent Schrodinger equation (TISE)**

1D PARTICLE WAVE FUNCTION IN A POTENTIAL

What about the time-independent equation?

$$-\frac{\hbar^2}{2m}\frac{\partial^2\,\psi(x)}{\partial \mathrm{x}^2} + U(x)\,\psi(x) = E\,\psi(x)$$

This is the famous **time-independent Schrodinger equation (TISE)**

- Need to know the potential $U(x)$ to solve it
- Both constant (energy) E and function $\psi(x)$ are unknown
- If we can solve it our complete solution is:

$$\Psi(x,t) = \psi(x)\,\mathrm{e}^{-iEt/\hbar}$$

Before going to specific potentials:

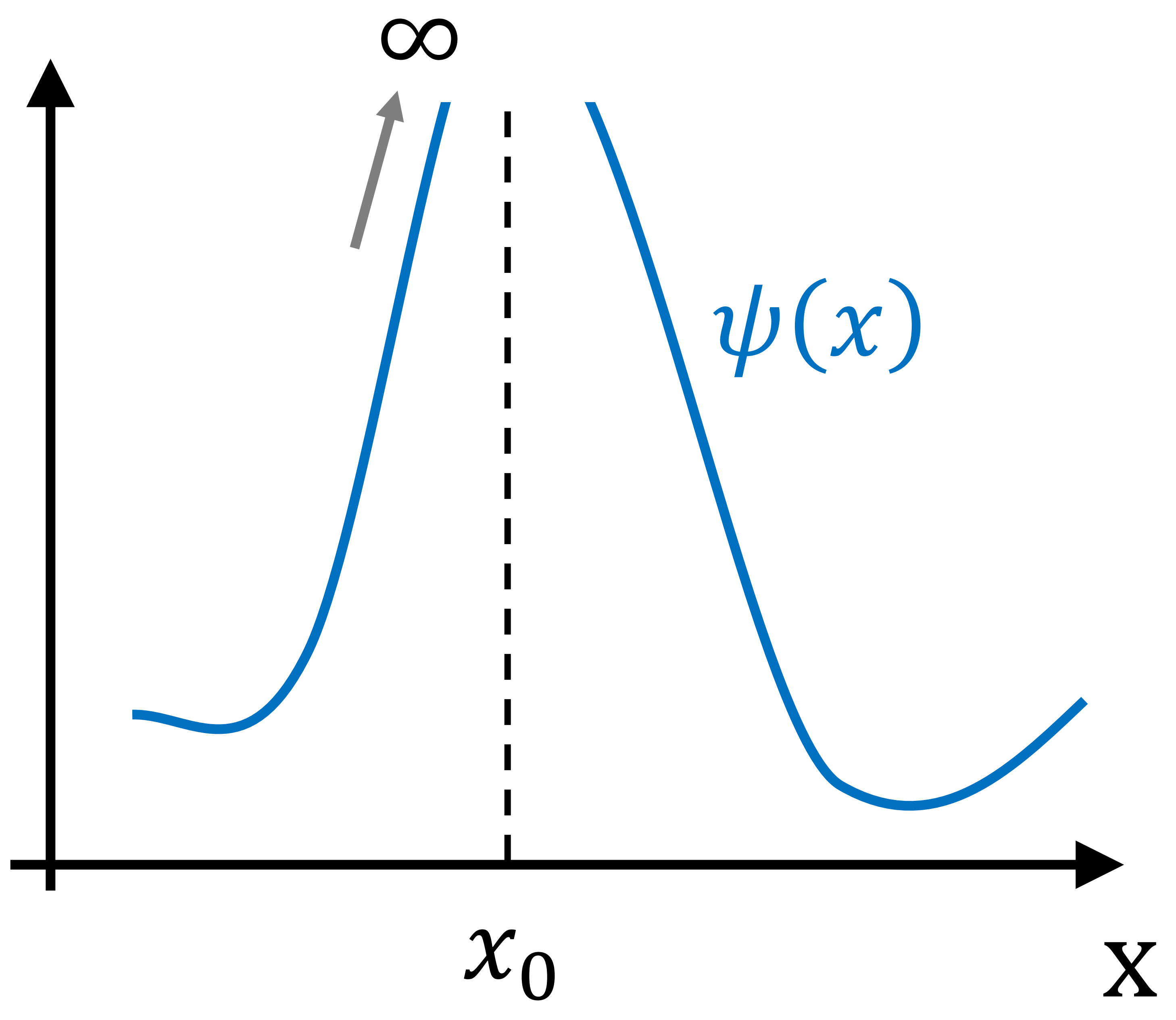
Conditions on the wave function

CONSEQUENCES FOR THE WAVE FUNCTION

- The probability $\int_{-\infty}^{\infty} |\psi(x)|^2 \ dx = 1$
- Wave function needs to be normalizable
- Therefore $\psi(x)$ needs to fulfill:

$$\lim_{x \to \pm\infty} \psi(x) \ \to \ 0$$

Other x: $\psi(x)$ finite



CONSEQUENCES FOR THE WAVE FUNCTION

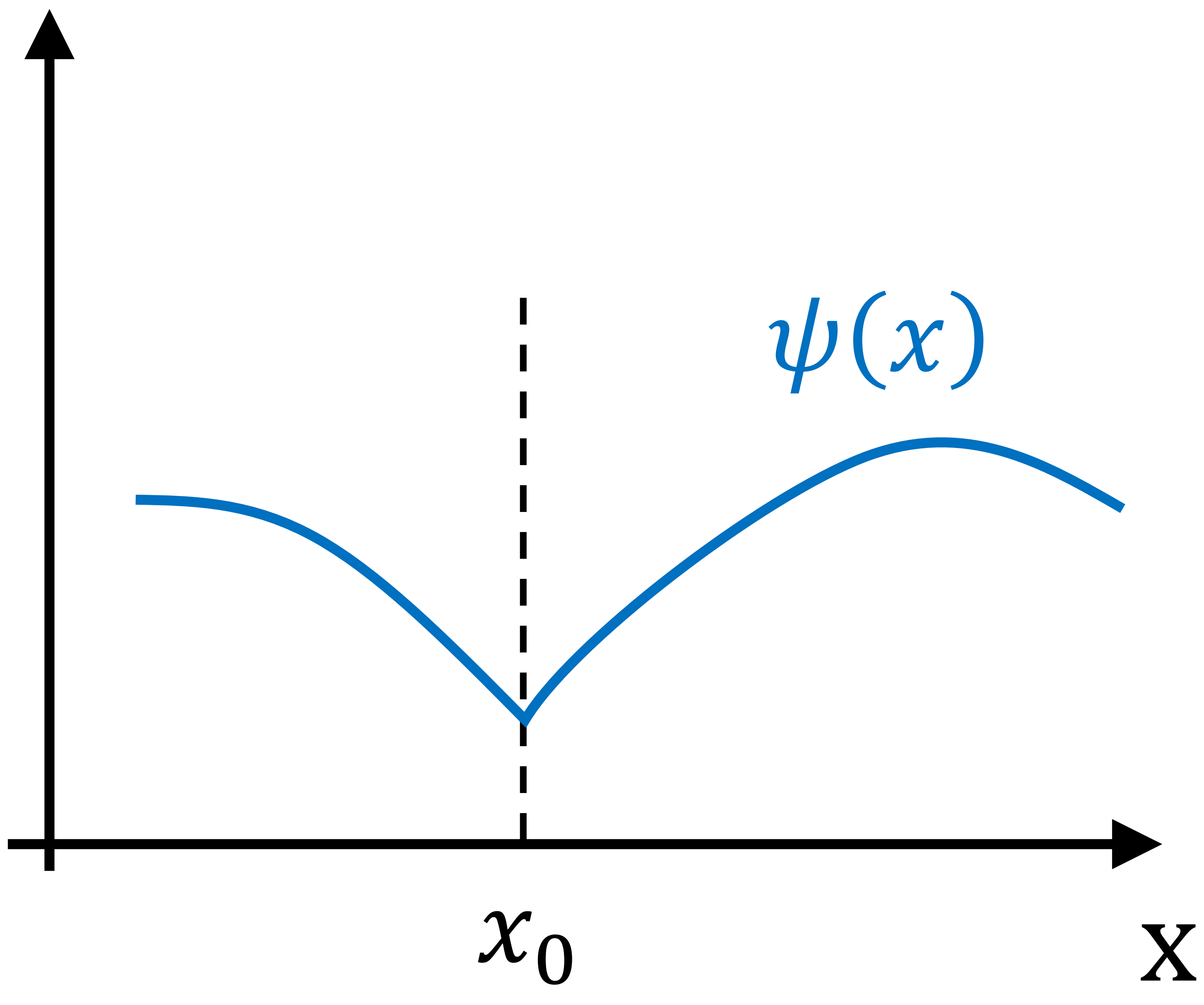
- Schrodinger's equation for a particle :

$$-\frac{\hbar^2}{2m}\frac{\partial^2\,\psi(x)}{\partial \mathrm{x}^2}+U(x)\,\psi(x)=E\,\psi(x)$$

- And wave function $\psi(x)$ is finite

Derivative $\psi' = \frac{\partial\psi(x)}{\partial x}$ continuous

Unless at x_0: $U(x_0) = \pm\infty$



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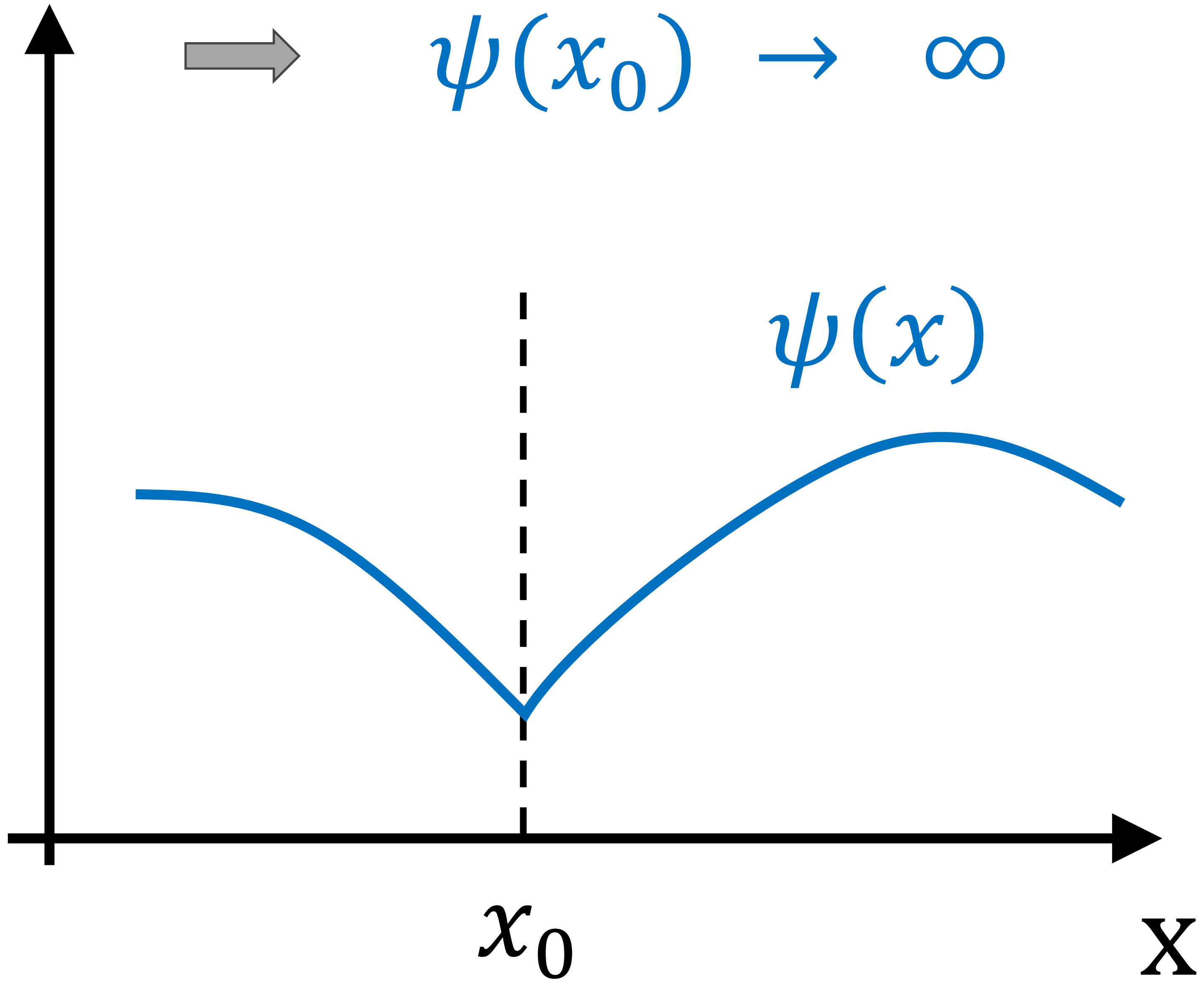
Unless at x_0: $U(x_0) = \pm\infty$

$$\frac{\partial\psi(x_0-)}{\partial x} \neq \frac{\partial\psi(x_0+)}{\partial x}$$

$$\Rightarrow \frac{\partial^2\psi(x_0)}{\partial x^2} \rightarrow \infty$$

$$\Rightarrow \psi(x_0) \rightarrow \infty$$



First example potential: $U(x) = 0$

Free particle revisited

THE WAVE FUNCTION FOR A FREE PARTICLE

- Schrodinger's equation of a free particle

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

- We had solutions of the form:

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

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

$$\Rightarrow \quad \Psi(\mathrm{x,t}) = A\, e^{ikx}\, e^{-i\omega t}$$

DISPERSION RELATION: ENERGY AND MOMENTUM

- Schrodinger's equation of a free particle

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

- Fill in the solution $\Psi(x,t) = A\,e^{ikx}\,e^{-i\omega t}$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 A\,e^{ikx}\,e^{-i\omega t}}{\partial \mathrm{x}^2} = i\hbar\frac{\partial A\,e^{ikx}\,e^{-i\omega t}}{\partial t}$$

$$\Rightarrow \quad -\frac{\hbar^2 i^2 k^2}{2m}\left(A\,e^{ikx}\,e^{-i\omega t}\right) = -i^2\omega\hbar\,\left(A\,e^{ikx}\,e^{-i\omega t}\right)$$

DISPERSION RELATION: ENERGY AND MOMENTUM

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$$-\frac{\hbar^2}{2m}\frac{\partial^2 A\,e^{ikx}\,e^{-i\omega t}}{\partial \mathrm{x}^2} = i\hbar\frac{\partial A\,e^{ikx}\,e^{-i\omega t}}{\partial t}$$

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

DISPERSION RELATION: ENERGY AND MOMENTUM

- Schrodinger's equation of a free particle

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

- Fill in the solution $\Psi(x,t) = A\, e^{ikx}\, e^{-i\omega t}$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 A\, e^{ikx}\, e^{-i\omega t}}{\partial \mathrm{x}^2} = i\hbar\frac{\partial A\, e^{ikx}\, e^{-i\omega t}}{\partial t}$$

$\Rightarrow$ $$K = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \hbar\omega = hf = E$$

TIME DEPENDENCY AND ENERGY

- Solution of a free particle: $\Psi(x,t) = A\, e^{ikx}\, e^{-i\omega t}$

Kinetic energy term: $K = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

Total energy $(K + U)$: $E = \hbar\omega$

Compare the time-dependent part for a stationary problem:

$$\Psi(x,t) = \psi(x)\, \mathrm{e}^{-iEt/\hbar} \longrightarrow \psi(x) = A\, e^{ikx}$$

NORMALIZABLE SOLUTIONS: WAVE PACKETS

- Schrodinger's equation free particle

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

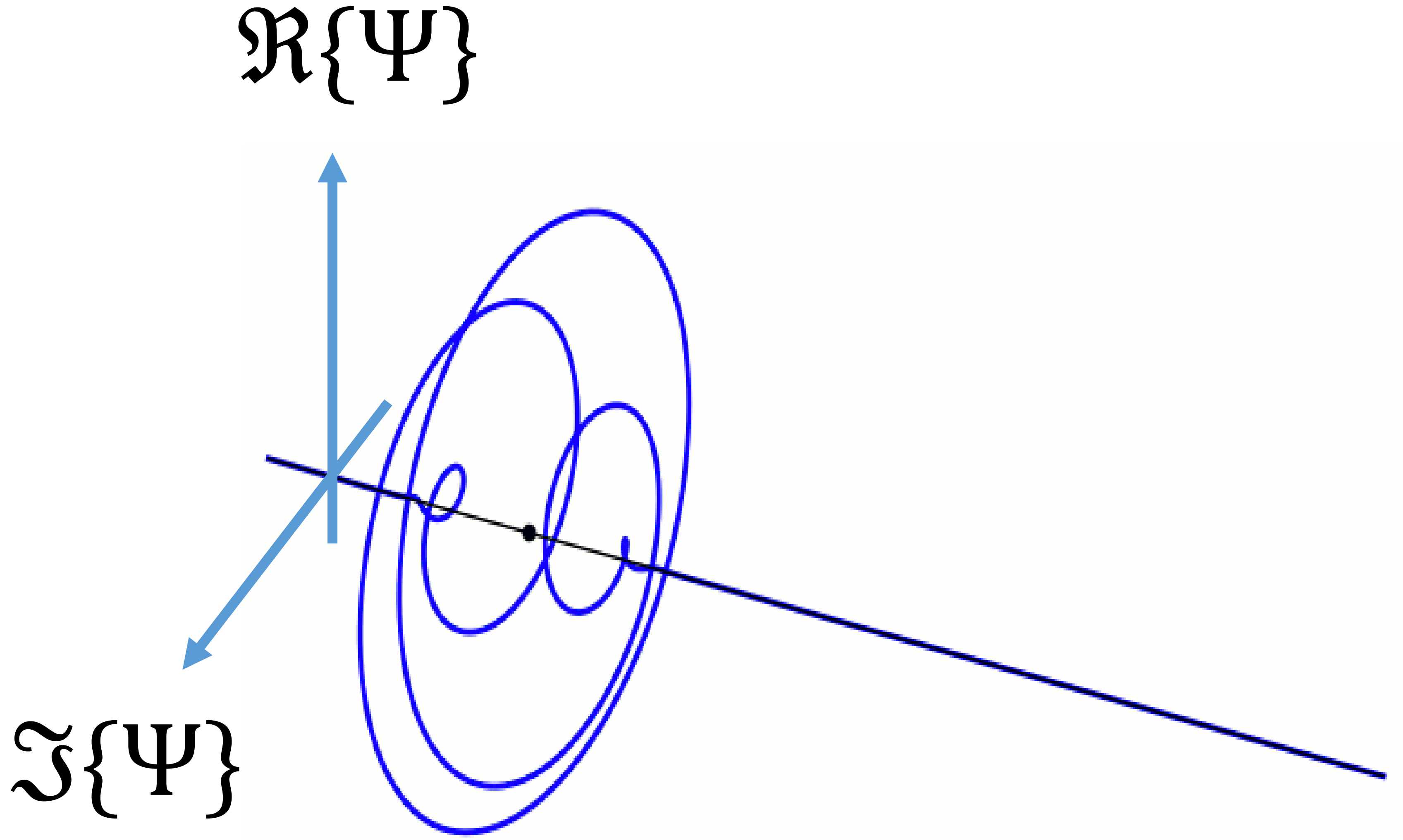
- Solutions of the form:

$$\Psi(x,t) = \int_{\infty}^{\infty} A(k)\, \mathrm{e}^{i(kx-\omega t)}\; dk$$

- Here $\omega = \omega(k)$ depends also on k
- Time-dependency: rotating phase
- Complex wave packet

Complex wave packet

$$\Psi = x + i\,y$$
$$= \Re\{\Psi\} + i\,\Im\{\Psi\}$$



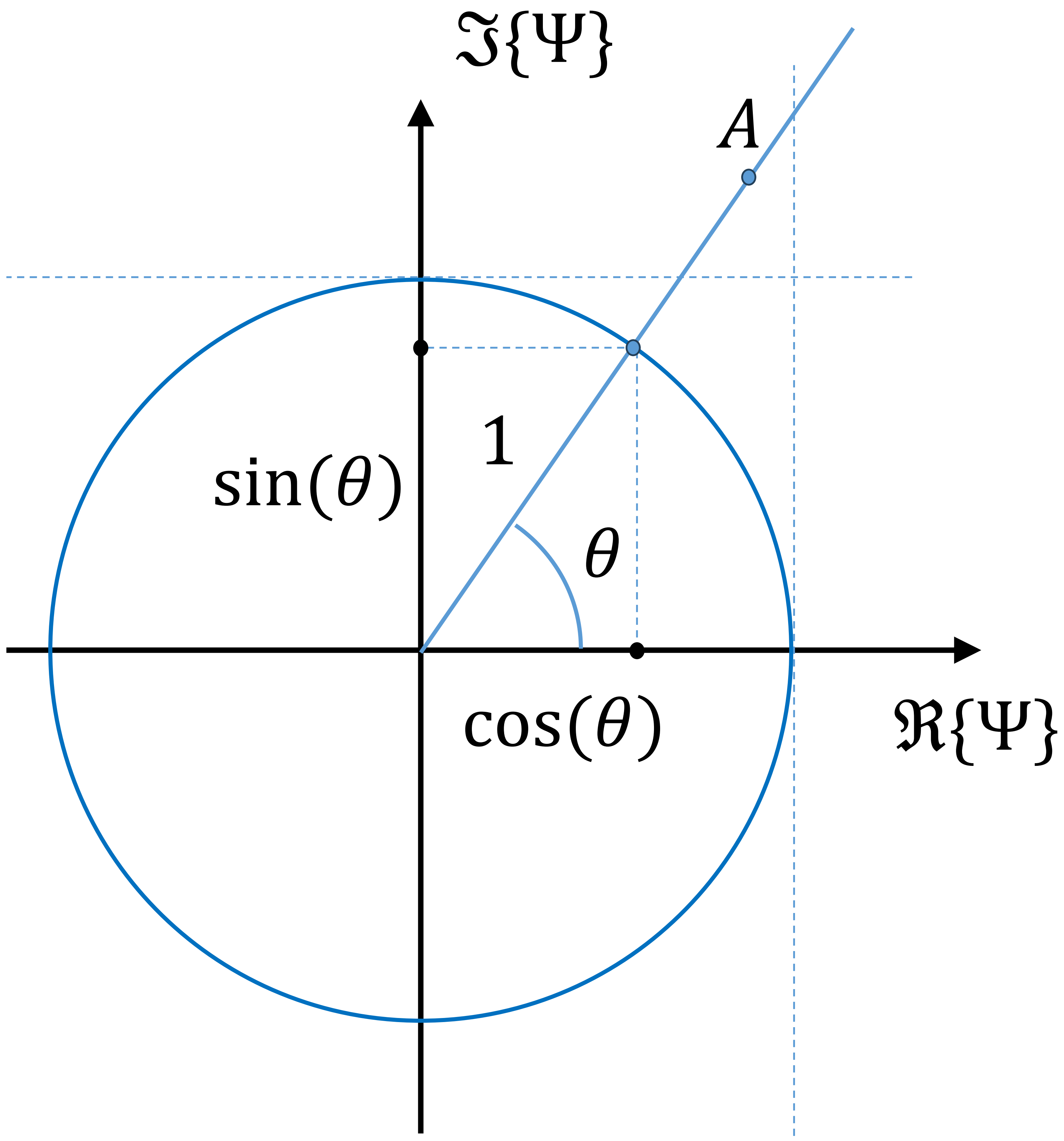
Adapted from Wikipedia: Gaussian wave packet with a=2, k=4

INTERMEZZO: COMPLEX NUMBERS AND WAVES

- Complex numbers:

$$\Psi = x + i\,y = \Re\{\Psi\} + i\,\Im\{\Psi\}$$

$$e^{i\theta} = \cos\theta + i\sin\theta \quad \begin{cases} \cos\theta = \dfrac{e^{i\theta} + e^{-i\theta}}{2} \\ \sin\theta = \dfrac{e^{i\theta} - e^{-i\theta}}{2i} \end{cases}$$



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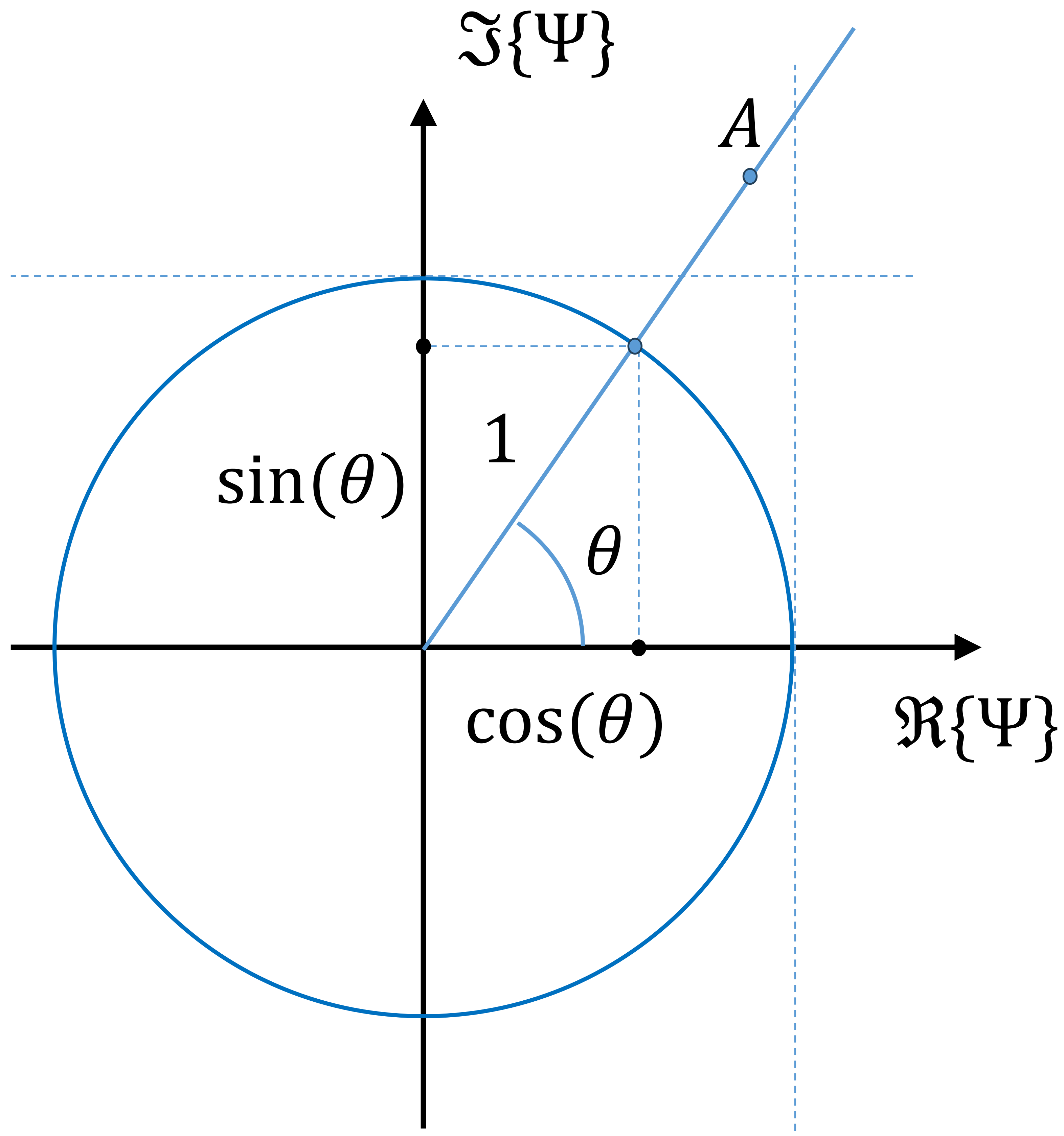


Standing waves:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Propagating waves:

$$\psi(x) = A\,e^{ikx}$$

INTERMEZZO: COMPLEX NUMBERS AND WAVES

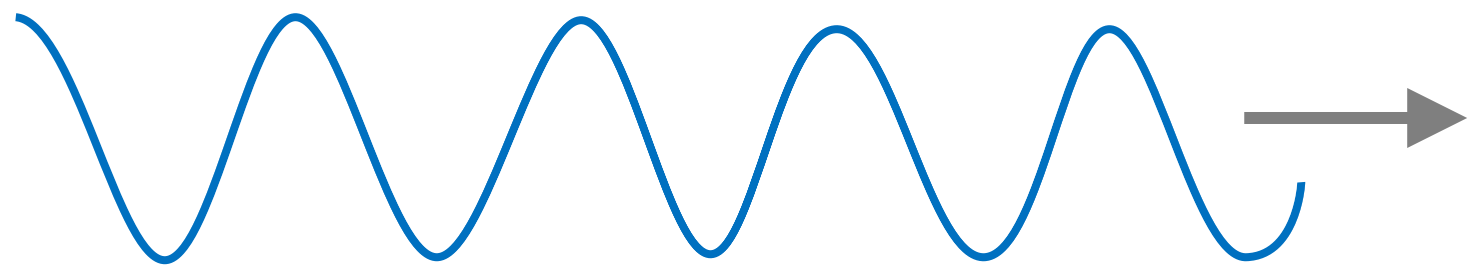
Propagating waves

Right: $\Psi(x,t) = A\, e^{ikx} e^{-i\omega t}$

$$= A\, e^{i(kx-\omega t)}$$

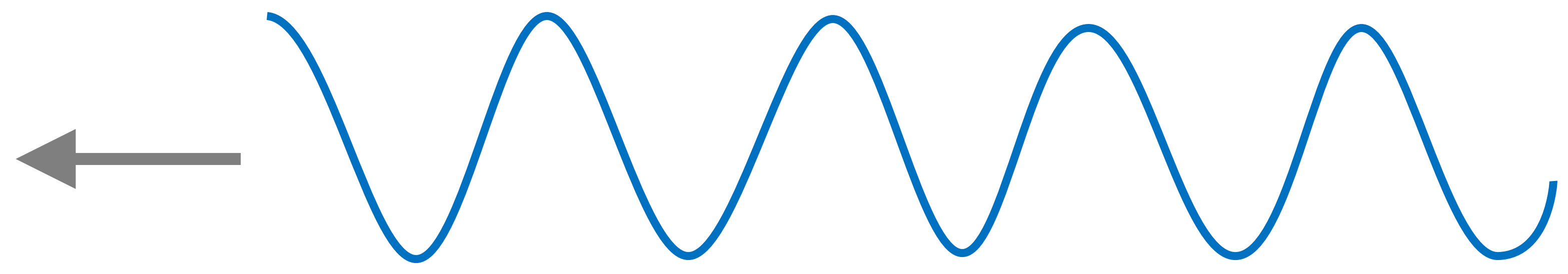
$$= A \cos\,(kx - \omega t) + i \sin(kx - \omega t)$$

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



Left: $\psi(x) = A\, e^{-ikx} e^{-i\omega t}$

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



INTERMEZZO: COMPLEX NUMBERS AND WAVES

Propagating waves

Right: $\Psi(x,t) = A\, e^{ikx} e^{-i\omega t}$

$$= A\, e^{i(kx-\omega t)}$$

$$= A \cos(kx - \omega t) + i \sin(kx - \omega t)$$

Left: $\psi(x) = A\, e^{-ikx} e^{-i\omega t}$

Standing waves (choose sine)

$$\psi(x) = A \sin(kx)$$

$$\Psi(x,t) = A \sin(kx)\, e^{-i\omega t}$$

$$= A\, \frac{\mathrm{e}^{ikx} - \mathrm{e}^{-ikx}}{2i}\, e^{-i\omega t}$$

$$= \frac{A}{2i}\left(\mathrm{e}^{ikx-i\omega t} - \mathrm{e}^{-ikx-i\omega t}\right)$$

THE WAVE FUNCTION

- Simple waves:

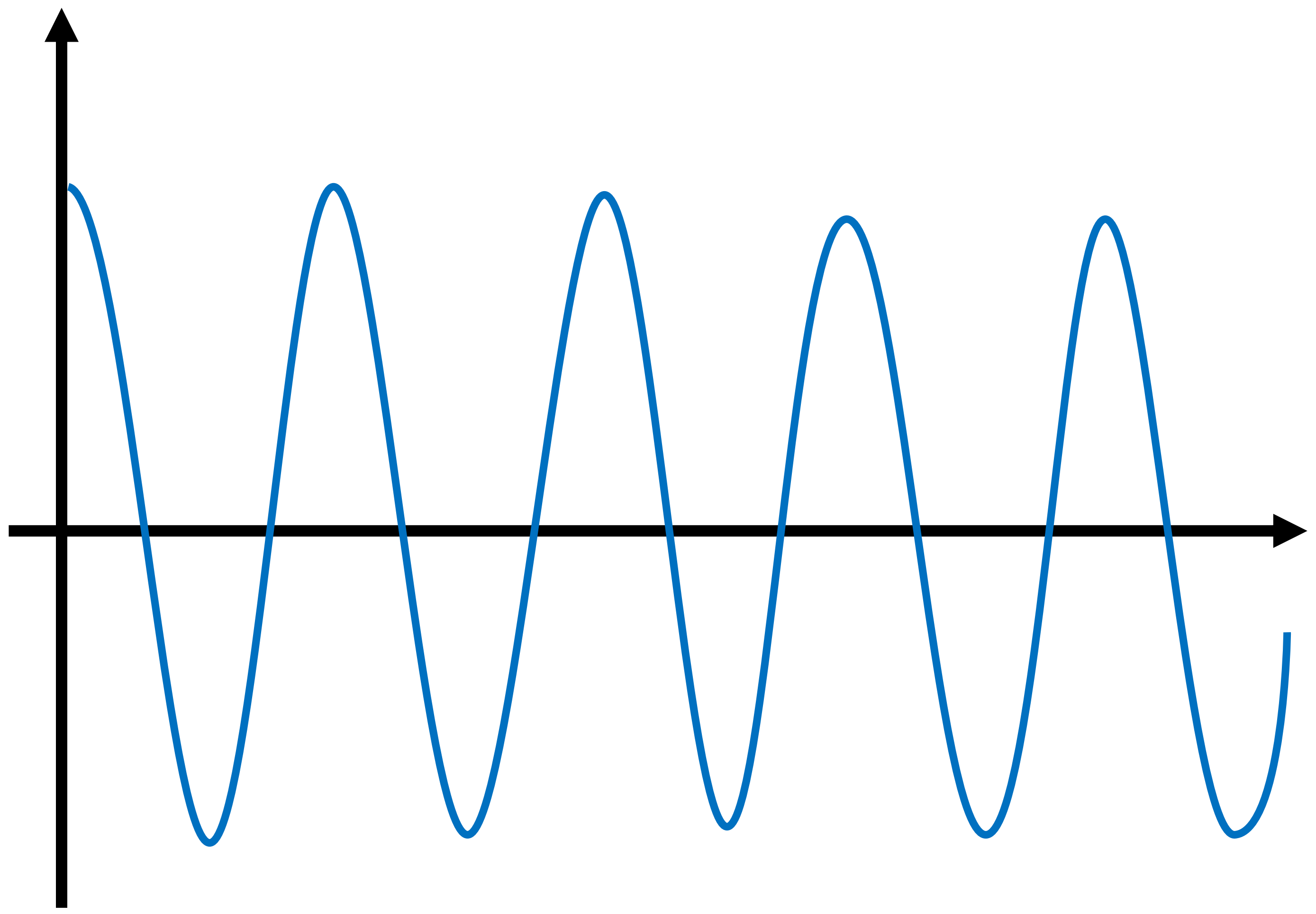
$$\Psi(x,t) = A\, e^{ikx}\, \mathrm{e}^{-i\omega t}$$

$$= \; A \cos\,(kx - \omega t) + i \sin(kx - \omega t)$$

- Represent the complex wave function by the **real and imaginary part**
- The solution to the time-independent wave equation **can often be chosen real**

Complex wave packet

$$\Psi = a + i\, b$$
$$= \Re\{\Psi\} + i\, \Im\{\Psi\}$$



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

PARTICLES WITH NONZERO MASS: WAVE PACKETS BROADEN

- Dispersion relation (massive)

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

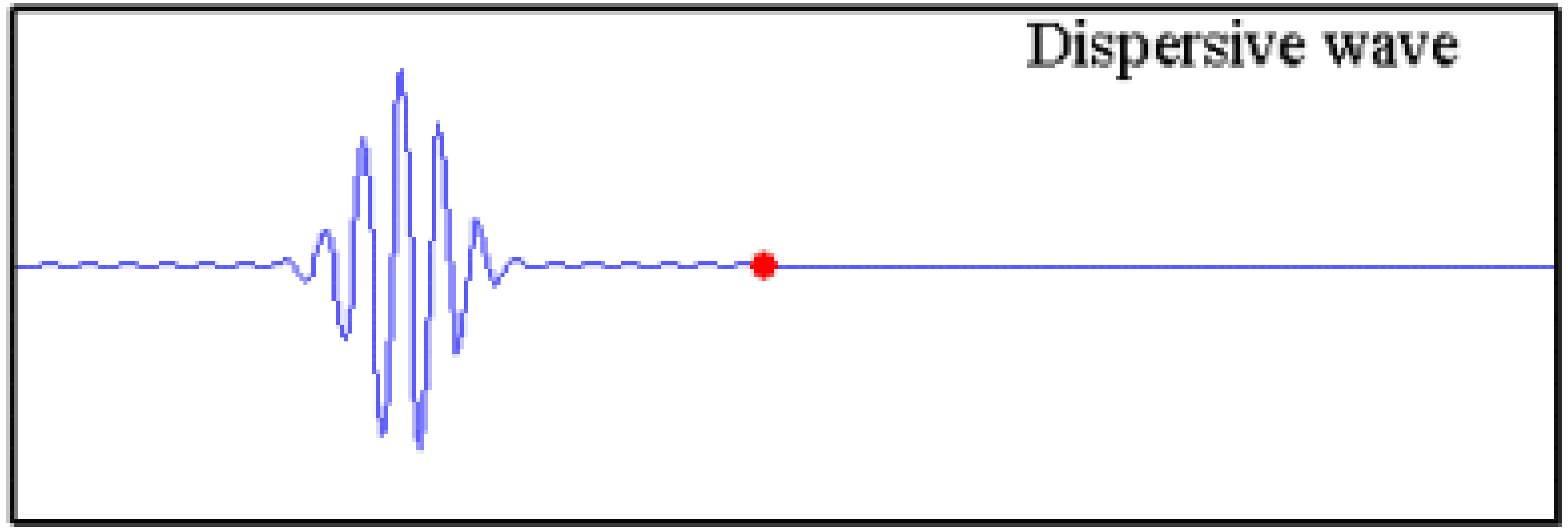
- Phase velocity

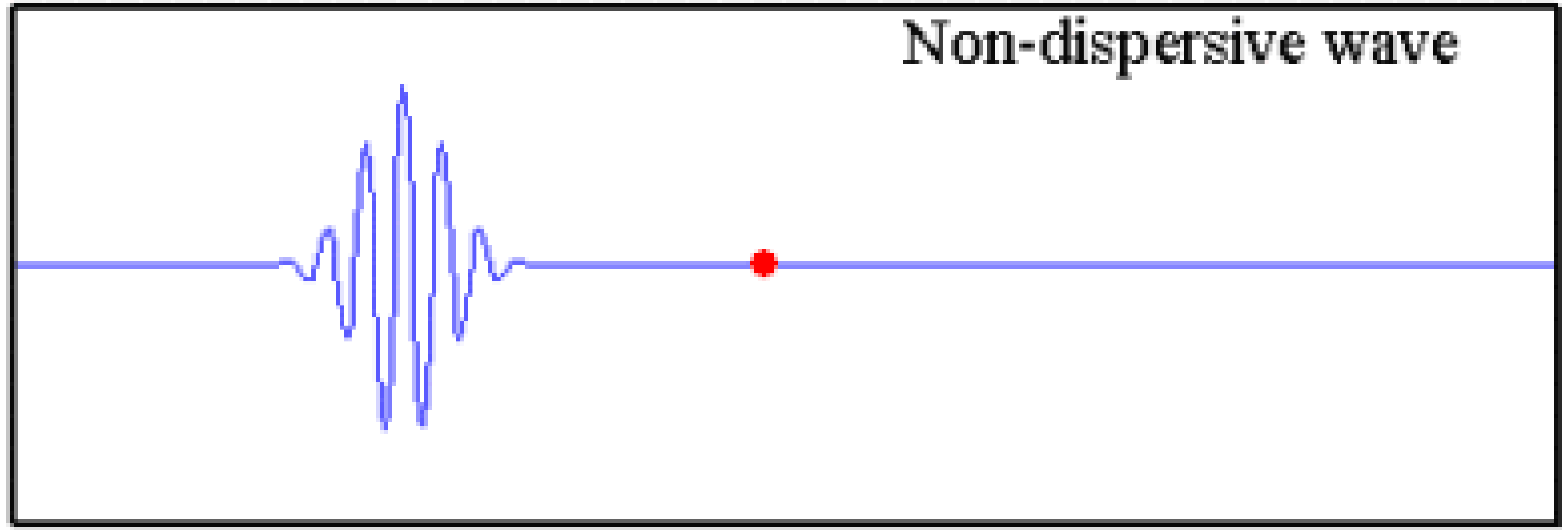
$$v_{\text{phase}} = \frac{\omega}{k} = \frac{\hbar^2 k}{2m}$$

- Group velocity

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

- Velocity dependent on k
- Wave packets broaden in time





Adapted from ISVR (University of South Hampton): Dispersive vs nondispersive wave packet

THE UNCERTAINTY RELATIONS

- Wave packets are superpositions of many waves (many wave numbers)

- Uncertainty relation:

$$\Delta p_x \, \Delta x \geq \frac{\hbar}{2}$$

- Uncertainty relation for energy-time

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$