Attendance Monitoring

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PHAS1202 16th October 2017:

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

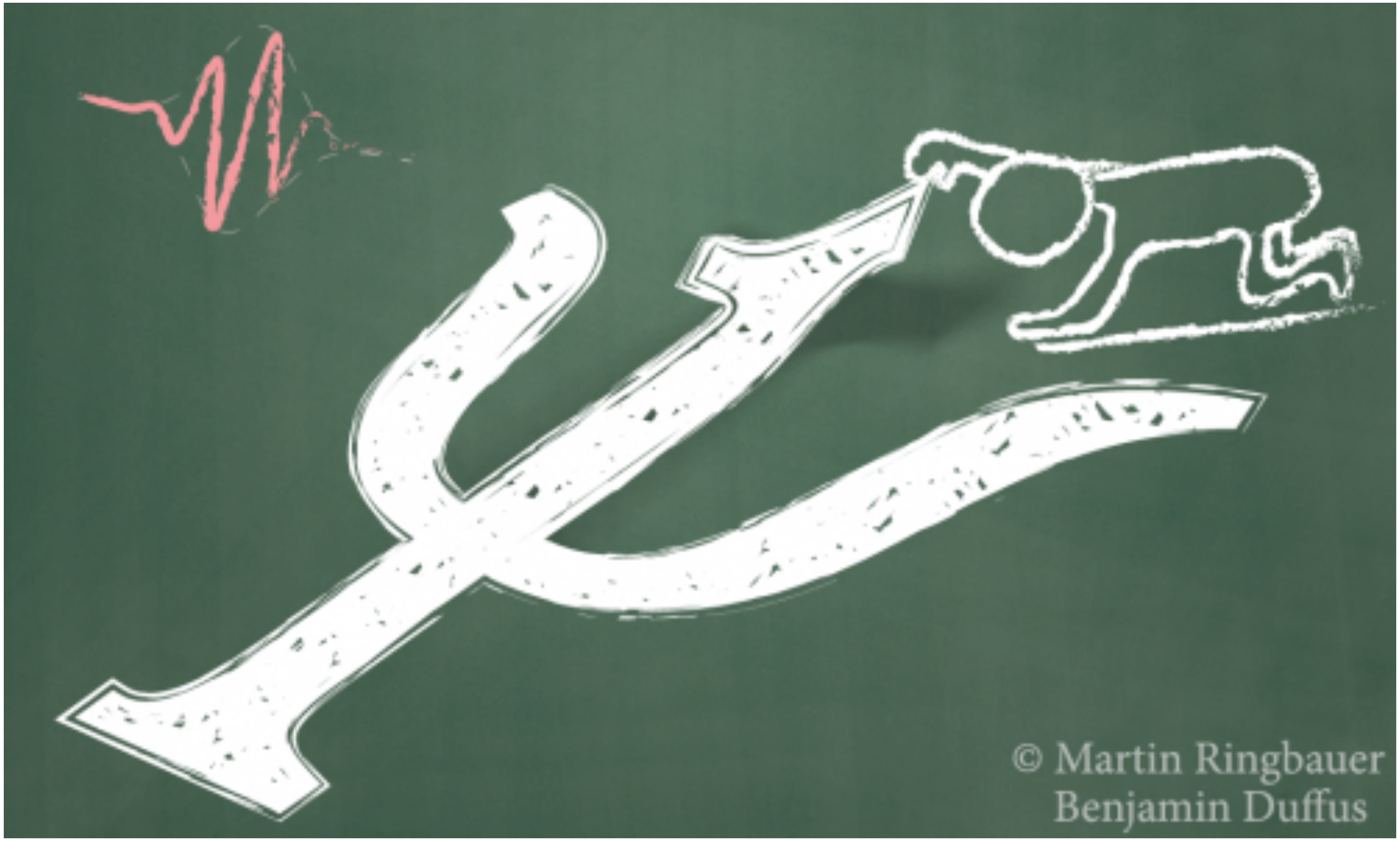


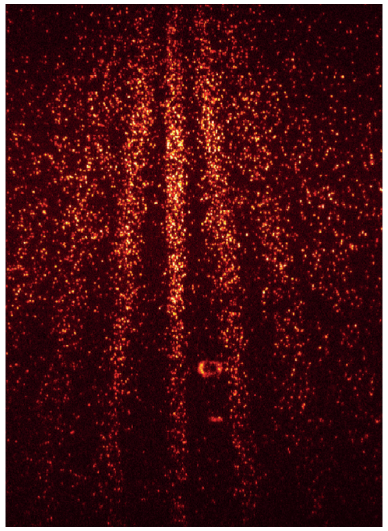
Image from: http://phys.org/news/2015-02-wavefunction-schroedinger-cat.html

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]

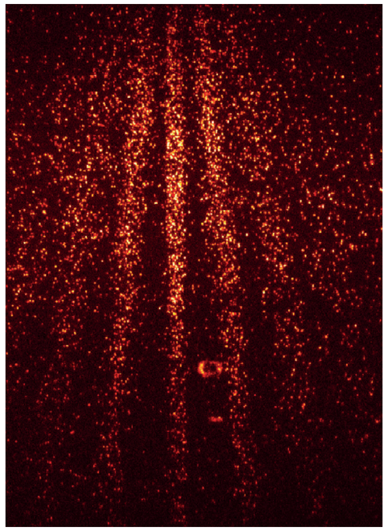
This lecture

- 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**
  - Introduction of the **wave-function**



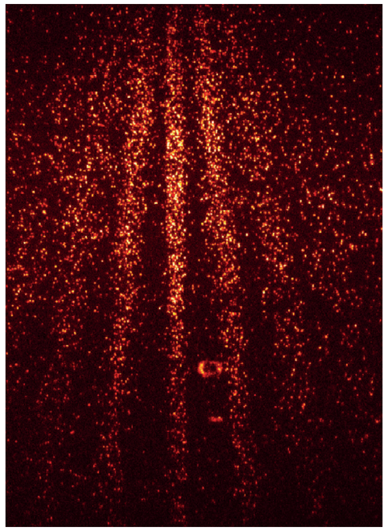
Elements of Quantum Mechanics

– 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**.

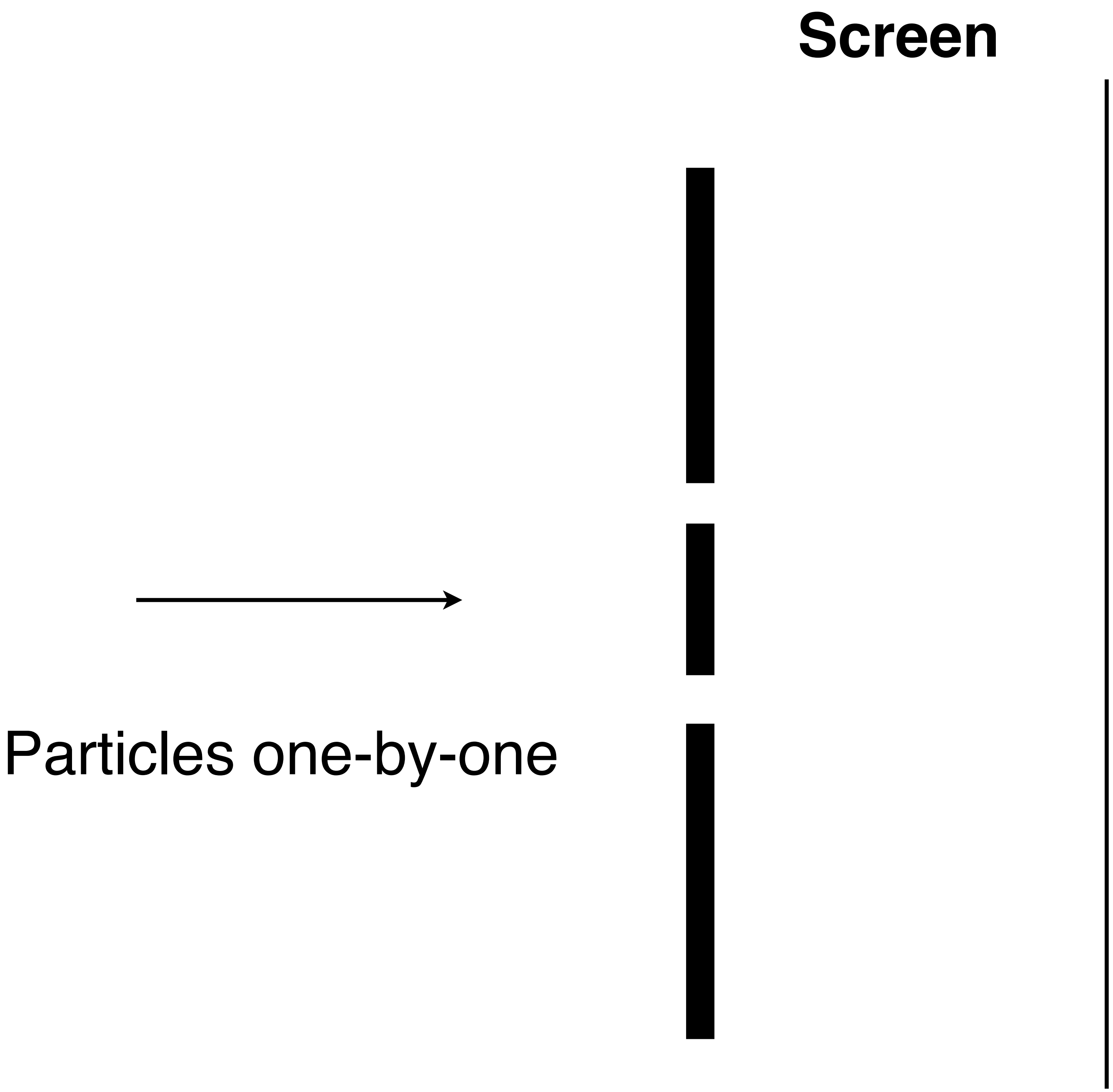


In Part 4, we will:

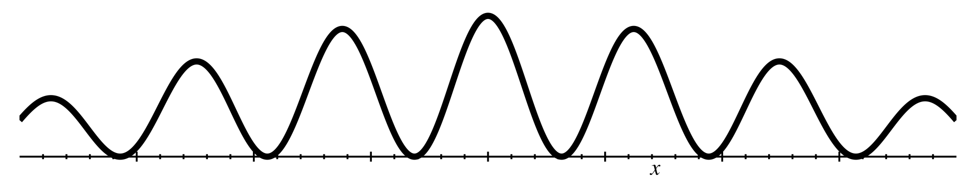
- Briefly revise the **wave-particle duality** in the **double slit** experiment.
  - And consider what happens if we **measure which slit** the particle travels through.
- Argue that to explain this we need **something** which incorporates
  - **wave-like** behaviour (**interference**)
  - **probabilities** (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**.

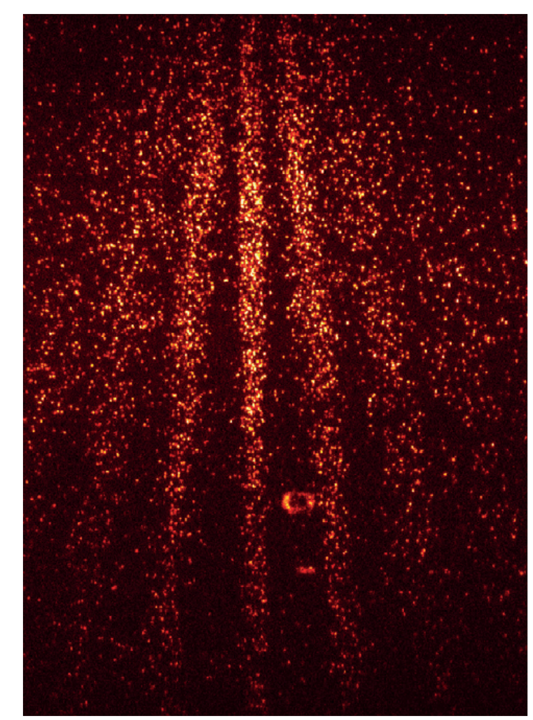
Double-slit experiment

–**Jönsson** (1961): **Electrons**



One-by-one, random clicks build Interference Pattern

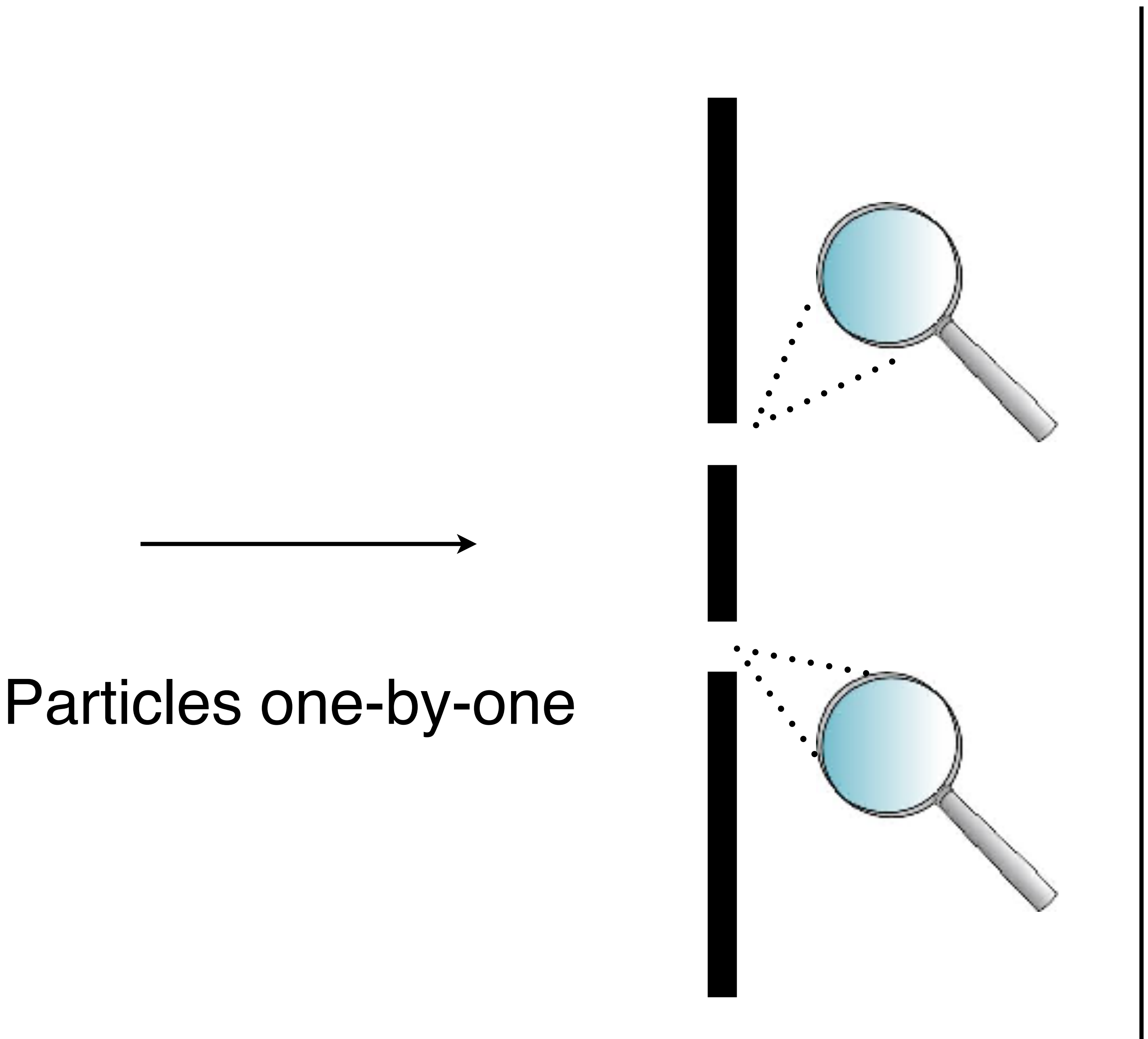




Double-slit experiment

- **Jönsson** (1961): **Electrons**

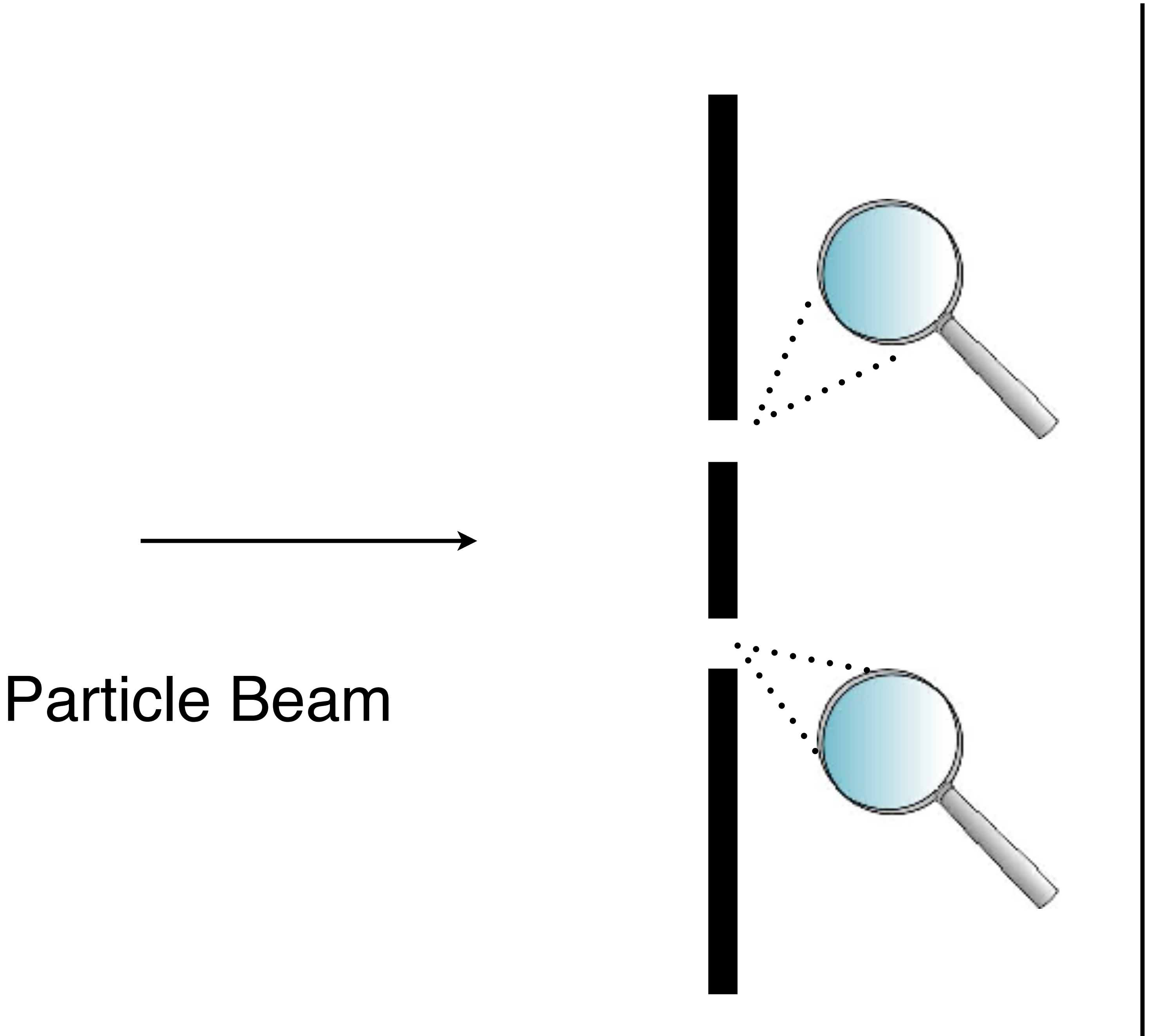
- Does particle go through both slits?
- What happens if we measure?



Quiz?

–**Jönsson** (1961): **Electrons**

- Will we see:

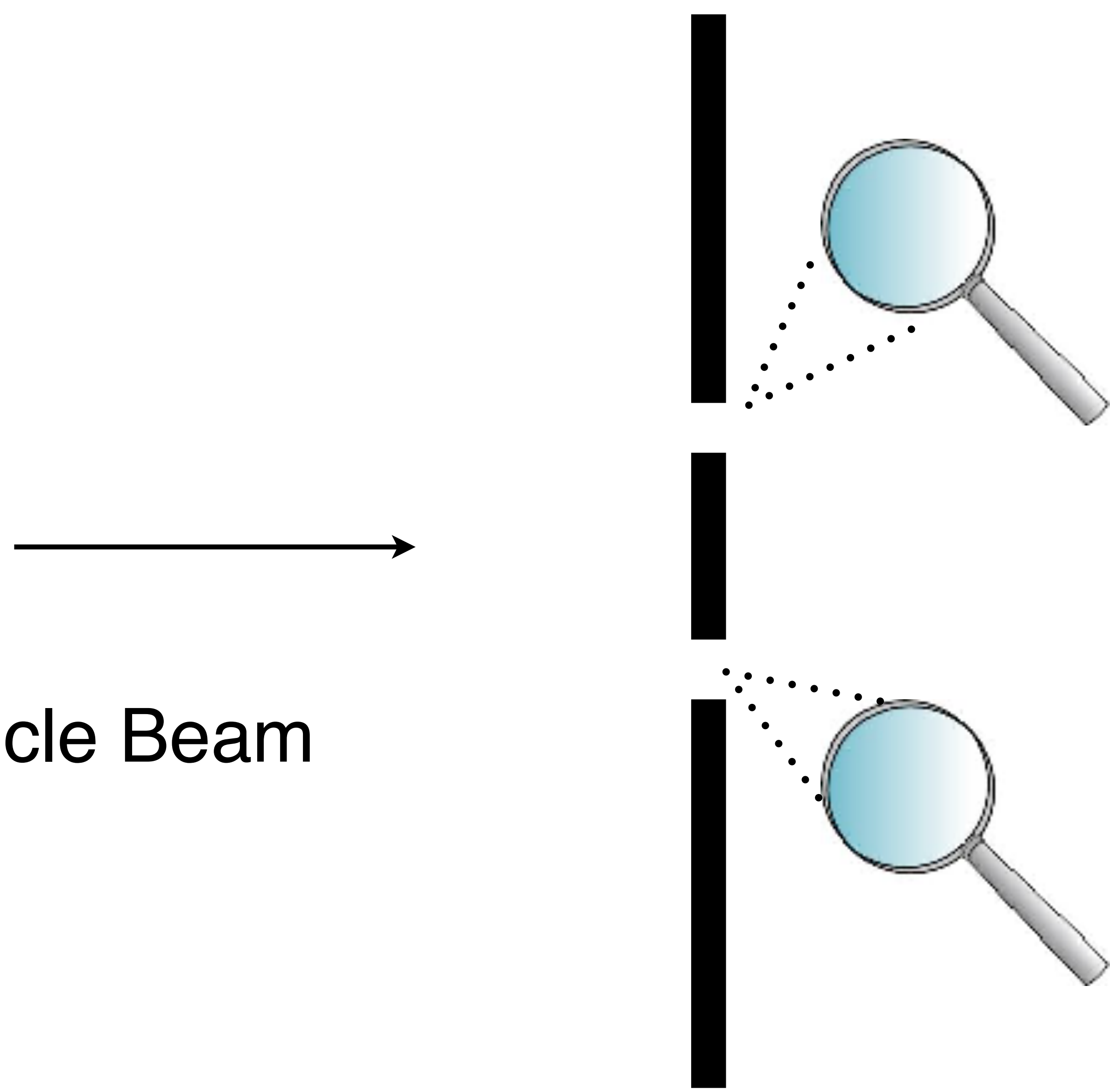


- 1. Particles in **both** slits?
- 2. Particle in just **one** slit?
- 3. Something else?

Double-slit experiment

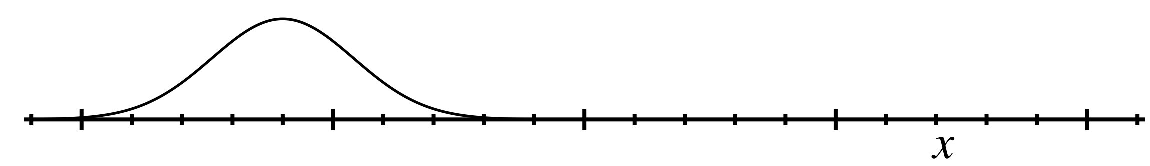
−**Jönsson** (1961): **Electrons**

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

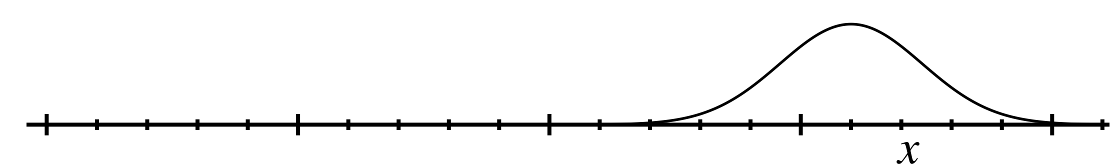


Particle Beam

Particle seen in **left** slit



Particle seen in **right** slit

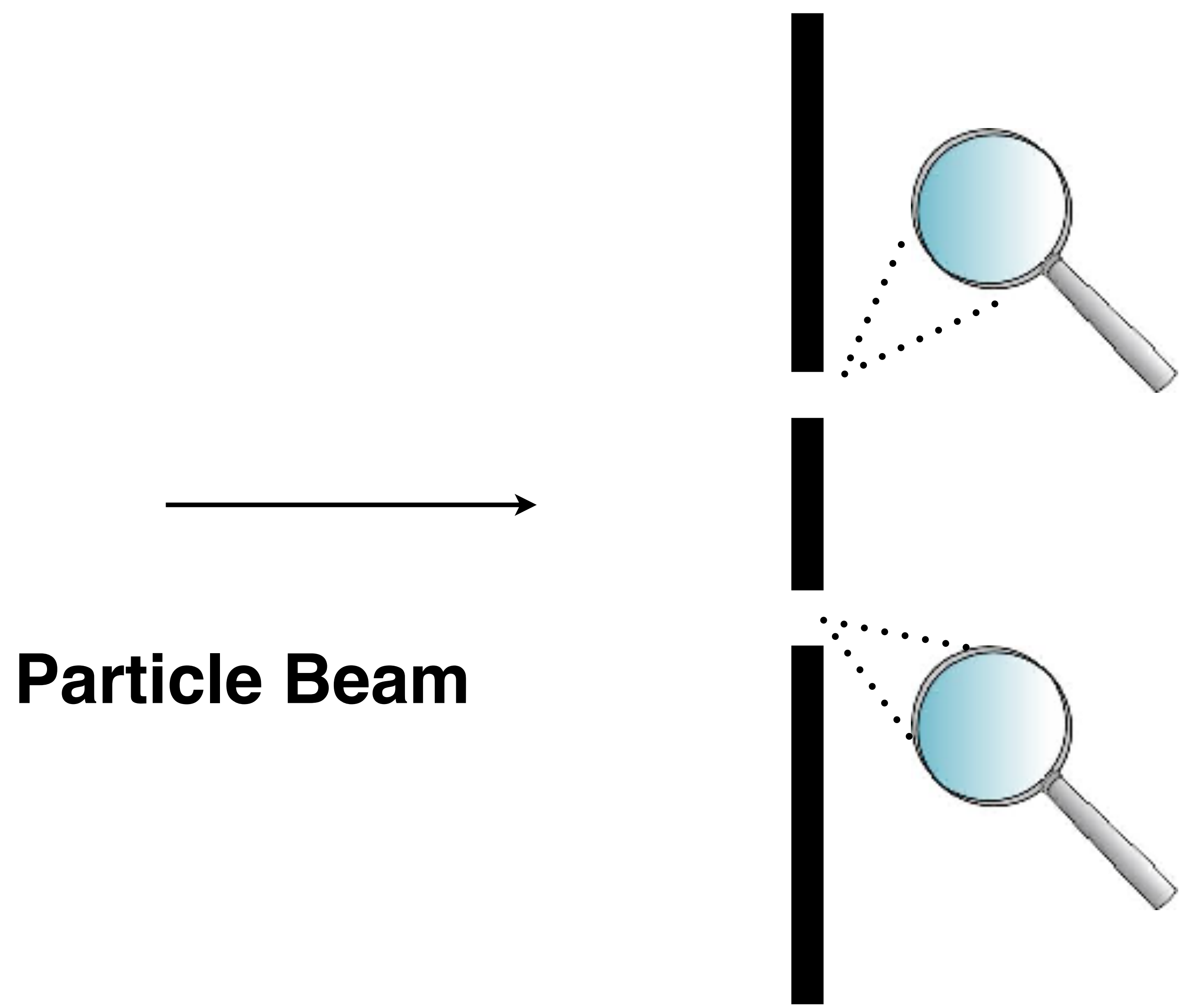


No interference fringes

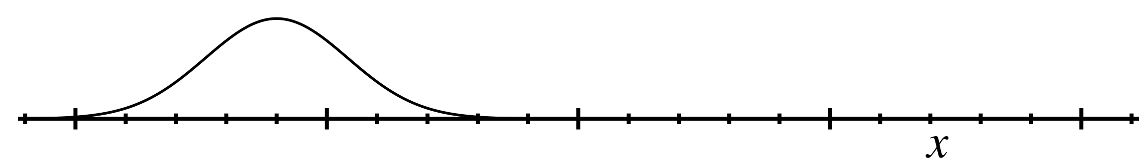
Double-slit experiment

– **Jönsson** (1961): **Electrons**

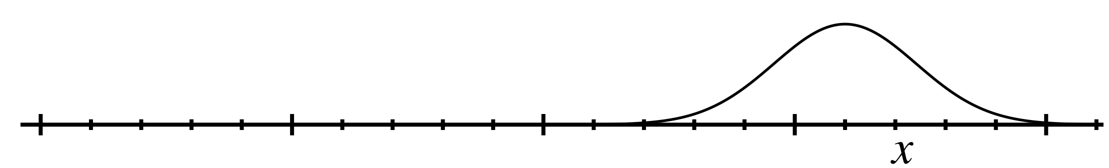
- Measuring **which-path** destroys the interference.



Particle seen in **left** slit



Particle seen in **right** slit

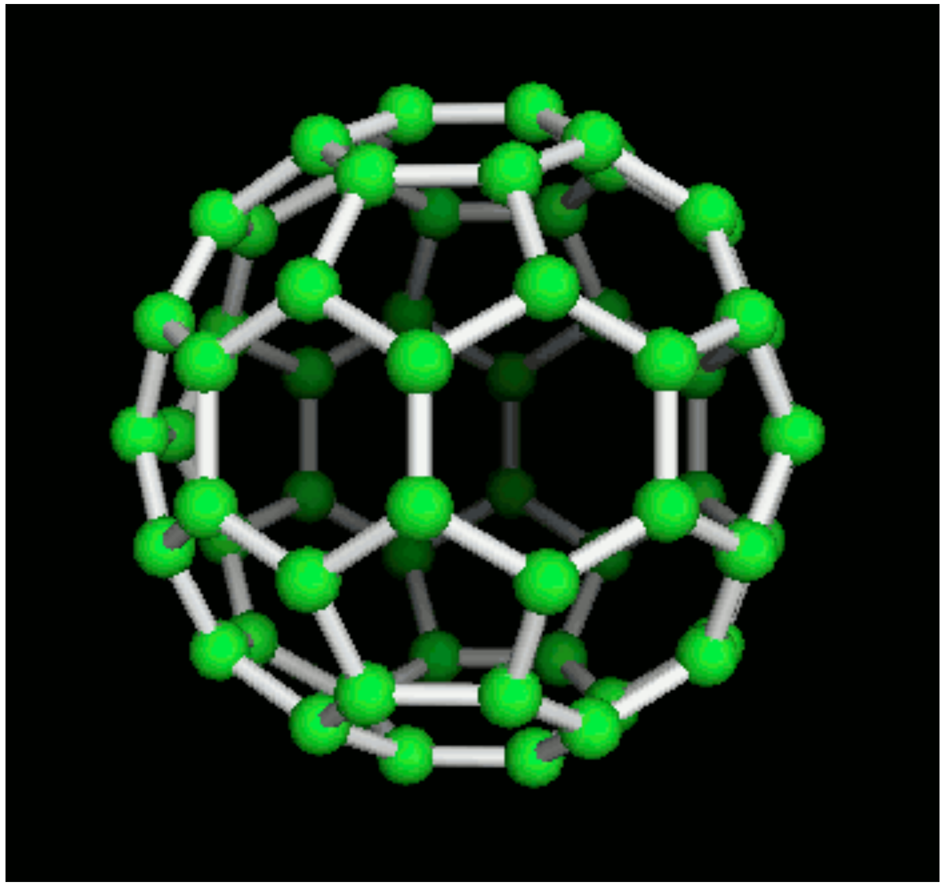


No interference fringes

Double-slit experiment

– **Jönsson** (1961): **Electrons**

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



- Carbon-60
- 60 atoms of carbon in a "football"-shaped molecule

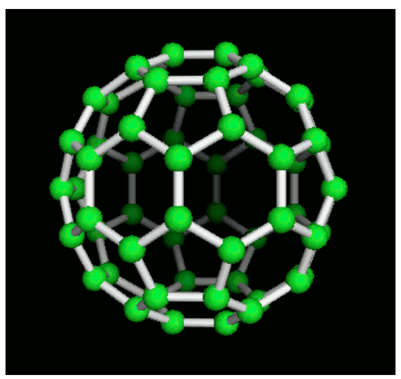
- If heated, C-60 molecules glow like a black body.

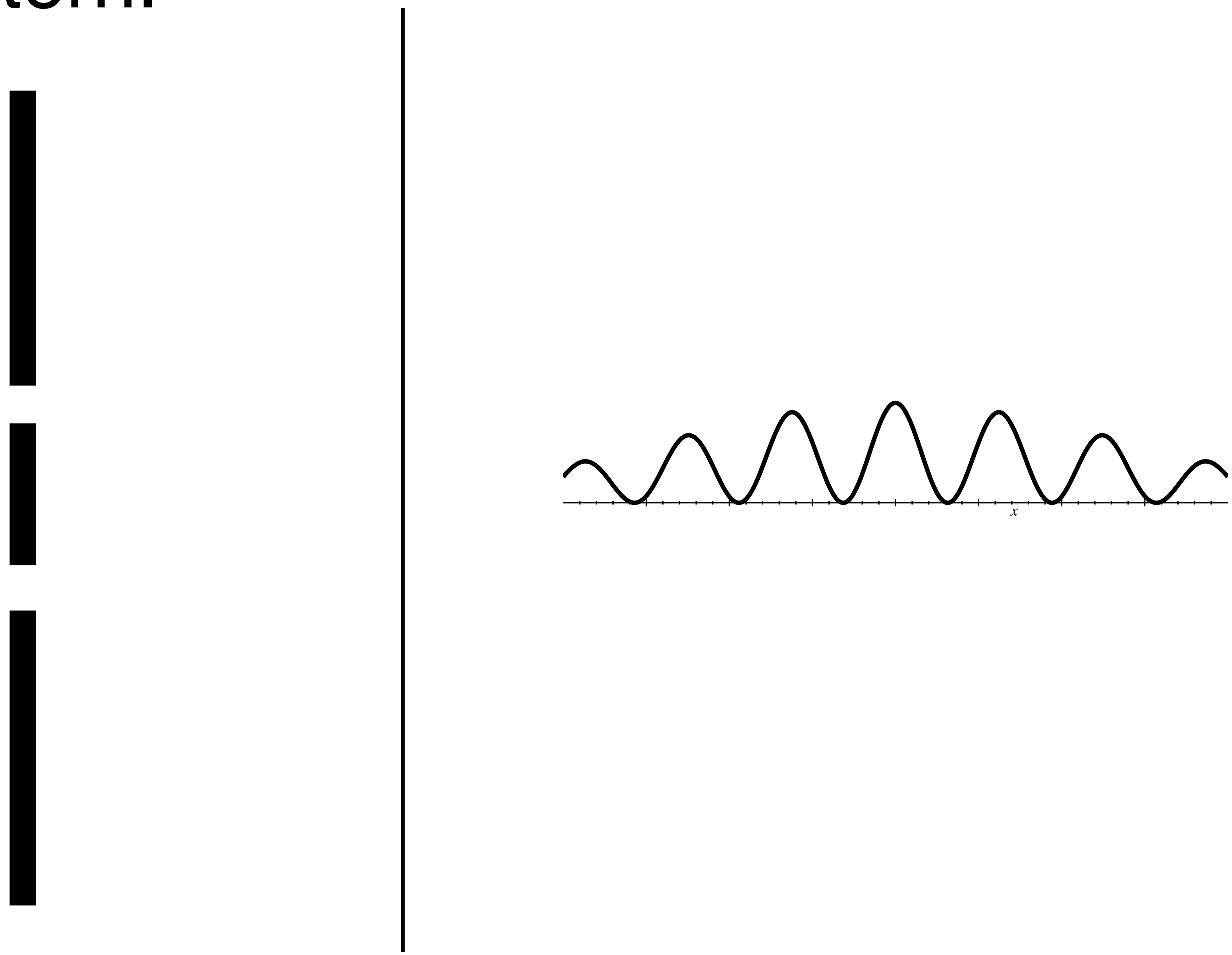
- Experiment (M. Arndt) performed in 1999.

Double-slit experiment

– **Jönsson** (1961): **Electrons**

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





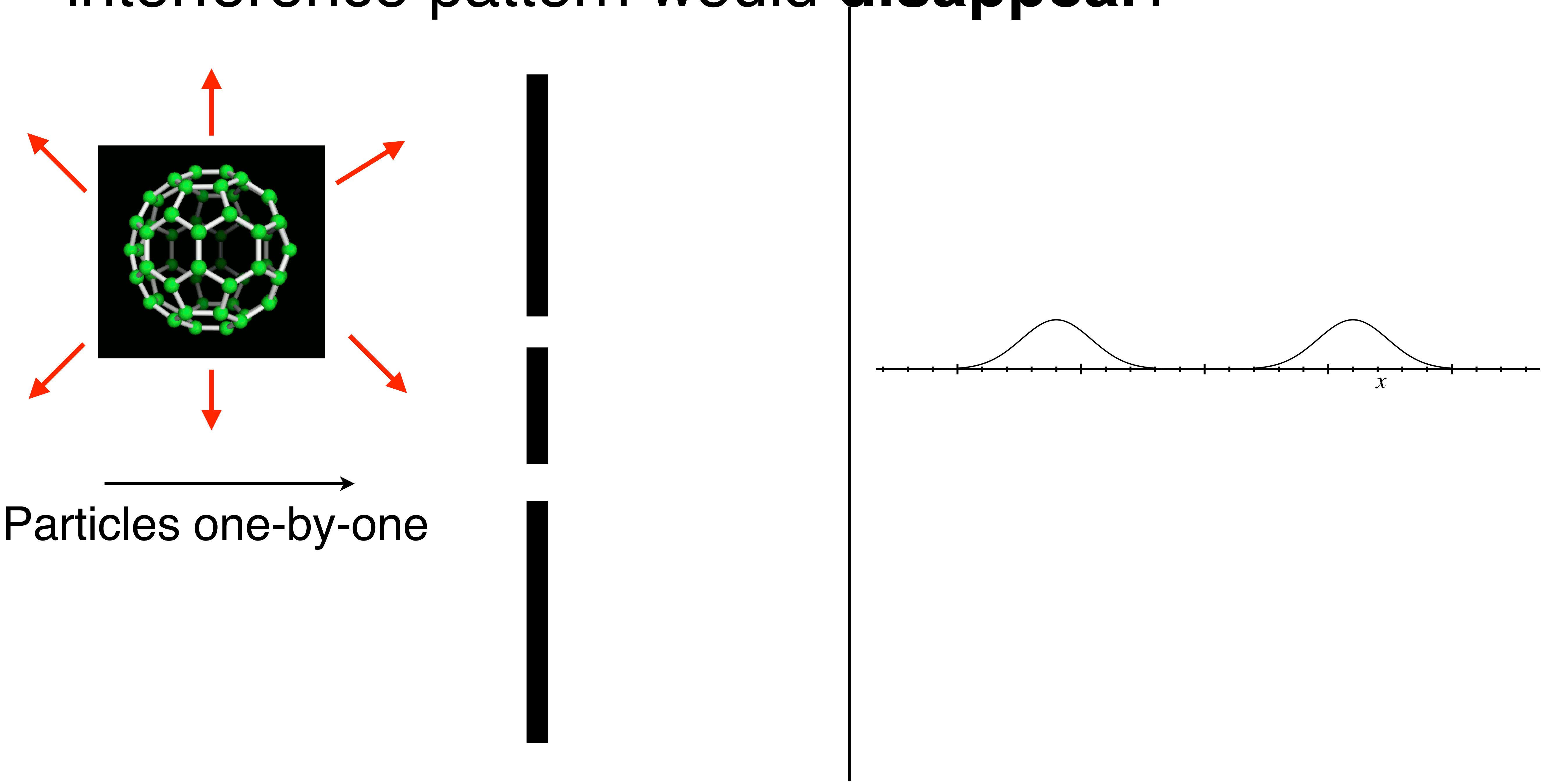
Particles one-by-one

Markus Arndt, et al., Nature (1999)

Double-slit experiment

– **Jönsson** (1961): **Electrons**

- With **hot** bucky balls the double slit interference pattern would **disappear**!



Markus Arndt, et al., Nature (1999)

Double-slit experiment

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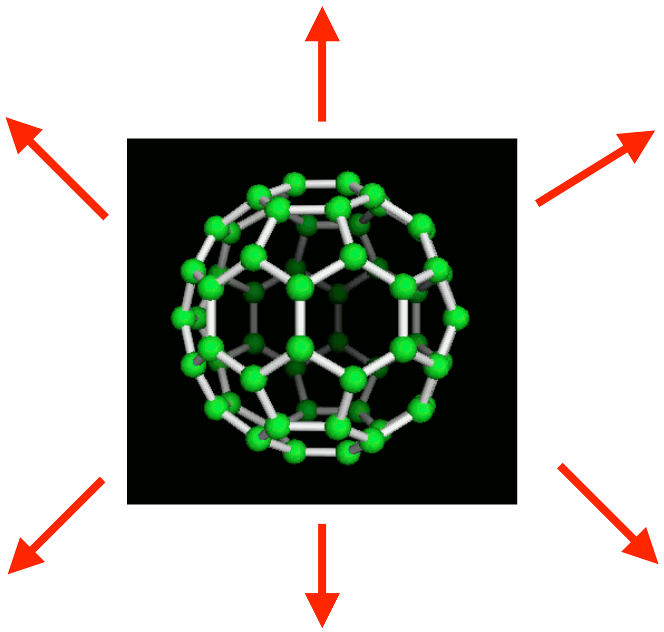
– **Jönsson** (1961): **Electrons**

- With **hot** bucky balls the double slit interference pattern would **disappear**!



- The hot bucky balls **emit** light, so you could "**see**" which slit they travelled through.
- The interference pattern is 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".

Markus Arndt, et al., Nature (1999)

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

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

Heads

Tails

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%**

Heads

Tails

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
  Tails: 0.5
– Monday: 1/7
  Tuesday: 1/7
  Wednesday: 1/7
  Thursday: 1/7
  Friday: 1/7
  Saturday: 1/7
  Sunday: 1/7

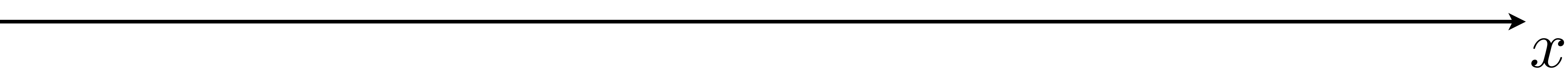
Probability for continuous values

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

heads	tails

Mon	Tue	Wed	Thu	Fri	Sat	Sun

- 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?

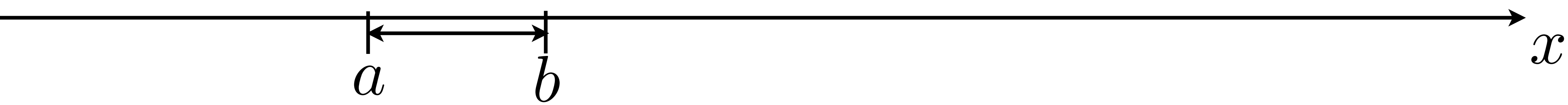
Resolution

- 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.



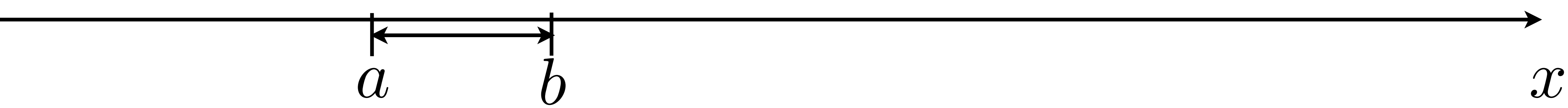
- We write:

$$\mathrm{Prob}(a \le x \le b) \;\; \textbf{:}$$

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**?



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

- **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.

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

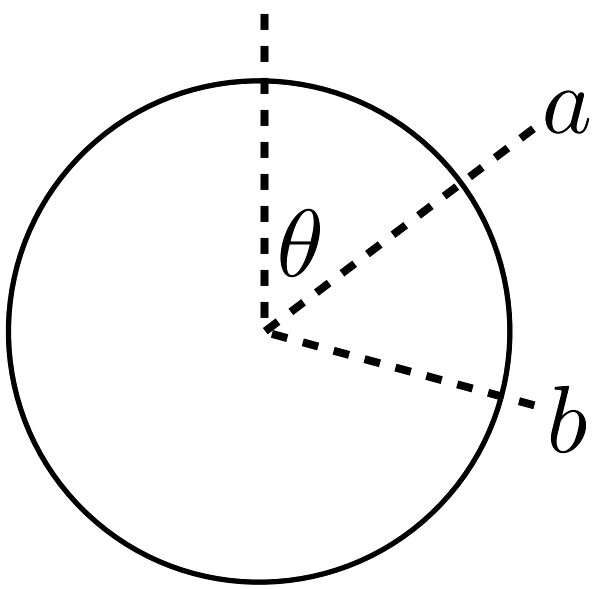
Normalisation

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

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

Examples

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

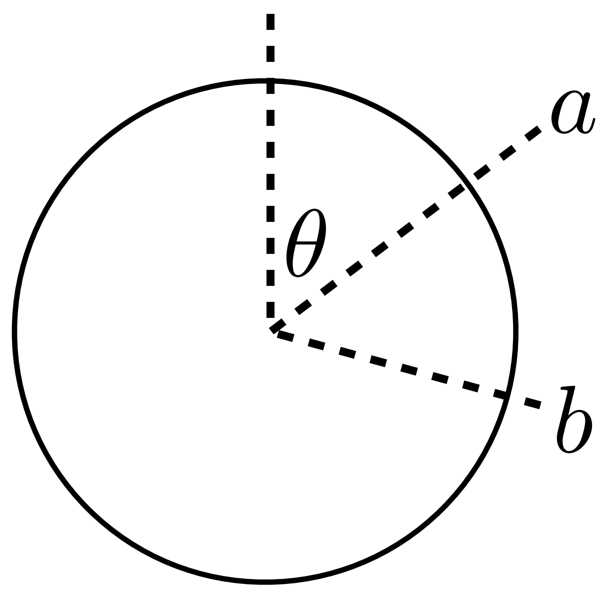


  – The probability of **theta** lying between ***a*** radians and ***b*** radians is

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

Examples

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



– The probability of **theta** lying between ***a*** radians and ***b*** radians is

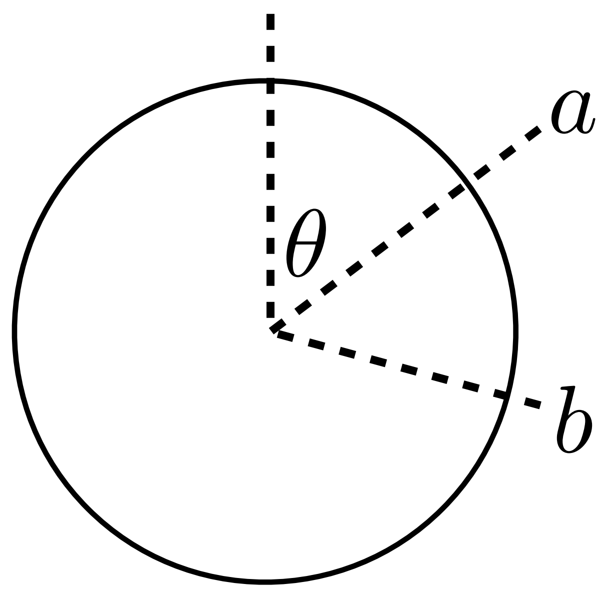
$$\mathrm{Prob}(a \leq \theta \leq b) = \frac{b-a}{2\pi}$$

– 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:

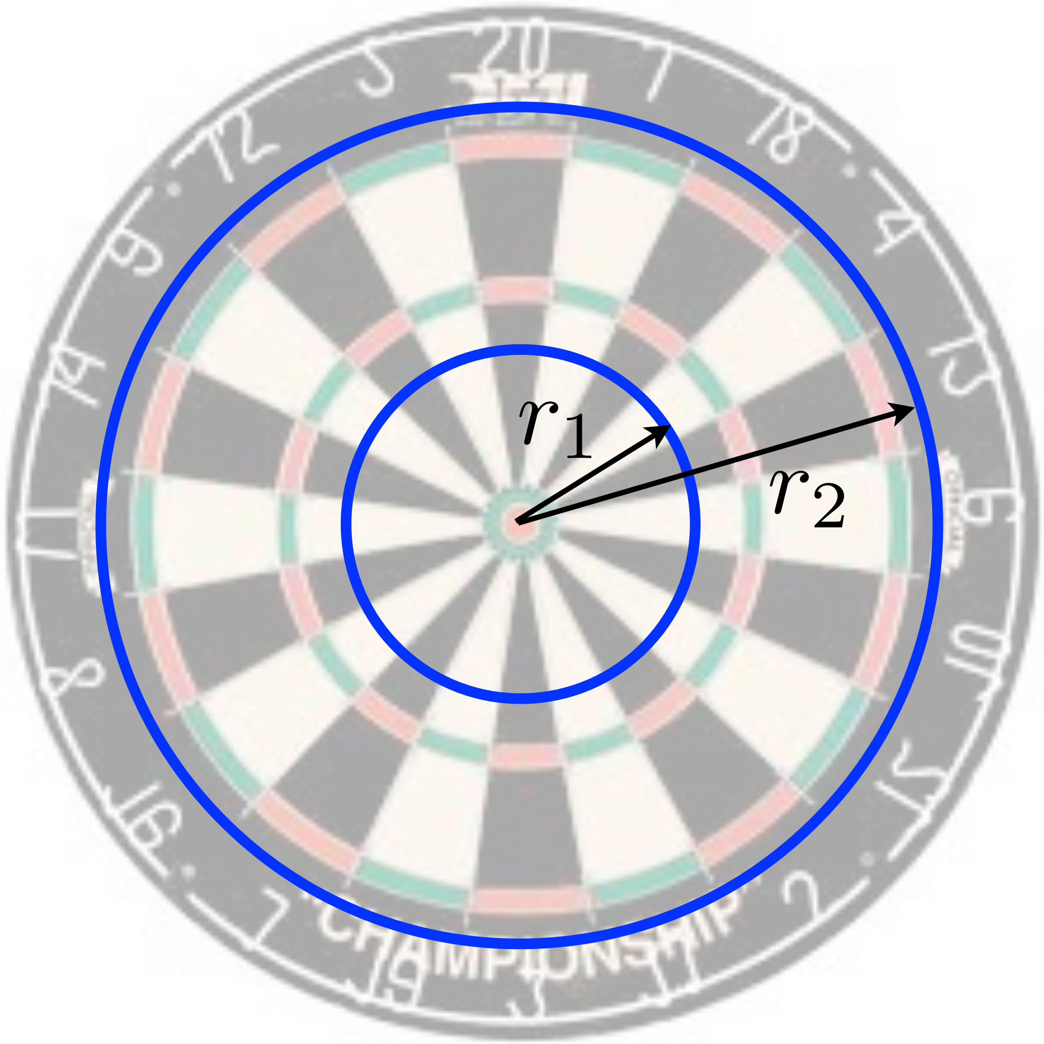
$$\int_0^{2\pi} \frac{1}{2\pi} = 1$$

Examples

– Consider the probability density of a dart landing between radius $\mathbf{r_1}$ and radius $\mathbf{r_2}$ from the centre of a dartboard of area $\boldsymbol{A}$.

– The probability is equal to the **area of the slice** divided by $\boldsymbol{A}$.

total
area A



- Probability density is:

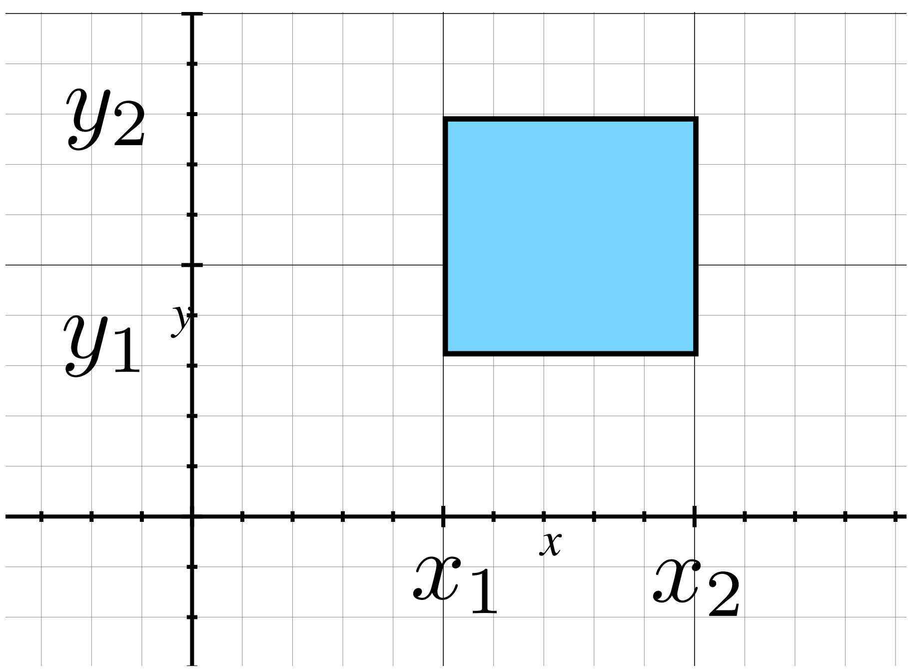
$$\rho(r) = \frac{2\pi r}{A}$$

- We confirm that

$$\mathrm{Prob}(r_1 \leq r \leq r_2) = \int_{r_1}^{r_2} \rho(r)dr$$

$$= \frac{\pi r_2^2 - \pi r_1^2}{A}$$

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

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

- 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

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

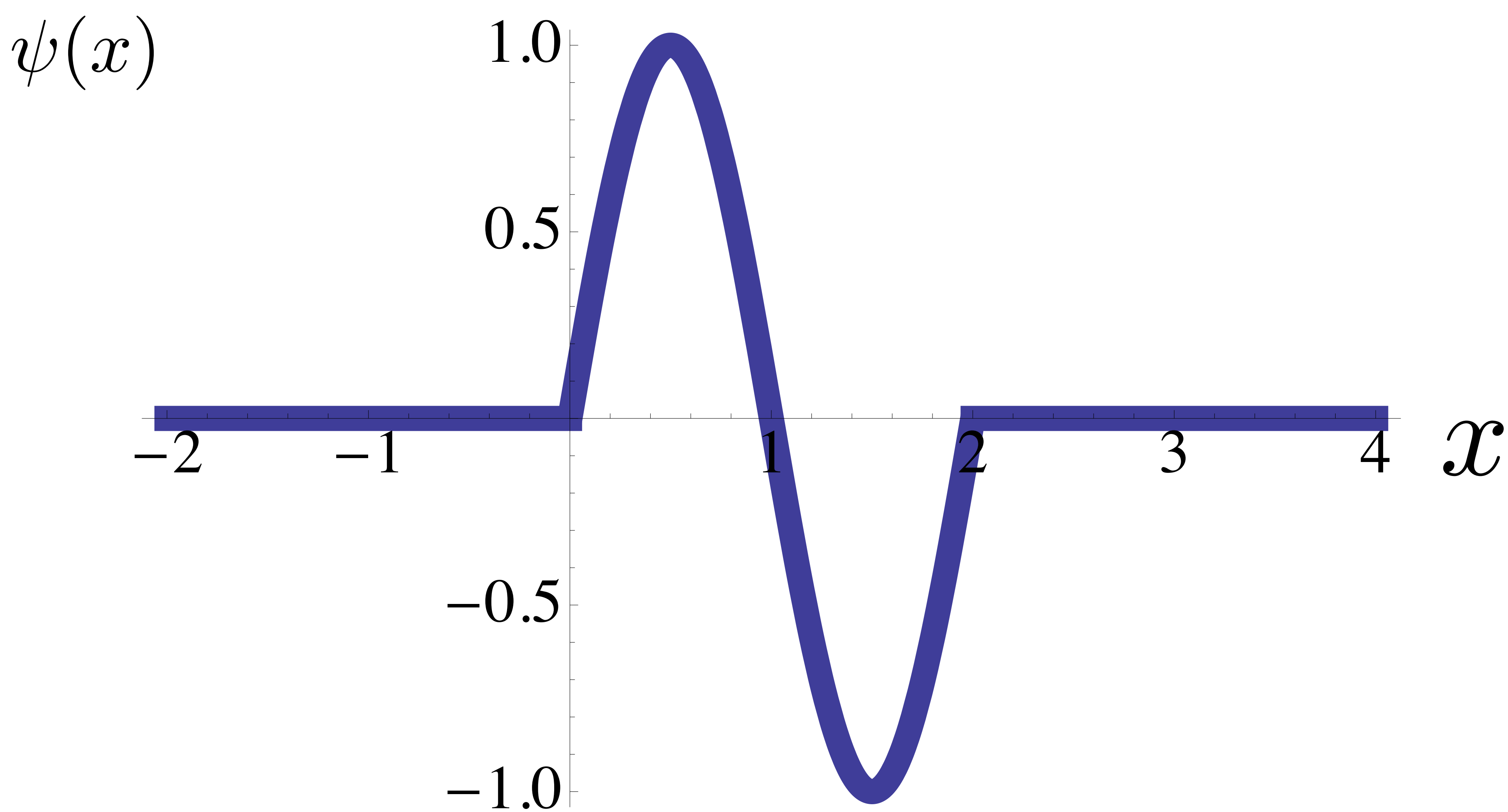
  is the **probability density** for **position**.
- NB The | | signs indicate the absolute value of ψ(x).

The wavefunction

- An example wave-function:

$$\psi(x) = \sin(\pi x) \quad \textbf{for} \quad 0 \le x \le 2$$

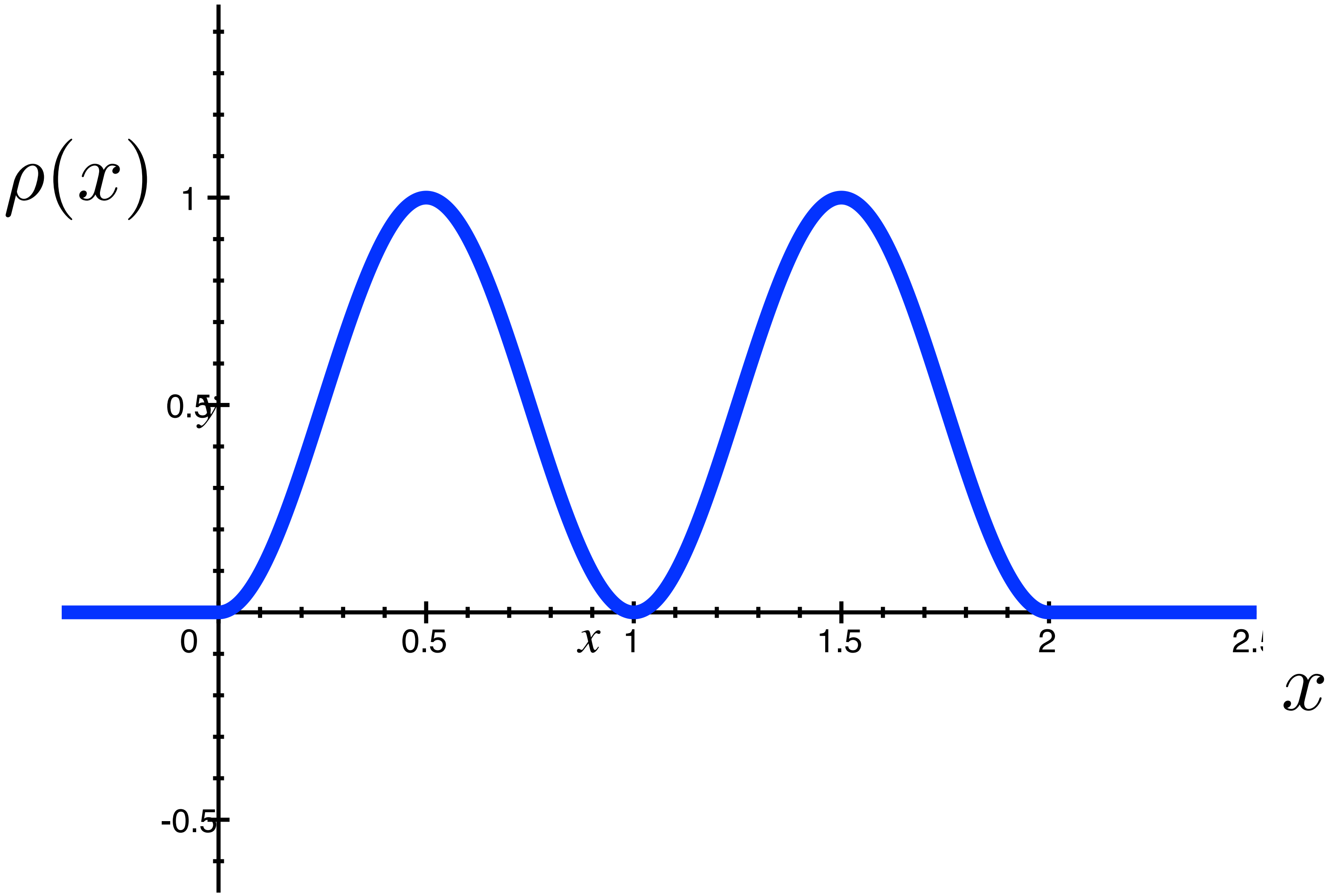
$$\psi(x) = 0 \quad \textbf{elsewhere}$$



The wavefunction

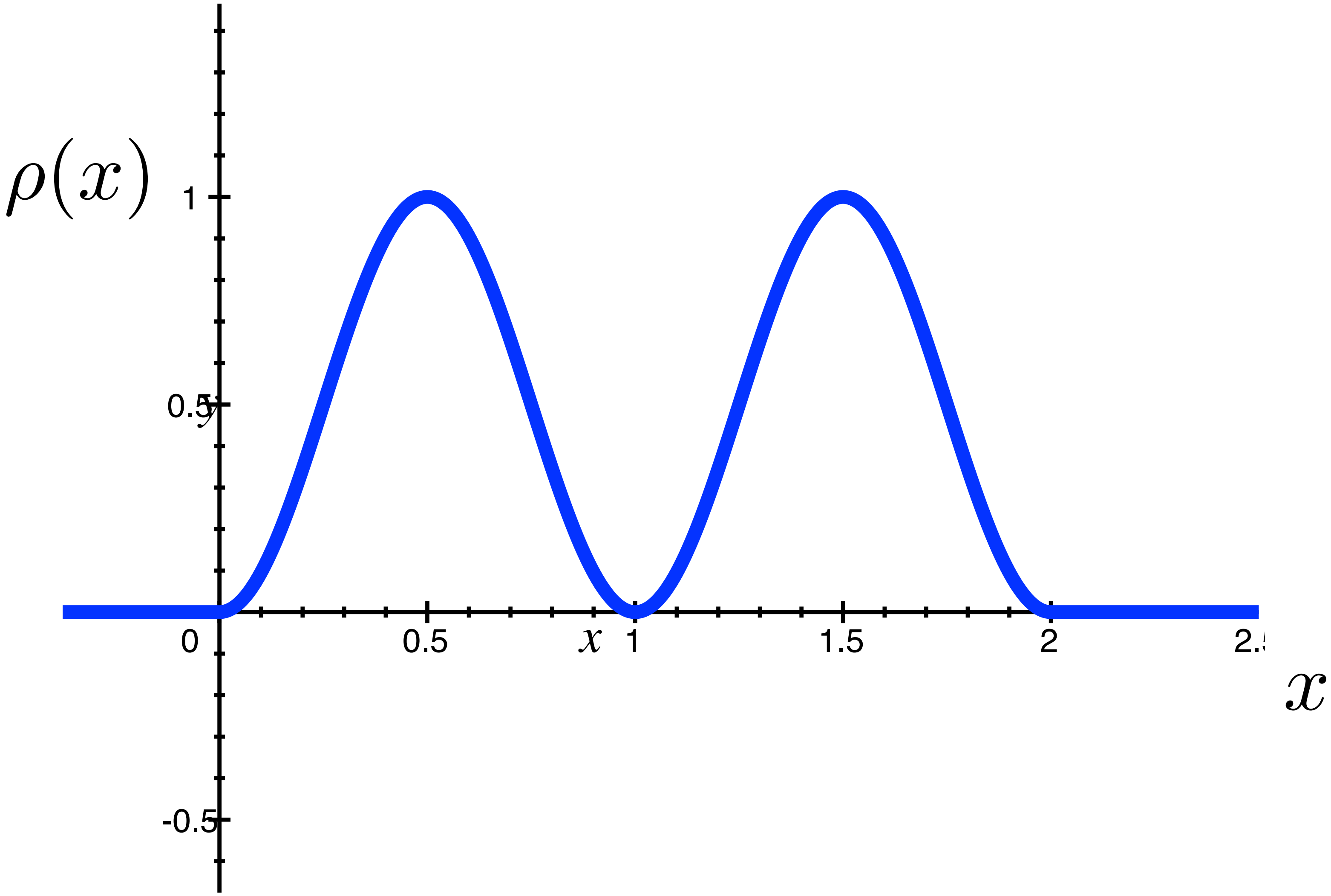
- The probability density for particle position is

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



Quiz

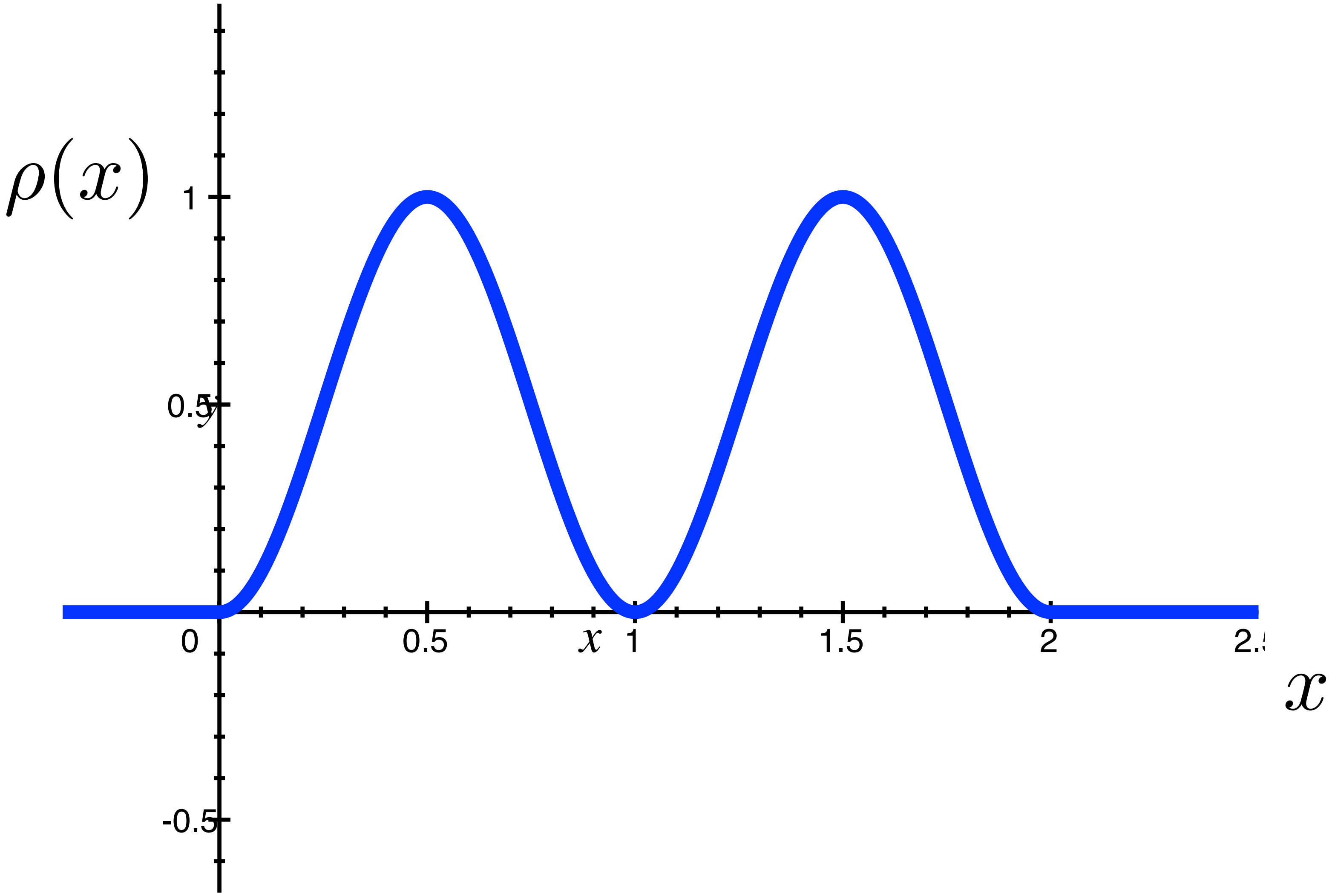
- By inspection, what is the probability for finding the particle in the region x = 0.5 to x = 1?



- 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?



- 1. 0
- 2. 1/2
- 3. 1

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**.

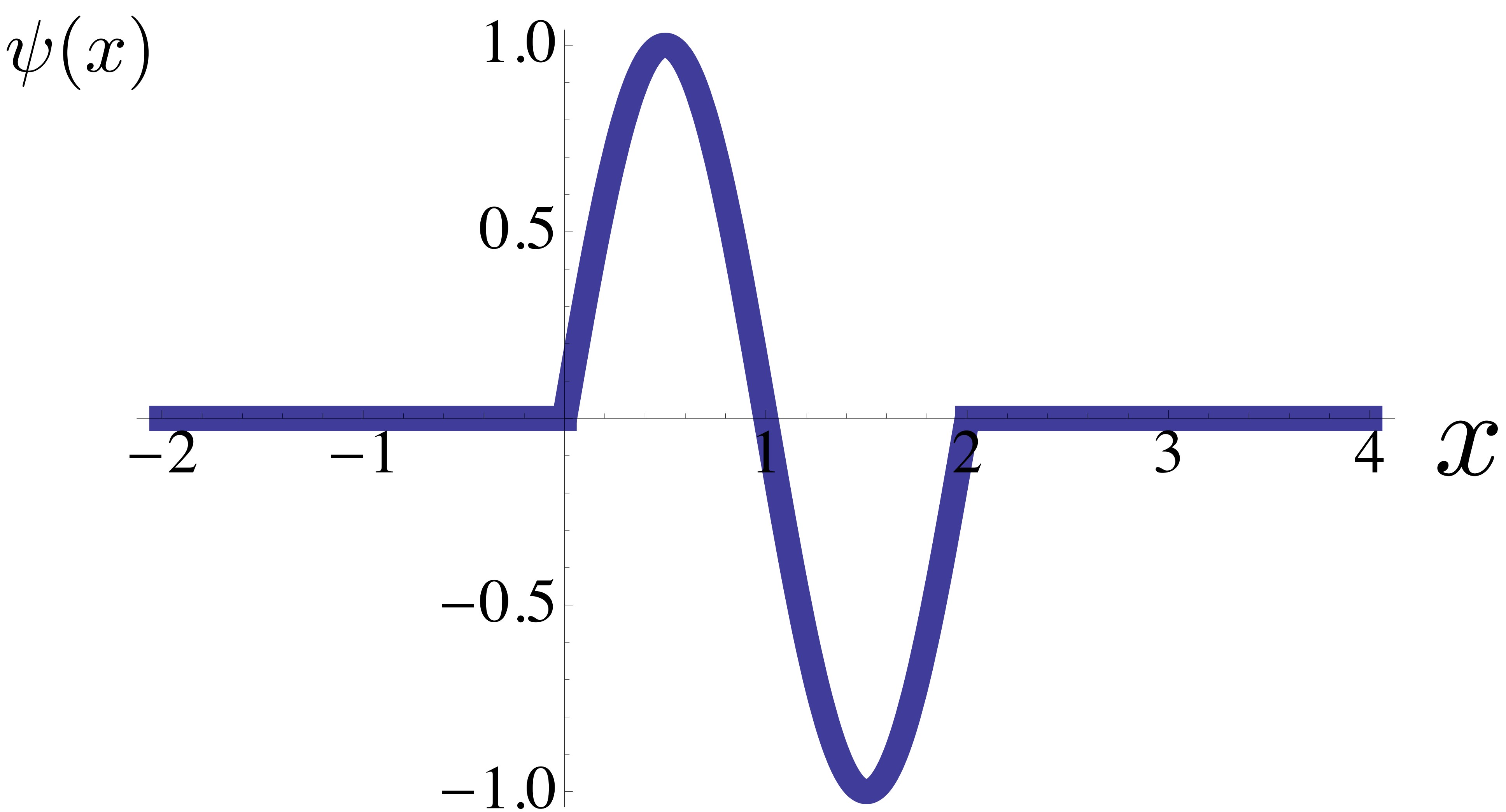
$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

- 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.

- Let us **verify** that this wavefunction is **normalised**:

$$\psi(x) = \sin(\pi x) \qquad \textbf{for } 0 \le x \le 2$$

$$\psi(x) = 0 \qquad \textbf{elsewhere}$$



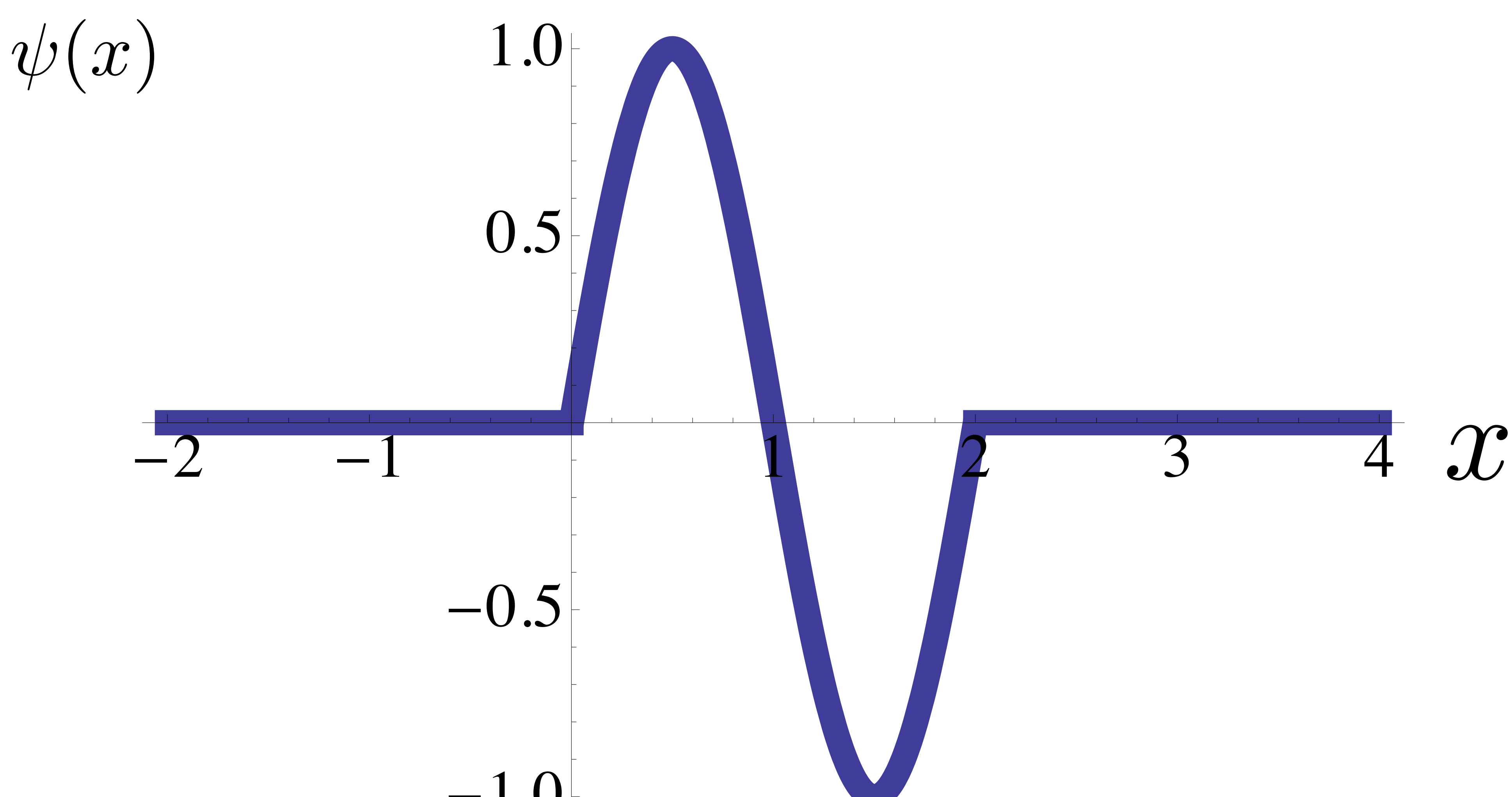
Hand-written Calculations

The wavefunction

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

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

$$\psi(x) = 0 \qquad \textbf{elsewhere}$$



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

$$\psi_2(x) = \frac{\psi_1(x)}{\sqrt{N}}$$

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

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

Quiz

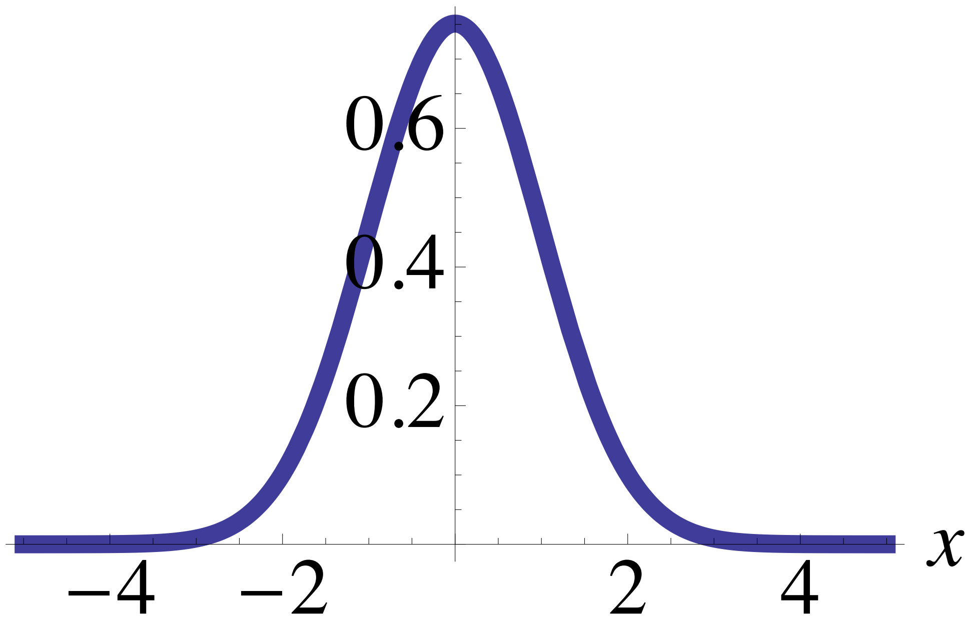
- Given the following mathematical identity, which of the following wave-functions is normalised?

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

1) $$\psi_1(x) = \frac{e^{-x^2}}{\pi^{1/2}}$$

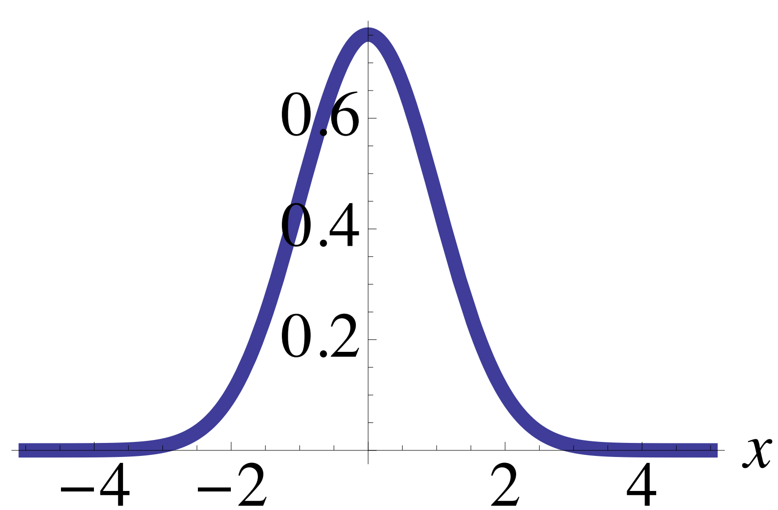
2) $$\psi_2(x) = \frac{e^{-x^2/2}}{\pi^{1/4}}$$

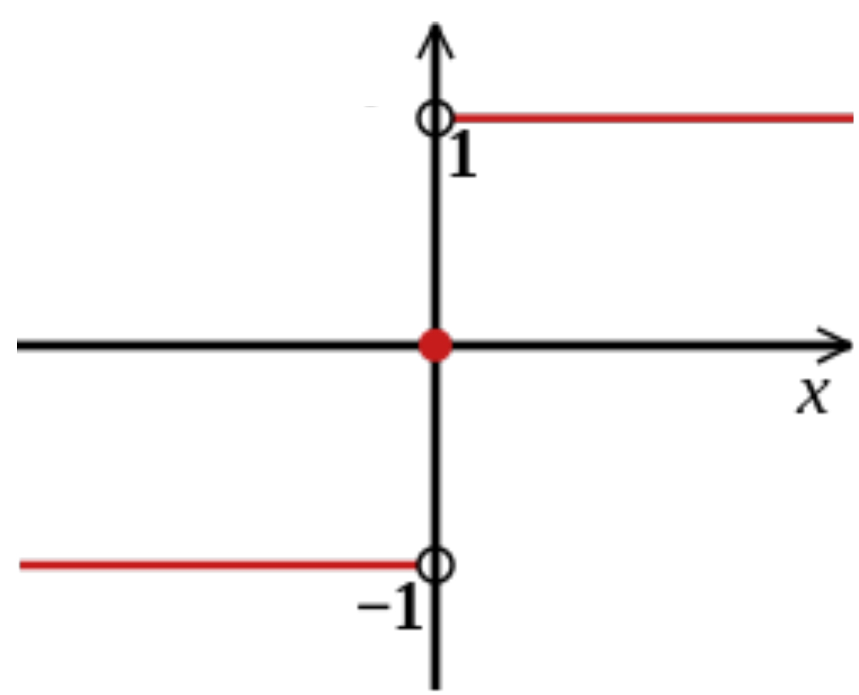
3) $$\psi_3(x) = \frac{e^{-x^2/2}}{\pi^{1/2}}$$



The wavefunction

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

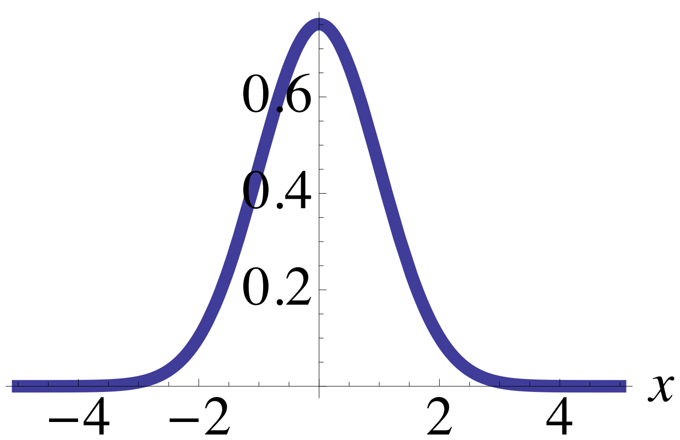


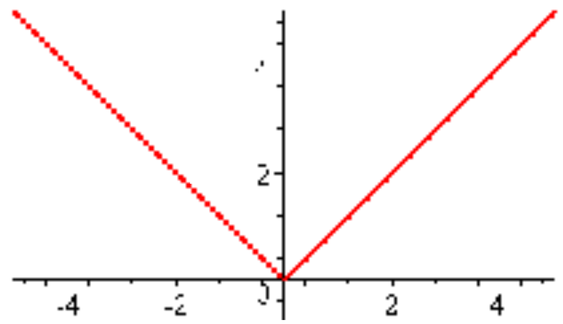


- This ensures that the **first derivative** of **Ψ(x)** is **finite**.

The wavefunction

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





- This ensures that the **second derivative** of **Ψ(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).
  - ψ(x) is **normalised**.
  - ψ(x) is **continuous**.
  - Probability of position measurement via the **Born rule**:

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

Poll

Expectation values

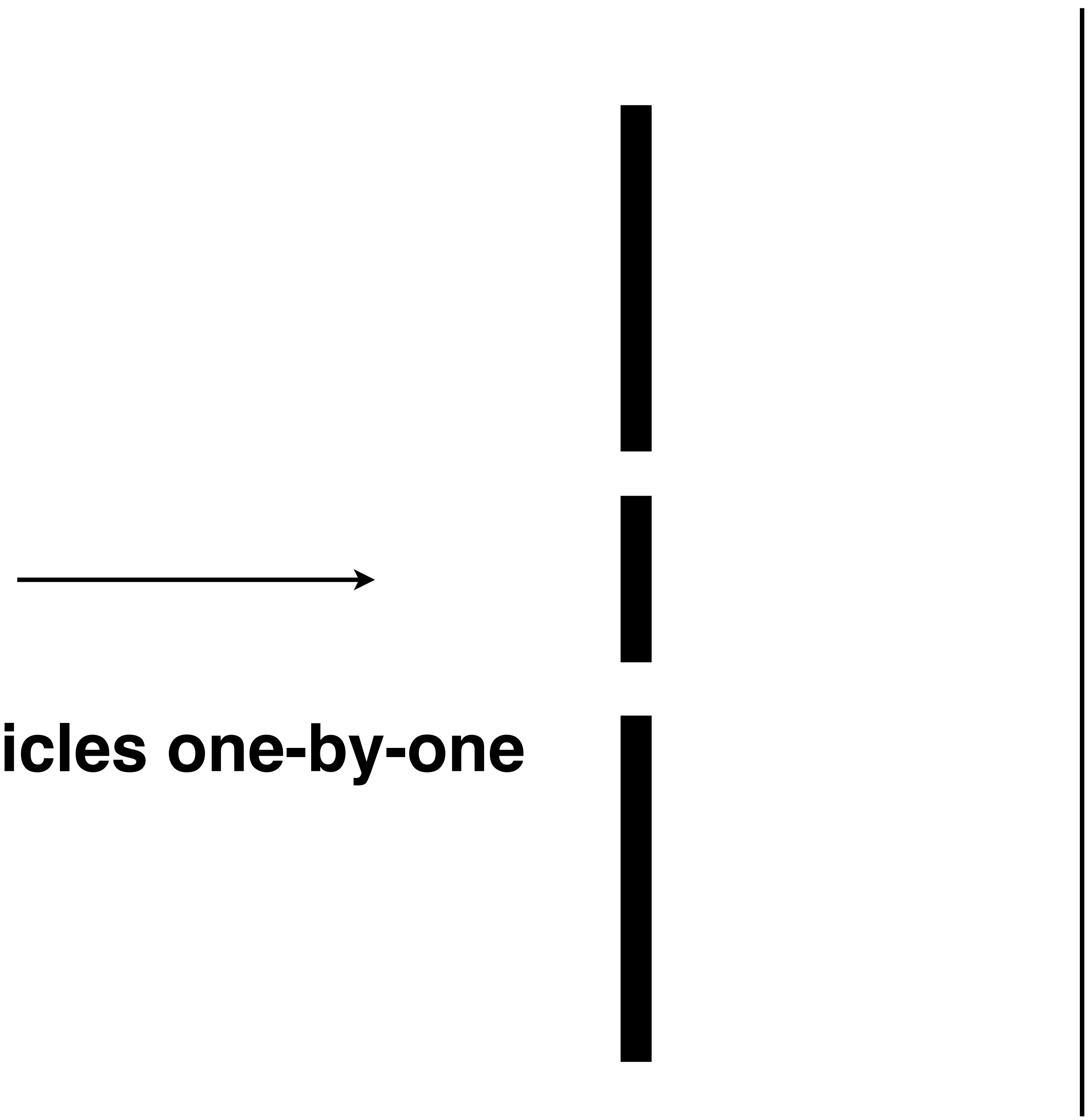
- Have you studied expectation values before?

  » 1. Yes
  » 2. No

Double-slit experiment

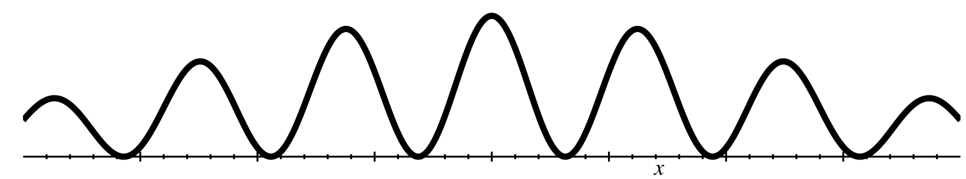
– **Jönsson** (1961): **Electrons**

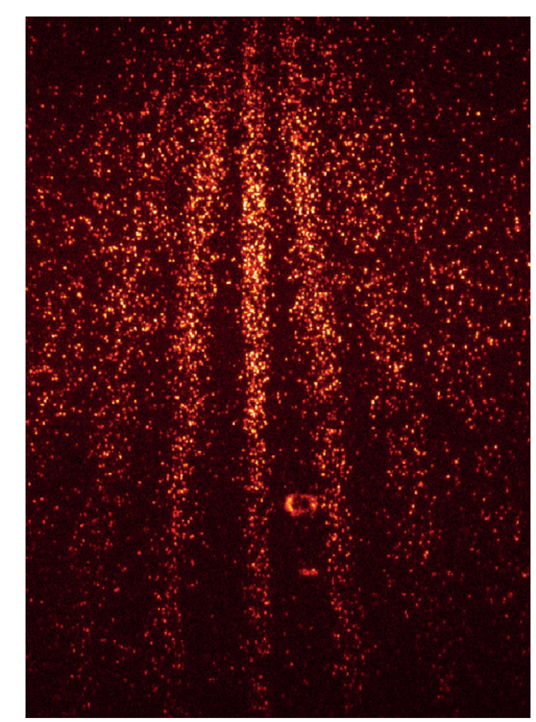
Screen



Particles one-by-one

One-by-one, random clicks build Interference Pattern

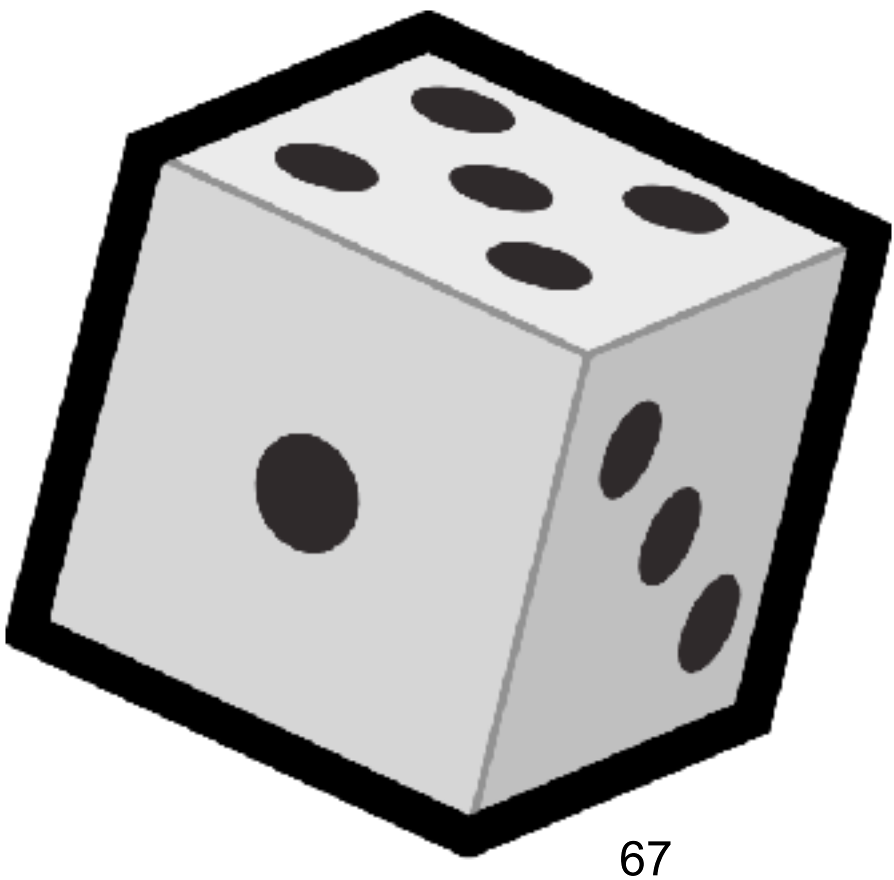




Expectation values

- 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.
  - $\boldsymbol{p_1}$=1/6, $\boldsymbol{p_2}$=1/6, $\boldsymbol{p_3}$=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
- ***p₁*=**1/6, ***p₂*=**1/6, ***p₃*=**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

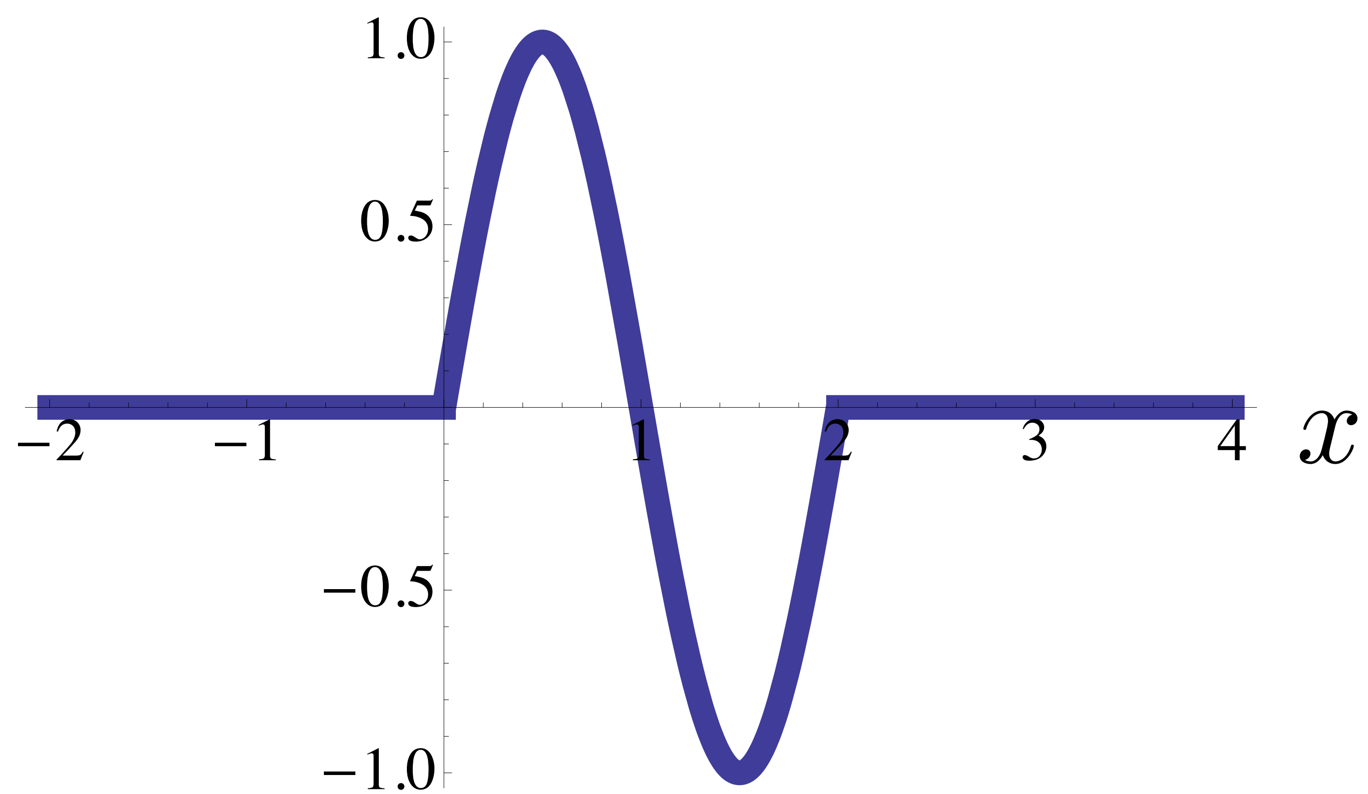
- Consider our example wavefunction:

$$\psi(x) = \sin(\pi x) \qquad \textbf{for } 0 \le x \le 2$$
$$\psi(x) = 0 \qquad \textbf{elsewhere}$$

- We can compute the expectation value:

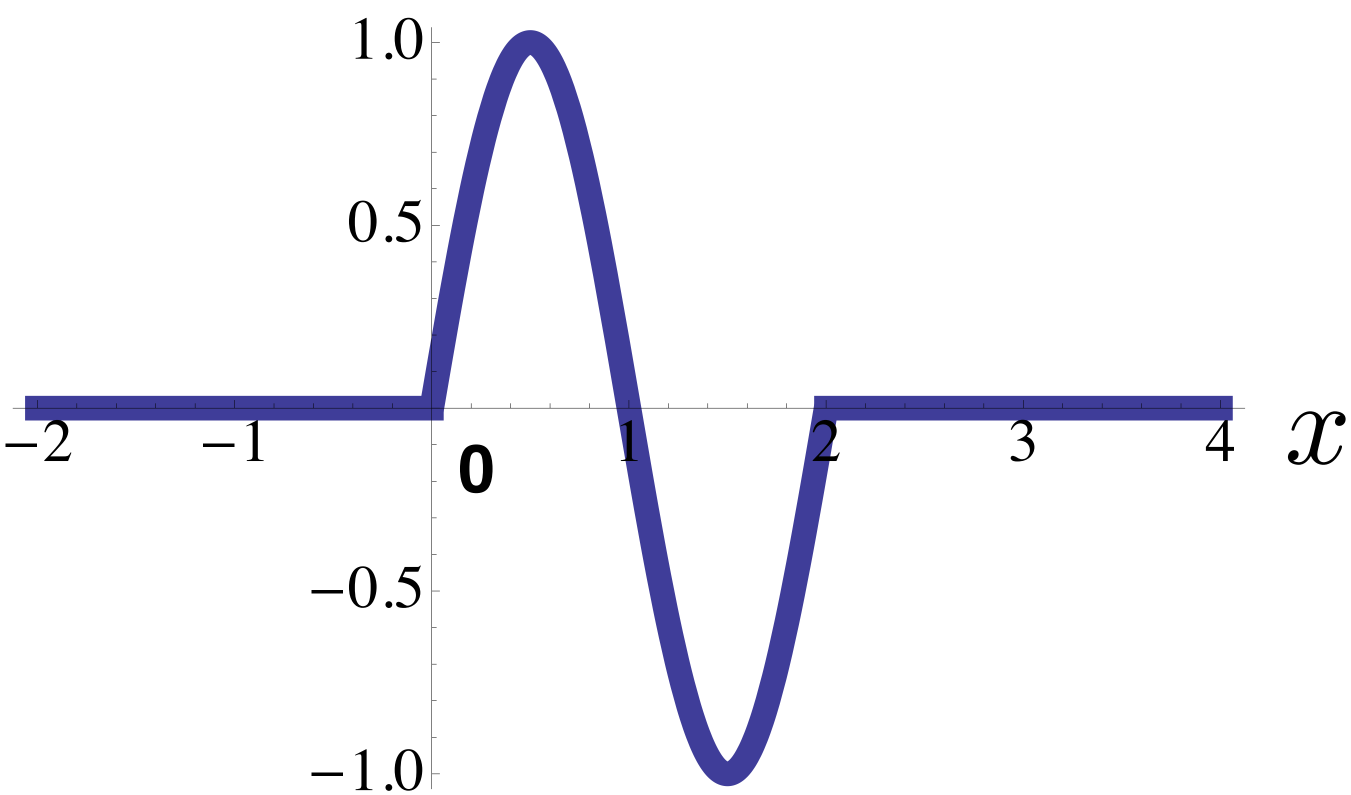
$$\langle x \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 x \; dx$$

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



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

- 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 **p** would have a wave-function:

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

- 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:

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!

$$\text{“}\frac{1}{\sqrt{\infty}} = 0\text{“}$$

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

- 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

Werner Heisenberg

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:

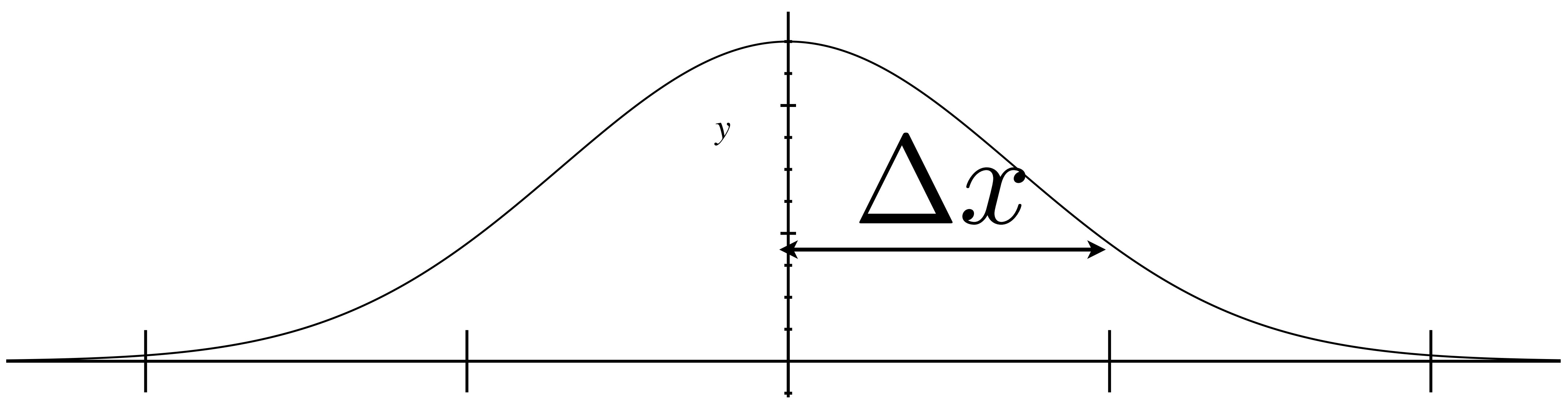
$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

- 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

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

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

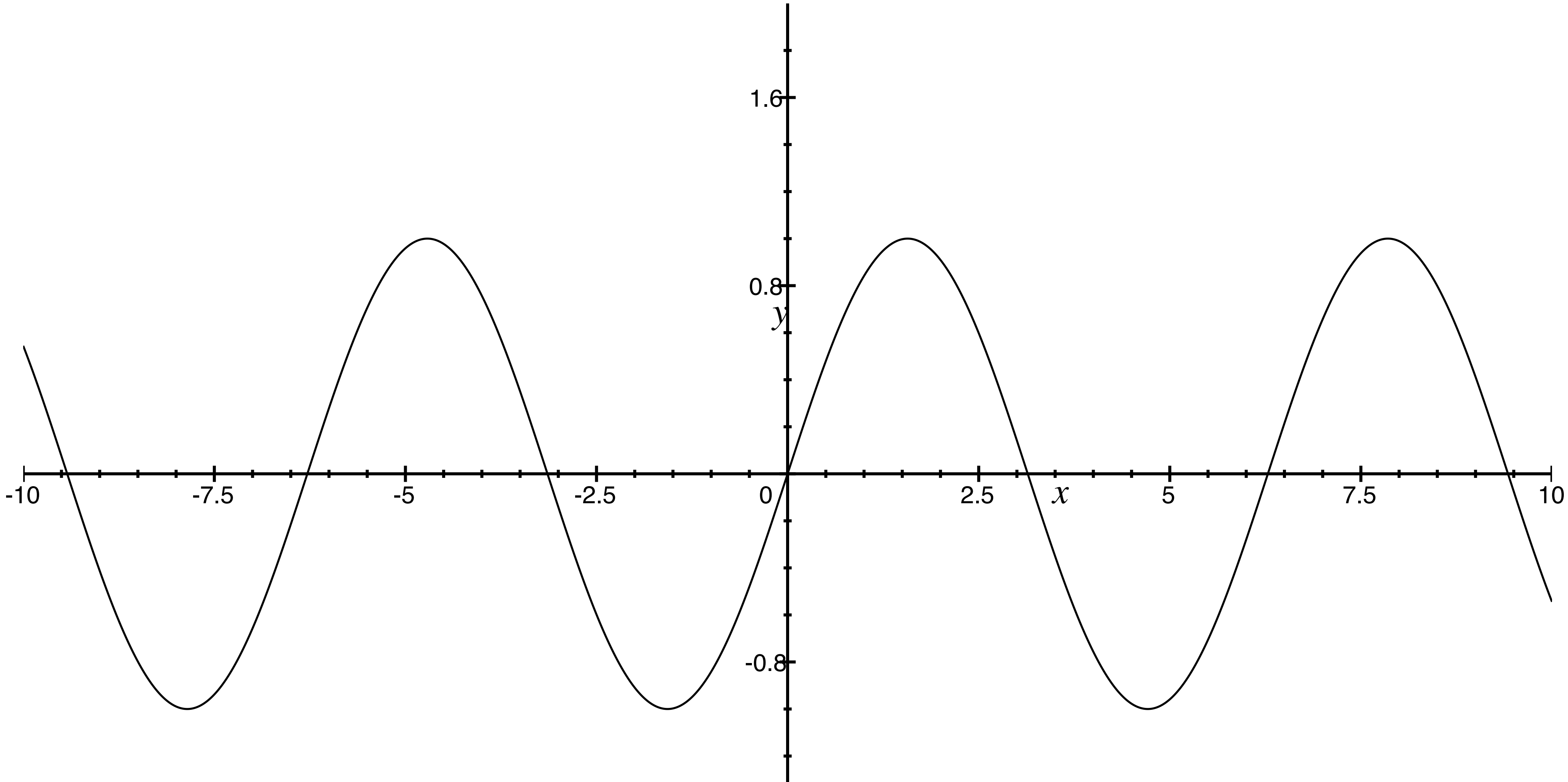
- The de Broglie waves represent a particle with **exact** momentum **p**.
- Exact momentum = **zero** uncertainty.
- This **violates** Heisenberg's relation.
- And is why such wavefunctions cannot be **normalised**, they are **not physical wavefunctions.**

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

Wave-packets

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

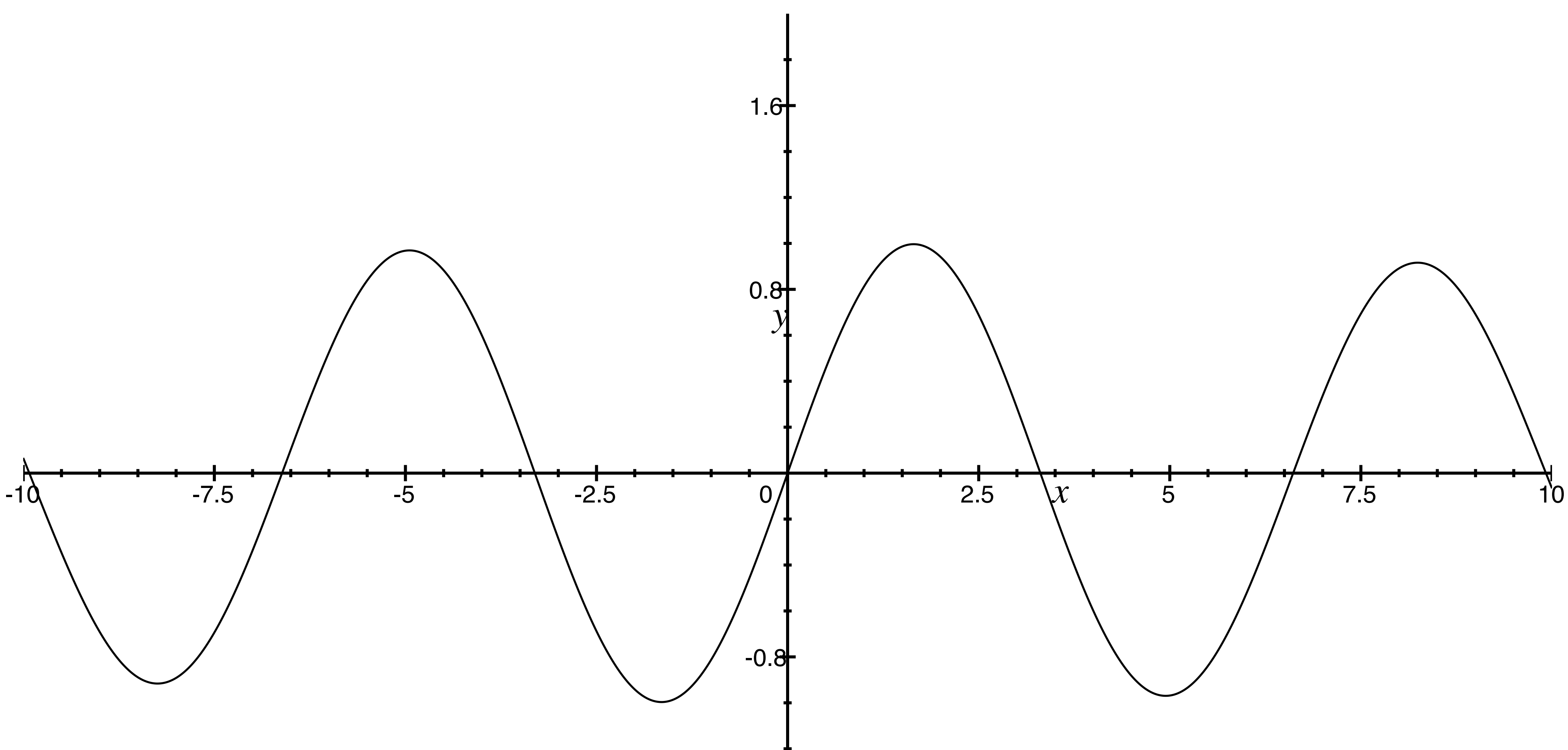
$$\sin(x)$$



Wave-packets

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

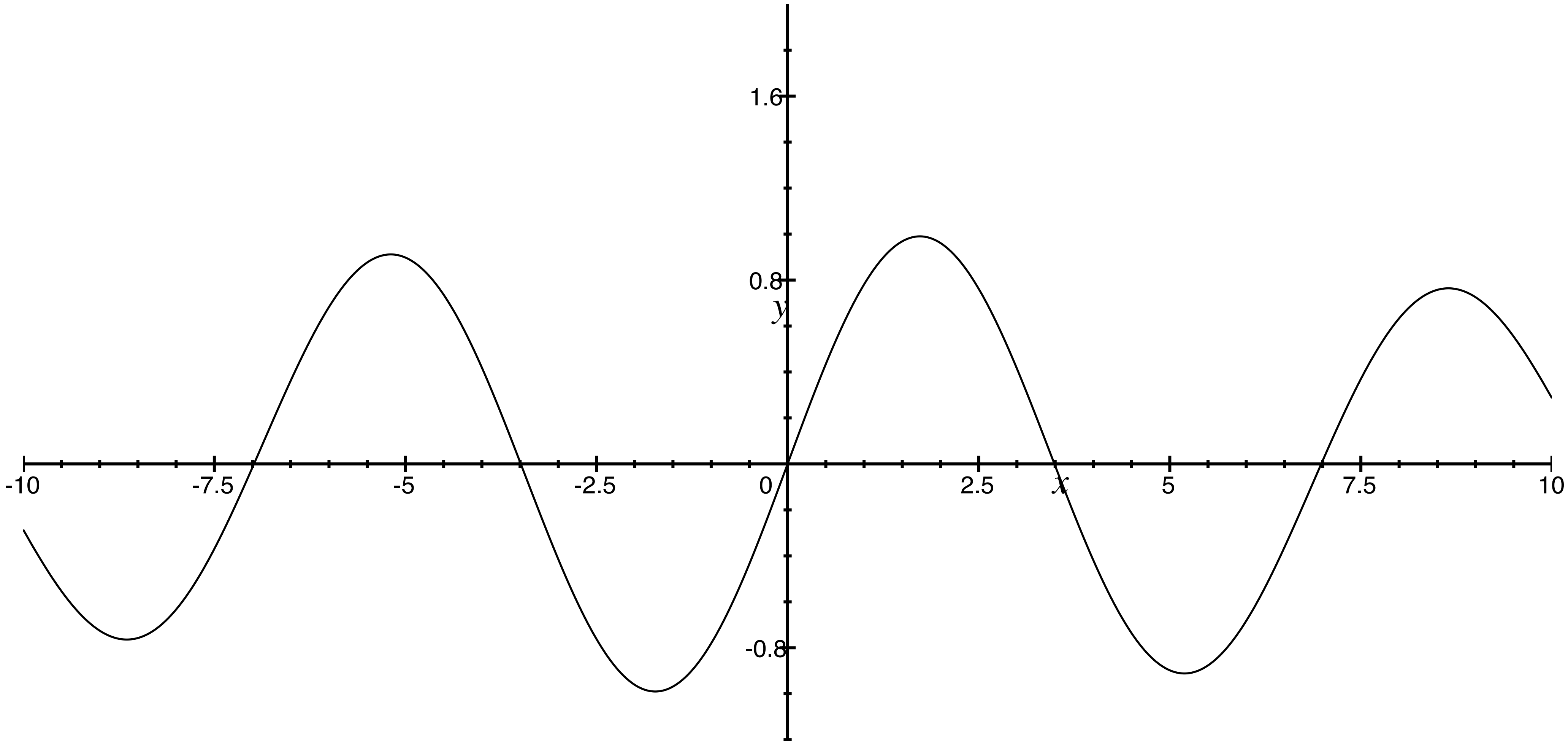
$$\frac{\sin(x) + \sin(0.9x)}{2}$$



Wave-packets

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

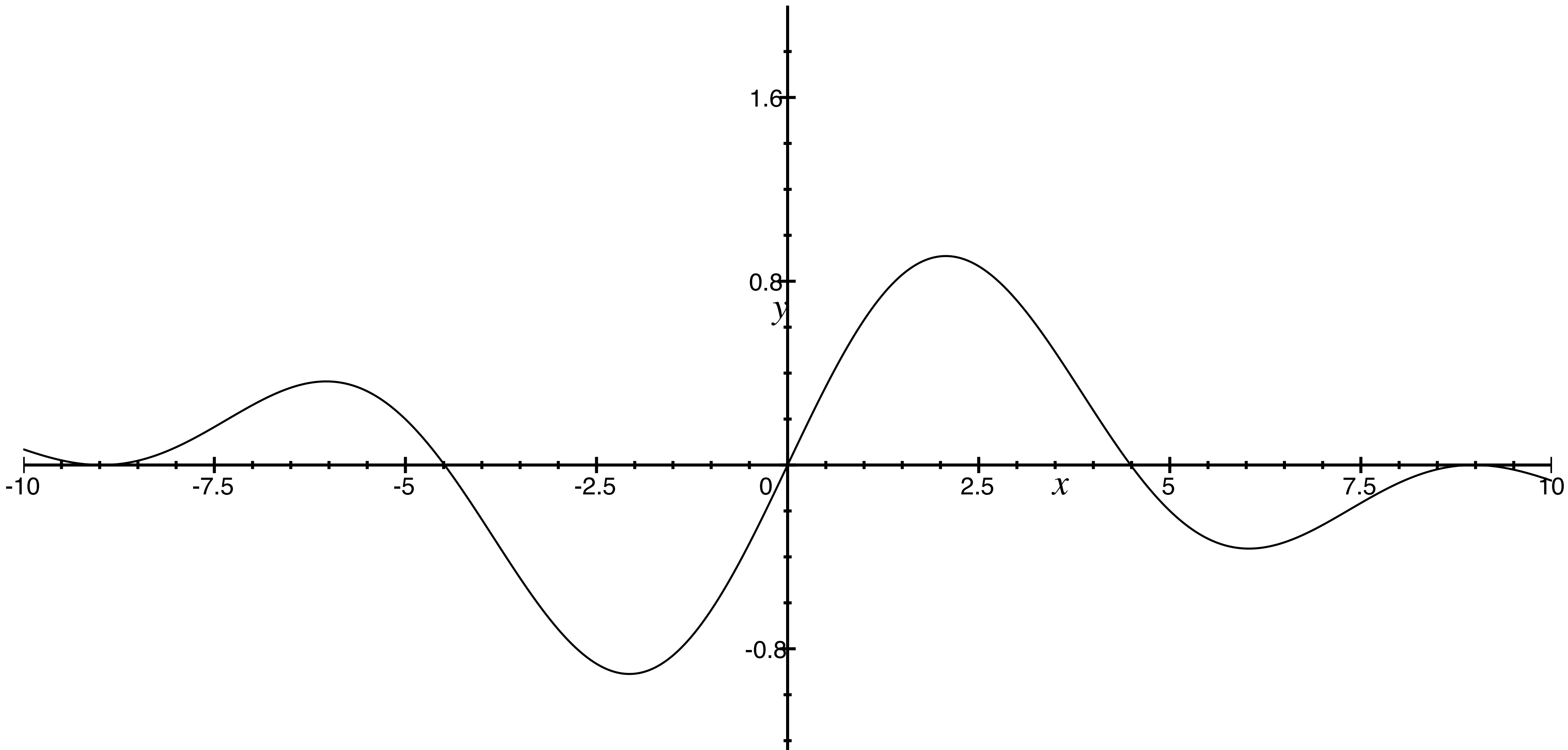
$$\frac{\sin(x) + \sin(0.9x) + \sin(0.8x)}{3}$$



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**.

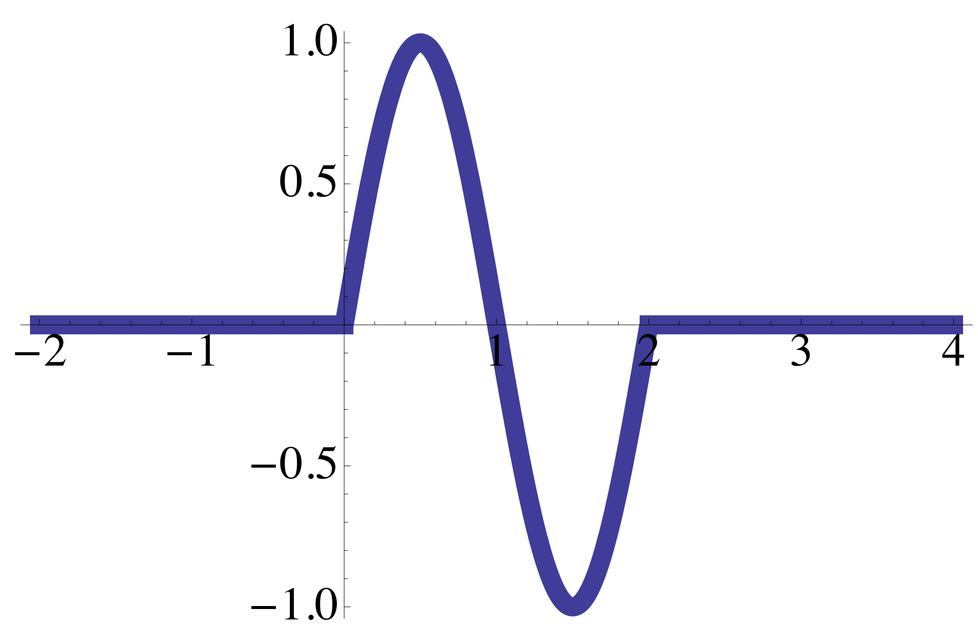
$$\Delta x \Delta p \gtrsim \frac{\hbar}{2}$$

- Heisenberg's principle in action!

Why the wave function?

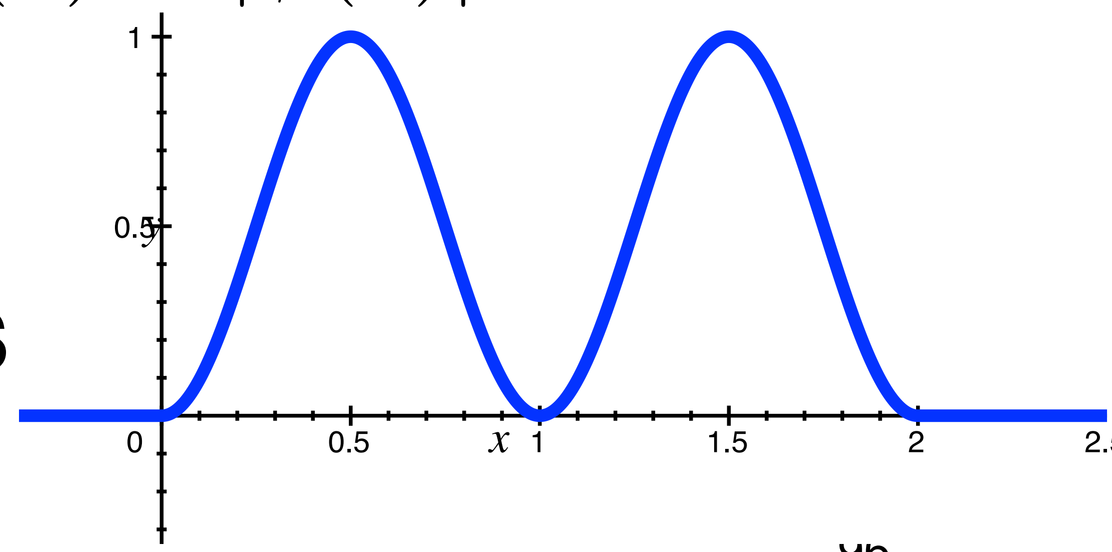
- So far, we have done nothing with the wave function other than **calculate probabilities**.
- So why use wave functions at all?
- Why not just work with **probabilities**?
  - We need **negative values** to achieve **destructive interference**!

$\psi(x)$



vs

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



Evolution in time

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

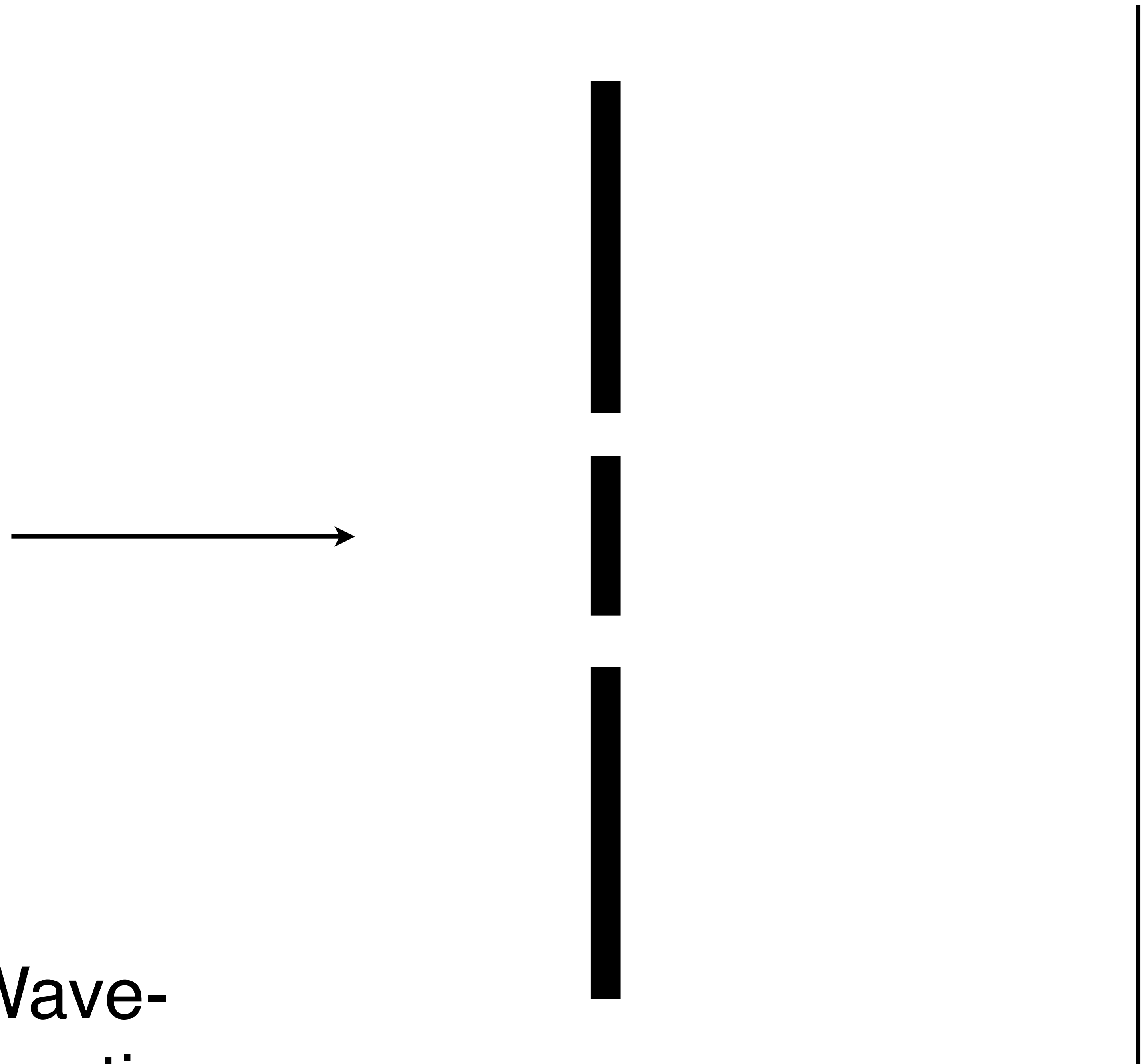
Erwin Schrödinger

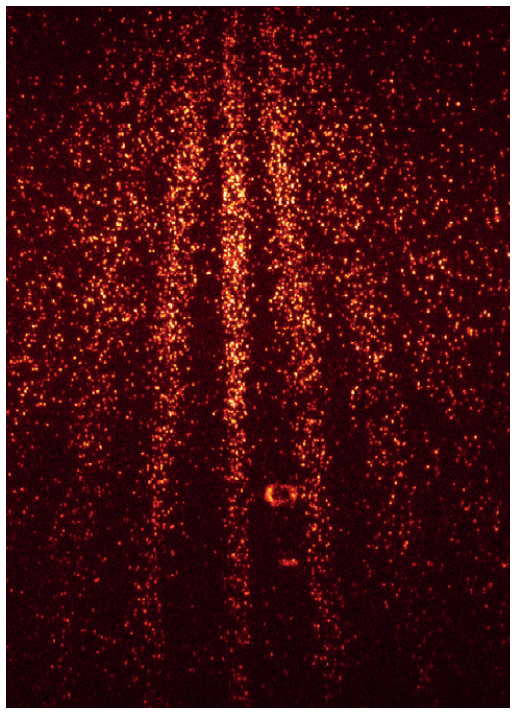
$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x^2} + V(x,t)\right)\psi(x,t)$$

- 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 = √(-1))
- For the purposes of this course, it suffices to think of the wave function "**evolving like a wave**".

Double-slit experiment

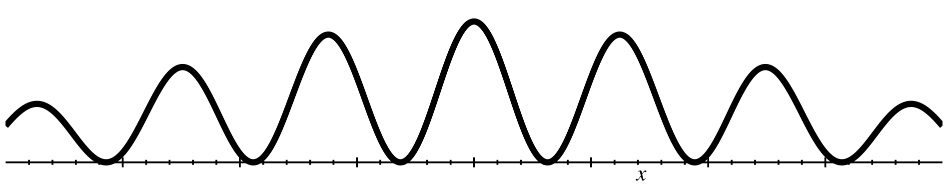
–**Jönsson** (1961): **Electrons**





Probability density:

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



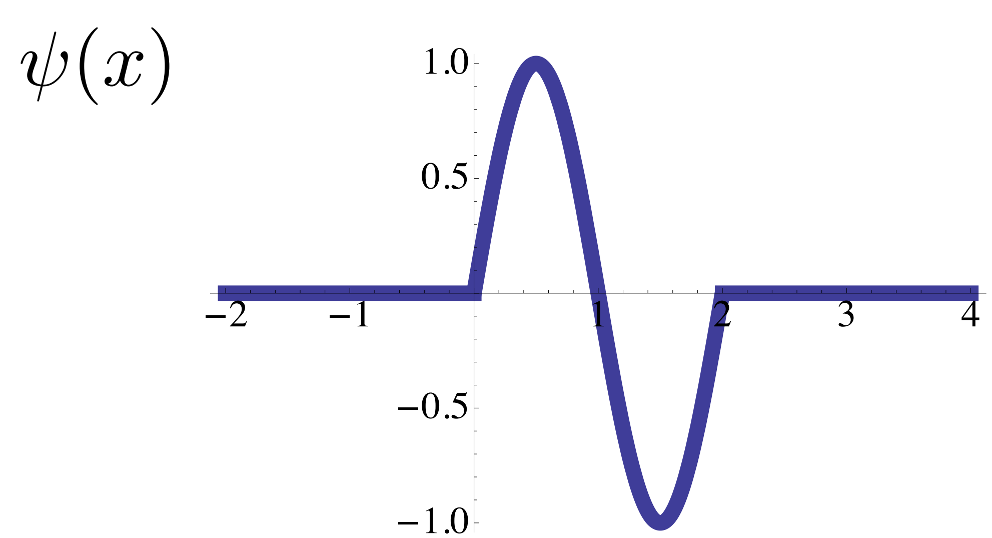
Wave-
function
evolves
"as a wave"

Experiences
wave
interference

Clicks on
screen follow
Born rule.

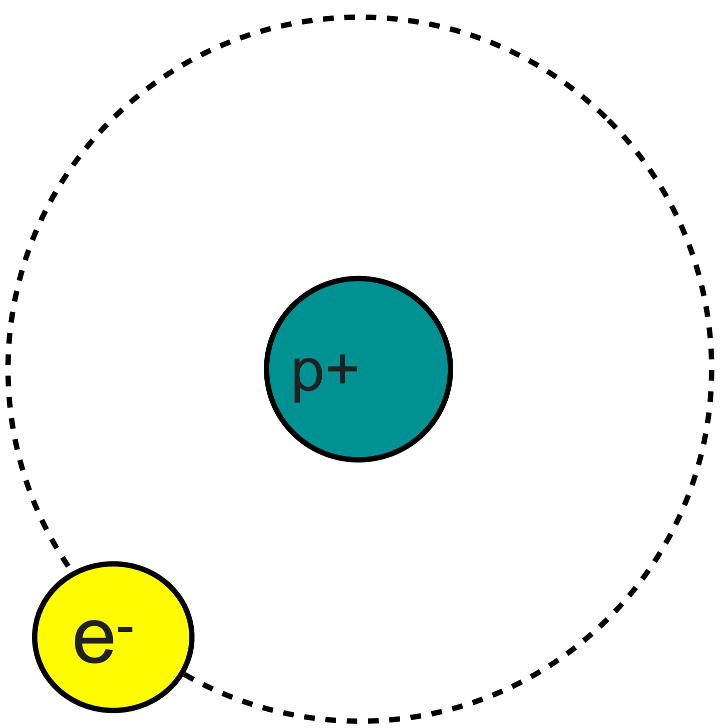
Importance of ψ(x)

- 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.



$$\longrightarrow \qquad \psi(x)$$

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.