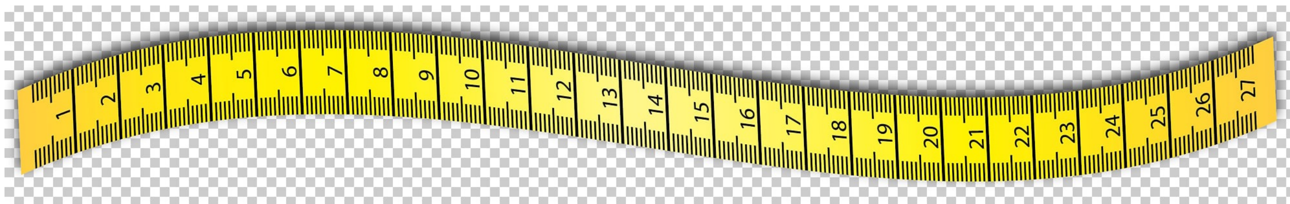
Section 2: How QM Works, Part 2

In these slides we will cover:

- The momentum operator and its eigenfunctions
- The position and energy operators
- The time-independent Schrödinger equation and energy eigenfunctions
- Commutation between operators
- Implication for simultaneous (or compatible) observables
- The uncertainty principle
- The time-dependent Schrödinger equation
- Solving the time-evolving wavefunction

Momentum, position & energy operators

Recipe for measurement in Quantum Mechanics (recap)



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 $\phi_n(x)$ 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 $|c_n|^2$

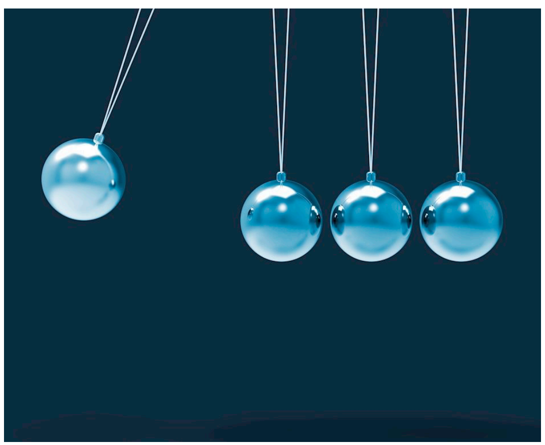
Perform the measurement → Obtain one of the eigenvalues, a_1 → The wavefunction collapses to the corresponding eigenfunction, $\phi_1(x)$

Momentum, position & energy operators

The key observables for a particle

- We saw in the last section that **observables are represented by operators** in Quantum Mechanics. Let's consider:

Momentum ***Position*** ***Energy***



- *Which operators represent these observables, and what does this imply for measurements of these quantities?*

Momentum, position & energy operators

The momentum operator

- The **momentum** operator for a particle moving in 1D is

$$\hat{p} = -i\hbar\frac{d}{dx}$$

- The momentum operator $\hat{p}$ differentiates a function with respect to x, then multiplies the result by the constant $-i\hbar$

- The "i" seems strange, but remember that the operator acts on a wavefunction, which can be a complex number

- Using the definition of eigenfunctions and eigenvalues, $\hat{p}\phi(x) = a\phi(x)$, we can see that $\phi(x) = e^{ipx/\hbar}$ is an eigenfunction of momentum with eigenvalue $a = p$

Momentum, position & energy operators

Momentum eigenfunctions

- To determine which values of momentum can be measured from a given wavefunction, and their corresponding probabilities, we can apply the usual QM rules

- We express the (normalised) wavefunction $\psi(x)$ of a particle as a sum over the eigenfunctions of momentum:

$$\psi(x) = \sum_n c_n \, \phi_n(x) = \sum_n c_n \, e^{ip_n x/\hbar}$$

- The probabilities of obtaining values p_n are then $|c_n|^2$

Momentum, position & energy operators

Momentum eigenfunctions

- **Example**: what momentum values can be measured for a particle in the ground state of an infinite well in the region $|x| < L$, which has wavefunction $\psi(x) = \frac{1}{\sqrt{L}} \cos\left(\frac{\pi x}{2L}\right)$?

- To express this wavefunction as a sum of complex exponentials, we can use the mathematical relation $\cos\theta = \left(e^{i\theta} + e^{-i\theta}\right)/2$. We find: $\psi(x) = \frac{1}{2\sqrt{L}}\left(e^{i\pi x/2L} + e^{-i\pi x/2L}\right)$. [Also useful: $\sin\theta = \left(e^{i\theta} - e^{-i\theta}\right)/2i$]

- Now let's compare this expression with the momentum eigenfunctions $\phi(x) \propto e^{ipx/\hbar}$. We can see that $\psi(x)$ is a sum of two eigenfunctions, with eigenvalues $p = \pm\frac{\pi\hbar}{2L}$, and **these are the 2 possible momentum values**

Momentum, position & energy operators

The position operator

- The operator for the **position** of a particle, $\hat{x}$, has a particularly simple form:

$$\hat{x} = x$$

- Applying $\hat{x}$ to a function just involves multiplying the function by x : $\hat{x}\, f(x) = x \cdot f(x)$

- [In case you're wondering, the eigenfunctions of $\hat{x}$ are the "Dirac delta functions" of x, $\delta_D(x)$, but this piece of maths isn't part of our course.]

- We'll soon return to the position operator when we discuss the uncertainty principle in upcoming slides!

Momentum, position & energy operators

The energy operator

- The **energy operator** has a special role in Quantum Mechanics and is also known as the **Hamiltonian**, $\hat{H}$

- The form of the energy operator can be deduced by analogy with classical mechanics. For a **free particle**, $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

- For a **particle moving in a potential**, $E = \frac{p^2}{2m} + V(x)$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Momentum, position & energy operators

Energy eigenfunctions

- The eigenfunctions of the energy operator are solutions of

$$\hat{H}\,\psi(x) = E\,\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)$$

- This is known as the **time-independent Schrödinger equation**, and its solutions are the energy eigenfunctions $\psi_n(x)$ with corresponding energy eigenvalues E_n

- The time-independent Schrödinger equation is a typical starting point for QM problems, and we'll see some examples of this in the next Section

Commuting operators & compatible observables

Compatible observables

- We have discussed the rules for measuring a single observable such as the momentum, position or energy of a particle
- The outcome of measuring an observable is uncertain, **unless the wavefunction is an eigenfunction of the operator** – in which case we'll always measure the corresponding eigenvalue
- **Can more than one observable be simultaneously known?** Can a function be an eigenfunction of multiple operators?
- This question will involve a short mathematical detour into the idea of **commuting operators**

Commuting operators & compatible observables

Commuting operators

- Two operators $\hat{A}$ and $\hat{B}$ **commute** if for any function $f(x)$

$$\hat{A}\,\hat{B}\,f(x) = \hat{B}\,\hat{A}\,f(x)$$

- If two operators commute, it doesn't matter in which order we apply the operators to a function, we'll find the same result

- **Example of commuting operators**: $\hat{A} = \frac{d}{dx}$ and $\hat{B} = \frac{d^2}{dx^2}$. These operators commute because $\hat{A}\hat{B}f = \hat{B}\hat{A}f = \frac{d^3 f}{dx^3}$

- **Example of non-commuting operators**: $\hat{A} = \frac{d}{dx}$ and $\hat{B} = x$. In this case, $\hat{A}\hat{B}f = \frac{d}{dx}(xf) = f + x\frac{df}{dx}$; and $\hat{B}\hat{A}f = x\frac{df}{dx} \neq \hat{A}\hat{B}f$

Commuting operators & compatible observables

Commutators

- Whether or not operators commute is so important that we define a special symbol, the **commutator** of the operators:

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\,\hat{B}\; - \hat{B}\;\hat{A}$$

- If $\hat{A}$ and $\hat{B}$ commute then the operator $\left[\hat{A}, \hat{B}\right]$ will give **zero** when applied to a function, since $\hat{A}\hat{B}f - \hat{B}\hat{A}f = 0$

- **Example 1**: if $\hat{A} = \frac{d}{dx}$ and $\hat{B} = \frac{d^2}{dx^2}$, then $\left[\hat{A}, \hat{B}\right] = 0$ because $\hat{A}\hat{B}f - \hat{B}\hat{A}f = 0$, for any function f

- **Example 2**: if $\hat{A} = \frac{d}{dx}$ and $\hat{B} = x$, then $\left[\hat{A}, \hat{B}\right] = 1$ because $\hat{A}\hat{B}f - \hat{B}\hat{A}f = f + x\frac{df}{dx} - x\frac{df}{dx} = f$, for any function f

Commuting operators & compatible observables

Commutators

- Here are some key results concerning the commutators of the position operator $\hat{x}$, momentum operator $\hat{p}$ and energy operator $\hat{H}$:

$$[\hat{x}, \hat{p}] = i\hbar$$

$$[\hat{H}, \hat{p}] = 0 \quad \text{if } V(x) = \text{constant}$$

- The position and momentum operators **do not commute**
- The position and energy operators **do commute** for a particle moving in a constant potential $V(x) = V_0$

Commuting operators & compatible observables

Simultaneous eigenfunctions and observables

- If two operators $\hat{A}$ and $\hat{B}$ commute, then **an eigenfunction of operator $\hat{A}$ is simultaneously an eigenfunction of operator $\hat{B}$**

- Non-examinable: let's write a quick proof of this result. Any function may be expanded as a sum of eigenfunctions, $f(x) = \sum_n c_n \phi_n(x)$

- Now we use the relations $\hat{A}\phi_n = a_n \phi_n$ and $\hat{B}\phi_n = b_n \phi_n$:

$$[\hat{A}, \hat{B}]f = \hat{A}\hat{B}f - \hat{B}\hat{A}f = \hat{A}\hat{B}\sum_n c_n \phi_n(x) - \hat{B}\hat{A}\sum_n c_n \phi_n(x)$$

$$= \sum_n c_n \left[\hat{A}\hat{B}\phi_n(x) - \hat{B}\hat{A}\phi_n(x)\right] = \sum_n c_n \left[\hat{A} b_n \phi_n(x) - \hat{B} a_n \phi_n(x)\right]$$

$$= \sum_n c_n \left[b_n \hat{A}\phi_n(x) - a_n \hat{B}\phi_n(x)\right] = \sum_n c_n \left[b_n a_n \phi_n(x) - a_n b_n \phi_n(x)\right] = 0$$

Commuting operators & compatible observables

Simultaneous eigenfunctions and observables

- **If two operators $\hat{A}$ and $\hat{B}$ commute, what happens when we measure their corresponding observables?**

Particle initially has any wavefunction Ψ

→ We measure observable A and obtain result a_n, an eigenvalue of $\hat{A}$

→ Particle now has wavefunction ϕ_n, the eigenfunction of $\hat{A}$ corresponding to a_n

→ Observable B is now measured

→ Since $\hat{A}$ and $\hat{B}$ commute, the wavefunction ϕ_n is also an eigenfunction of $\hat{B}$

→ We obtain result equal to eigenvalue b_n, wavefunction doesn't change

→ We measure observable A again and obtain an unchanged result a_n

A and B can be simultaneously known

Commuting operators & compatible observables

Simultaneous eigenfunctions and observables

- Relating this to our previous examples …

$[\hat{x}, \hat{p}] = i\hbar$ → The position and momentum operators **do not commute** → Position and momentum **cannot** be simultaneously known

$[\hat{H}, \hat{p}] = 0$ (if $V(x) =$ constant) → The energy and momentum operators **do commute** (if $V(x) =$ constant) → Energy and momentum **can** be simultaneously known (if $V(x) =$ constant)

Commuting operators & compatible observables

Simultaneous eigenfunctions and observables

- We can summarise it as follows:
- **Certain pairs of observables can be simultaneously known, i.e. repeated measurements will produce the same values**
- These have commuting operators (are "compatible")
- **Certain pairs of observables can't be simultaneously known, i.e. repeated measurements will produce different values**
- These observables have non-commuting operators

Commuting operators & compatible observables

The uncertainty principle

- The concept that two observables cannot be simultaneously known, if their corresponding operators do not commute, is known as the **uncertainty principle** (for pairs of observables)

- A good example is **momentum** and **position**. We have seen that a particle with a precisely known momentum p has a wavefunction $\psi(x) = e^{ipx/\hbar}$ (an eigenfunction of momentum)

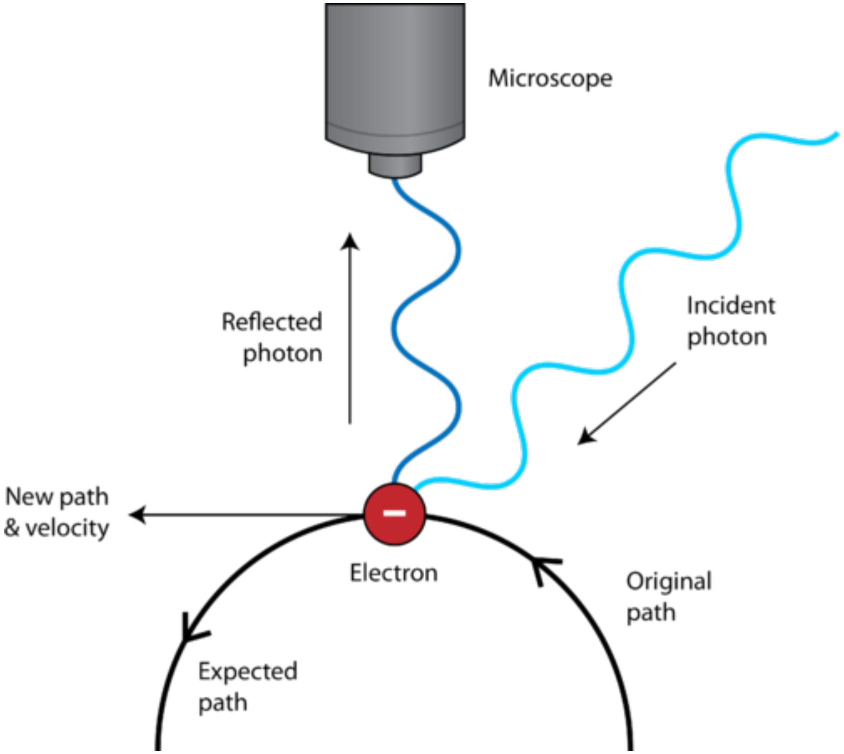
- The probability of finding the particle in space is then, $|\psi(x)|^2 = 1$ – the particle is infinitely extended in space!

- **Exact knowledge of momentum means no knowledge of position** – this is the uncertainty principle

Commuting operators & compatible observables

The uncertainty principle

- The uncertainty principle is sometimes described as the act of measuring a particular property (such as position) causes an uncertainty in another property (such as momentum)



If an electron is prepared in a state of known momentum, the act of measuring its position perturbs its momentum

Commuting operators & compatible observables

Relation of the uncertainty principle to commutators

- The uncertainty principle can be precisely described mathematically using commutators and expectation values:

If $\left[\hat{A},\hat{B}\right]=i\hat{C}$, the spread of measurements of observables A and B are related by $\sigma_A\,\sigma_B\geq\frac{1}{2}\langle\hat{C}\rangle$. (Note: the spread of measurements means their standard deviation, $\sigma_A=\sqrt{\langle A^2\rangle-\langle A\rangle^2}$.)

- For the example of position and momentum: since $[\hat{x},\hat{p}]=i\hbar$, then $\sigma_x\sigma_p\geq\hbar/2$, where $\sigma_x=\sqrt{\langle x^2\rangle-\langle x\rangle^2}$

Time-evolution of the wavefunction

Postulate for the time-evolution of $\boldsymbol{\Psi}$

- The time-development of the wavefunction $\Psi(x,t)$ is given by the **time-dependent Schrödinger equation**, which we can write in the form

$$\hat{H}\,\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

- $\hat{H}$ is the Hamiltonian or energy operator, which for a particle moving in 1D is $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ [i.e., a function of x]

- We consider a **separable solution** to this equation, in which x and t are separated into different functions:

$$\Psi(x,t) = \psi(x)\,T(t)$$

Time-evolution of the wavefunction

Separable solutions and stationary states

- After substituting in this solution we obtain:

$$\frac{1}{\psi(x)}\,\hat{H}\,\psi(x) = \frac{i\hbar}{T(t)}\,\frac{dT(t)}{dt} = E$$

- We obtain the final equality using $\hat{H}\psi(x) = E\psi(x)$, if ψ is an eigenfunction of energy with eigenvalue E. In this case, we can solve the equation for T and find $T(t) = e^{-iEt/\hbar}$

- Separated solutions $\Psi(x,t) = \psi(x)\,e^{-iEt/\hbar}$ are states of **definite total energy** (i.e., they are eigenfunctions of $\hat{H}$)

- These are also called **"stationary states"**, since the probability distribution $|\Psi(x,t)|^2 = \Psi^*\Psi = |\psi(x)|^2$ is time-independent

Time-evolution of the wavefunction

The time-evolving wavefunction

- Suppose we are given the wavefunction of a particle at $t = 0$, $\Psi(x, 0)$. **How do we determine its time-evolution $\boldsymbol{\Psi(x, t)}$?**

Step 1	Express $\Psi(x, 0)$ as a linear combination of the energy eigenfunctions, $\Psi(x, 0) = \sum_n c_n \, \psi_n(x)$
Step 2	Each eigenfunction (with energy E_n) evolves forward in time according to the previous slide: $\psi_n(x) \, e^{-iE_n t/\hbar}$
Step 3	The full solution is then the linear combination $\Psi(x, t) = \sum_n c_n \, \psi_n(x) \, e^{-iE_n t/\hbar}$

Time-evolution of the wavefunction

The time-evolving wavefunction

***Example**: a particle in an infinite potential well in the range $|x| < L$ is in an the wavefunction $\Psi(x,0) = \frac{1}{\sqrt{5L}}\left[\cos\left(\frac{\pi x}{2L}\right) + 2\sin\left(\frac{\pi x}{L}\right)\right]$. What is the wavefunction at later times, $\Psi(x,t)$?*

- We have seen this example in Sec 1, where we expressed the wavefunction in terms of the energy eigenfunctions, $\Psi(x,0) = \frac{1}{\sqrt{5}}\phi_1(x) + \frac{2}{\sqrt{5}}\phi_2(x)$
- If these eigenfunctions have associated energies E_1 and E_2, we can find the time-dependent wavefunction using the rule on the previous slide, such that $\Psi(x,t) = \frac{1}{\sqrt{5}}\phi_1(x)\, e^{-iE_1 t/\hbar} + \frac{2}{\sqrt{5}}\phi_2(x)\, e^{-iE_2 t/\hbar}$
- The new $e^{-iEt/\hbar}$ factors do not change the overall normalisation of the wavefunction, such that $\int_{-\infty}^{\infty}|\Psi(x,t)|^2\, dx = 1$ at all times!

Summary

Momentum, position and energy operators

- The momentum operator is $\hat{p} = -i\hbar \frac{d}{dx}$
- The position operator is $\hat{x} = x$ (i.e., multiply by x)
- The energy operator is $\widehat{H} = \frac{\hat{p}^2}{2m} + V = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V$
- Energy eigenfunctions satisfy the time-independent Schrödinger equation, $\widehat{H}\psi_n(x) = E\psi_n(x)$

Commuting operators and compatible observables

- Two operators commute if $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$
- Commuting operators have joint eigenfunctions, whose observables can be simultaneously known
- The observables of non-commuting operators are governed by the uncertainty principle

Time evolution of the wavefunction

- The time-evolution of Ψ is given by $\widehat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$
- The solutions are $\Psi(x,t) = \sum_n c_n\, \psi_n(x)\, e^{-iE_nt/\hbar}$, where $\psi_n(x)$ are the energy eigenfunctions