

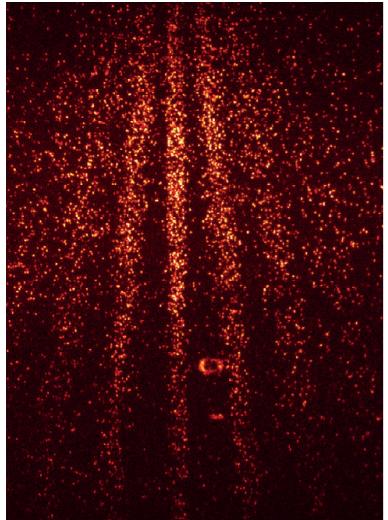
Part 4: Elements of Quantum Mechanics I - The Wave-function

Course Structure

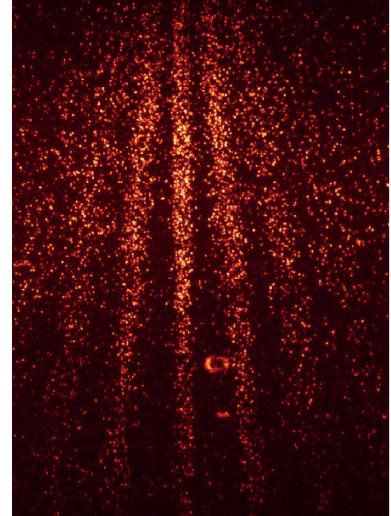
- 1 - Waves as particles - the Photon [3 hours]
- 2 - Atomic theory from 400 BC to 1913 [2 hours]
- 3 - Particles as Waves [1 hour]
- **4 - Elements of Quantum Mechanics I -
The wave-function [3 hours]**
- 5 - Elements of Quantum Mechanics II -
Energy in quantum mechanics [6 hours]

This lecture

- We will begin Part 4:
 - Elements of Quantum Mechanics I - The Wave-function
 - and focus on
 - **Motivations** for the “wave-function” of a particle
 - Revision of **probability**
 - (**Time permitting:**) Introduction of the **wavefunction**



Elements of Quantum Mechanics



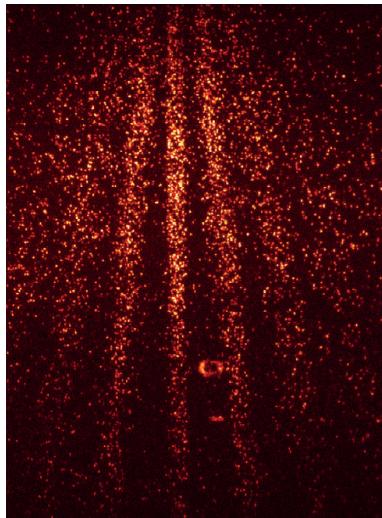
- We have seen that **wave-particle duality** cannot be explained by a **classical wave-picture** or a **particle description**.
- Quantum mechanics provides
 - a **new way** to describe the **properties** of systems
 - to calculate **physical quantities** (e.g. energy)
 - to compute the **evolution** of systems **in time**.
 - and predict **outcomes** of experiments (e.g. measurements).
- In each of these aspects, it is **completely different** to classical physics!

Elements of Quantum Mechanics

- The **full theory** of quantum mechanics (2nd year and 3rd year courses), requires
 - Complex numbers
 - Vectors and Matrices
 - Partial Differential Equations

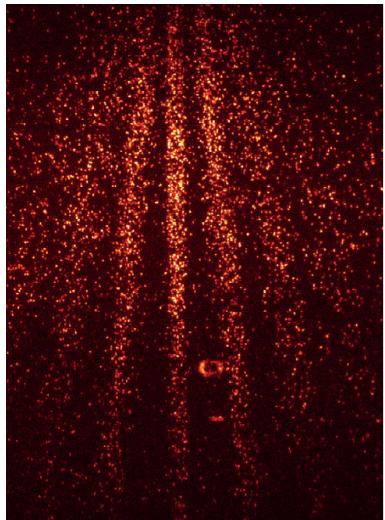
Nevertheless **many** of the key features can be explored with **A-level Maths** techniques including:

- **Wave-functions** (Part 4 of course)
- **Energy** in Quantum Mechanics (Part 5 of course)
- These will provide the **basis** for a **quantum mechanical** model of the **atom**.

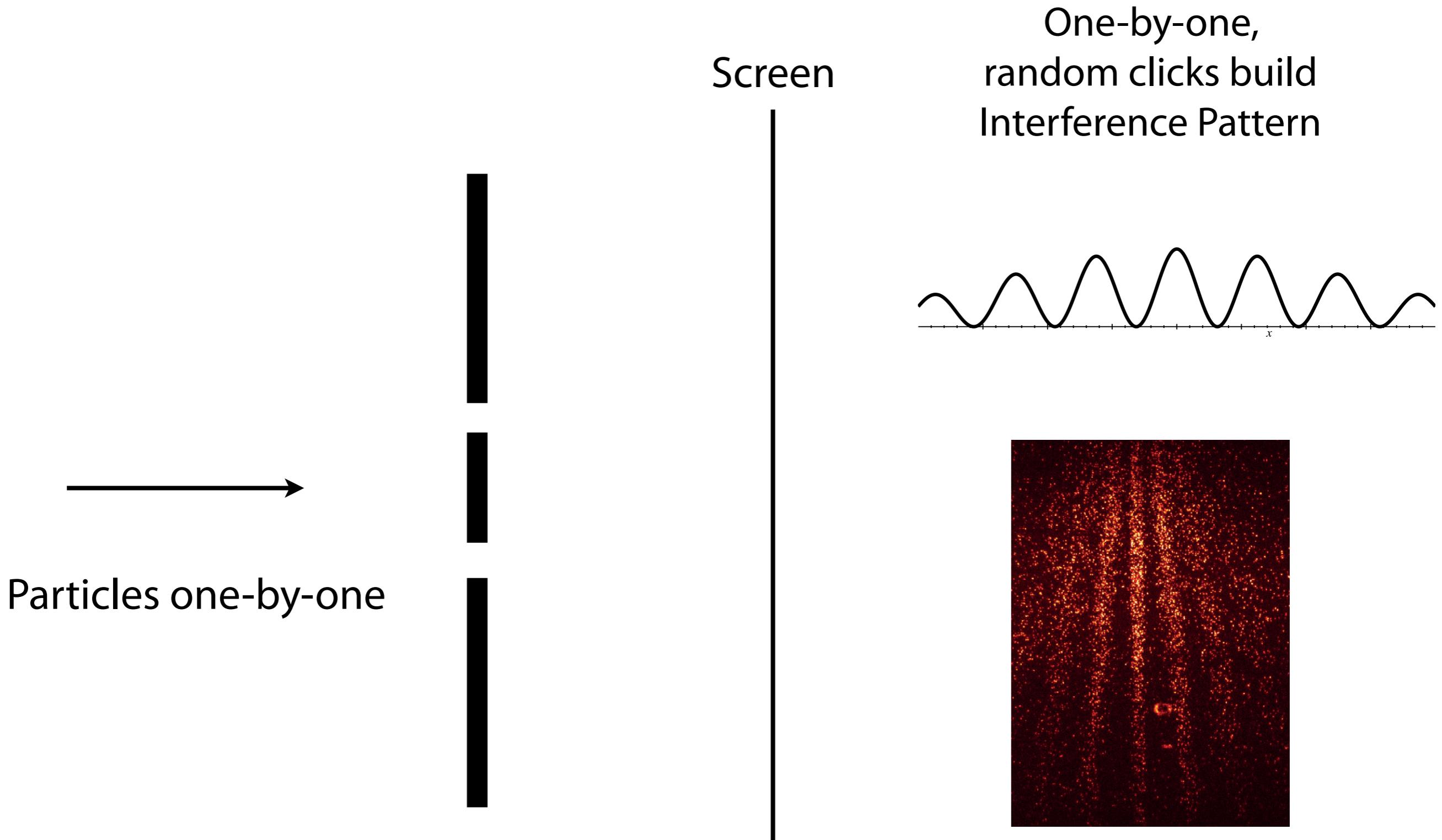


In Part 4, we will:

- Briefly revise the **wave-particle duality** in the **double slit experiment**.
 - And consider what happens if we **measure which slit** the particle travels through.
- Argue that to explain this we need **something** which incorporates
 - **wave-like behaviour (interference)**
 - **probabilities (in measurement)**
- We will revise **probability** and study **continuous probability distributions**.
- Then introduce the **wave-function** - our first element of **quantum mechanics** - and study its **properties**.

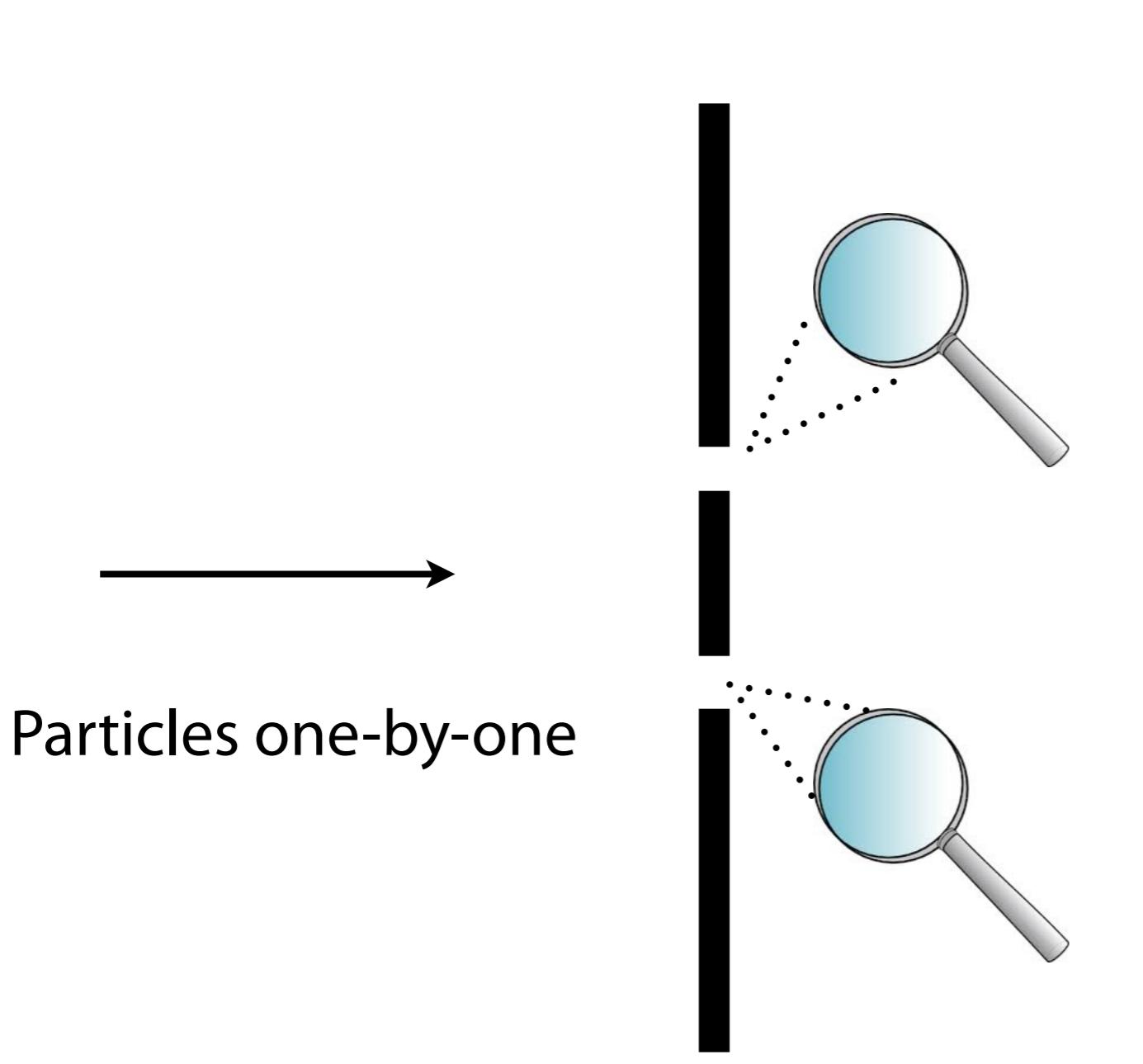


Double-slit experiment



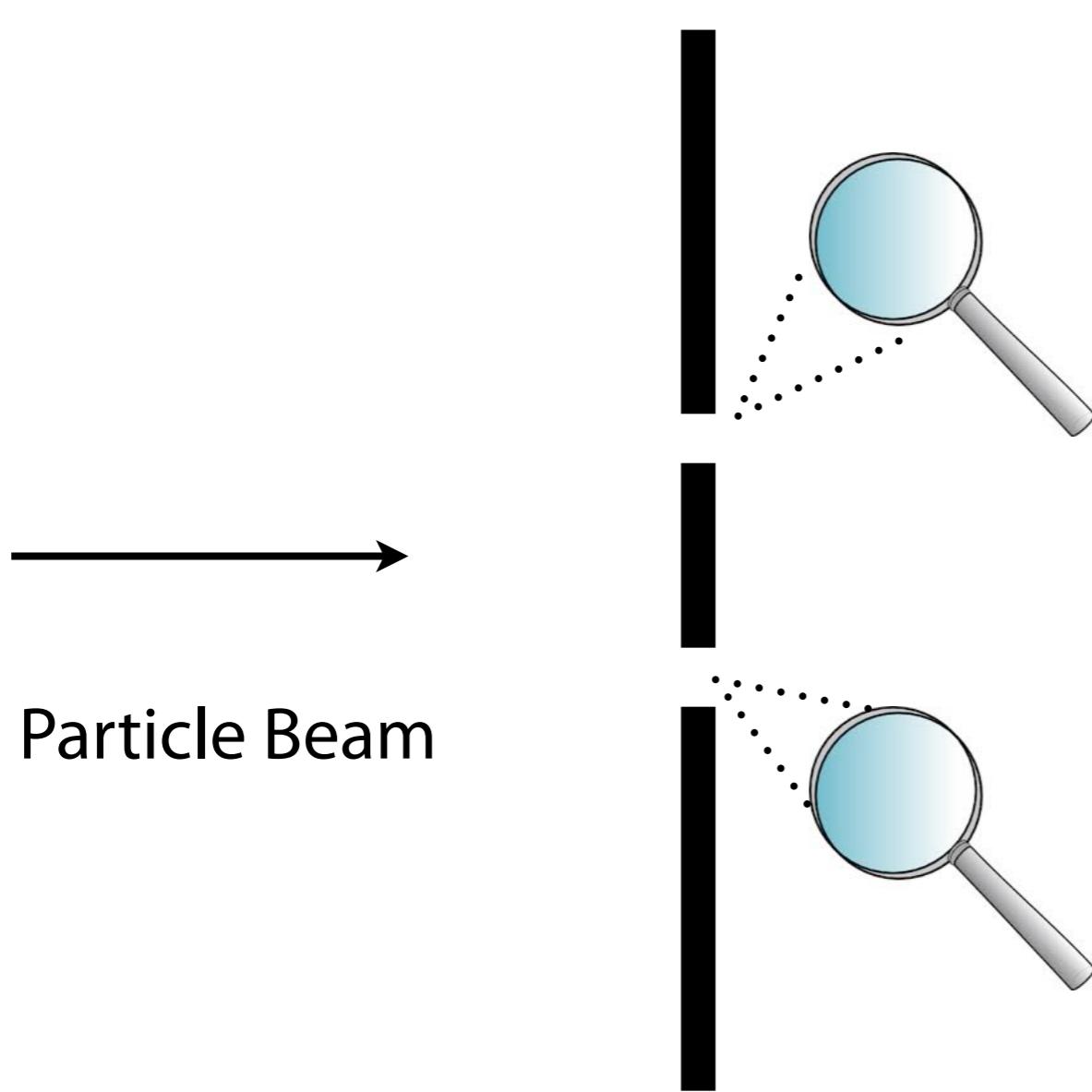
Double-slit experiment

- Does particle go through both slits?
- What happens if we measure?



Quiz?

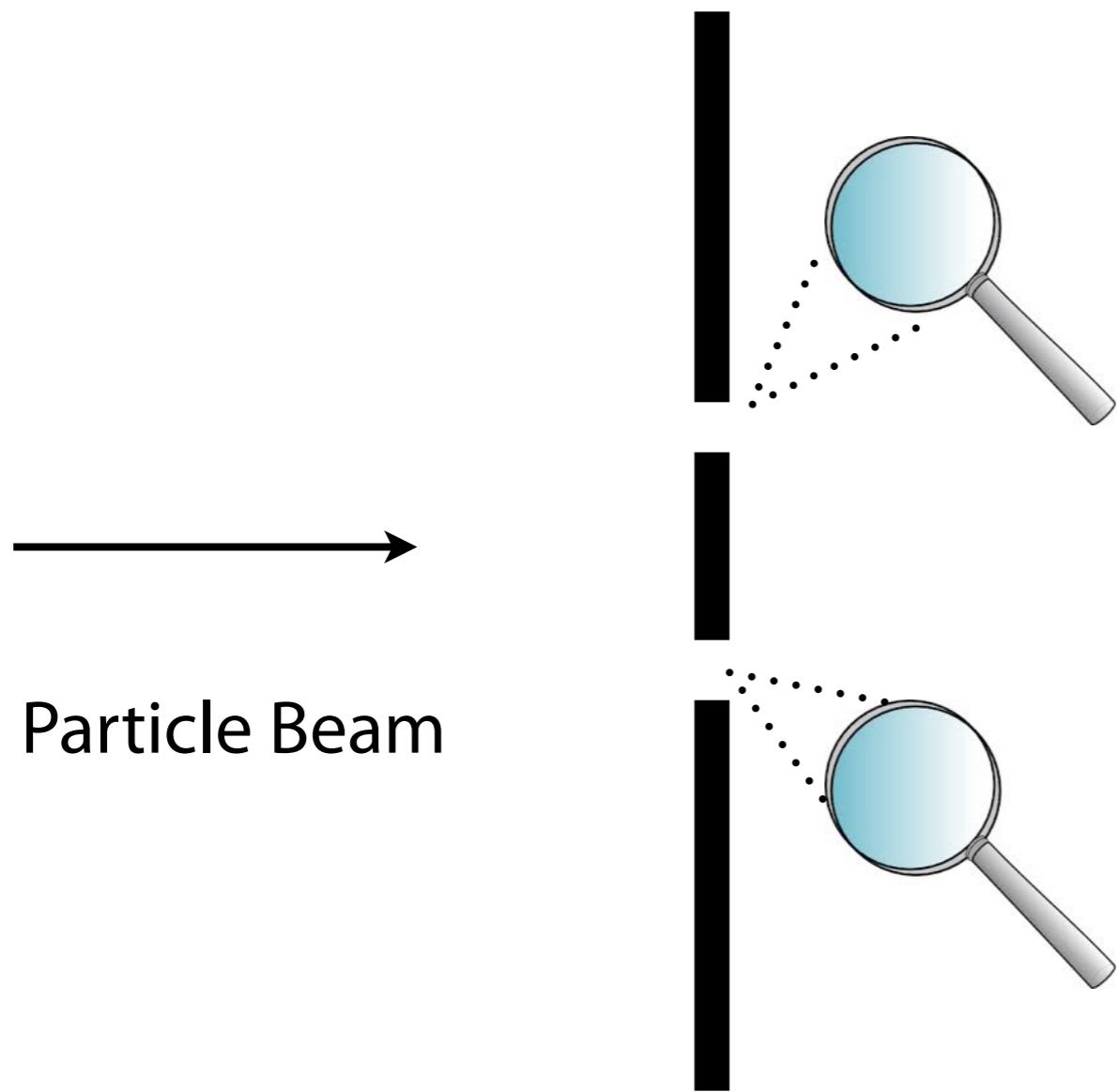
- Will we see:



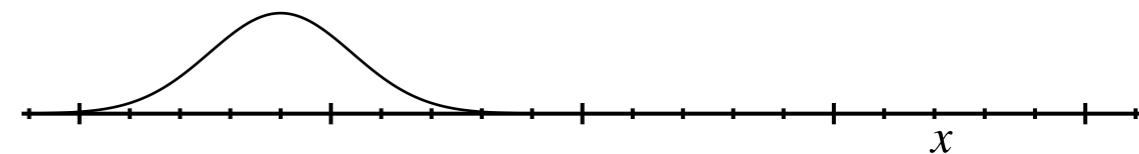
- 1. Particles in both slits?
- 2. Particle in just one slit?
- 3. Something else?

Double-slit experiment

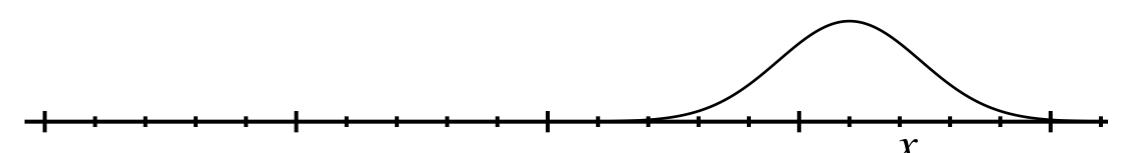
- We always just see **one** particle.
- And pattern on screen **changes**.



Particle seen in left slit



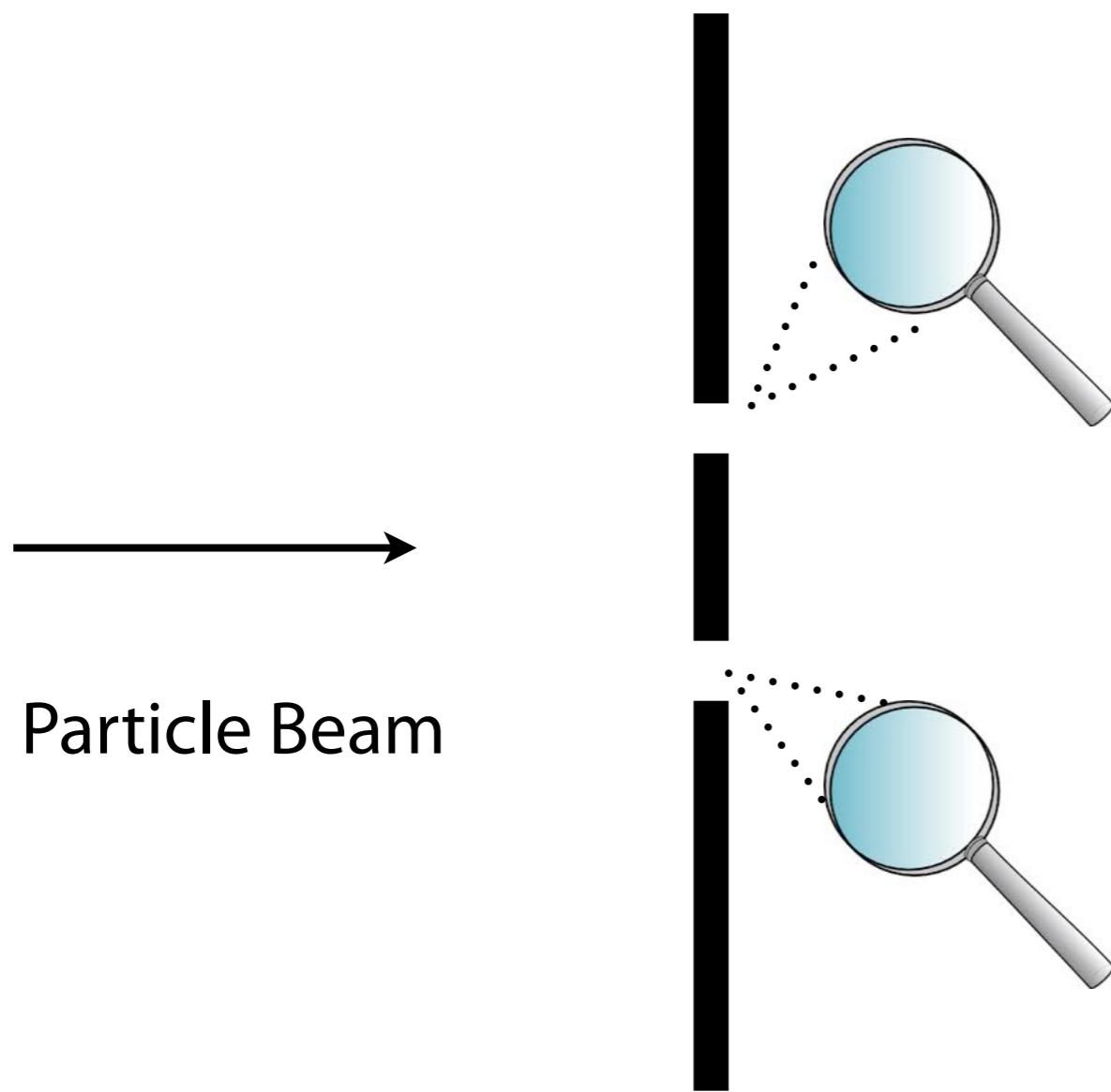
Particle seen in right slit



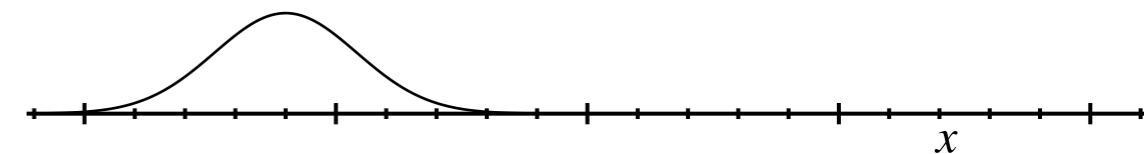
No interference fringes

Double-slit experiment

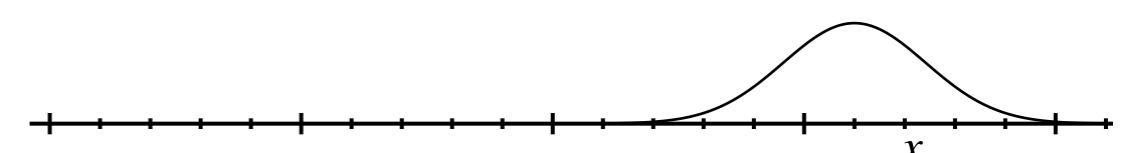
- Measuring which-path destroys the interference.



Particle seen in left slit



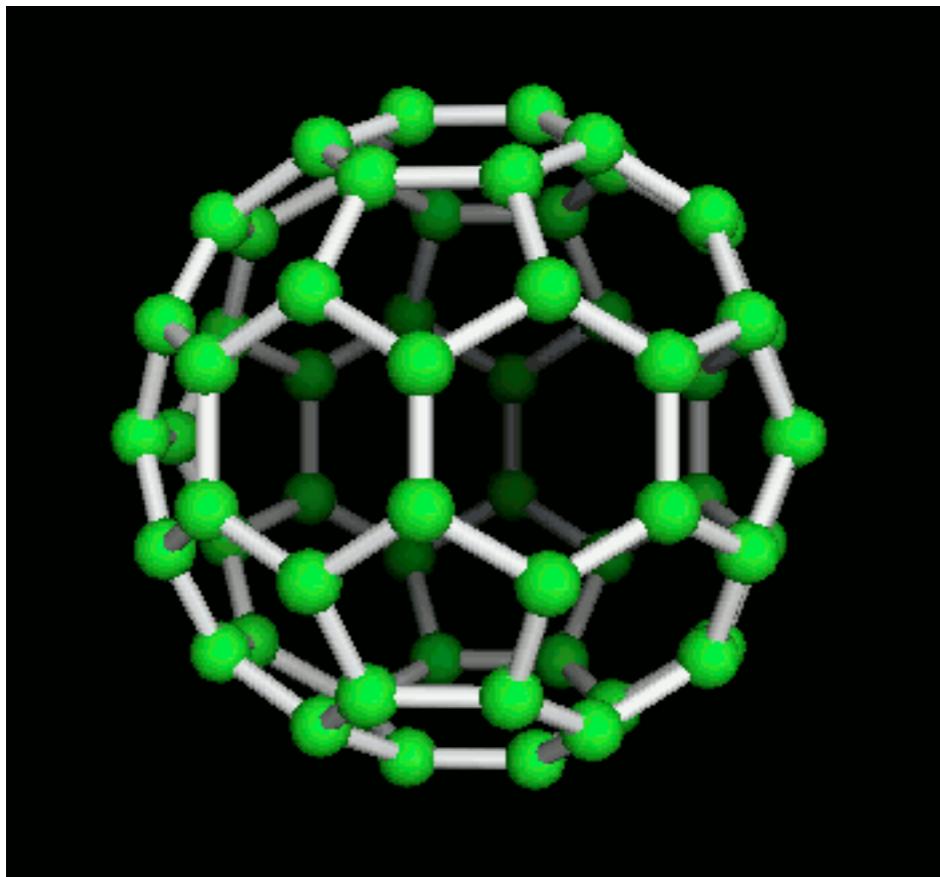
Particle seen in right slit



No interference fringes

Double-slit experiment

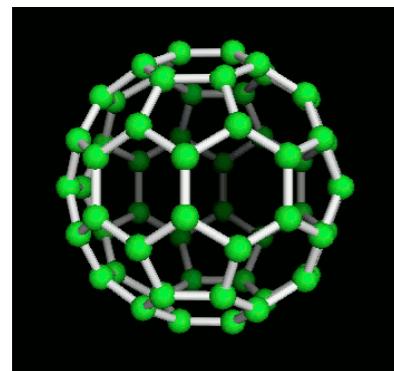
- A beautiful demonstration of this effect.
- Interference of Bucky Balls.



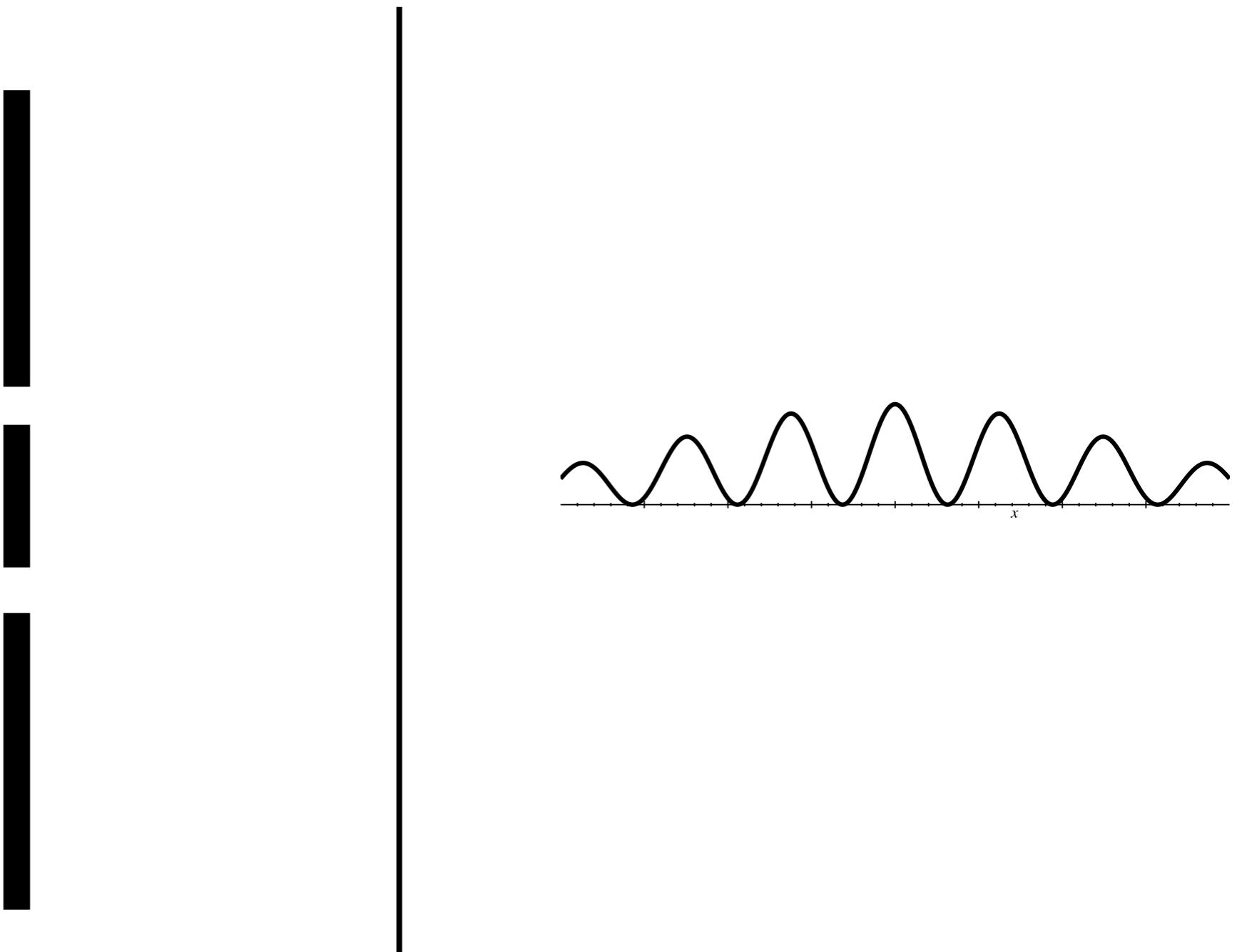
- Carbon-60
 - 60 atoms of carbon in a “football”-shaped molecule
 - If heated, C-60 molecules glow like a black body.
-
- Experiment (M. Arndt) performed in 1999.

Double-slit experiment

- With cold bucky balls they saw the double slit interference pattern.

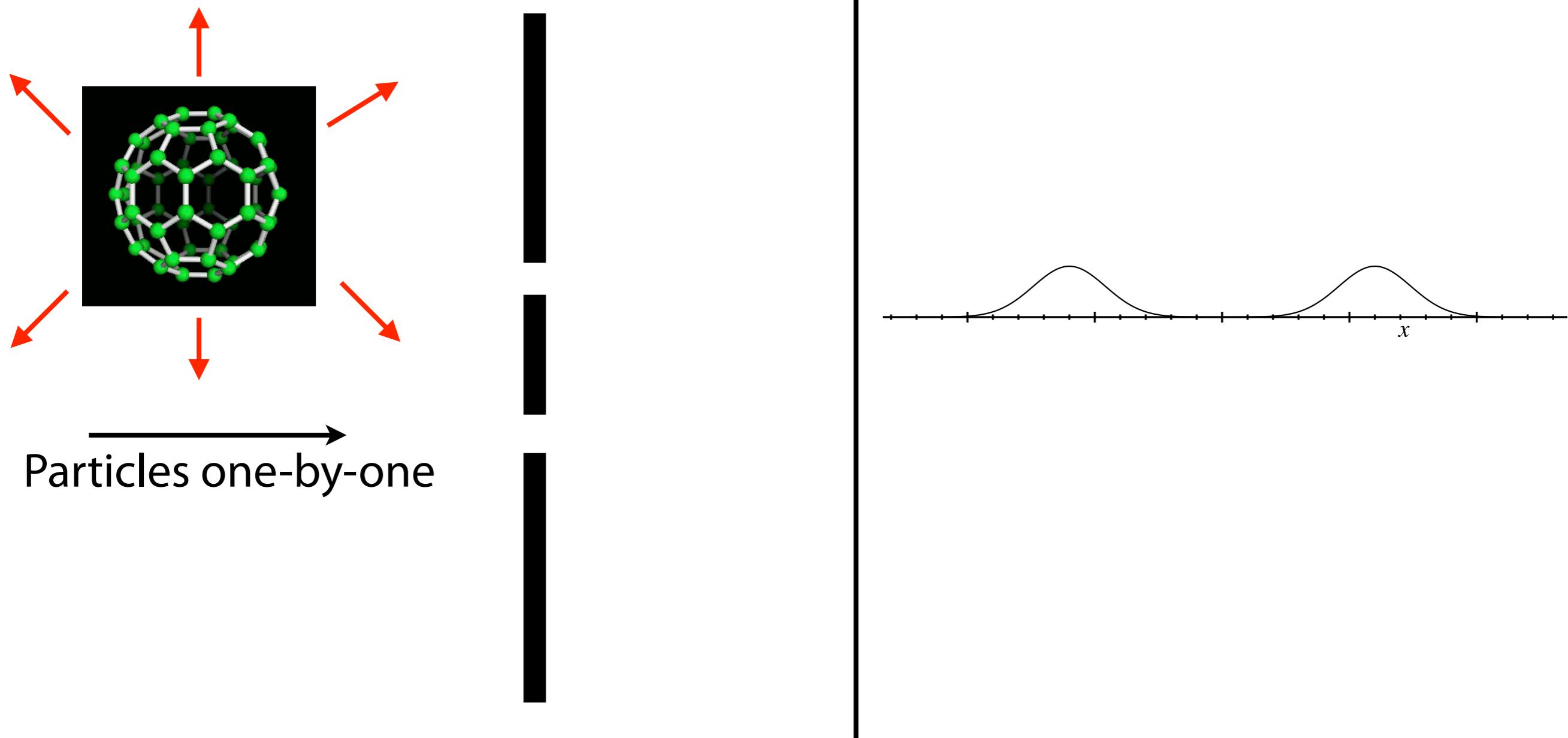


Particles one-by-one



Double-slit experiment

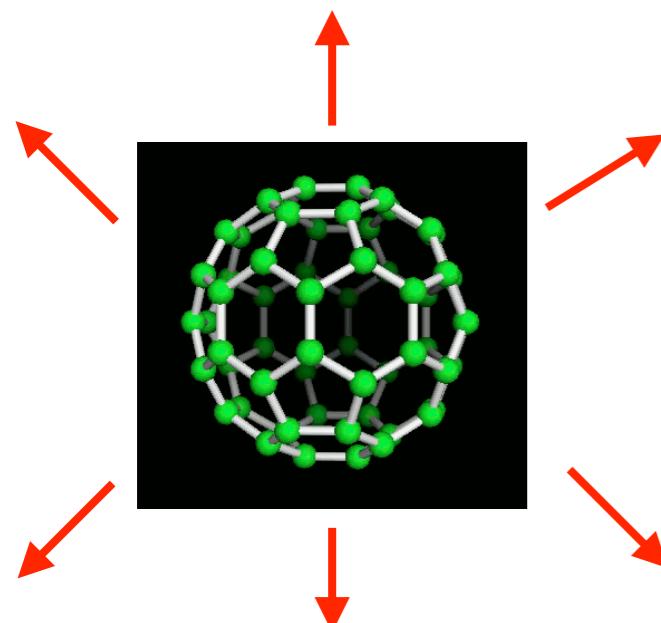
- With hot bucky balls the double slit interference pattern disappeared!



Markus Arndt, et al., Nature (1999)

Double-slit experiment

- With hot bucky balls the double slit interference pattern disappeared!



- The hot bucky balls **emitted light**, so you could “see” which slit they travelled through.
- The interference pattern was **destroyed**.
- Measuring path of particle** “forces the particle to choose” a slit.
- NB **Any physical process** which leaves a record of a physical property (e.g. glowing) can be considered a “**measurement**”.

Lessons from the two-slit experiment

- Quantum particles are not particles.
 - They travel as waves - experiencing interference and travelling through two slits.
 - Measurement outcomes are probabilistic.
 - E.g which slit
 - Which point on the screen the particle lands.
 - Measurement changes the future evolution.
(Measuring which slit destroys interference).

Lessons from the two-slit experiment

- Quantum particles are not particles.
 - These seemingly contradictory properties of wave-particle duality are captured by the **wavefunction**.
 - To understand **wave-functions** - an essential role is played by **probabilities**.
 - So first - we revise **probability theory**.

Poll

- Have you studied **probability** before?
 - 1. Yes
 - 2. No

Poll

- Have you studied **probability density** before?
 - 1. Yes
 - 2. No

Probability revised



Heads



Tails

- Probability allows us to **quantify** the **likelihood** of an outcome a repeatable event.

Probability revised

- Consider an event with two possible outcomes.
 - E.g. a coin toss
- Repeated 100 times
- See approx. 50 heads
- See approx. 50 tails
- Probability of “heads”: 50%
- Probability of “tails”: 50%



Probability revised

- Meaning of probability:
- If an outcome of an experiment (e.g. heads) has probability p
 - after repeating the experiment (tossing the coin) N times
 - when N is a large number, we expect the event to occur pN times.
- A probability is number between 0 and 1.



Heads



Tails

Probability revised

- Example: A child has a **1/7** chance of being born on a Tuesday.
 - If we survey all **62 million** inhabitants of the UK, we expect to find approx **9 million** born on a Tuesday.

Probability revised

- A **probability distribution** is a **list of the probabilities** for **all** outcomes.
- Heads: 0.5
Tails: 0.5
- Monday: 1/7
Tuesday: 1/7
Wednesday: 1/7
Thursday: 1/7
Friday: 1/7
Saturday: 1/7
Sunday: 1/7

Probability revised

- If we are consider two **mutually exclusive** events,
 - the probability of one **OR** the other happening is the **sum** of their probabilities.
 - E.g. the probability that you were born on Monday **or** Tuesday is

$$1/7 + 1/7 = 2/7.$$

Probability revised

Normalisation

A **probability distribution** (for mutually exclusive events) always must add up to 1.

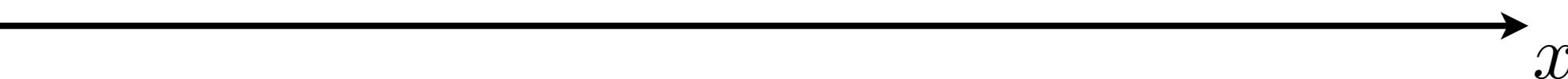
- Heads: 0.5
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- Monday: 1/7
Tuesday: 1/7
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Thursday: 1/7
Friday: 1/7
Saturday: 1/7
Sunday: 1/7

Probability for continuous values

- Properties such as **heads / tails**, the **day of the week** are **discrete**.

heads	tails	Mon	Tue	Wed	Thu	Fri	Sat	Sun
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- In Physics, however, many of the quantities we study are **continuous**.



- E.g. position, momentum, energy, temperature, entropy.
- Probability for continuous quantities** can be studied, but with some **important differences** from the discrete case.

Poll

- Have you studied **probability for continuous variables** before?
 - 1. Yes
 - 2. No

Probability for continuous values

- Continuous quantities are represented by real numbers.
 - This can lead to important differences to the discrete case.
- *Consider a game of darts.*



Quiz

- *Consider a game of darts.*
 - The area of the bullseye is approx. 0.5% of the area of the board.



- If I throw darts **randomly**, but they are guaranteed to hit the board what is the **probability** of hitting **bullseye**?
 - 1. 0.5%
 - 2. 0%
 - 3. 50%

Quiz

- *Consider a game of harder darts.*
 - Imagine I shrink the bullseye, so it now only consists of 0.0005% of the board (!)



- What now is the probability of hitting bullseye?
 - 1. 0.0005%
 - 2. 0%
 - 3. 50%

Probability for continuous values

- The trend is clear - if the darts are thrown fairly at random
 - the **probability** of hitting an area is **proportional** to that area.



Quiz

- *Now consider a much harder game of darts.*
- What is the probability of hitting the **exact centre** of the board?
 - 1. 0%
 - 2. A small finite number close to but not equal to 0%.
 - 3. There is not enough information in the question to compute this.



Quiz

- *Now consider a much harder game of darts.*
- What is the probability of hitting the **exact centre** of the board?
 - 1. 0%
 - 2. A small finite number close to but not equal to 0%.
 - 3. There is not enough information in the question to compute this.



A paradox?

- An **exact point** has zero area.
- Thus the probability of hitting **any exact point** is zero!
- Nevertheless the dart always lands at a point! Doesn't it?



Resolution

- For continuous quantities it is **meaningless** to assign probabilities to a point (it would always be zero).
- We can only consider the probability of achieving a **finite** range of values.



- We can only measure the dart's position to **finite precision**.
- I.e. we can also only measure the **frequency** of the dart reaching a **finite** area of the board.

Probability for continuous values

- This is the **always** the case for any probabilistic behaviour over continuous variables.
- To achieve **meaningful probabilities** for continuous numbers we always need to consider a **range** of values.



- We write:

$$\text{Prob}(a \leq x \leq b) :$$

The probability that x lies in the range between (and including) a and b .

Probability density

- We could in principle ask for the probability for **any finite region**?



$$\text{Prob}(a \leq x \leq b)$$

- **How can we calculate that?**
- We'd like some way of representing **any probability for any region.**
- The answer: We use a **probability density** function.

x

Probability for continuous values

- The **probability density** function for a continuous random variable x

$$\rho(x)$$

is a function which allows us to compute the probability of any finite region (between a and b) via the integral

$$\text{Prob}(a \leq x \leq b) = \int_a^b \rho(x)dx$$



Probability for continuous values

Normalisation

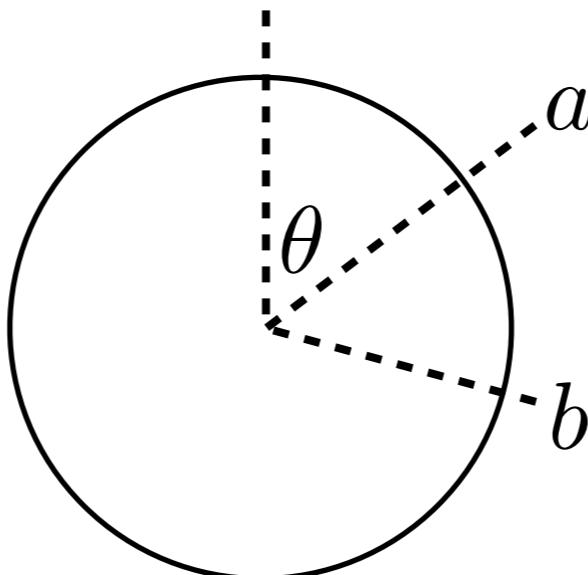
- Similarly to **discrete probability distributions**, if the region spans all values of x , the probability must be 1.
 - E.g. The probability that a particle is found somewhere is 1.
- Thus, **probability densities** satisfy:

$$\int_{-\infty}^{\infty} \rho(x)dx = 1$$

- We call this a **normalisation condition**.

Examples

- Consider a **randomly chosen angle** (in radians)
(eg the angle of the queen's head when you toss a coin.)

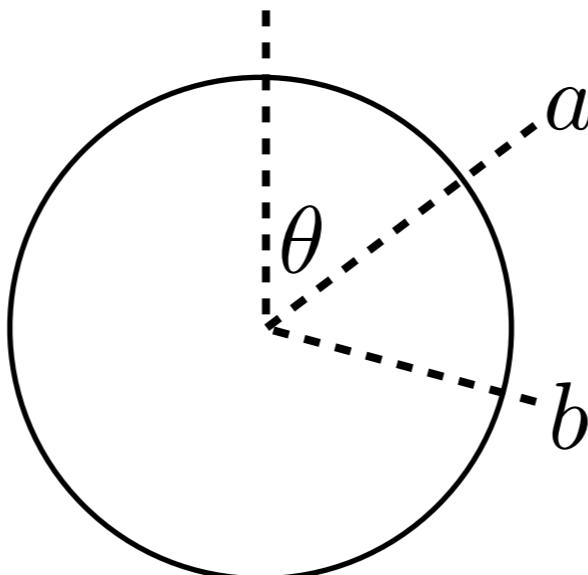


- The probability of θ lying between a radians and b radians is

$$\text{Prob}(a \leq \theta \leq b) = \frac{b - a}{2\pi}$$

Examples

- Consider a **randomly chosen angle** (in radians)
(eg the angle of the queen's head when you toss a coin.)



- The probability of θ lying between a radians and b radians is

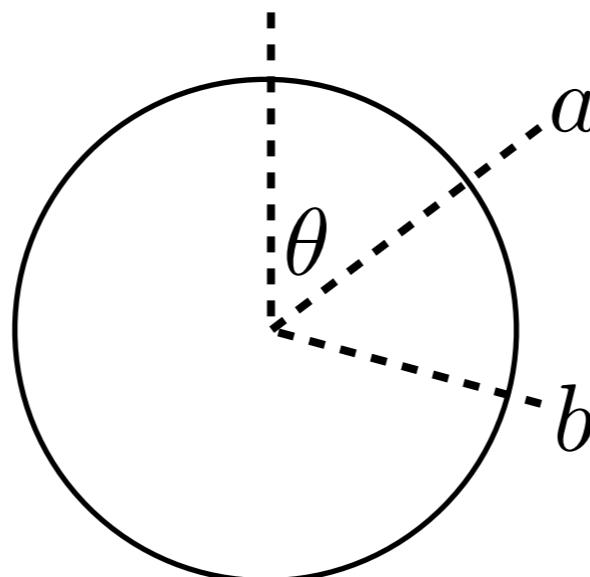
$$\text{Prob}(a \leq \theta \leq b) = \frac{b - a}{2\pi}$$

- The **probability density** is:

$$\rho(\theta) = \frac{1}{2\pi}$$

Examples

- Consider a **randomly chosen angle** (in radians)
(eg the angle of the queen's head when you toss a coin.)



- The **probability density**:
$$\rho(\theta) = \frac{1}{2\pi}$$
- satisfies the normalisation condition:

$$\int_0^{2\pi} \frac{1}{2\pi} = 1$$

For future reference

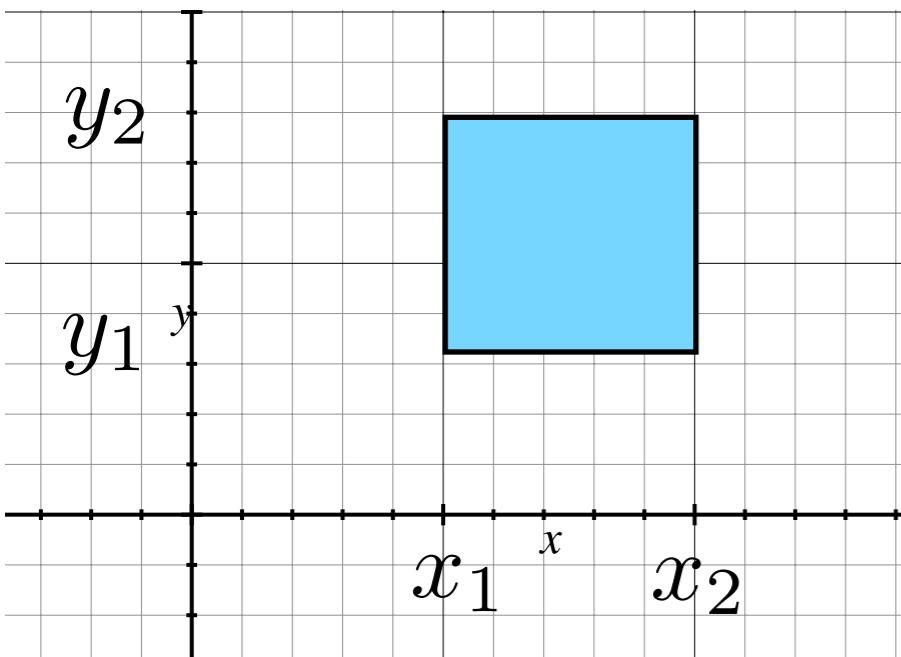
- Probability density functions can be constructed for more than one variable, e.g. 2-D coords x, y .

$$\rho(x, y)$$

- Then probability is then given by a **multiple integral**

$$\text{Prob} = \int_{x_1}^{x_2} \int_{y_1}^{y_2} \rho(x, y) dx dy$$

- You will **not** need multiple integrals on this course, but will encounter them in your Maths course this year.



Summary of probability density

- The **probability density** function for a continuous random variable x

$$\rho(x)$$

is a function which allows us to compute the probability of any finite region (between a and b) via the integral

$$\text{Prob}(a \leq x \leq b) = \int_a^b \rho(x)dx$$



- It satisfies a **normalisation condition**

$$\int_{-\infty}^{\infty} \rho(x)dx = 1$$

The Wave-function

The wavefunction

- The **wavefunction** for a particle is the **quantum mechanical representation of the particle's position**.
- The wave-function is a **function of position**, which can be both **positive** and **negative** (or even **complex**, see Y2 course).

E.g.

$$\psi(x, y, z) = \sin(x) \cos(y) e^{-z}$$

- It is usually labelled with the greek letter **Ψ (psi)**.
- In this course, we will mainly assume that the world is **1-dimensional** and study **1-d** wave-functions.
- E.g.

$$\psi(x) = \sin(x) e^{-2x}$$

The wavefunction

- How does a wave-function represent **position**?
- The wave-function tells us the **probability** of finding the particle in a **region of space**, via the **Born rule**:



Max Born

$$\text{Prob}(a \leq x \leq b) = \int_a^b |\psi(x)|^2 dx$$



- In other words

$$|\psi(x)|^2$$

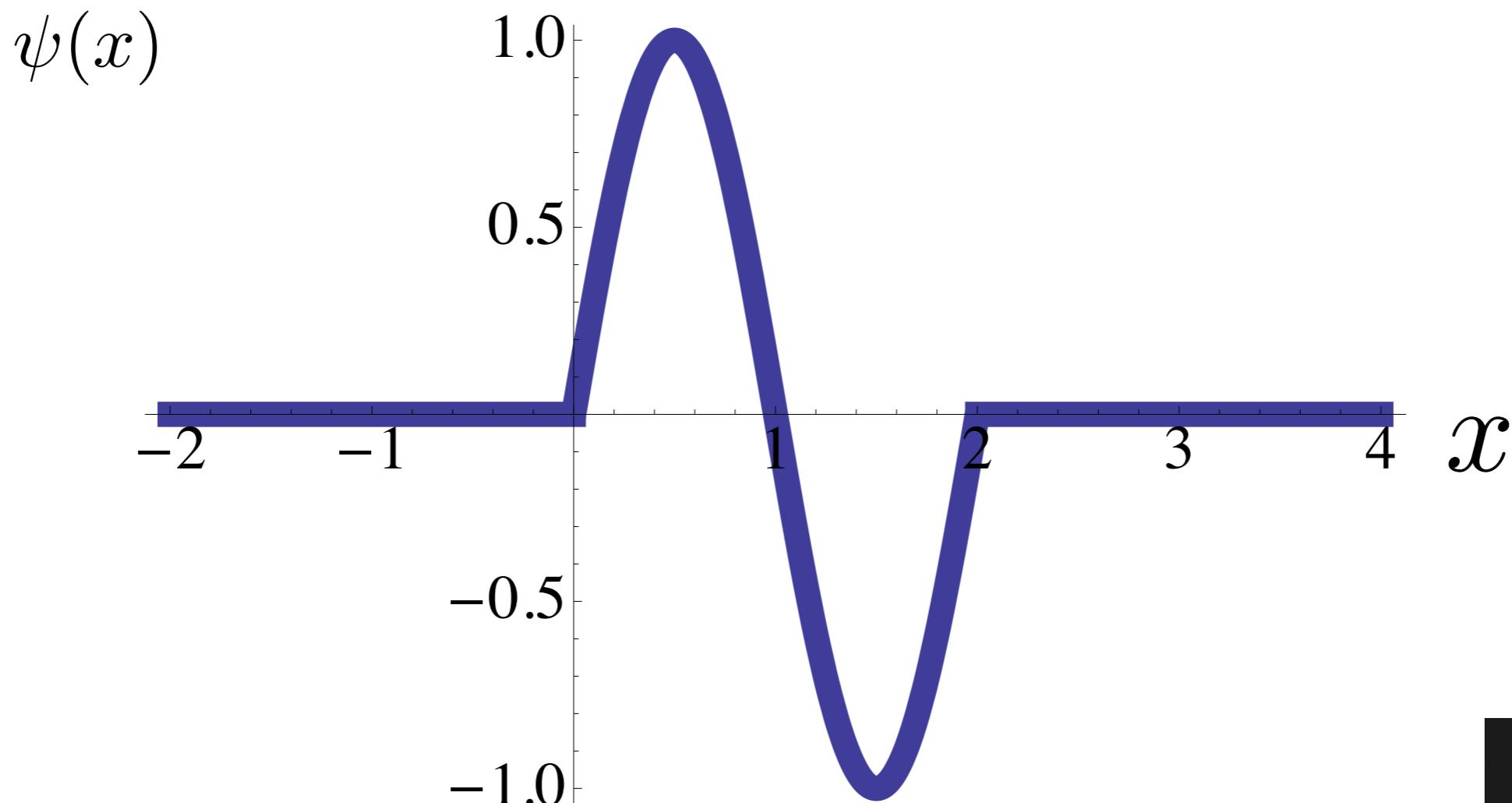
is the **probability density** for position.

The wavefunction

- An example wave-function:

$$\psi(x) = \sin(\pi x) \quad \text{for } 0 \leq x \leq 2$$

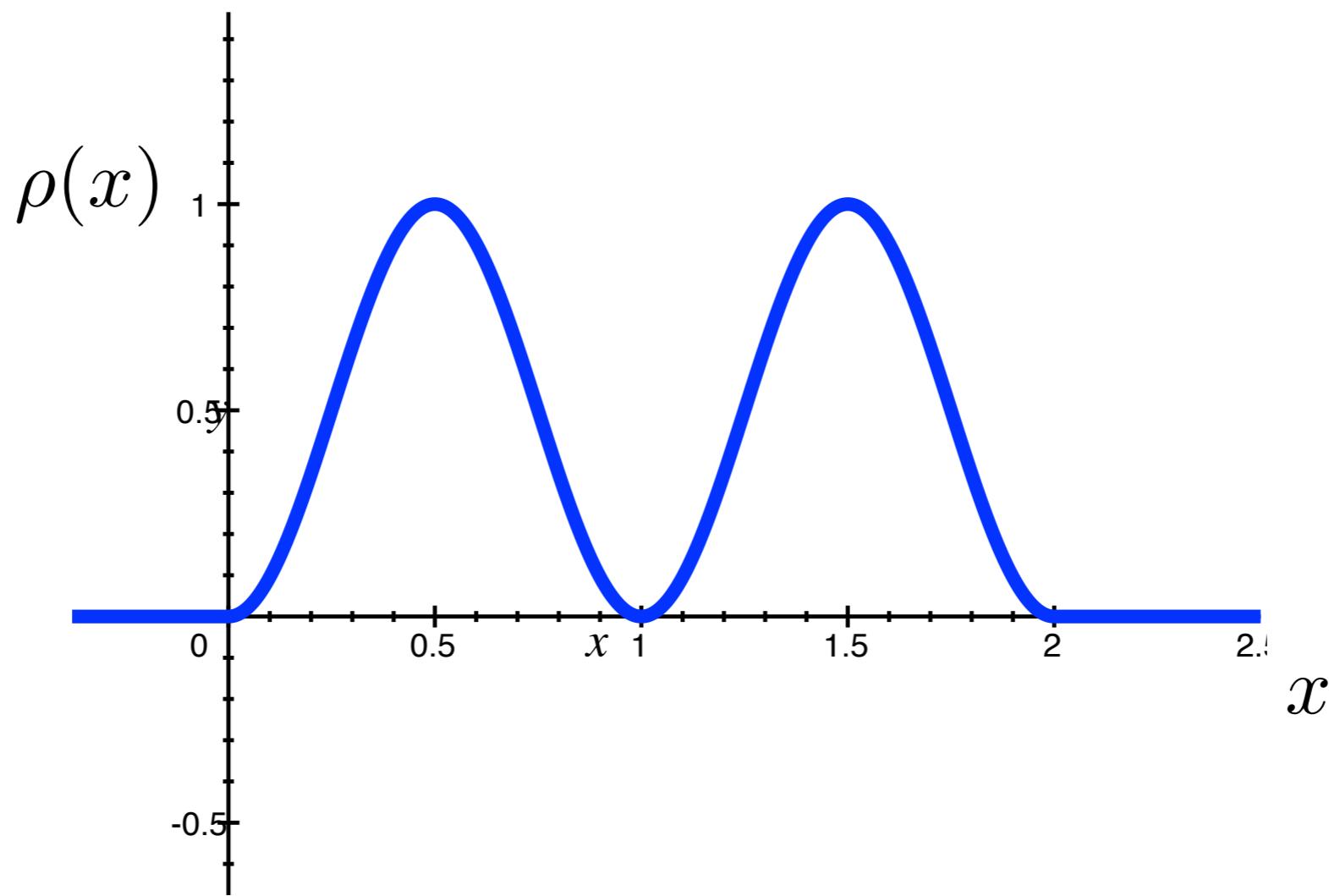
$$\psi(x) = 0 \quad \text{elsewhere}$$



The wavefunction

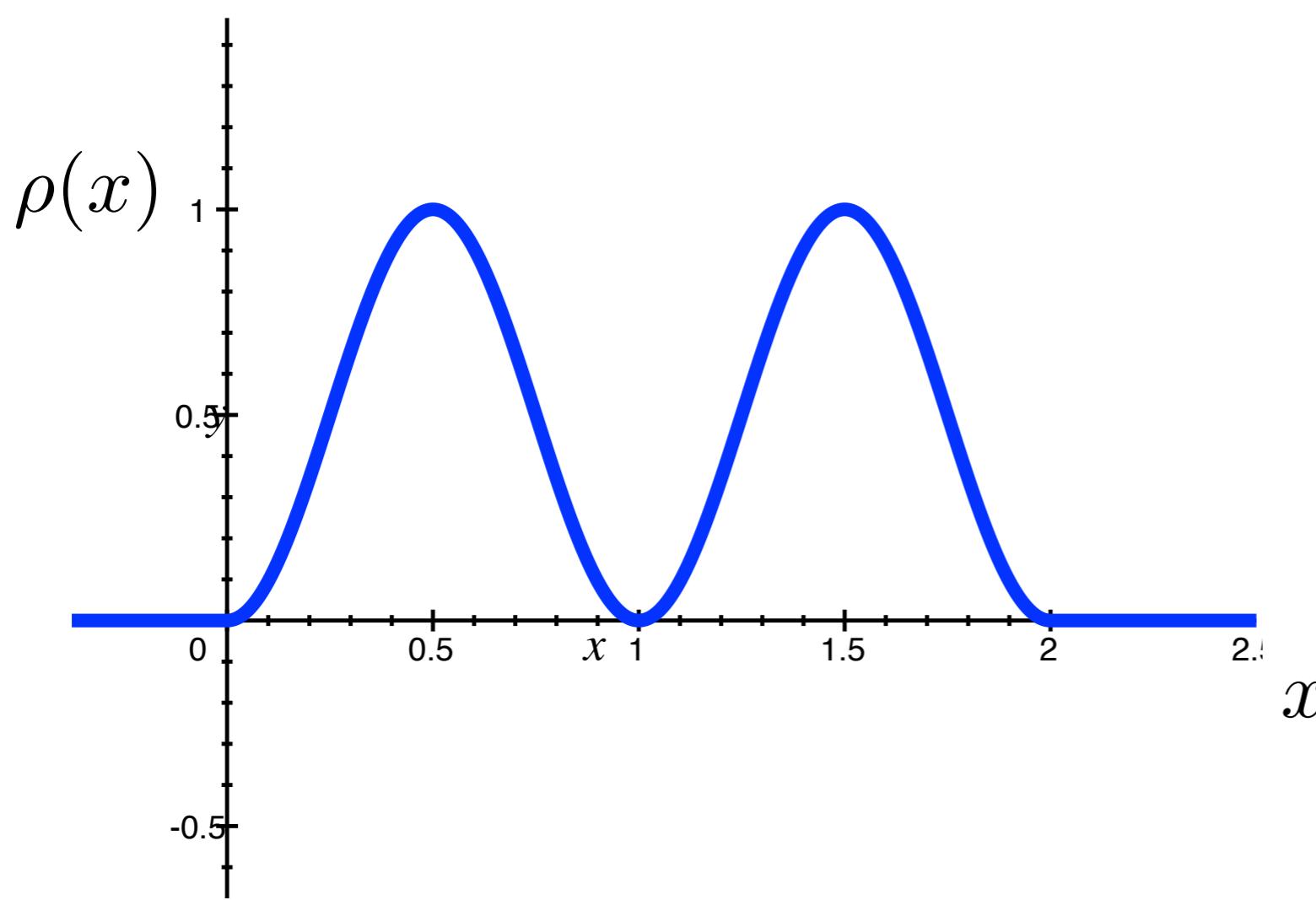
- The probability density for particle position is

$$\rho(x) = |\psi(x)|^2 = \sin^2(\pi x)$$



Quiz

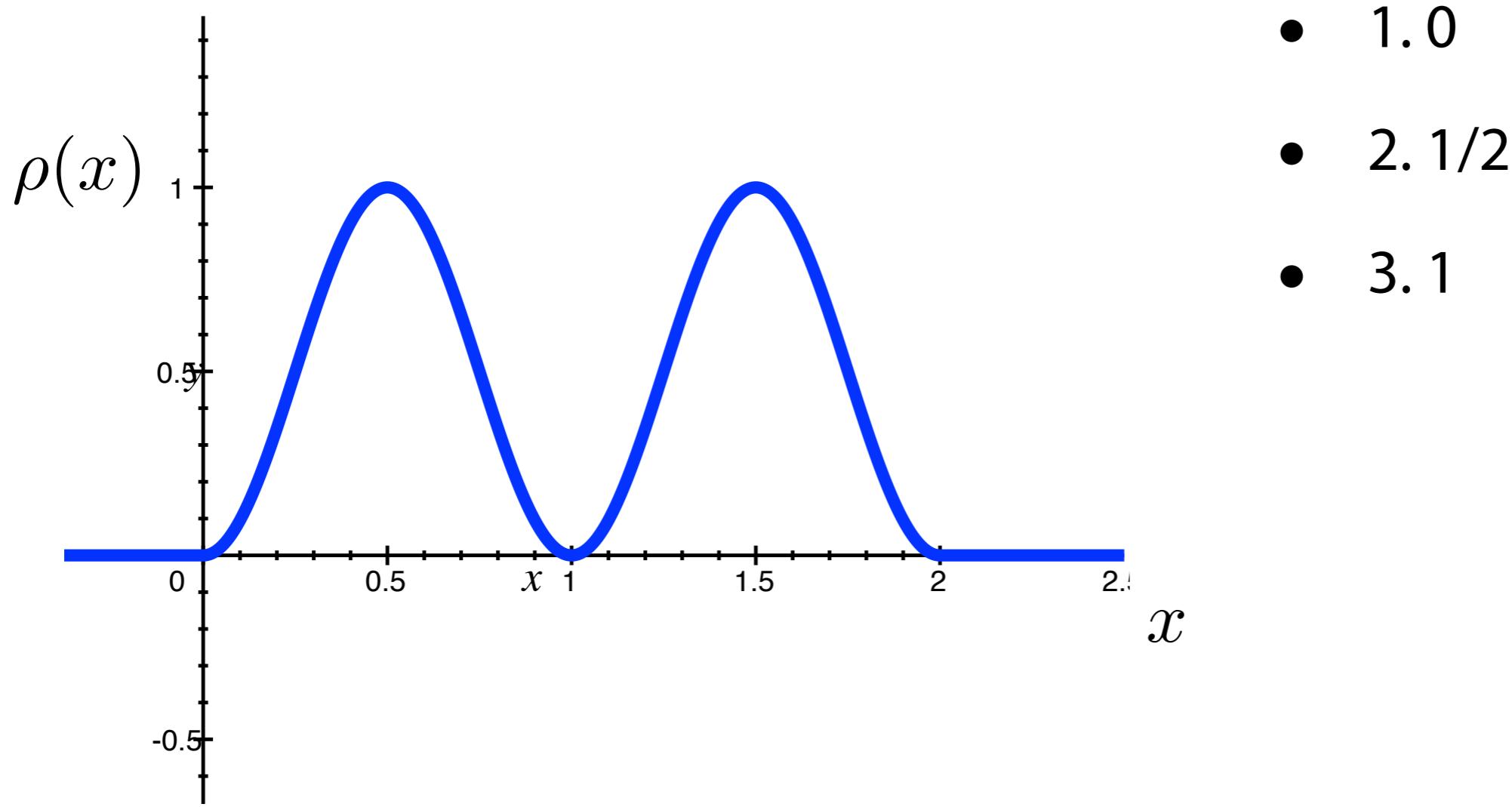
- By inspection, what is the probability for finding the particle in the region $x = 0.5$ to $x = 1$?



- 1. $1/2$
- 2. $1/4$
- 3. $1/8$
- 4. 0

Quiz

- By inspection, what is the probability for finding the particle in the region $x = 0$ to $x = 2$?



The normalisation condition

- A probability density must satisfy

$$\int_{-\infty}^{\infty} \rho(x) dx = 1$$

- Similarly **all** physical wave-functions must satisfy a **normalisation condition**.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

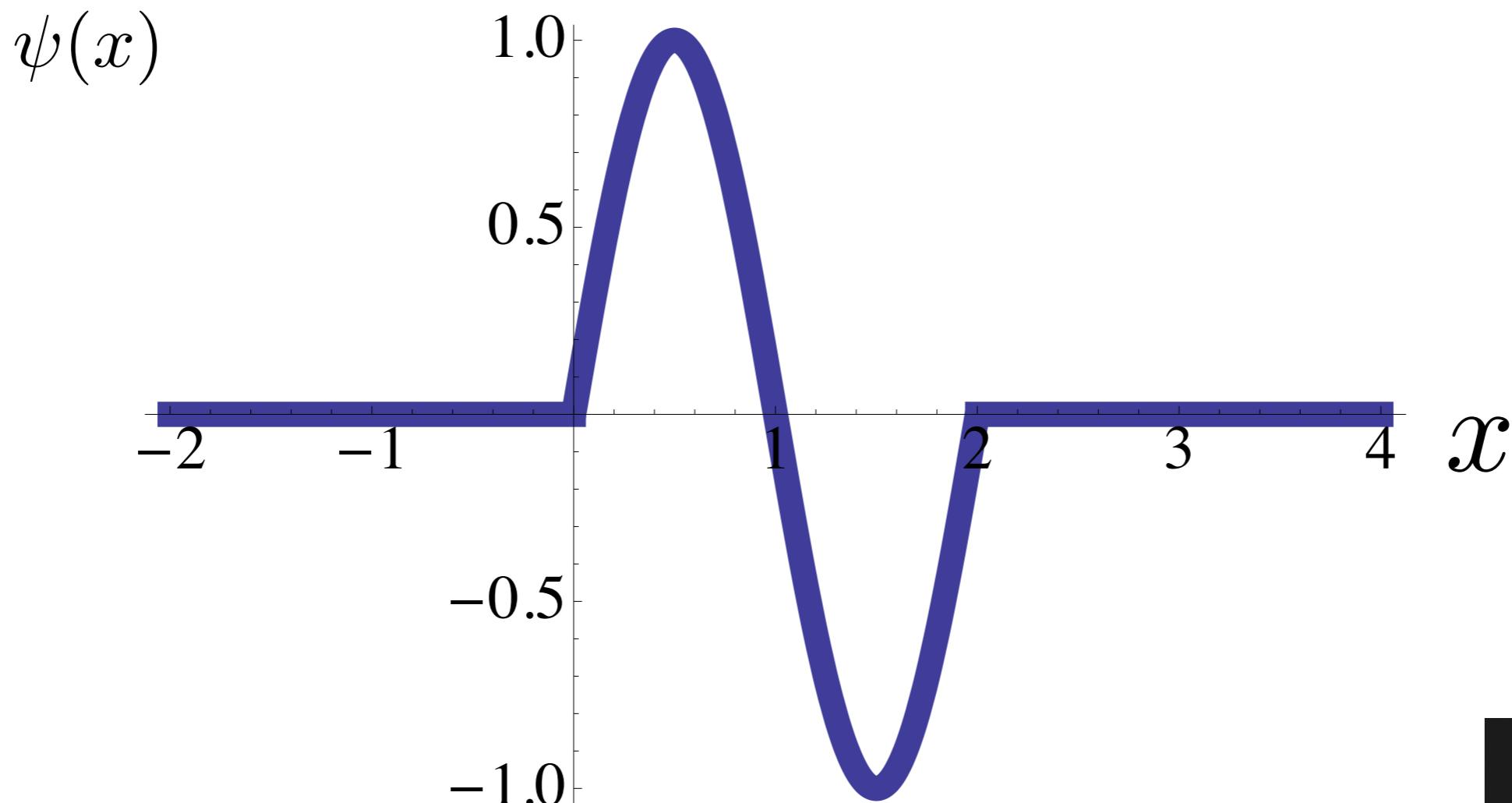
- Any wave-function which satisfies this condition is called **normalised**.
- It is sometimes convenient to work with wave-functions which are not normalised - we will see examples later.

The wavefunction

- Let us verify that this wavefunction is normalised:

$$\psi(x) = \sin(\pi x) \quad \text{for} \quad 0 \leq x \leq 2$$

$$\psi(x) = 0 \quad \text{elsewhere}$$



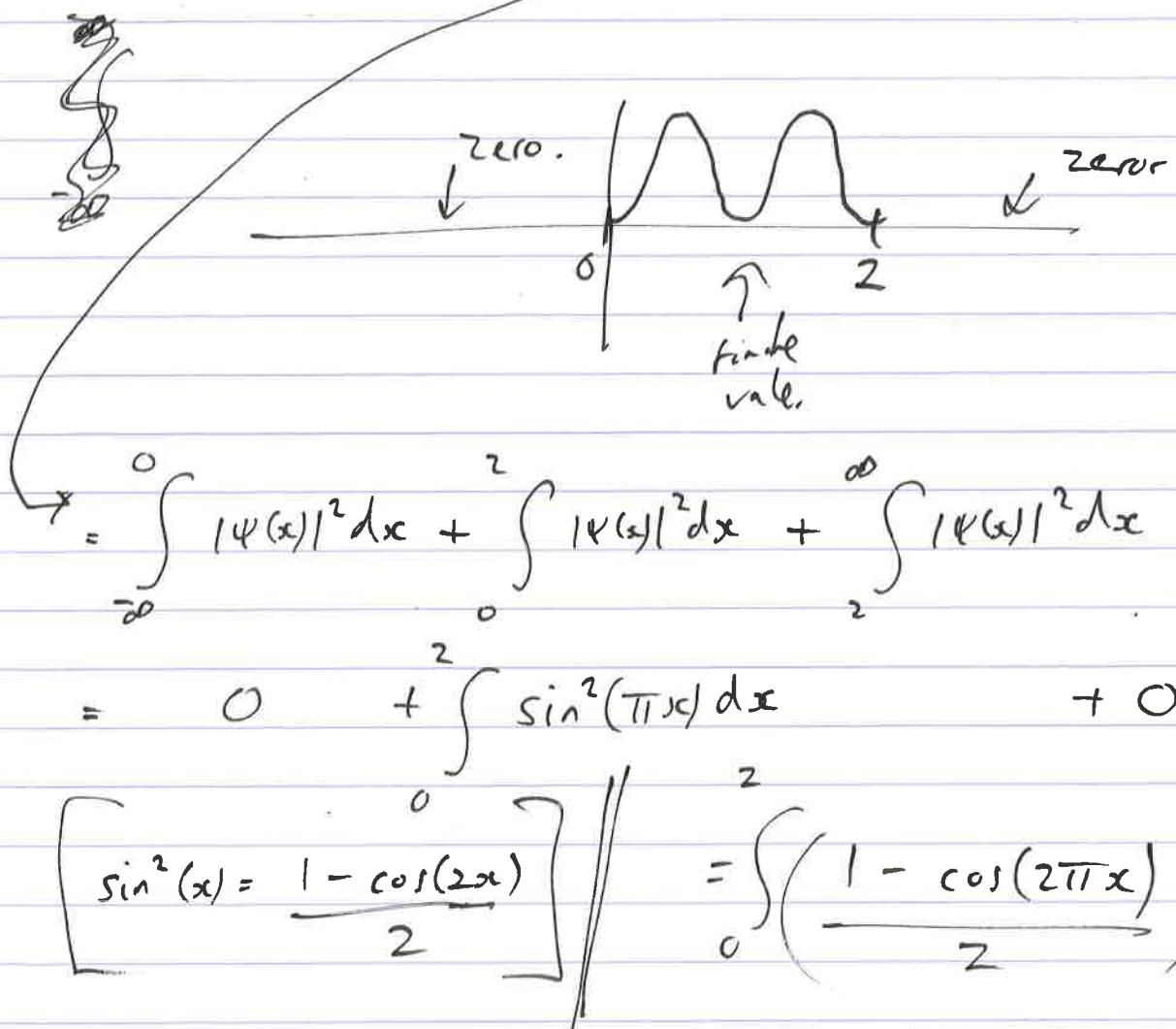
Hand-written Calculations



$$\Psi(x) = \begin{cases} \sin(\pi x) & \text{for } 0 \leq x \leq 2, \\ 0 & \text{elsewhere.} \end{cases}$$

Want to check:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$$



$$= \int_{-\infty}^0 |\Psi(x)|^2 dx + \int_0^2 |\Psi(x)|^2 dx + \int_2^{\infty} |\Psi(x)|^2 dx$$

$$= 0 + \int_0^2 \sin^2(\pi x) dx + 0$$

$$\left[\sin^2(x) = \frac{1 - \cos(2\pi x)}{2} \right] \parallel \int_0^2 \left(\frac{1 - \cos(2\pi x)}{2} \right) dx$$

$$= \frac{1}{2} (2 - 0) - \frac{1}{2} \left[\frac{\sin(2\pi x)}{2\pi} \right]_0^2$$

$$= 1 - \frac{1}{2} (0 - 0) = 1 \quad \therefore$$

\uparrow Normalised

$$\text{Prob}(a \leq x \leq b) = \int_a^b |\psi(x)|^2 dx.$$

(assume $a > 0$ $b < 2$ $b > a$)

$$= \int_a^b \sin^2(\pi x) dx = \int_a^b \frac{1 - \cos(2\pi x)}{2} dx$$

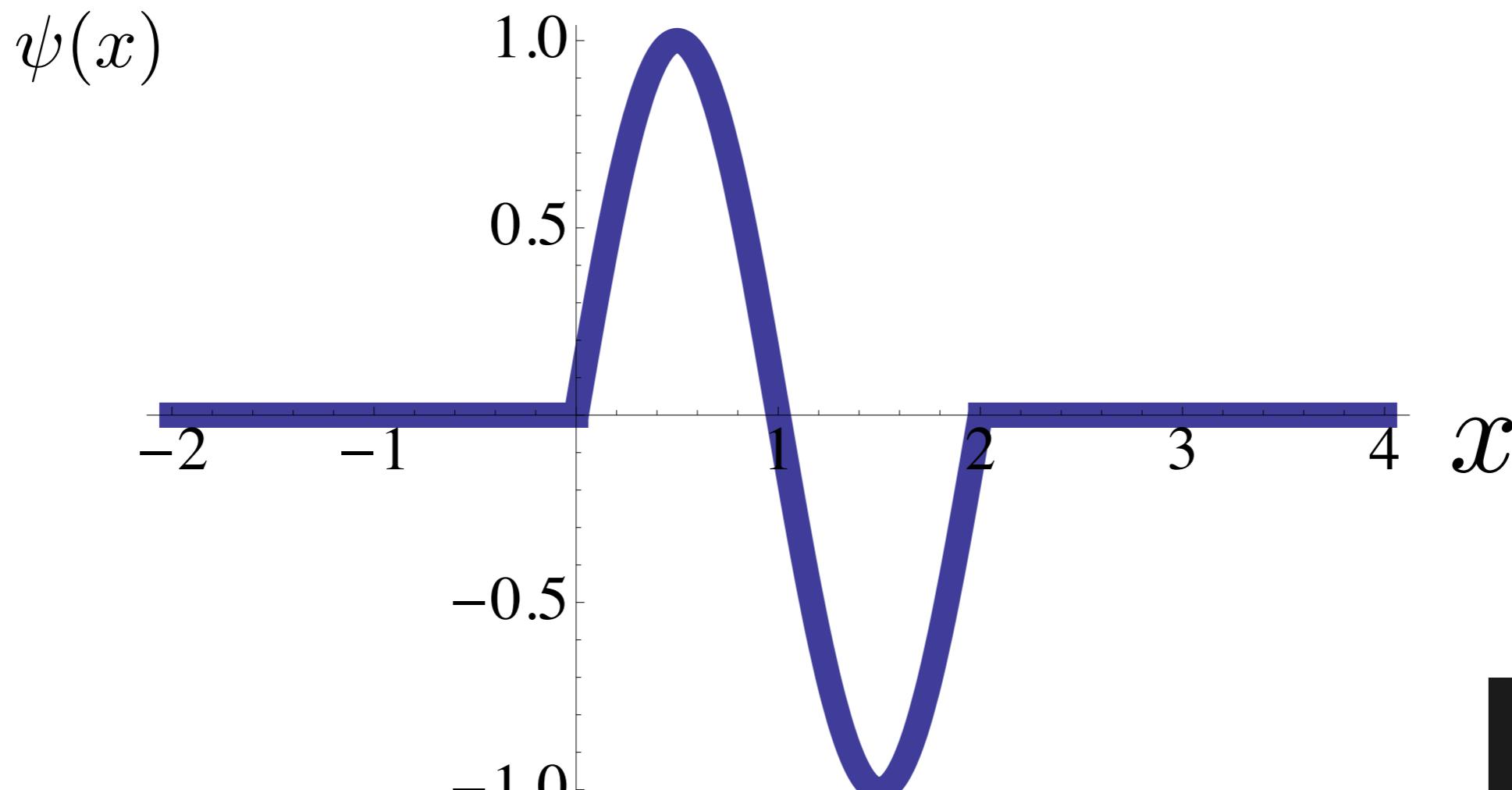
$$= \frac{1}{2} (b-a) - \frac{1}{2} \left(\frac{1}{2\pi}\right) \left(\sin(2\pi b) - \sin(2\pi a) \right)$$

The wavefunction

- We can compute via integration, the probability to find the particle between any limits a and b .

$$\psi(x) = \sin(\pi x) \quad \text{for } 0 \leq x \leq 2$$

$$\psi(x) = 0 \quad \text{elsewhere}$$



Hand-written Calculations



Normalisation

- Sometimes we calculate wave-functions, but they are **not normalised** (a common result of standard calculation techniques).
- Fortunately, for most functions, we can **convert** them into **normalised wavefunctions** by a **simple method**:
- Consider function $\psi_1(x)$ which satisfies:

$$\int_{-\infty}^{\infty} |\psi_1(x)|^2 dx = N \neq 1$$

- If we divide $\psi_1(x)$ with \sqrt{N} we achieve a **normalised function**

$$\psi_2(x) = \frac{\psi_1(x)}{\sqrt{N}} \quad \int_{-\infty}^{\infty} |\psi_2(x)|^2 dx = \frac{N}{N} = 1$$

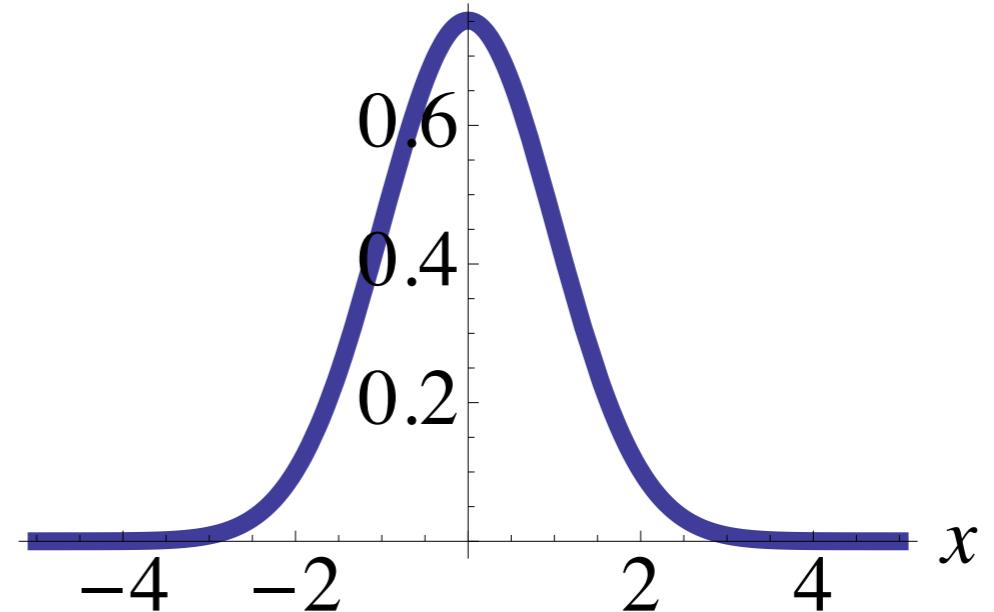
- $\psi_2(x)$ is **normalised**.

Quiz

- Given the following mathematical identity, which of the following wave-functions is normalised?

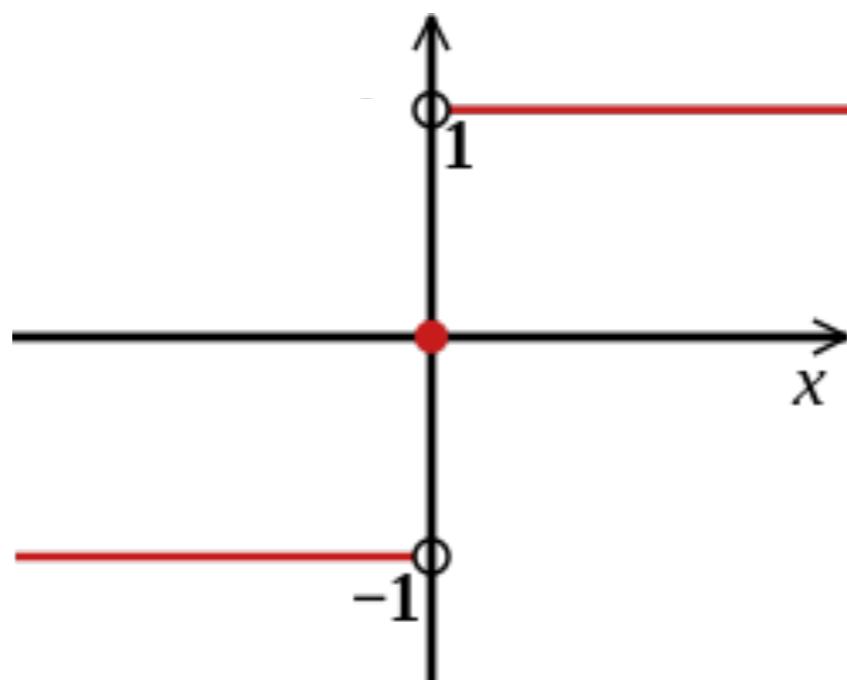
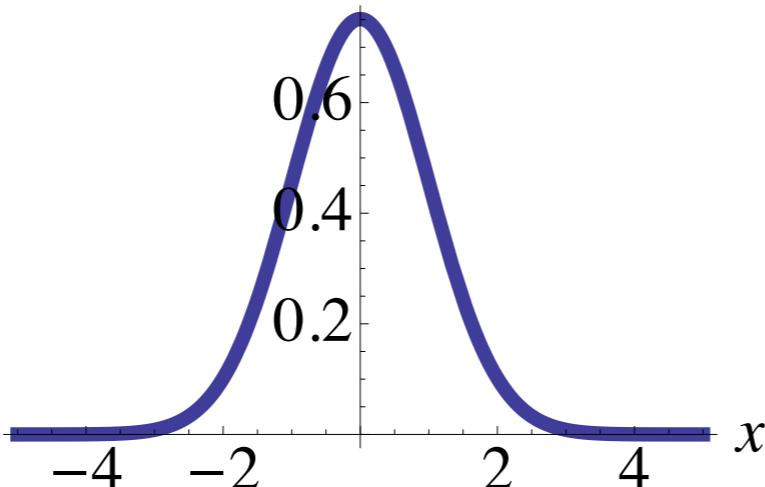
$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

- 1. $\psi_1(x) = \frac{e^{-x^2}}{\pi^{1/2}}$
- 2. $\psi_2(x) = \frac{e^{-x^2/2}}{\pi^{1/4}}$
- 3. $\psi_3(x) = \frac{e^{-x^2/2}}{\pi^{1/2}}$



The wavefunction

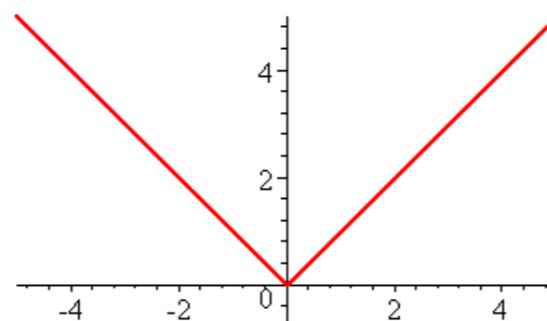
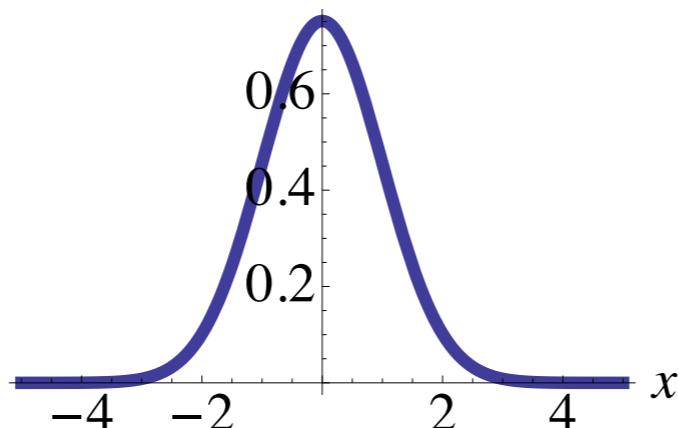
- There is a final property wave-functions must satisfy. The functions must be **continuous**. No “jumps”.



- This ensures that the **first derivative** of $\Psi(x)$ is finite.

The wavefunction

- Wave-functions (usually) must also be **continuous** in their **first derivatives**. No “kinks”.



- This ensures that the **second derivative** of $\Psi(x)$ is **finite**.
- For future reference only. We will not consider (or enforce!) this condition in this course.

Wavefunctions - Summary of properties

- A **wavefunction** is a function of position which:
 - is a **positive** and / or **negative** (and/or complex) number for all values of x (can be zero).
 - $\psi(x)$ is **normalised**.
 - $\psi(x)$ is **continuous**.
 - Probability of position measurement via the **Born rule**:

$$\text{Prob}(a \leq x \leq b) = \int_a^b |\psi(x)|^2 dx$$

Poll

- Have you studied expectation values before?
 - 1. Yes
 - 2. No

Expectation values

- For any random variable with a probability distribution, we can compute the **expectation value**.
- Consider a **discrete** probability distribution $x = x_j$ with probability p_j .
- Example
 - A fair 6 sided dice, will return integers from 1 to 6, each with probability $1/6$.
 - $p_1=1/6, p_2=1/6, p_3=1/6$, etc.



Expectation values

- If we repeatedly poll from this probability distribution, we can compute the **mean value** of the values obtained so far.
- The **expectation value** represents this **mean** value in the **limit** of a **very large number** of repetitions.
- The **expectation value** of x , written $\langle x \rangle$ is given by the formula:

$$\langle x \rangle = \sum_j p_j x_j$$

Expectation values

- Let n_j be the number of times value x_j is returned.
- The **mean value** of x , written $\langle x \rangle$ is given by the formula:

$$\bar{x} = \frac{\sum_j n_j x_j}{\sum_k n_k}$$

- In the limit of many repetitions, we expect n_j to converge to

$$n_j = p_j \sum_k n_k$$

- And thus the mean converges to

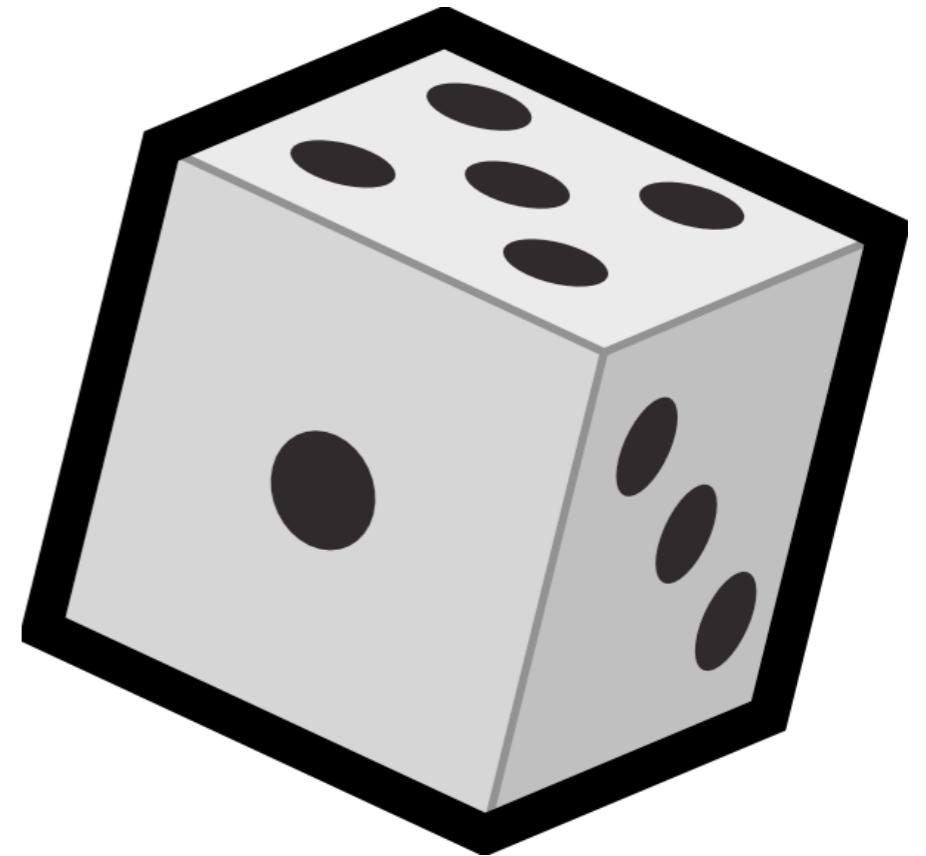
$$\langle x \rangle = \sum_j p_j x_j$$

Expectation values

- Example
- $p_1=1/6, p_2=1/6, p_3=1/6$, etc.

$$\langle x \rangle = \sum_j p_j x_j$$

$$\langle x \rangle = \sum_{n=1}^6 \frac{1}{6} n = \frac{21}{6} = 3.5$$



Expectation values

- We can also compute **expectation values** for **continuous random variables**.
- We replace the **sum** by an **integral** and use the **probability density**.

$$\langle x \rangle = \int_{-\infty}^{\infty} \rho(x) x \, dx$$

Expectation values

- We can therefore compute the expectation value for position of **quantum particles**.
- From:

$$\langle x \rangle = \int_{-\infty}^{\infty} \rho(x) x \, dx$$

- We obtain:

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

Example

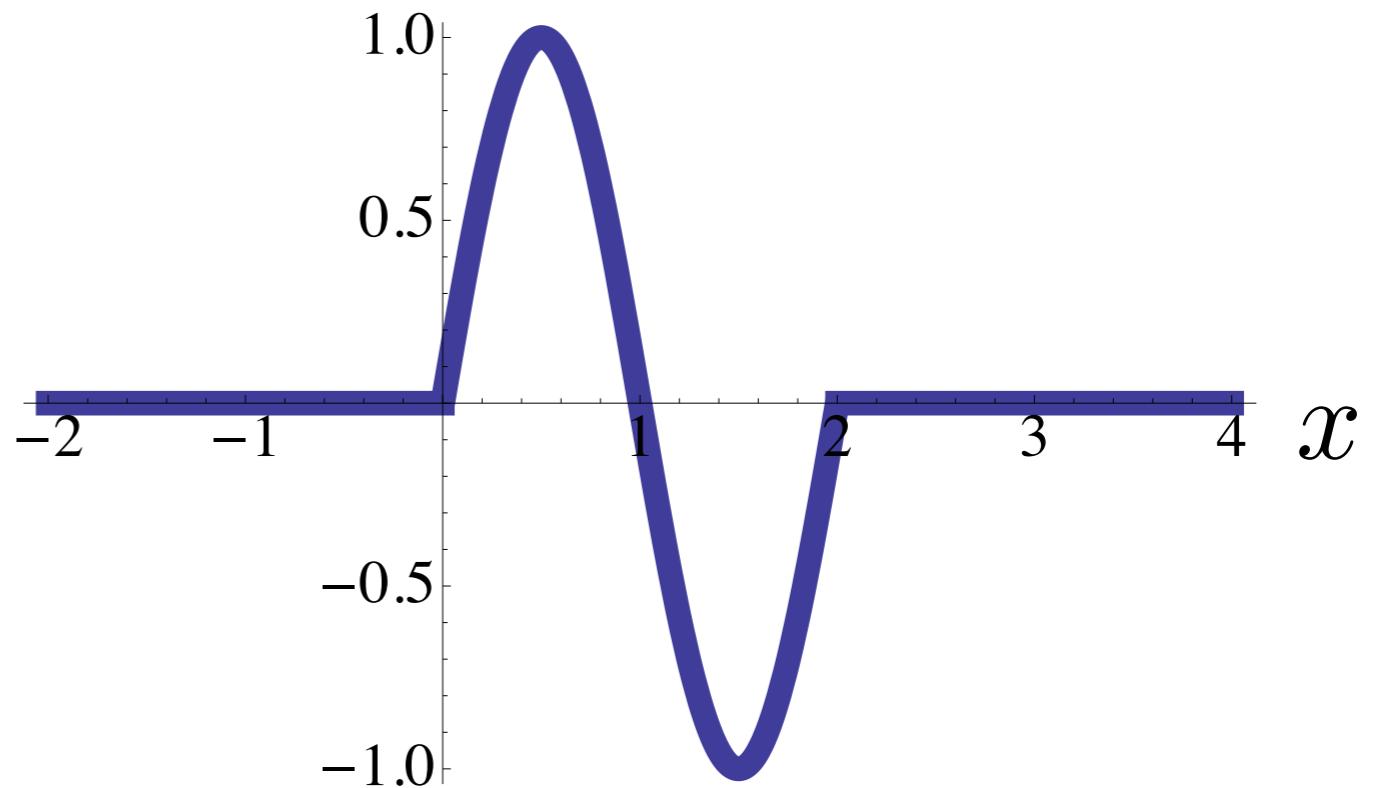
- Consider our example wavefunction:

$$\begin{aligned}\psi(x) &= \sin(\pi x) && \text{for } 0 \leq x \leq 2 \\ \psi(x) &= 0 && \text{elsewhere}\end{aligned}$$

- We can compute the expectation value:

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

$$= \int_0^2 \sin(\pi x)^2 x \, dx$$



Quiz

- Without doing the integral, what is the expectation value of x ?

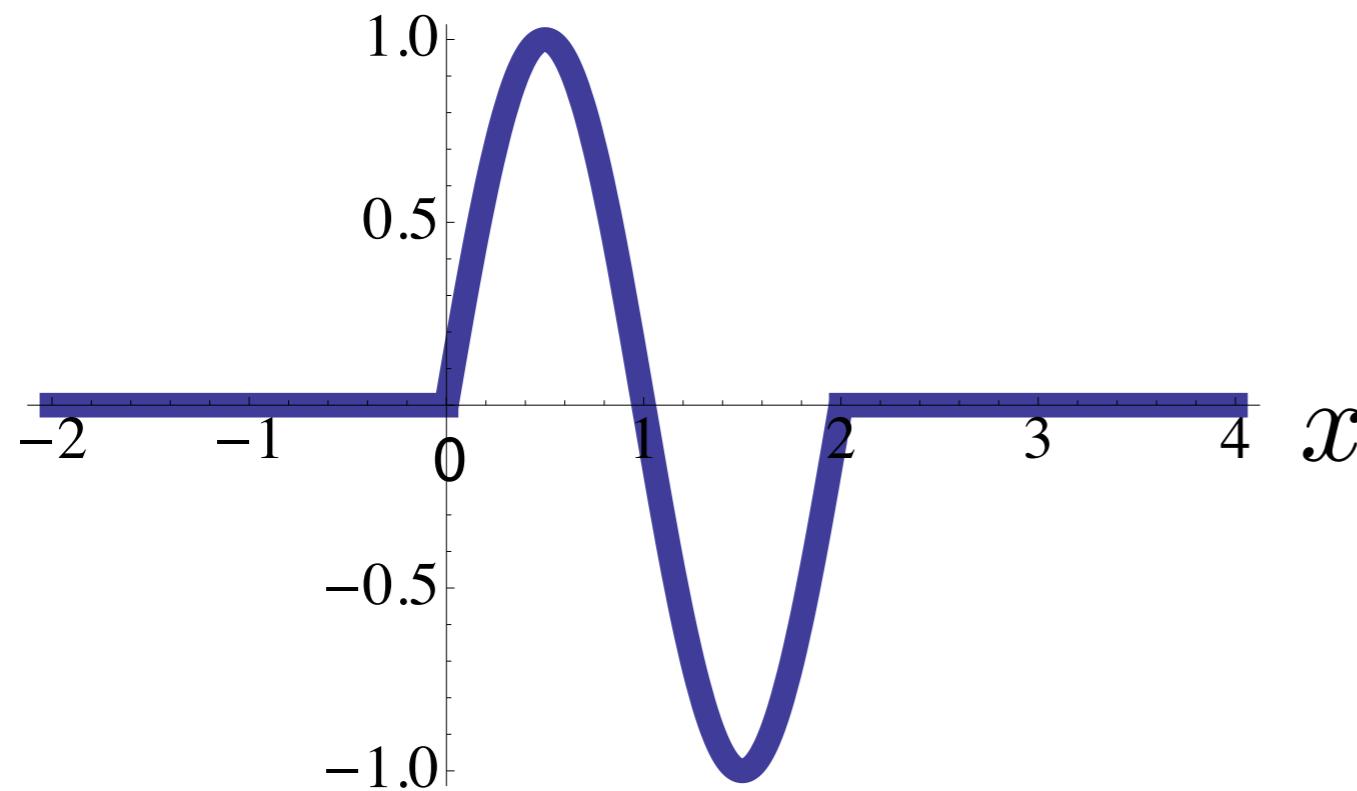
- 1. 0.0

- 2. 0.5

- 3. 1.0

- 4. 1.5

- 5. 2.0



Hand-written Calculations



$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx$$

$\psi(x) = \sin(\pi x) \quad 0 \leq x \leq 2$
 elsewhere.

$$= \int_0^2 x \sin^2(\pi x) dx = \int_0^2 x \left(1 - \frac{\cos(2\pi x)}{2} \right) dx$$

$$= \int_0^2 \frac{x}{2} dx - \underbrace{\frac{1}{2} \int_0^2 x \cos(2\pi x) dx}_{\text{Integration by parts}}$$

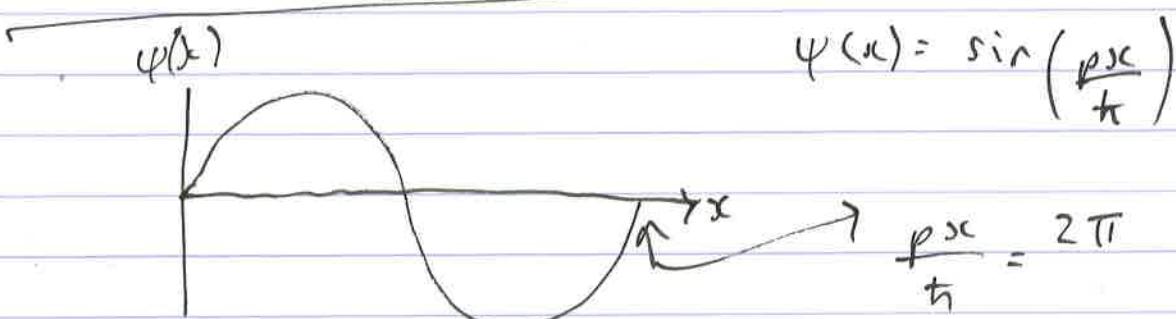
Integration by parts: $\int_a^b u(x)v'(x) dx = \left[u(x)v(x) \right]_{x=a}^{x=b} - \int_a^b v(x)u'(x) dx$

$$u(x) = x \quad u'(x) = \frac{du}{dx} = 1 \quad v'(x) = \cos(2\pi x) \quad v(x) = \frac{1}{2\pi} \sin(2\pi x)$$

$$\int_0^2 x \cos(2\pi x) dx = \left[x \frac{\sin(2\pi x)}{2\pi} \right]_0^2 - \int_0^2 \frac{1}{2\pi} \sin(2\pi x) dx$$

$$= 0 - 0 + \frac{1}{2\pi} \frac{1}{2\pi} \left[\cos(2\pi x) \right]_0^2 = \frac{1}{(2\pi)^2} (1 - 1) = 0$$

$$= \int_0^2 \frac{x}{2} dx - \frac{1}{2} \frac{(4-0)}{2} = \frac{4}{4} = 1$$

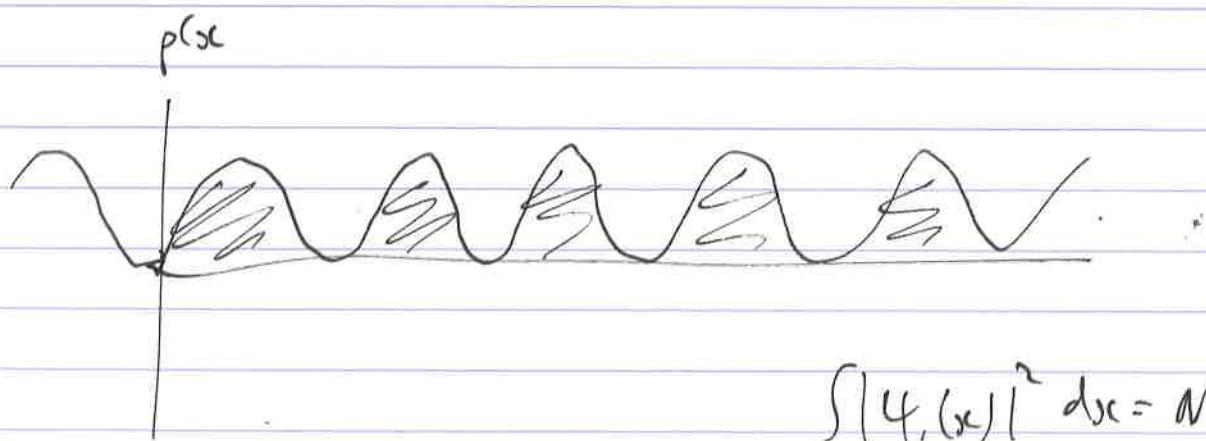
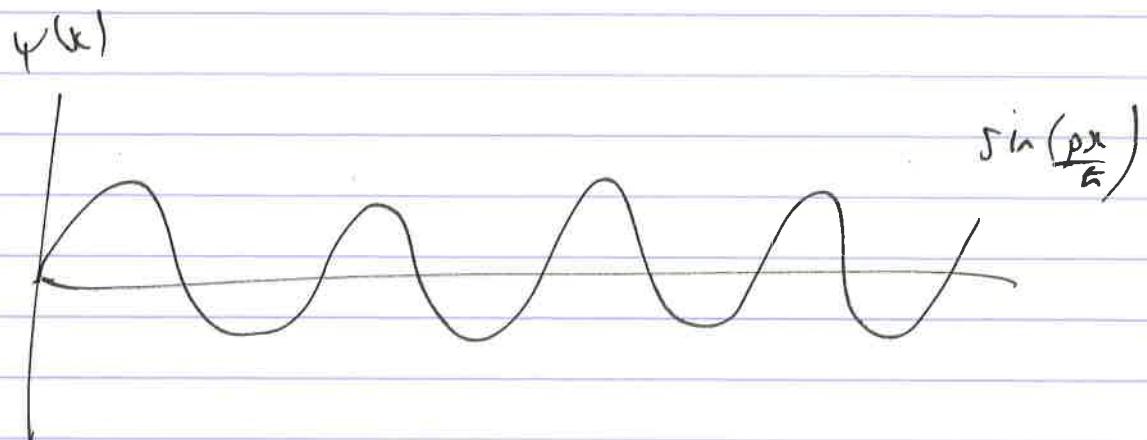


$$\frac{p\lambda}{\hbar} = 2\pi$$

$$\frac{p\lambda}{\hbar} = 2\pi$$

$$\boxed{\lambda = \frac{\hbar}{p}}$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \quad \psi(x) = \sin\left(\frac{px}{\hbar}\right)$$



$$\int |\psi(x)|^2 dx = N$$

$$\int_{-P}^P p(x) dx = \infty \quad \psi_2(x) = \frac{\psi_1(x)}{\sqrt{N}}$$

$$\frac{1}{\sqrt{N}} = \text{---}$$

de Broglie waves



- Do de Broglie waves arise in wave-functions?
- Yes - they do!
- In 1-d, in free space, a particle with exact momentum p would have a wave-function:

de Broglie waves



- Do de Broglie waves arise in wave-functions?
- Yes - they do!
- In 1-d, in free space, a particle with exact momentum \mathbf{p} would have a wave-function:

$$\psi(x) = e^{\frac{i p x}{\hbar}}$$

- This wave-function has **complex numbers**, so we won't study it this year!

de Broglie waves



- But there is a **very similar** wave-function we can study.

$$\psi(x) = \sin(px/\hbar)$$

- This has **many** of the same features as the **de Broglie wave-function**.
- Let's check its wavelength:

de Broglie waves



- But there is a **very similar** wave-function we can study.

$$\psi(x) = \sin(px/\hbar)$$

- This has **many** of the same features as the **de Broglie wave-function**.
- Let's check its wavelength:

Hand-written Calculations

de Broglie waves



$$\psi(x) = \sin(px/\hbar)$$

- The wave-function has wave-length

$$\lambda = \frac{h}{p}$$

- It has energy

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

as we shall see in the next chapter.

de Broglie waves



$$\psi(x) = \sin(px/\hbar)$$

- Is this wave-function **normalised?**

Hand-written Calculations

de Broglie waves



$$\psi(x) = \sin(px/\hbar)$$

- Is this wave-function **normalised?**
- Since

$$\int_{-\infty}^{\infty} \sin^2(px/\hbar) dx$$

diverges (is infinite), not only is this not normalised, it **cannot** be normalised!

$$\frac{''1''}{\sqrt{\infty}} = 0$$

de Broglie waves



$$\psi(x) = \sin(px/\hbar)$$

- The **same** is true of the **complex de Broglie wave**.

$$\psi(x) = e^{\frac{ipx}{\hbar}}$$

- This function also **cannot** be **normalised**.
- What is the problem? Are these wavefunctions **physical**?

Heisenberg's Uncertainty Relation



Werner
Heisenberg

- In 1927, Heisenberg proposed his **uncertainty relation** (uncertainty principle).

$$\Delta x \Delta p \gtrsim \frac{\hbar}{2}$$

- Where
 - Δx represents uncertainty in position
 - Δp represents uncertainty in momentum

Uncertainty

- We quantify **uncertainty** in terms of the **standard deviation**.

Poll

- Have you studied the standard deviation before?
 - 1. Yes
 - 2. No

Uncertainty

- We quantify **uncertainty** in terms of the **standard deviation**.
- It is defined in terms of expectation values:

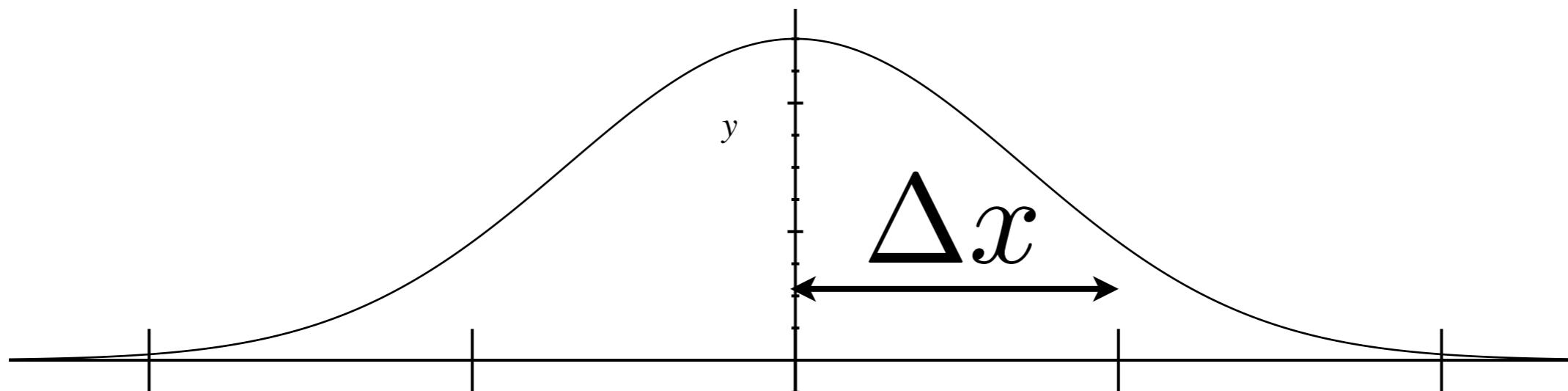
$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

- where

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx$$

Uncertainty

- The standard deviation quantifies the **breadth** of a probability distribution.
- E.g. For a **Gaussian** distribution.



Heisenberg's Uncertainty Relation



Werner
Heisenberg

- The **uncertainty relation** places limits on the uncertainty in **position** and **momentum**.

$$\Delta x \Delta p \gtrsim \frac{\hbar}{2}$$

- Where
 - Δx represents uncertainty in position
 - Δp represents uncertainty in momentum

de Broglie waves



$$\psi(x) = \sin(px/\hbar)$$

$$\psi(x) = e^{\frac{ipx}{\hbar}}$$

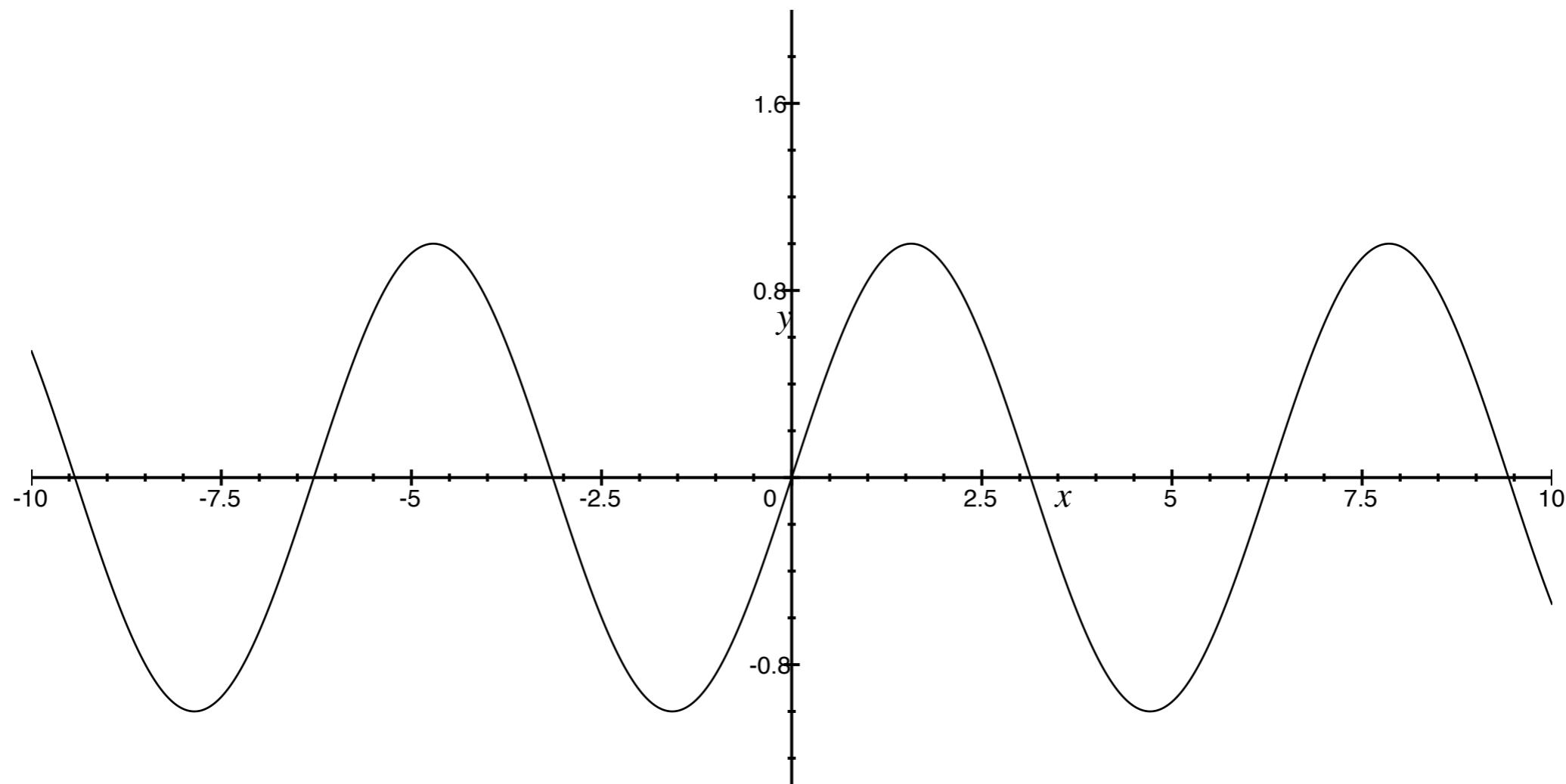
- The de Broglie waves represent a particle with **exact** momentum p .
- Exact momentum = **zero** uncertainty.
- This **violates** Heisenberg's relation.
- And is why such wavefunctions cannot be **normalised**, they are **not physical wavefunctions**.

$$\Delta x \Delta p \gtrsim \frac{\hbar}{2}$$

Wave-packets

- What happens when we add waves with different wave-lengths together?

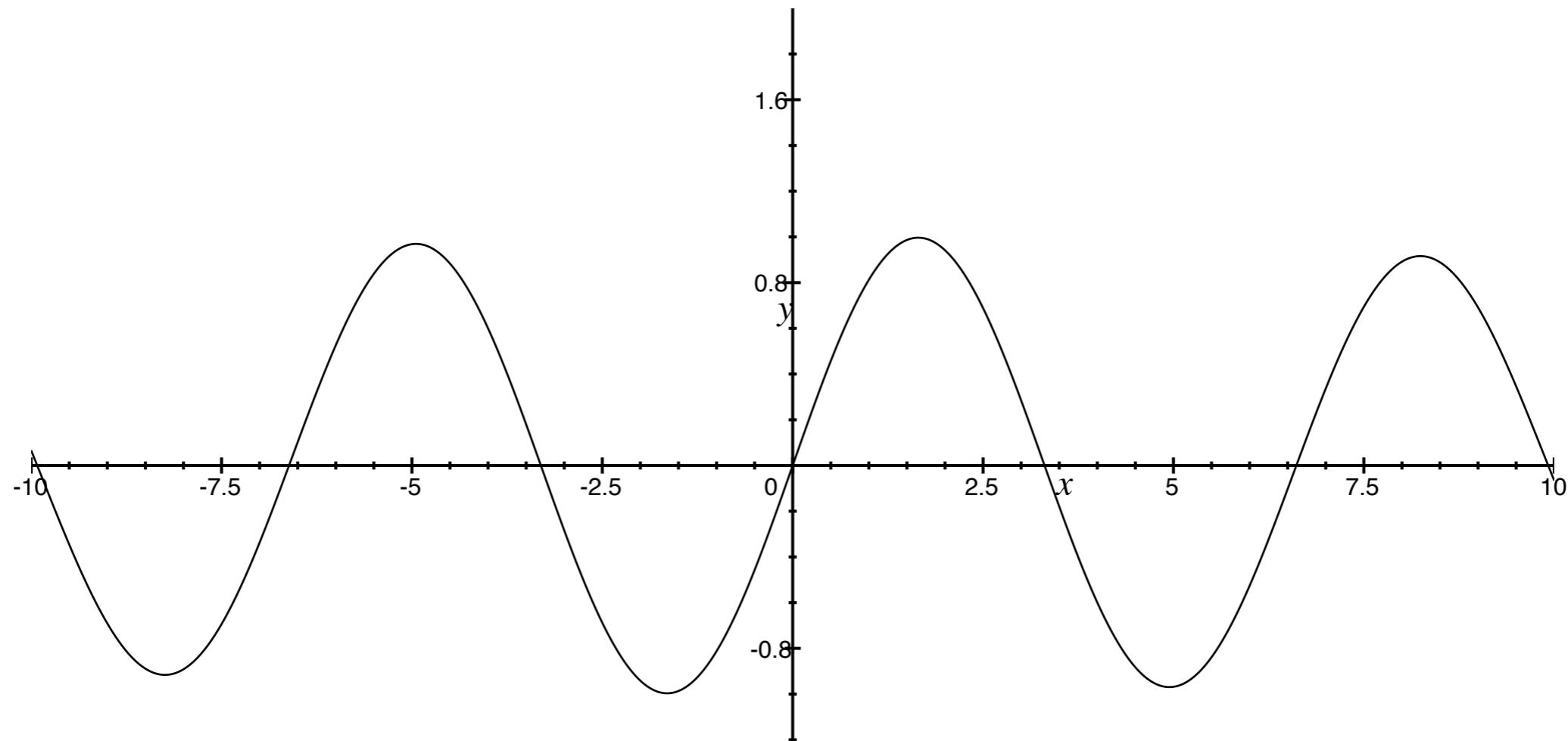
$$\sin(x)$$



Wave-packets

- What happens when we add waves with different wave-lengths together?

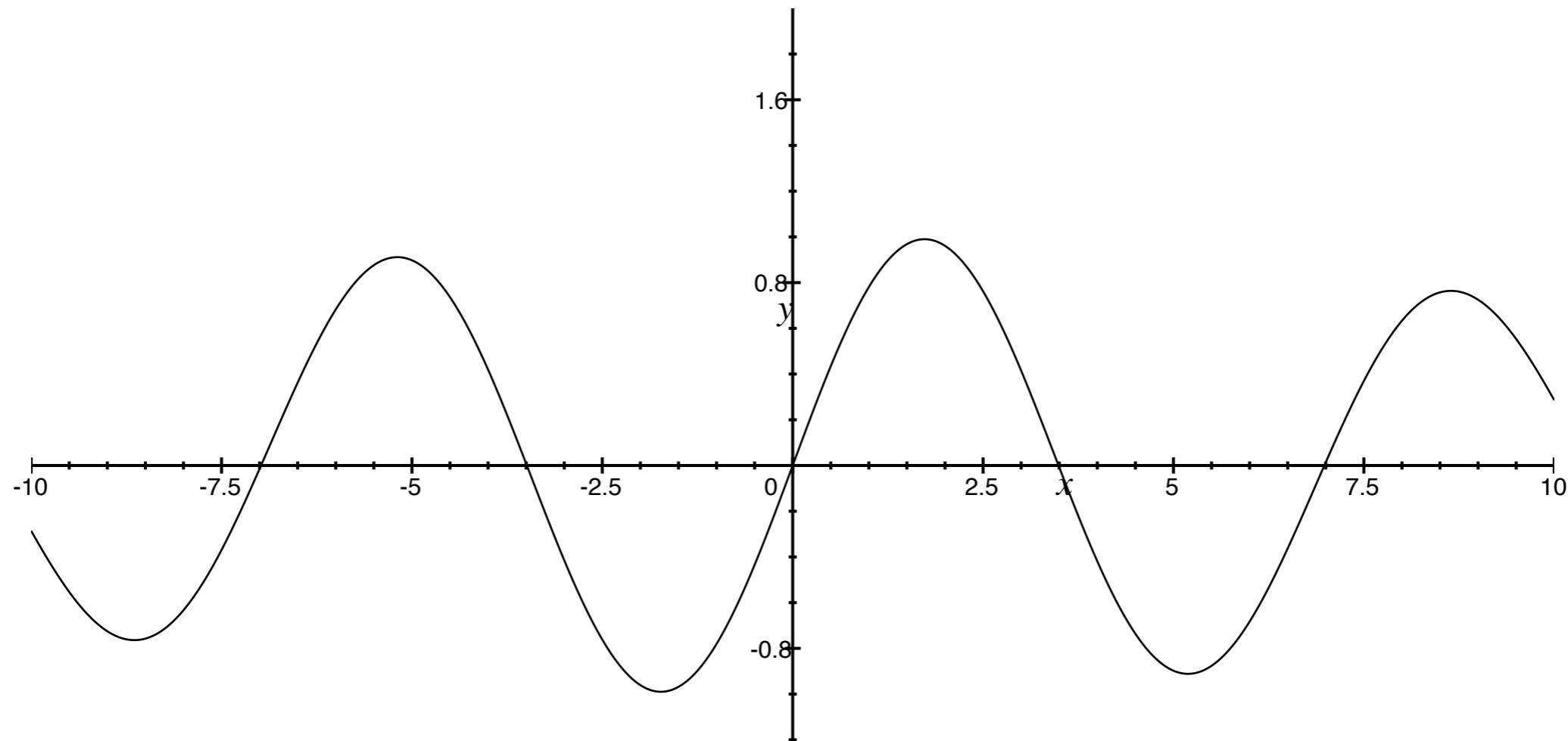
$$\frac{\sin(x) + \sin(0.9x)}{2}$$



Wave-packets

- What happens when we add waves with different wave-lengths together?

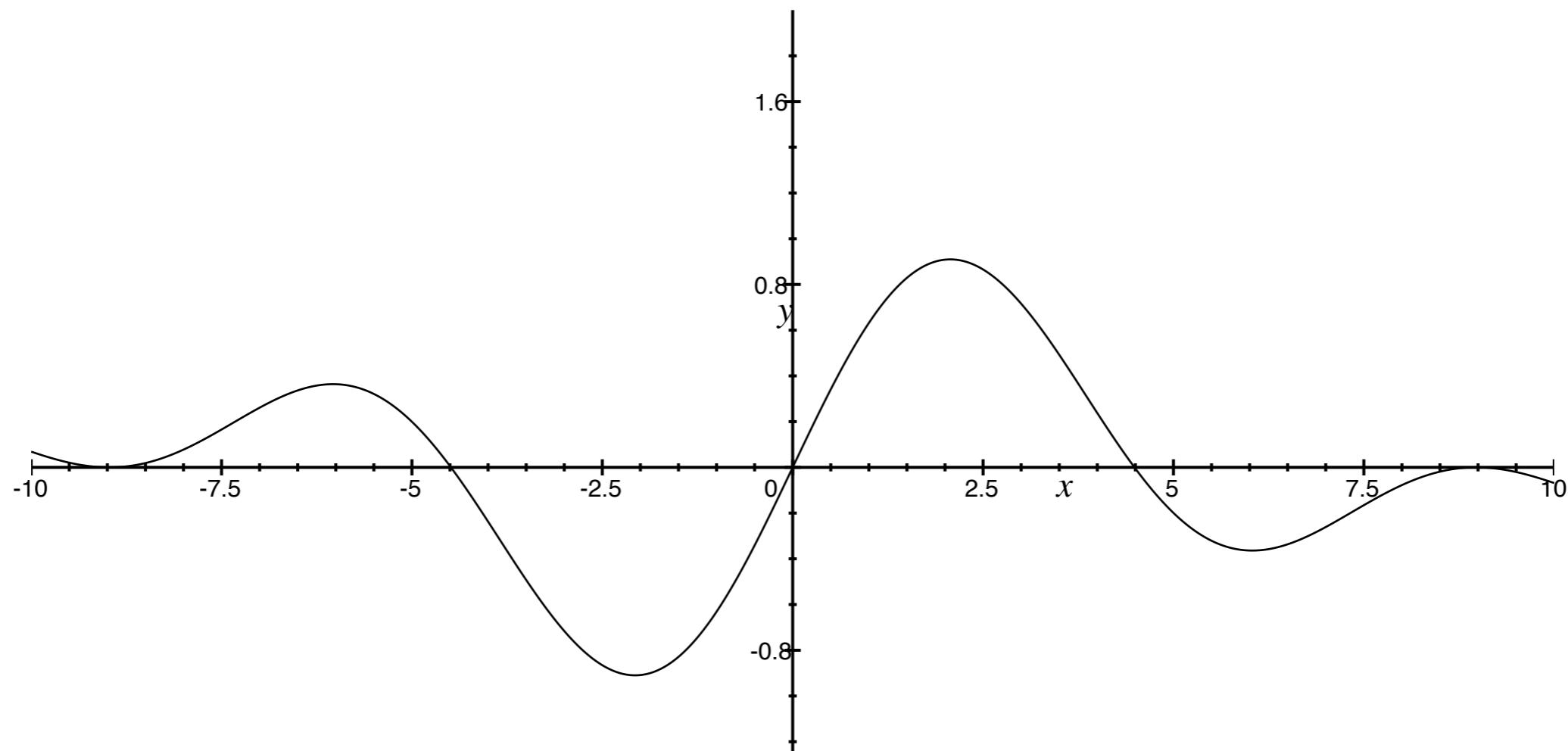
$$\frac{\sin(x) + \sin(0.9x) + \sin(0.8x)}{3}$$



Wave-packets

- What happens when we add waves with different wave-lengths together?

$$\frac{\sin(x) + \sin(0.9x) + \sin(0.8x) + \sin(0.7x) + \sin(0.6x) + \sin(0.5x) + \sin(0.4x)}{7}$$



Wave-packets

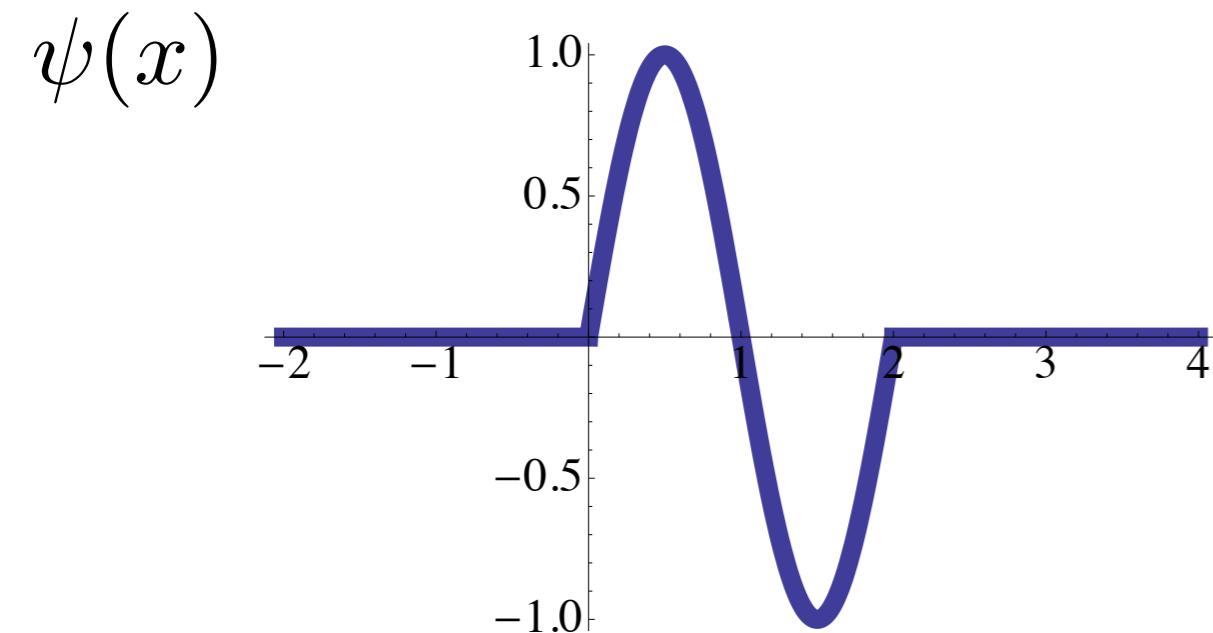
- A **wave-packet** is a collection of waves of **different frequencies, localised in space**.
- As **more and more wavelengths** are added, the wavepacket becomes more **localised**.
- More **wavelengths** = more different values of **momentum**.
- Increasing the spread of momentum is decreasing the spread of position.

$$\Delta x \Delta p \gtrsim \frac{\hbar}{2}$$

- Heisenberg's principle in action!

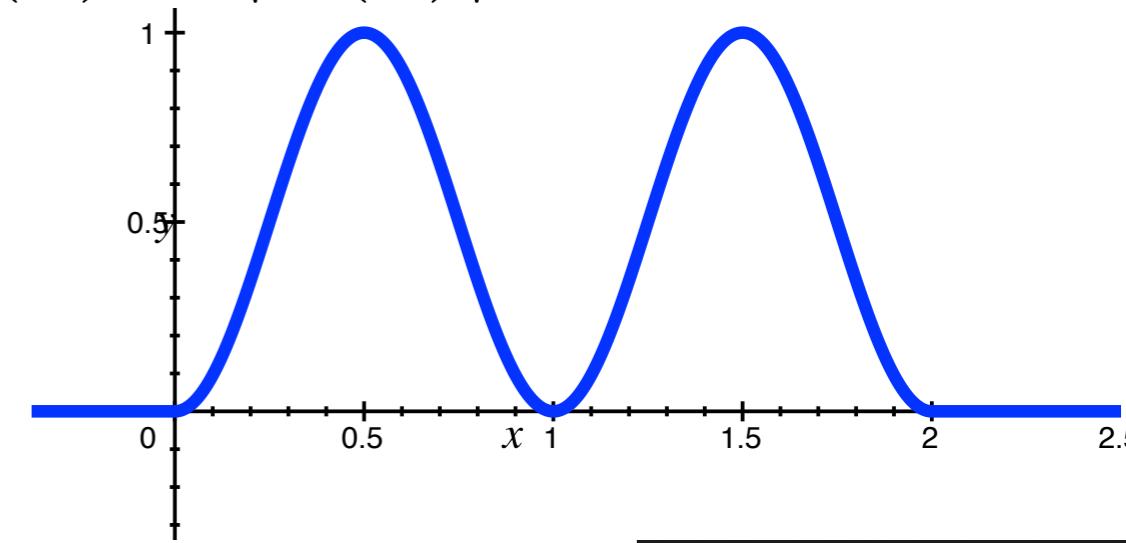
Why the wave function?

- So far, we have done nothing with the wave function other than **calculate probabilities**.
- So why use wave functions at all?
- Why not just work with **probabilities**?
- We need **negative values** to achieve **destructive interference**!



$$\rho(x) = |\psi(x)|^2$$

VS



Evolution in time



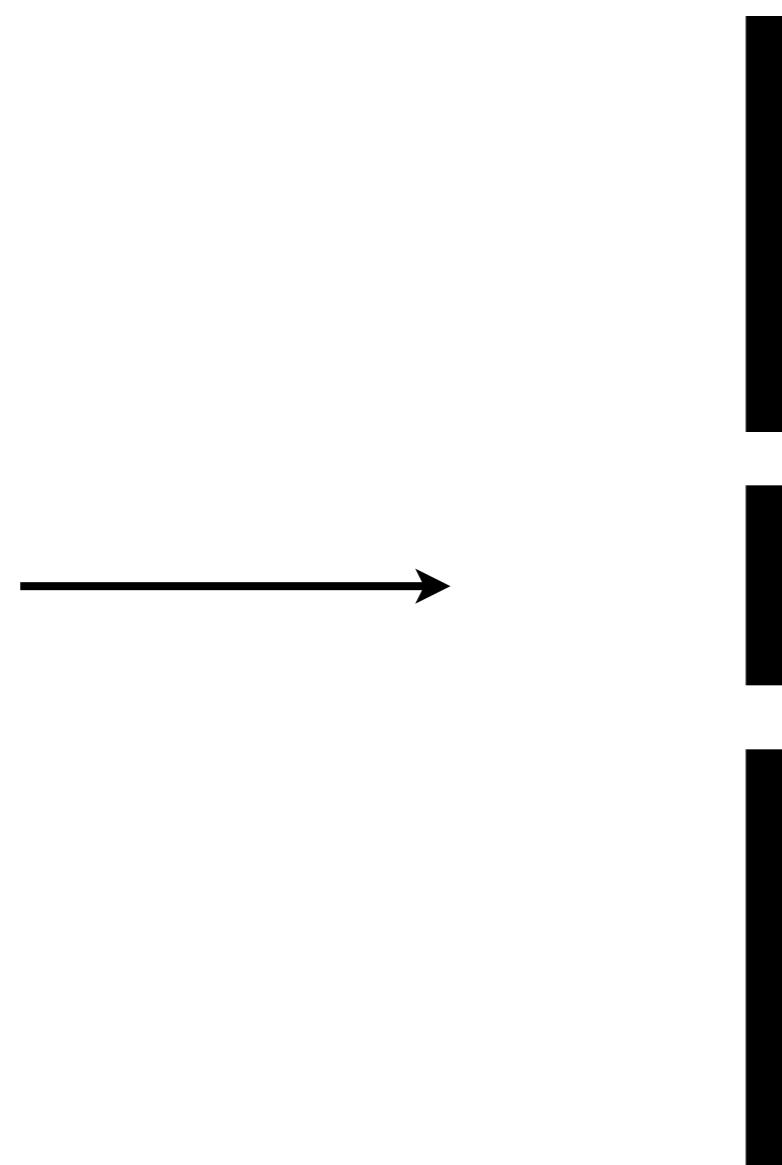
- When not being measured, wave-functions evolve in time according to the **Time Dependent Schrödinger Equation.**

Erwin
Schrödinger

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

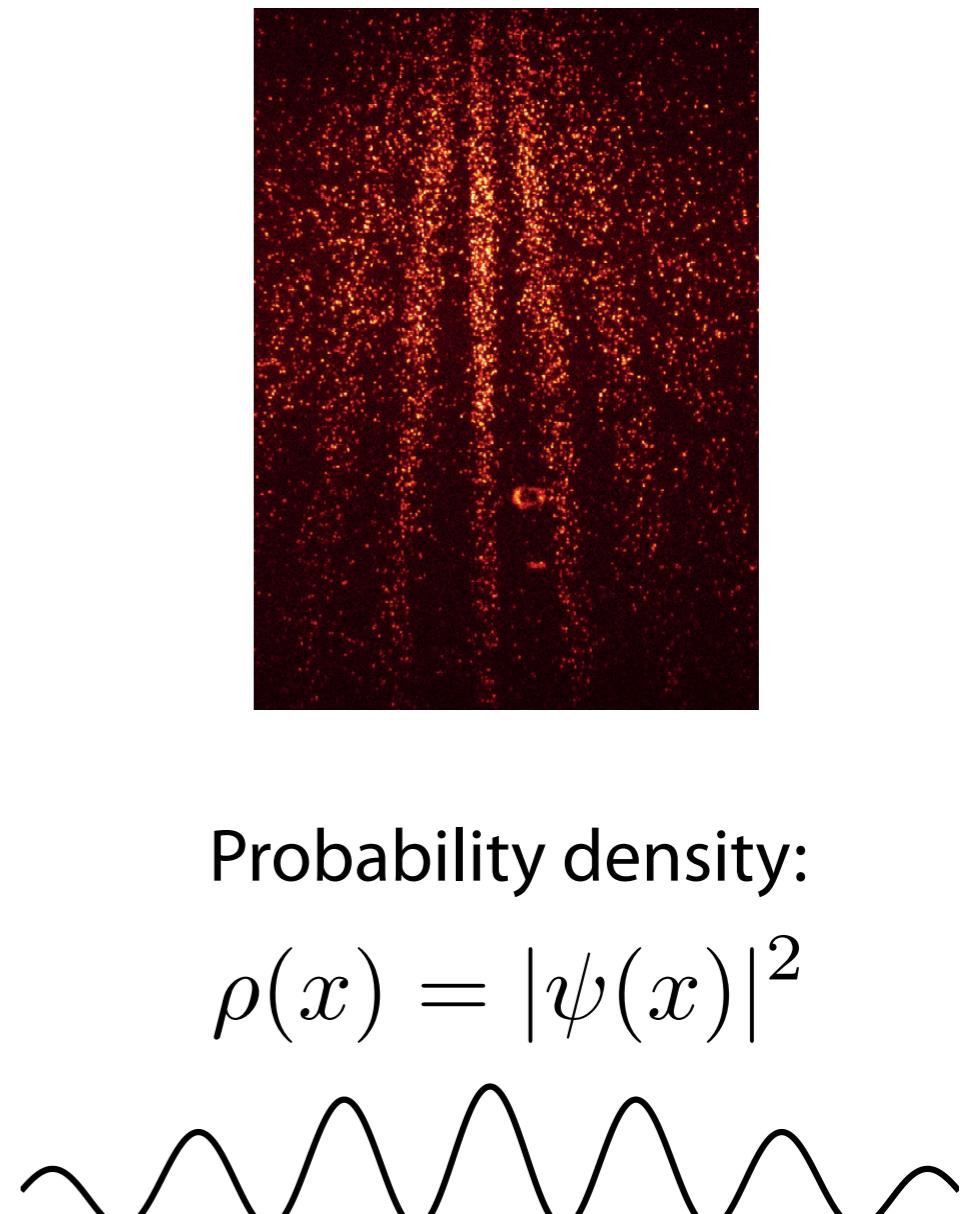
- We will **not** study this in this course! (2nd year)
- It is **similar** to the equation followed by **classical waves** (e.g water), but with some important differences.
 - E.g. It contains the **complex number i** ($i = \sqrt{(-1)}$)
 - For the purposes of this course, it suffices to think of the wave function “**evolving like a wave**”.

Double-slit experiment



Wave-function
evolves
“as a wave”

Experiences
wave
interference



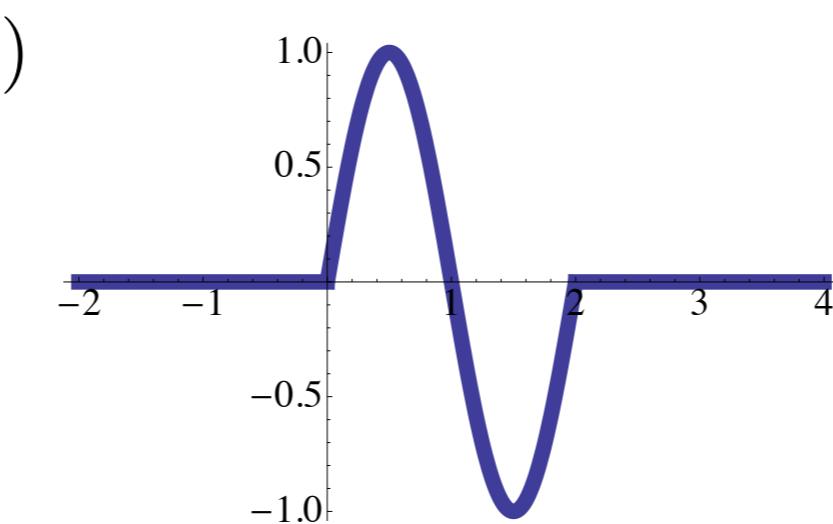
Probability density:

$$\rho(x) = |\psi(x)|^2$$

Clicks on screen
follow Born rule.

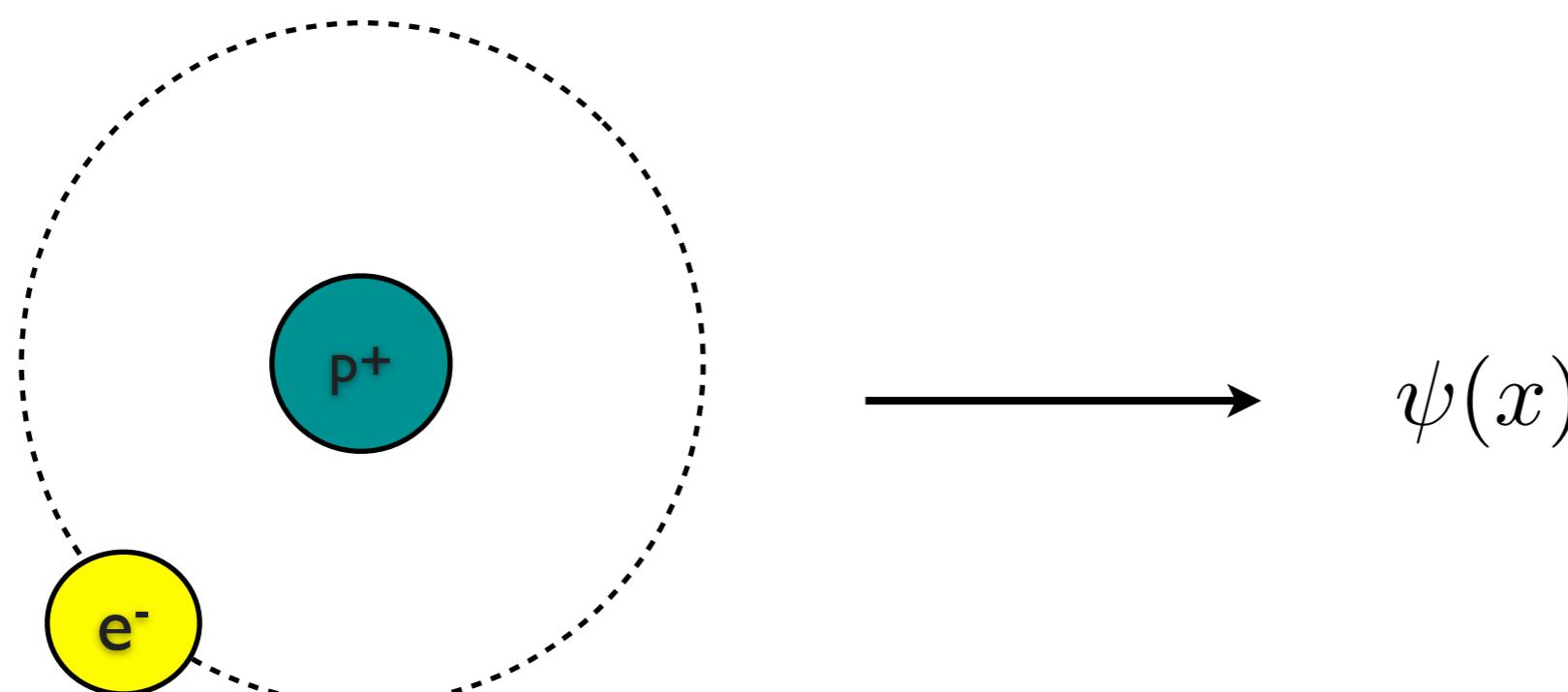
Importance of $\psi(x)$

- Quantum particles **do not** have a “position” in a classical sense.
- Instead, they have a **wave-function**, from which probabilities of position can be computed from the Born rule.
- In quantum mechanics, we don’t ask
 - what is the position of a particle?
 - what is its orbit (e.g. Bohr model)?
- To **characterise** a particles position and motion, we must determine its **wave-function**.



Towards a quantum atomic model

- We wish to construct a **quantum model** of the atom.
- This means, for example, in a **Hydrogen atom**, we wish to identify the allowed **wave-functions** of the electron.
- The **wave-function** of the electron which will replace the **orbit** of the Bohr model.
- To calculate this - we need to study **Energy in Quantum Mechanics**.
- The theme of **Part 5** of this course.



Summary of Part 4

- We revised **probability** for discrete variables and introduced **probability density** for **continuous variables**.
- We introduced the wave-function, studied its properties, and the **Born rule** for calculating **probabilities**.
- We saw how the combination of **wave evolution** with **Born rule** probabilities explains the double-slit experiment with particles.
- We explored **de Broglie** waves, and saw that the **Heisenberg uncertainty principle** forbids particles from having a perfectly defined momentum.

