Section 1: How QM Works, Part 1

In these slides we will cover:

- The Schrödinger Equation
- The probability interpretation of the wavefunction
- The discrete nature of observables
- The correspondence between observables and operators
- Eigenfunctions, eigenvalues and their properties
- Measurement in Quantum Mechanics
- Expectation values

The wavefunction

Particles and waves

- In classical physics, we use **Newton's Laws** to determine the equation of motion $x(t)$ of a particle of mass m moving in a potential $V(x)$:

$$F = m\frac{d^2x}{dt^2} = -\frac{dV}{dx}$$

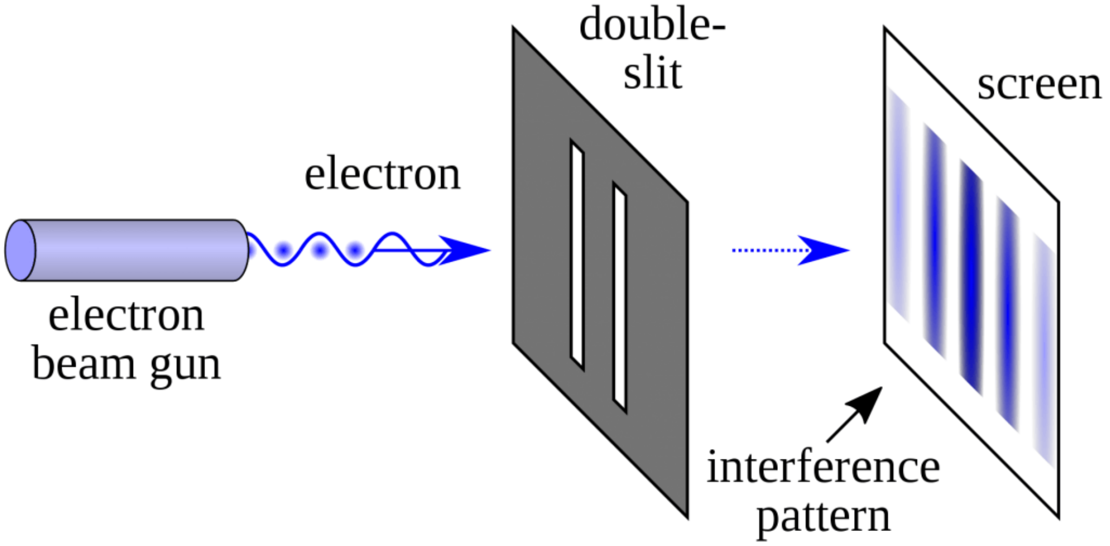
- Equivalently, we can **conserve the energy** of the particle:

$$\frac{1}{2}mv^2 + V(x) = \text{Energy}$$

The wavefunction

Particles and waves

- This picture cannot apply in the Quantum world, because **particles behave like waves** (see: the double-slit experiment)



- Since a wave is an **object extended in space**, we need to change how we describe a particle

The wavefunction

The Schrödinger equation

- In Quantum Mechanics, the equation of motion of a particle in a potential $V(x)$ is replaced by the **Schrödinger equation**:

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

- The symbol $\hbar = h/2\pi$, where h is Planck's constant
- It's an equation for the **wavefunction of the particle** $\Psi(x,t)$. This looks complicated, but we'll soon see it's the same as:

$$\text{Kinetic energy} + \text{Potential energy} = \text{Total energy}$$

- The $i = \sqrt{-1}$ appearing in the Schrödinger equation looks strange – the wavefunction is a complex number in general!

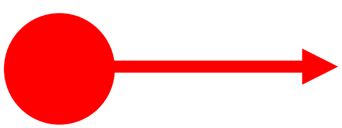
The wavefunction

The wavefunction

- The **wavefunction** Ψ – that's the Greek letter "psi" – is how we describe the state of a particle in Quantum Mechanics

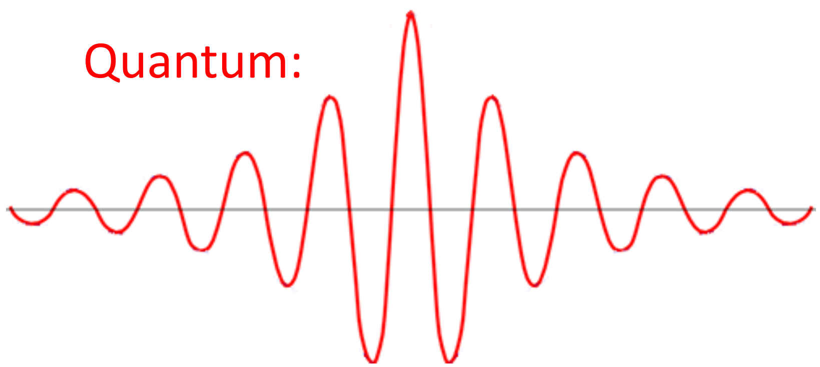
- At a given time t, a particle is not at a fixed position $x(t)$, but is in a state described as a **function of position**, $\Psi(x, t)$

Classical:



becomes

Quantum:



- The wavefunction depends on the co-ordinates of a system and contains **all the information about the system**

The wavefunction

Probability interpretation of the wavefunction

- **What does the wavefunction mean?** It's connected to the **probability** of the particle being in a particular position:

Probability of finding a particle in a range $x \rightarrow x + dx$ $= |\Psi|^2 \, dx$

Note: although Ψ can be a complex number, $|\Psi|^2 = \Psi \cdot \Psi^*$ is real, as it should be for a probability!

- The particle must be somewhere! Hence, these probabilities must sum to 1.0, which is known as the **normalisation** of Ψ:

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

- The probability interpretation of the wavefunction implies that Quantum Mechanics has a **statistical** or **indeterminate** nature

Operators, eigenfunctions & eigenvalues

Discrete nature of observables

- In Quantum Mechanics, a measurement of a quantity **can only produce discrete (specific) outcomes**, not any value

- You have previously studied a particle in an **infinite potential well**, which has certain allowed energy levels (see recap on next slide)

- Another example is poor Schrödinger's cat, which only has 2 possible states …

Operators, eigenfunctions & eigenvalues

Discrete nature of observables

- In Physics 2A QM, you studied that a particle enclosed in an infinite potential well has discrete energies and wavefunctions
- We'll see this example again in Section 3!

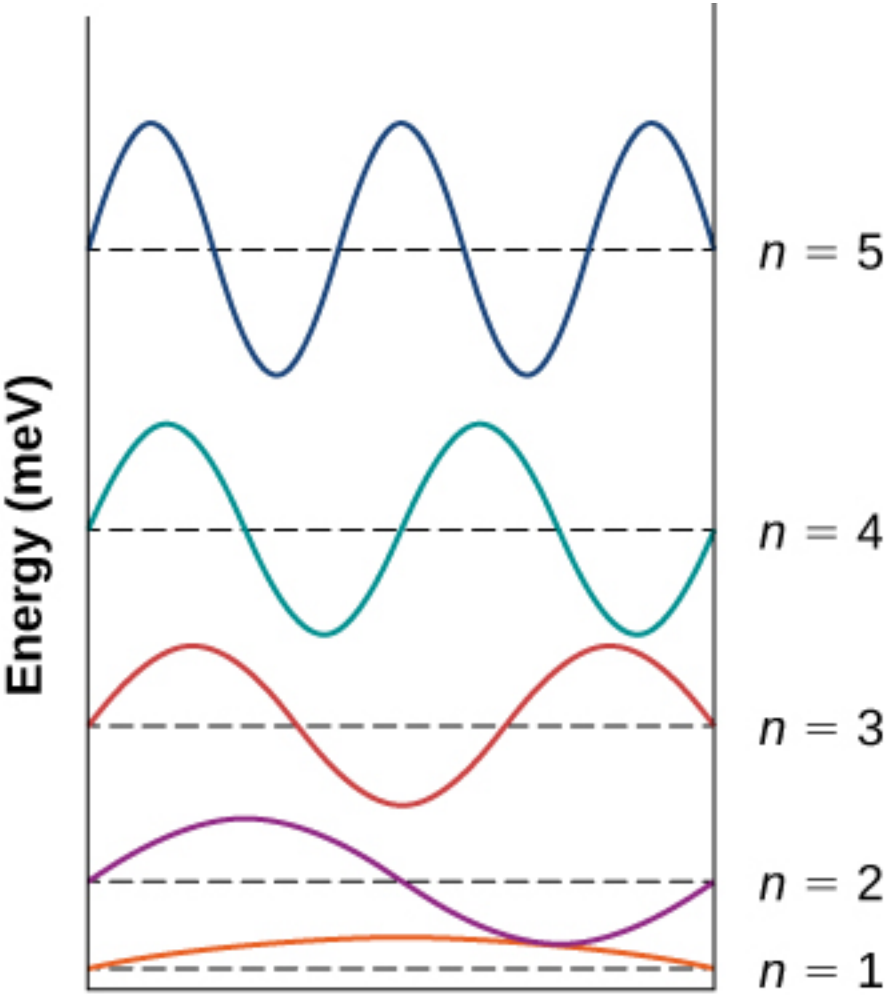


Image credit: https://opentextbc.ca/universityphysicsv3openstax/chapter/the-quantum-particle-in-a-box/

Operators, eigenfunctions & eigenvalues

Discrete nature of observables

- Physics is described in the language of mathematics; so we need a mathematical structure in which discrete values appear
- Welcome to the world of **operators**, **eigenfunctions** and **eigenvalues**! Please do not turn back!
- We can describe the mathematical framework of Quantum Mechanics by the following statement:

Each quantity we can observe is represented by a corresponding operator. If we measure that observable, we will always obtain a result which is one of the eigenvalues of the operator

- What do these words mean??

Operators, eigenfunctions & eigenvalues

What is an operator?

- An operator is a **mathematical instruction which acts on a function to produce another function**:

Operator acts on Function $f(x)$ to produce Function $g(x)$

- **Example**: $\frac{d}{dx}$ is an operator which acts on a function $f(x)$ to produce the derivative function $g(x) = \frac{df}{dx}$
- **Example**: $x \cdot$ ("multiply by x") is an operator which acts on a function $f(x)$ to produce another function $g(x) = x\, f(x)$

Operators, eigenfunctions & eigenvalues

Eigenfunctions and eigenvalues

- When an operator acts on some special functions – called the **eigenfunctions** of the operator – it returns the same function, scaled by a number – called an **eigenvalue**

$$\hat{A}\,\phi_n(x) = a_n\,\phi_n(x)$$

$\hat{A}$ is an **operator** – these are usually written with little hats!

$\phi_n(x)$ is an **eigenfunction** – the subscript "n" labels the different eigenfunctions $(\phi_1, \phi_2, \phi_3, \ldots)$

a_n is the **eigenvalue** (number) corresponding to the eigenfunction $\phi_n(x)$

Operators, eigenfunctions & eigenvalues

Eigenfunctions and eigenvalues

- When an operator acts on some special functions – called the **eigenfunctions** of the operator – it returns the same function, scaled by a number – called an **eigenvalue**

$$\hat{A}\,\phi_n(x) = a_n\,\phi_n(x)$$

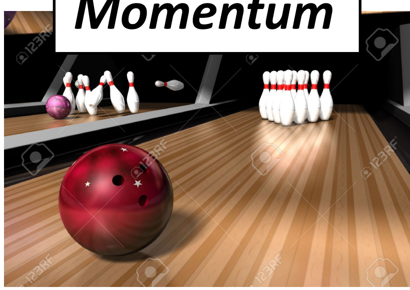
- As an example, let's consider the operator $\hat{A} = \frac{d}{dx}$ again
- $\phi(x) = e^{ax}$ is an eigenfunction of $\hat{A}$ with eigenvalue a
- **Why?** Because $\hat{A}\phi(x) = \frac{d\phi}{dx} = a\,e^{ax} = a\,\phi(x)$ – *the operator has returned the same function, scaled by a number*

Operators, eigenfunctions & eigenvalues

Properties of the operators representing observables

Each quantity we can observe is represented by a corresponding operator. If we measure that observable, we will always obtain a result which is one of the eigenvalues of the operator

Momentum

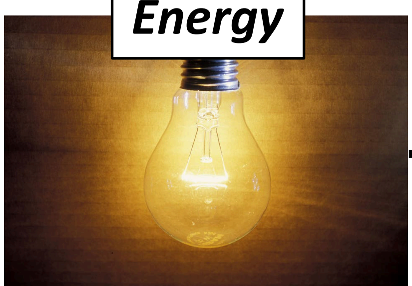


Represented by mathematical operator

Position

Represented by mathematical operator

Energy



Represented by mathematical operator

Angular momentum

Represented by mathematical operator

Operators, eigenfunctions & eigenvalues

Properties of the operators representing observables

- The operators representing observables have **3 key properties**:

1. Their **eigenvalues are real** (not complex) numbers, so they can correspond to the results of physical measurements

2. Different eigenfunctions are **orthogonal**, which is defined by:

$$\int_{-\infty}^{\infty} \phi_m^*(x)\, \phi_n(x)\, dx = \begin{cases} 1, & m = n \\ 0, & m \neq n \end{cases}$$

Note: ϕ^* means the complex conjugate of ϕ

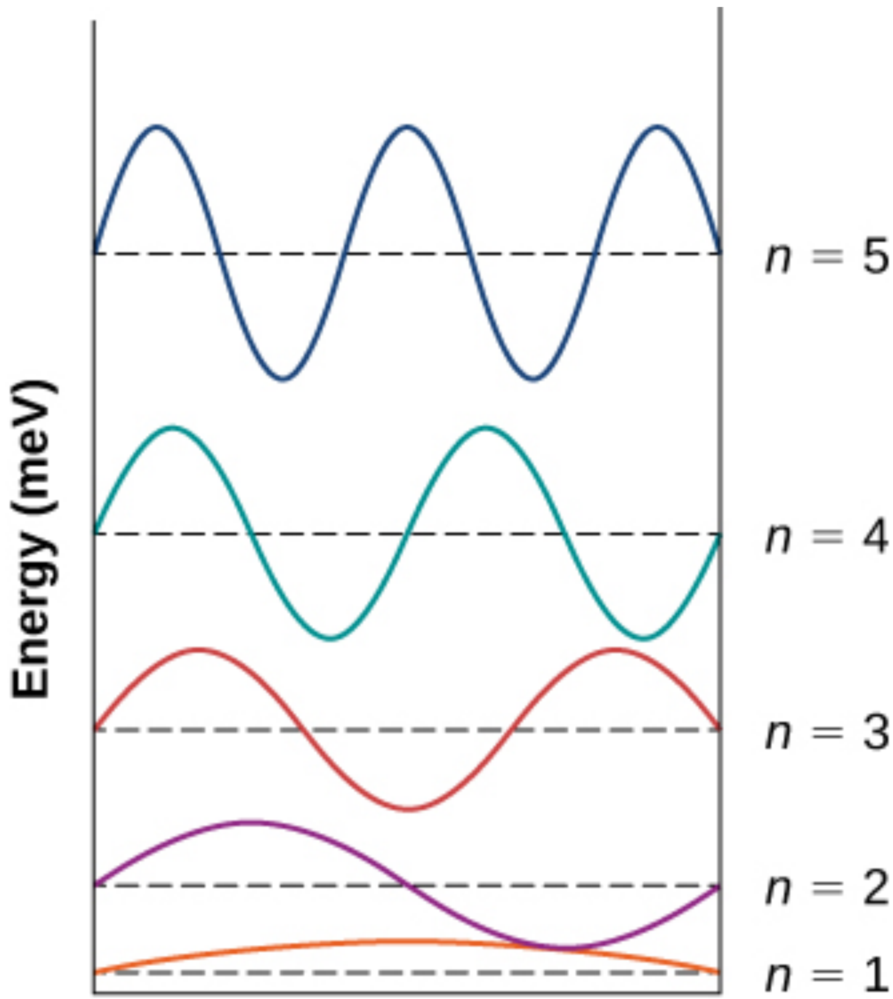
3. Any other function $f(x)$ can be expressed as a **linear combination of the eigenfunctions**, which we can write as:

$$f(x) = \sum_n c_n\, \phi_n(x)$$

Operators, eigenfunctions & eigenvalues

Properties of the operators representing observables

- We can use the energy eigenfunctions for the infinite potential well to illustrate **orthogonality**
- These sine functions average to zero if $m \neq n$, $\int_{-\infty}^{\infty} \phi_m^*(x)\, \phi_n(x)\, dx = 0$
- If $m = n$, then $\int_{-\infty}^{\infty} |\phi_n(x)|^2\, dx = 1$, which is the same as normalising the eigenfunctions



Operators, eigenfunctions & eigenvalues

Linear combinations of eigenfunctions

- We just mentioned that any function $f(x)$ can be expressed as a **linear combination of the eigenfunctions** of an operator:

$$f(x) = \sum_n c_n \, \phi_n(x)$$

- We can determine the coefficients c_n using the orthogonality property. We can derive them by considering:

$$\int_{-\infty}^{\infty} \phi_m^*(x) \, f(x) \, dx = \int_{-\infty}^{\infty} \phi_m^*(x) \sum_n c_n \, \phi_n(x) \, dx$$

Changing the order of the integral and sum …

$$= \sum_n c_n \boxed{\int_{-\infty}^{\infty} \phi_m^*(x) \, \phi_n(x) \, dx}$$

$$= c_m$$

This is equal to 1 if $m = n$ and 0 otherwise

Measurement in Quantum Mechanics

Measurement if Ψ is an eigenfunction

- At the heart of Quantum Mechanics is the how the wavefunction is related to **measurement of observables**

- Suppose we measure a particular observable of a system (e.g. momentum, position, energy, angular momentum, etc.)

- Recapping … this observable is represented by a corresponding **operator** (we will see some examples shortly)

- If the wavefunction of the system is an **eigenfunction** of the corresponding operator ($\Psi = \phi_n$), then the result of the measurement is the corresponding **eigenvalue**, a_n

Measurement in Quantum Mechanics

Measurement if $\boldsymbol{\Psi}$ is not an eigenfunction

- If the wavefunction Ψ is **not** an eigenfunction of the corresponding operator, it can always be expressed as a **linear combination** of the eigenfunctions:

$$\Psi(x) = \sum_n c_n\, \phi_n(x)$$

- In this case, **the result of the measurement may be any one of the eigenvalues a_n, with corresponding probabilities $|c_n|^2$**

- Following the measurement, **the wavefunction "collapses"** and becomes the eigenfunction, $\Psi(x) = \phi_n(x)$

- If the observable is measured again, we'll find value a_n again

Measurement in Quantum Mechanics

Measurement if Ψ is not an eigenfunction

Measurement changes the wavefunction, causing it to "collapse" into the eigenfunction corresponding to the result of the measurement. This ensures that future measurements of the quantity produce the same result.

- It is equivalent to opening the box containing Schrödinger's cat, and seeing the result!

[Yes, cat photos are an occupational hazard here.]

Measurement in Quantum Mechanics

Measurement if Ψ is not an eigenfunction

- This gives us the **recipe for measurement in Quantum Mechanics**, represented by the following flow chart!

The state of the particle is described by its wavefunction $\Psi(x)$

We want to measure an observable A → What is the operator $\hat{A}$ corresponding to this observable? → What are the eigenfunctions $\Psi_n(x)$ and eigenvalues a_n of this operator $\hat{A}$?

Express the wavefunction as a linear combination of the eigenfunctions, $\Psi(x) = \sum_n c_n \, \phi_n(x)$ → The possible results of the measurement are the eigenvalues a_n, with probabilities $|c_n|^2$

Perform the measurement → Obtain one of the eigenvalues, a_1 → The wavefunction collapses to the corresponding eigenfunction, $\phi_1(x)$

Measurement in Quantum Mechanics

Measurement if Ψ is not an eigenfunction

***Example**: a particle in an infinite potential well in the range $|x| < L$ is prepared in the wavefunction $\Psi(x) = \frac{1}{\sqrt{5L}}\left[\cos\left(\frac{\pi x}{2L}\right) + 2\sin\left(\frac{\pi x}{L}\right)\right]$. What energy states can be measured, and with what probabilities?*

- The factor $\frac{1}{\sqrt{5L}}$ is to ensure $\Psi(x)$ is normalised: $\int_{-\infty}^{\infty}|\Psi(x)|^2\,dx = 1$
- We notice that the terms in the square bracket are the 1st and 2nd energy eigenfunctions. Substituting these in, we find $\Psi(x) = \frac{1}{\sqrt{5}}\phi_1(x) + \frac{2}{\sqrt{5}}\phi_2(x)$
- Hence, the possible measurements of the energy state are E_1 (with probability $|c_1|^2 = \left|\frac{1}{\sqrt{5}}\right|^2 = \frac{1}{5}$) and E_2 (with probability $|c_2|^2 = \left|\frac{2}{\sqrt{5}}\right|^2 = \frac{4}{5}$)
- The probabilities $\frac{1}{5}$ and $\frac{4}{5}$ sum to 1, as they should!

Measurement in Quantum Mechanics

Expectation values

- Although we can't predict exactly which value will result from a measurement (only their probabilities), we can predict the **mean measurement**, also known as the **expectation value** – which has the symbol of angled brackets, $\langle a \rangle$

$$\langle a \rangle = \sum_n \mathrm{Prob}(n)\, a_n$$

- **Example**: what is the expectation value when a dice is thrown?

$$\langle a \rangle = \frac{1}{6} \cdot 1 + \frac{1}{6} \cdot 2 + \frac{1}{6} \cdot 3 + \frac{1}{6} \cdot 4 + \frac{1}{6} \cdot 5 + \frac{1}{6} \cdot 6 = 3.5$$

[Note: the value 3.5 *cannot be obtained for any individual throw of the dice, but is the average over many throws!]*

Measurement in Quantum Mechanics

Expectation values

- In Quantum Mechanics, we have seen that $\text{Prob}(n) = |c_n|^2$

$$\langle a \rangle = \sum_n \text{Prob}(n)\, a_n = \sum_n |c_n|^2\, a_n$$

- **Example**: for the particle in the infinite potential well 2 slides back, $\langle E \rangle = \frac{1}{5} E_1 + \frac{4}{5} E_2$
- We can also find a general relation by substituting in $c_n = \int_{-\infty}^{\infty} \Psi(x)\, \phi_n^*(x)$ and using the orthogonality relation:

$$\langle a \rangle = \int_{-\infty}^{\infty} \Psi^*(x)\, \hat{A} \Psi(x)\, dx$$

Summary

The rules of Quantum Mechanics

- The state of a particle is described by the wavefunction $\Psi(x,t)$, which satisfies the Schrödinger equation, $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\,\Psi = i\hbar\frac{\partial\Psi}{\partial t}$
- The probability of a particle being located at a position in the range $[x, x + dx]$ at time t is $|\Psi(x,t)|^2$
- Physical observables are represented by operators, and the possible results of measuring an observable are the eigenvalues a_n of those operators
- Any wavefunction can be expressed as a linear combination of the eigenfunctions of these operators: $\Psi = \sum_n c_n \phi_n$. The probability of measuring the eigenvalue a_n is then $|c_n|^2$
- If a measurement of an observable yields a result a_n, the wavefunction collapses into the corresponding eigenfunction, $\Psi = \phi_n$