UC3
Mathematical formalism of Quantum Mechanics

UC3 contents:

- Linear algebra, Hermitian operators, and Hilbert space.
- Eigenfunctions, eigenvectors, and eigenvalues for discrete and continuous spectra.
- Dirac notation and the generalised statistical interpretation.
- Operators of position and momentum and the uncertainty principle.

Mathematical Formalism of QM: vectors

QM theory is based on linear algebra:

i) Wavefunctions : states → abstract vectors (functions in ∞-dim. spaces)

ii) Operators : observables → linear transformations

Vectors in QM: $|\alpha\rangle$

They are represented by the N-tuple of its components $\{a_n\}$ with respect to a specified orthonormal basis:

$$|\alpha\rangle = a = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

Inner product: $\langle\alpha|\beta\rangle$

It's a complex number:

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \cdots + a_N^* b_N$$

Linear transformations: T

They are represented by matrices (wrt the specified basis)

$$|\beta\rangle = \hat{T}|\alpha\rangle \rightarrow b = Ta = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ t_{21} & t_{22} & & \\ \vdots & \vdots & \ddots & \\ t_{N1} & & & t_{NN} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

Hilbert space

What is new / different in QM?

- Vectors live in ∞-dim. spaces
- Manipulations that work in N-dim, may not work in ∞-dim.

Vector space:

It is the collection of all functions of x.
Wave functions must be normalized to represent possible physical states.

$$\int |\psi|^2 dx = 1$$

$\Rightarrow$ they must be square-integrable functions, on an interval.

Hilbert space: $L^2(a,b)$

It is a vector space that contains the set of all square-integrable functions

Wave functions in QM $\in$ Hilbert space.

$$f(x) \rightarrow \int_a^b |f(x)|^2 dx < \infty$$

Inner products

Inner product of 2 functions: $f(x)$ ^ $g(x)$

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\,dx$$

if $f, g \in H \Rightarrow \langle f|g\rangle$ is guaranteed to exist.

converges to a finite number.

Schwarz inequality:

$$\left|\int_a^b f(x)^* g(x)\,dx\right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$$

Properties:

1) $\langle g|f\rangle = \langle f|g\rangle^*$

2) $\langle f|f\rangle = \int_a^b |f(x)|^2 dx. \Rightarrow \langle f|f\rangle \in \mathbb{R}\ , >0$ (unless $f(x)=0$)

3) A function is normalised if $\langle f|f\rangle = 1$

Inner products

4) Two functions are orthogonal if $\langle f|g\rangle = 0$

5) $\{f_n\}$ (a set of functions) is orthonormal if normalised and mutually orthogonal.

$$\langle f_m|f_n\rangle = \delta_{mn}$$

6) A set of functions is complete if any other function, $\in H$, can be expressed as a linear combination:

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

If $\{f_n\}$ are orthonormal, $c_n = \langle f_n|f\rangle$ (Fourier's trick)

Observables

Observables: $Q(x,p)$ constructed from Q with $p \to i\hbar \frac{d}{dx}$

Hermitian Operators:

Expectation value of $Q(x,p)$ is an inner product:

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi \, dx = \langle \Psi | \hat{Q} \Psi \rangle$$

This is the outcome of a measurement, so:

$$\langle Q \rangle = \langle Q \rangle^*$$

$$\Rightarrow \langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle \quad \text{for any } \Psi.$$

Operators representing observables:

$$\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle \quad \text{for all } f(x).$$

We call $\hat{Q}$ Hermitian operators.

Hermitian Operators and Determinate States

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}g|f\rangle \text{ for all } f(x) \wedge g(x).$$

Hermitian conjugate/adjoint: $\hat{Q}^\dagger$ of $\hat{Q}$

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}^\dagger f|g\rangle \text{ for all } f \wedge g.$$

$$\Rightarrow \hat{Q} = \hat{Q}^\dagger$$

Determinate states:

- Ensemble of identically prepared systems, all in Ψ.
- We don't get the same answer due to Q.M. indeterminacy.

Can we prepare determinate states for Q?

- Stationary states are determinate states of $\hat{H}$.
- A measurement of E for Ψ_n returns E_n.

Determinate States

1) σ of $Q = 0$: (every measurement gives q) $\Rightarrow \langle Q \rangle = q$

$$\sigma^2 = \langle (Q - \langle Q \rangle)^2 \rangle = \langle \Psi | (\hat{Q} - q)^2 \Psi \rangle$$

$$= \langle (\hat{Q} - q)\Psi | (\hat{Q} - q)\Psi \rangle = 0$$

2) $\hat{Q}$ and $\hat{Q} - q$ are Hermitian operators.

3) The only vector whose inner product with itself vanishes is 0

$\Rightarrow \hat{Q}\psi = q\psi$ (eigenvalue eq.)

eigenvalue ↗ ↖ eigenfunction of $\hat{Q}$

4) The determinate states of Q are eigenfunctions of $\hat{Q}$

5) A measurement of Q on such states yields q.

6) $\Psi = 0$ excluded as eigenfunction. $\hat{Q}\,0 = q\,0 = 0$

7) q could be zero

Spectrum

It is the collection of all eigenvalues;
When 2 or more linearly independent share the same eigenvalue, spectrum is degenerate.
Determinate states of the total E are eigenfunctions of $\hat{H}$

$$\hat{H}\psi = E\psi$$

(time-independent Sch. eq)

Eigenfunctions of a Hermitian operator:

These are determinate states of observables
There are 2 categories:
① Discrete spectra

② Continuous spectra

Types of Spectra

① Discrete spectra ⇒ eigenfunctions $\in H$
they are physically realisable states.

② Continuous spectra ⇒ eigenfunctions are not normalisable
do not represent wave functions.
linear combinations may be normalisable

Example of 1: Hamiltonian for harmonic oscillator.

Example of 2 Hamiltonian for free particles.

Both 1 and 2: Hamiltonian for finite square well.

I) Discrete Spectra:

Inner products are guaranteed to exist.
We have eigenvectors of a Hermitian matrix.

Discrete Spectra

Normalisable eigenfunctions have two properties:

1) Their eigenvalues are $\mathbb{R}$.

Suppose: $\hat{Q}f = qf$, $f(x)$ is an eigenfunction of $\hat{Q}$ with eigenvalue q.

$\langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle$, $\hat{Q} \equiv$ Hermitian, $f(x) \in \mathbb{H}$

$$\langle f|\hat{Q}f\rangle = \int f(x)^* \hat{Q} f(x)\, dx = \int f^* q f\, dx =$$

$$= q\int f^* f\, dx = q\langle f|f\rangle = \int [\hat{Q}f]^* f\, dx = \int q^* f^* f\, dx$$

$$= q^* \int f^* f\, dx = q^* \langle f|f\rangle$$

$$\Rightarrow q\langle f|f\rangle = q^* \langle f|f\rangle$$

$$\Rightarrow (q - q^*)\langle f|f\rangle = 0 \Rightarrow \boxed{q = q^*} \Rightarrow q \in \mathbb{R}$$

Discrete Spectra

Normalisable eigenfunctions have two properties:

2) Eigenfunctions belonging to distinct eigenvalues are orthogonal.

Suppose: $\hat{Q}f = qf$; $\hat{Q} \equiv$ Hermitian ; $f, g \in \mathbb{H}$
$\hat{Q}g = q'g$

$$\Rightarrow \langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$$

$$\langle f|\hat{Q}g\rangle = \int f^*\hat{Q}g\,dx = \int f^* q' g\,dx = q'\int f^* g\,dx = q'\langle f|g\rangle$$

$$\langle \hat{Q}f|g\rangle = \int [\hat{Q}f]^* g\,dx = \int q^* f^* g\,dx = q^*\int f^* g\,dx = q^*\langle f|g\rangle$$

$$\Rightarrow q'\langle f|g\rangle = q^*\langle f|g\rangle$$

$$\Rightarrow (q' - q^*)\langle f|g\rangle = 0 \Rightarrow \boxed{\langle f|g\rangle = 0} \Rightarrow f \wedge g \text{ are orthogonal.}$$

<u>Notes</u>:

① Stationary states of the ∞ □ well or harmonic oscillator are orthogonal because they are eigenfunctions of $\hat{H}$ with distinct eigenvalues.

Discrete Spectra

2) This holds for any determinate state of any observable.

3) If 2 or more eigenfunctions share the same eigenvalue ($q = q'$), any linear combination of them is itself an eigenfunction with the same eigenvalue (degenerate states)
We can use the Gram-Schmidt orthogonalisation procedure to construct orthogonal eigenfunctions within each degenerate subspace.

1) Eigenfunctions can always be chosen to be orthonormal, so we can use the Fourier's trick.

In a finite-dimensional vector space:

3) Eigenfunctions of an observable operator are <u>complete</u>: any function $\in \mathbb{H}$ can be expressed as a linear combination of them
This is an axiom, or restrictions on the class of Hermitian op. that can represent observables.

Gramm-Schmidt orthogonalisation procedure

We start out with a basis that is not orthonormal

$|e_1\rangle, |e_2\rangle, |e_3\rangle, \ldots, |e_n\rangle$

The Gram-Schmidt procedure allows us to generate an orthonormal basis

$|e_1'\rangle, |e_2'\rangle, |e_3'\rangle, \ldots |e_n'\rangle$

Method:

i) Normalise the first vector basis:

$$|e_1'\rangle = \frac{|e_1\rangle}{\|e_1\|}$$ by dividing by its norm.

ii) Find the projection of the second vector along the first, and subtract it off:

$$|e_2\rangle - \langle e_1'|e_2\rangle|e_1'\rangle$$

which is orthogonal to $|e_1'\rangle$

Gramm-Schmidt orthogonalisation procedure

iii) Normalise it to get $|e_2'\rangle$

iv) subtract from $|e_3\rangle$ its projections along $|e_1'\rangle$ and $|e_2'\rangle$:

$$|e_3\rangle - \langle e_1'|e_3\rangle|e_1'\rangle - \langle e_2'|e_3\rangle|e_2'\rangle$$

which is orthogonal to $|e_1'\rangle \wedge |e_2'\rangle$

v) Normalise to get $|e_3'\rangle$, and so on.

Problem:

What is the Fourier transform of $\delta(x)$?

Plancherel's theorem:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-ikx}\, dx$$

$$\Rightarrow \quad F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x)\, e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}}$$

$$\therefore \quad \delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}}\, e^{ikx}\, dk = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx}\, dx$$

Gramm-Schmidt orthogonalisation procedure

Problem:

Knowing that: $\int_{-\infty}^{+\infty} f(x) D_1(x)\,dx = \int_{-\infty}^{+\infty} f(x) D_2(x)\,dx$

where $D_1(x) \wedge D_2(x)$ are expressions involving delta functions.

show that: $\delta(cx) = \frac{1}{|c|}\delta(x)$; $c \in \mathbb{R}$

$$\int_{-\infty}^{+\infty} f(x)\,\delta(cx)\,dx = \int_{-\infty}^{+\infty} \frac{1}{|c|} f\left(\frac{y}{c}\right)\delta(y)\,dy = \frac{1}{|c|} f(0) = \int_{-\infty}^{+\infty} f(x)\frac{1}{|c|}\delta(x)\,dx$$

$y = cx$

$\Rightarrow dy = c\,dx$

$$\Rightarrow \boxed{\delta(cx) = \frac{1}{|c|}\delta(x)}$$

Continuous Spectra

If the spectrum of a Hermitian operator is continuous, the eigenfunctions are not normalisable.

Proofs of theorems 1 ^ 2 fail because inner products may not exist.

Three essential properties:

① Reality

② Orthogonality

③ Completeness

still hold.

Let's see via examples:

Exercise:

Find the eigenfunctions and eigenvalues of the momentum operator on the interval $-\infty < x < \infty$

Let $f_p(x)$ be the eigenfunction and p the eigenvalue:

$$-i\hbar \frac{d}{dx} f_p(x) = p f_p(x)$$

Continuous Spectra

$$\Rightarrow \frac{df_p}{dx} = \frac{ip}{\hbar} f_p \Rightarrow \frac{df_p}{f_p} = \frac{ip}{\hbar} dx \Rightarrow \ln(f_p) = \frac{ipx}{\hbar} + C_1$$

$$\Rightarrow \boxed{f_p = A e^{\frac{ip}{\hbar}x}}$$

This is not square-integrable for any $\mathbb{C}$ value of p.
The momentum operator has no eigenfunctions in $\mathbb{H}$ space.

But, if we restrict ourselves to $\mathbb{R}$ eigenvalues:

$$\int_{-\infty}^{+\infty} f_{p'}^*(x) f_p(x)\, dx = |A|^2 \int_{-\infty}^{+\infty} e^{\frac{i(p-p')x}{\hbar}} dx = |A|^2 (2\pi)\hbar\, \delta(p-p')$$

Remember that:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk$$

$$\delta(cx) = \frac{1}{|c|} \delta(x)$$

↳ orthonormality

$$\Rightarrow \boxed{A = \frac{1}{\sqrt{2\pi\hbar}}}$$

Continuous Spectra

Therefore:

$$f_p = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ip}{\hbar}x}$$

$$\Rightarrow \boxed{\langle f_{p'} | f_p \rangle = \delta(p-p')}$$

Kronecker delta → Dirac delta

Dirac orthonormality

indices are continuous variables

Eigenfunctions with $\mathbb{R}$ eigenvalues are complete.

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x) \Rightarrow f(x) = \int_{-p}^{p} c(p) f_p(x) dp$$

$$f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} c(p) e^{\frac{ipx}{\hbar}} dp$$

(This expansion is a Fourier transform)

The coefficients $c(p)$ are obtained via Fourier's trick.

$$\langle f_{p'} | f \rangle = \int_{-\infty}^{+\infty} c(p) \langle f_{p'} | f_p \rangle dp = \int_{-\infty}^{+\infty} c(p) \delta(p-p') dp = c(p')$$

Continuous Spectra

I) $\int \psi_m(x)^* f(x)\,dx = \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \psi_n(x)\,dx = \sum_{n=1}^{\infty} c_n \delta_{nm} = c_m$

with: $f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$

II) Plancherel's theorem:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx}\,dk \iff \overbrace{F(k)}^{\text{F.T.}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx}\,dx$$

↳ i.F.T.

The eigenfunctions of momentum are sinusoidal with:

$$\lambda = \frac{2\pi\hbar}{p} \qquad \text{(de Broglie formula)}$$

There are no particles with determinate p, but we can construct a normalisable wavepacket with a narrow set of p, to which the above formula applies.

Continuous Spectra

None of the eigenfunctions of $\hat{p}$ lives in $\mathbb{H}$, but a certain family of them with $\mathbb{R}$ eigenvalues reside nearby with quasi-normalisability.

They do NOT represent possible physical states, but are useful.

Exercise:

Find the eigenfunctions and eigenvalues of $\hat{x}$:

Let $g_y(x) \to$ eigenfunction

$y \to$ eigenvalue (fixed number)

$$\Rightarrow \hat{x} g_y(x) = \underset{\substack{\uparrow \\ \text{continuous}}}{x}\, g_y(x) = \underset{\substack{\uparrow \\ \text{fixed}}}{y}\, g_y(x)$$

What function has the property that multiplying it by x is the same as multiplying it by a constant?

$\hookrightarrow g_y(x) = 0$, except at $x = y$

$\Rightarrow g_y(x) = A\,\delta(x-y) \quad \to$ Dirac delta

Continuous Spectra

Notes:

① $y \in \mathbb{R}$

② $g_y(x)$ are not square integrable.

③ they admit Dirac orthonormality, e.g. $\left\{ \begin{matrix} y \\ y' \end{matrix} \right\}$ are eigenvalues:

$$\Rightarrow \int_{-\infty}^{+\infty} g_{y'}^*(x)\, g_y(x)\, dx = |A|^2 \int_{-\infty}^{+\infty} \delta(x-y')\,\delta(x-y)\, dx$$

$$= |A|^2\, \delta(y-y')$$

Let's pick $A = 1$: $\quad g_y(x) = \delta(x-y)$

$$\Rightarrow \langle g_{y'} | g_y \rangle = \delta(y-y')$$

What about completeness?

$$f(x) = \int_{-\infty}^{+\infty} c(y)\, g_y(x)\, dy = \int_{-\infty}^{+\infty} c(y)\, \delta(x-y)\, dy$$

$$\uparrow$$

$$c(y) = f(y)$$

Continuous Spectra

Notes:

If the spectrum of a Hermitian op. is continuous, the eigenvalues are labeled by a continuous variable (p), the eigenfunctions are not normalisable, they $\notin \mathbb{H}$, so they are not possible physical states

The eigenfunctions with $\mathbb{R}$ eigenvalues are Dirac normalisable and complete ($\Sigma \to \int$)

This is all that is required!

Note that the entire space of functions, including those in the "suburbs" of the Hilbert space, is sometimes called a "rigged Hilbert space".

Generalised Statistical Interpretation

This allows us to study the possible results of any measurement and their probabilities.

It is the foundation of QM (jointly with Sch. eq).

It states the following:

"If you measure an observable $Q(x,p)$ on a particle in state $\Psi(x,t)$, you are certain to get one of the eigenvalues of the Hermitian operator $\hat{Q}\left(x, -i\hbar\frac{d}{dx}\right)$. If the spectrum of $\hat{Q}$ is discrete, the probability of getting the particular q_n associated with the orthonormalised eigenfunction $f_n(x)$ is:

$$|c_n|^2, \quad \text{where} \quad c_n = \langle f_n | \Psi \rangle$$

If the spectrum is continuous, with $\mathbb{R}$ eigenvalues $q(z)$ and associated (Dirac-orthonormalised) eigenfunctions $f_z(x)$, the probability of getting a result in the range dz is:

$$|c(z)|^2 dz, \quad \text{where} \quad c(z) = \langle f_z | \Psi \rangle$$

Upon measurement, the Ψ collapses to the corresponding eigenstate."

Generalised Statistical Interpretation

The eigenfunctions of an observable operator are complete.

$$\Psi(x,t) = \sum_n c_n(t) f_n(x) \qquad (\text{when } \hat{Q} = \hat{H},\ c_n \equiv \text{constants})$$

The coefficients are given by Fourier's trick:

$$c_n(t) = \langle f_n | \Psi \rangle = \int f_n(x)^* \, \Psi(x,t)\, dx$$

c_n tells us how much f_n is contained in Ψ.

$$\boxed{\sum_n |c_n|^2 = 1}\ , \qquad |c_n|^2 \equiv \text{prob. that measuring } \hat{Q} \text{ gives } q_n.$$

particle in Ψ will be in f_n

Proof:

$$\langle \Psi | \Psi \rangle = 1 \Rightarrow \left\langle \left(\sum_{n'} c_{n'} f_{n'} \right) \middle| \left(\sum_n c_n f_n \right) \right\rangle = \sum_{n'} \sum_n c_{n'}^* c_n \langle f_{n'} | f_n \rangle =$$

$$= \sum_{n'} \sum_n c_{n'}^* c_n \delta_{n'n} = \sum_n c_n^* c_n = \sum_n |c_n|^2 = 1$$

Expectation value of Q:

$$\boxed{\langle Q \rangle = \sum_n q_n |c_n|^2}$$

$|c_n|^2$ → prob. of getting q_n

q_n: all possible outcomes of q_n

Generalised Statistical Interpretation

Proof:

$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle = \langle \left(\sum_{n'} c_{n'} f_{n'} \right) \Big| \left(\hat{Q} \sum_{n} c_n f_n \right) \rangle$, knowing that $\hat{Q} f_n = q_n f_n$

$\Rightarrow \langle Q \rangle = \sum_{n'} \sum_{n} c_{n'}^* c_n q_n \langle f_{n'} | f_n \rangle = \sum_{n'} \sum_{n} c_{n'}^* c_n q_n \delta_{n'n} = \sum_{n} |c_n|^2 q_n$ //

Can we reproduce the original statistical interpretation?

every $\mathbb{R}$ "y" is an eigenvalue of $\hat{x}$.

The Dirac orthonormalised eigenfunction is $g_y(x) = \delta(x-y)$

$\Rightarrow c(y) = \langle g_y | \Psi \rangle = \int_{-\infty}^{+\infty} \delta(x-y) \Psi(x,t)\, dx = \Psi(y,t)$

$\therefore$ the prob. of getting a result in the range dy is $|\Psi|^2 dy$
which is the original statistical interpretation.

Generalised Statistical Interpretation

For momentum?

Dirac orthonormalised eigenfunctions of p: $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}}$

$$\Rightarrow c_p = \langle f_p | \Psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-\frac{ipx}{\hbar}} \Psi(x,t)\, dx$$

which is called the "momentum space wave function", $\Phi(p,t)$

This is the Fourier transform of the (position space) wave function, $\Psi(x,t)$, which is its inverse Fourier transform.

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-\frac{ipx}{\hbar}} \Psi(x,t)\, dx$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{+\frac{ipx}{\hbar}} \Phi(p,t)\, dp$$

The prob. that a measurement of p yields a result with dp,

$$|\Phi(p,t)|^2 dp$$

The Generalised Uncertainty Principle

The uncertainty principle: $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

Generalised uncertainty principle:

Any observable A:

$$\sigma_A^2 = \langle (\hat{A} - \langle A \rangle)\Psi | (\hat{A} - \langle A \rangle \Psi \rangle = \langle f | f \rangle$$

where $f = (\hat{A} - \langle A \rangle)\Psi$

Any other observable B:

$$\sigma_B^2 = \langle g | g \rangle$$

where $g = (\hat{B} - \langle B \rangle)\Psi$

We can invoke Schwarz inequality

$$\sigma_A^2 \sigma_B^2 = \langle f | f \rangle \langle g | g \rangle \geq |\langle f | g \rangle|^2$$

Remember:

$$|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 \geq [\mathrm{Im}(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2$$

If $z = \langle f | g \rangle$,

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\left[\langle f | g \rangle - \langle g | f \rangle\right]\right]^2$$

The Generalised Uncertainty Principle

Hermiticity of $\hat{A} - \langle A \rangle$

$$\langle f|g\rangle = \langle (\hat{A} - \langle A\rangle)\Psi | (\hat{B} - \langle B\rangle)\Psi\rangle = \langle \Psi | (\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)\Psi\rangle$$

$$= \langle \Psi | (\hat{A}\hat{B} - \hat{A}\langle B\rangle - \hat{B}\langle A\rangle + \langle A\rangle\langle B\rangle)\Psi\rangle$$

$$= \langle \Psi | \hat{A}\hat{B}\Psi\rangle - \langle B\rangle\langle \Psi|\hat{A}\Psi\rangle - \langle A\rangle\langle \Psi|\hat{B}\Psi\rangle + \langle A\rangle\langle B\rangle\langle \Psi|\Psi\rangle$$

$$= \langle \hat{A}\hat{B}\rangle - \langle B\rangle\langle A\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle$$

$$\langle g|f\rangle = \langle \hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle$$

$$\langle f|g\rangle - \langle g|f\rangle = \langle \hat{A}\hat{B}\rangle - \langle \hat{B}\hat{A}\rangle = \langle [\hat{A},\hat{B}]\rangle,$$

where $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

Commutator of 2 operators:

$$\Rightarrow \quad \sigma_A^2 \sigma_B^2 \geq \Big(\underbrace{\frac{1}{2i}\langle [\hat{A},\hat{B}]\rangle}_{\in \mathbb{R}}\Big)^2 > 0$$

Uncertainty principle for every pair of observables whose operators do not commute **(incompatible observables).**

Compatible versus incompatible observables.

Incompatible observables:
They do not have a complete set of common eigenfunctions.

Compatible observables:
They do admit a complete set of simultaneous eigenfunctions (states that are determinate for both observables).

Notes:
- The uncertainty principle is a consequence of the statistical interpretation.
- A second measurement makes the first one obsolete because the wave function is not an eigenstate of the p and x operators.

Can we recover the original uncertainty principle?

$$\hat{A} = \hat{x} \quad , \quad \hat{B} = \hat{p} = -i\hbar \frac{d}{dx}$$

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

$$\Rightarrow \quad \sigma_x^2 \sigma_p^2 \geq \left(\frac{1}{2i} i\hbar \right)^2 = \left(\frac{\hbar}{2} \right)^2$$

$$\Rightarrow \quad \sigma_x \sigma_p \geq \frac{\hbar}{2}$$ $\Rightarrow$ Heisenberg's uncertainty principle

Minimum Uncertainty Wave Packet

The minimum-uncertainty wave packet

We have seen examples where $\sigma_x \sigma_p \geq \frac{\hbar}{2}$ $\left\{ \begin{array}{l} \text{ground state of H. osc.} \\ \text{Gaussian w.p. for free particle} \end{array} \right.$

What is the minimum uncertainty wp?

$$\left.\begin{array}{l} ① \; \sigma_A^2 \sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq \langle f|g\rangle^2 \\ ② \; |z|^2 = [Re(z)]^2 + [Im(z)]^2 \geq [Im(z)]^2 \end{array}\right\} \text{ take eq., what happens to } \psi?$$

① $\sigma_A^2 \sigma_B^2 = \langle f|g\rangle^2$ if $g(x) = c f(x)$, $c \in \mathbb{C}$

② $|z|^2 = [Im(z)]^2$ if $Re(z) = 0 \Rightarrow Re\langle f|g\rangle = Re(\underset{\mathbb{C}}{\underset{\downarrow}{c}} \overset{\nearrow \mathbb{R}}{\langle f|f\rangle}) = 0$

$\Rightarrow c = ia$

The necessary and sufficient condition for minimum uncertainty is

$$g(x) = ia f(x) \quad , \quad a \in \mathbb{R}$$

Minimum Uncertainty Wave Packet

Position - momentum:

$$\left(-i\hbar\frac{d}{dx} - \langle p\rangle\right)\Psi = ia\left(x - \langle x\rangle\right)\Psi$$

$$\Rightarrow \frac{d\psi}{dx} = \frac{i}{\hbar}\left(iax - ia\langle x\rangle + \langle p\rangle\right)\Psi = \frac{a}{\hbar}\left(-x + \langle x\rangle + \frac{i}{a}\langle p\rangle\right)\psi$$

$$\Rightarrow \frac{d\psi}{\psi} = \frac{a}{\hbar}\left(-x + \langle x\rangle + \frac{i\langle p\rangle}{a}\right)dx$$

$$\Rightarrow \ln(\psi) = -\frac{a}{2\hbar}\left(x - \langle x\rangle\right)^2 + \frac{i\langle p\rangle x}{a}x + C_1$$

$$\Rightarrow \boxed{\Psi = A\,e^{-a\frac{(x-\langle x\rangle)^2}{2\hbar}}\,e^{i\frac{\langle p\rangle x}{\hbar}}}$$

The minimum uncertainty w.p is a Gaussian

Energy-time uncertainty principle

We have an observable $Q(x,p,t)$, how fast is the system changing?

$$\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle = \langle\frac{\partial\Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle\Psi|\frac{\partial\hat{Q}}{\partial t}\Psi\rangle + \langle\Psi|\hat{Q}\frac{\partial\Psi}{\partial t}\rangle$$

The Sch. eq states: $\quad i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \quad ; \quad \hat{H} = \frac{p^2}{2m} + V$

$$\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\langle\hat{H}\Psi|\hat{Q}\Psi\rangle + \frac{1}{i\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle$$

$\hat{H}$ is Hermitian, so $\langle\hat{H}\Psi|\hat{Q}\Psi\rangle = \langle\Psi|\hat{H}\hat{Q}\Psi\rangle$

$$\Rightarrow \boxed{\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle}$$

Generalised Ehrenfest theorem.

Energy-time uncertainty principle

Let us pick $A = H$, $B = Q$, Q does not explicitly depend on t

$$\sigma_H^2 \sigma_Q^2 \geq \left(\frac{1}{2i} \langle [\hat{H}, \hat{Q}] \rangle \right)^2 = \left(\frac{1}{2i} \frac{\hbar}{i} \frac{d\langle Q \rangle}{dt} \right)^2$$

$$= \left(\frac{\hbar^2}{2} \right) \left(\frac{d\langle Q \rangle}{dt} \right)^2$$

$$\Rightarrow \sigma_H \sigma_Q \geq \frac{\hbar}{2} \left| \frac{d\langle Q \rangle}{dt} \right|$$

If $\Delta E \equiv \sigma_H$, $\quad \Delta t \equiv \dfrac{\sigma_Q}{\left| \frac{d\langle Q \rangle}{dt} \right|}$

$$\Rightarrow \boxed{\Delta E \Delta t \geq \frac{\hbar}{2}}$$ energy-time uncertainty principle.

Note: Δt represents the amount of time it takes for the expectation value of Q to change by 1 standard deviation. (Mandelstam – Tamm formulation)

Small ΔE implies gradual change (long Δt)

Small Δt implies large E uncertainty.

Vectors and Operators

I) Vectors:

Bases in $\mathbb{H}$ (Hilbert) space:

2D vector: $\vec{A} = A_x \hat{i} + A_y \hat{j}$

Components $\begin{cases} A_x = \hat{i}\cdot\vec{A} \\ A_y = \hat{j}\cdot\vec{A} \end{cases}$ components' $\begin{cases} A_x' = \hat{i}'\cdot\vec{A} \\ A_y' = \hat{j}'\cdot\vec{A} \end{cases}$

bases $\{ \{\hat{i}, \hat{j}\}, \{\hat{i}', \hat{j}'\}$

Same happens in QM.

State of a system $\mapsto$ vector $|S(t)\rangle \in \mathbb{H}$

We can express it wrt any combination of bases.

$\Rightarrow \boxed{\Psi(x,t) = \langle x | S(t)\rangle}$ is the "x" component in the expansion of $S(t)$ in the basis of $\hat{x}$ eigenfunctions, $|x\rangle$.

$\hookrightarrow \hat{i}\cdot\vec{A}$

Vectors and Operators

$\Phi(p,t) = \langle p | S(t) \rangle$ → momentum eigenfunctions $|p\rangle$ with eigenvalue p.

$C_n(t) = \langle n | S(t) \rangle$ → energy eigenfunctions $|n\rangle$ of $\hat{H}$ for a discrete spectrum

↳ $\boxed{C_n(t) = \langle f_n | \Psi \rangle = \int f_n^* \Psi \, dx}$

They are all the same state: $\Psi, \Phi, \{C_n\}$ contain same information.

3 ways of identifying the same vector

$$|S(t)\rangle \to \int \Psi(y,t)\,\delta(x-y)\,dy = \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}\, e^{i\frac{px}{\hbar}}\,dp =$$

$$= \sum c_n\, e^{-i\frac{E_n t}{\hbar}}\, \psi_n(x)$$

II) Operators: (represent observables)

$$|\beta\rangle = \hat{Q}\,|\alpha\rangle$$

↑

linear transformations on $\mathbb{H}$ space

Vectors and Operators

Vectors are represented wrt an orthonormal basis $\{|e_n\rangle\}$ by comp.

$$|\alpha\rangle = \sum_n a_n |e_n\rangle, \qquad |\beta\rangle = \sum_n b_n |e_n\rangle$$

$\uparrow$ discrete basis

$$a_n = \langle e_n|\alpha\rangle \qquad b_n = \langle e_n|\beta\rangle$$

Operators are represented wrt a basis by matrix elements,

$$\langle e_m|\hat{Q}|e_n\rangle \equiv Q_{mn}$$, so $|\beta\rangle = \hat{Q}|\alpha\rangle$ becomes:

$$\Rightarrow \sum_n b_n |e_n\rangle = \sum_n a_n \hat{Q}|e_n\rangle$$

$$\Rightarrow \sum_n b_n \langle e_m|e_n\rangle = \sum_n a_n \langle e_m|\hat{Q}|e_n\rangle$$

Since $\langle e_m|e_n\rangle = \delta_{mn}$:

$$\Rightarrow \boxed{b_m = \sum_n Q_{mn} a_n} \qquad \boxed{\vec{b} = Q\,\vec{a}} \rightarrow \vec{b}_N = Q_{N\times N}\cdot \vec{a}_N$$

The matrix elements of $\hat{Q}$ tell us how the components transform.

Dirac notation

Operators look different in different basis (matrices look different)

$$\hat{x} \rightarrow \begin{cases} x \\ i\hbar \frac{\partial}{\partial p} \end{cases} \qquad \hat{p} \rightarrow \begin{cases} -i\hbar \frac{\partial}{\partial x} & \rightarrow \text{in } x \text{ space} \\ p & \rightarrow \text{in } p \text{ space} \end{cases}$$

Dirac Notation:

Inner product: $\langle \alpha | \beta \rangle$

bra: $\langle \alpha |$ → linear function of vectors
ket: $| \beta \rangle$ → vector

$\langle \alpha | \beta \rangle = \mathbb{C}$ #
instruction to integrate $\int$.

any function

$$\langle f | = \int f^* [\cdots\cdots] \, dx$$

In finite dimensional vector spaces: $\underset{\text{bra}}{\langle \beta} | \underset{\text{ket}}{\alpha \rangle}$, ket expressed as column:

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \quad \langle \beta | = \begin{pmatrix} b_1^* & b_2^* & \cdots & b_n^* \end{pmatrix},$$ bra is a row.

$$\Rightarrow \langle \beta | \alpha \rangle = b_1^* a_1 + b_2^* a_2 + \cdots + b_n^* a_n$$

Dirac notation

The collection of all bras constitutes the so-called dual space. Therefore, bras can be treated as separate entities, if $|\alpha\rangle$ is a normalised vector; the operator:

$$\hat{P} \equiv |\alpha\rangle\langle\alpha| \equiv \text{projection operator}$$

picks out the portion of any other vector that lies along $|\alpha\rangle$:

$$\hat{P}|\beta\rangle = (\langle\alpha|\beta\rangle)|\alpha\rangle$$

$\hat{P}$ is the projection operator onto a 1D subspace spanned by $|\alpha\rangle$.

If $\{|e_n\rangle\}$ is a discrete orthonormal basis,

$$\langle e_m|e_n\rangle = \delta_{mn} \quad \Rightarrow \quad \boxed{\sum_n |e_n\rangle\langle e_n| = 1} \equiv \text{identity operator.}$$

Example:

$$\sum_n (\langle e_n|\alpha\rangle)|e_n\rangle = |\alpha\rangle$$

If $\{|e_z\rangle\}$ is a Dirac-orthonormalised continuous basis:

$$\langle e_z|e_{z'}\rangle = \delta(z-z') \quad \Rightarrow \quad \boxed{\int |e_z\rangle\langle e_z|\,dz = 1} \equiv \text{identity op.}$$

Dirac notation

$$\boxed{\sum_n |e_n\rangle\langle e_n| = 1} \equiv \text{identity operator.}$$

$$\boxed{\int |e_z\rangle\langle e_z|\,dz = 1} \equiv \text{identity op.}$$

Both express completeness.

<u>Naming conventions:</u>

It is good to name vectors after the functions they represent: $|f\rangle$.

<u>Example:</u> (Hermitian operator)

$$\langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle$$

In Dirac notation:

LHS: $\langle f|\hat{Q}f\rangle = \langle f|\hat{Q}|f\rangle$

RHS: $\langle \hat{Q}f|$ is the bra dual of $\hat{Q}|f\rangle$

$\langle \hat{Q}f| = \langle f|\hat{Q}^{+}$, remember $\langle f|\hat{Q}g\rangle = \langle \hat{Q}^{+}f|g\rangle$

Hermitian conjugate / adjoint

Dirac notation

An operator takes one vector $\in \mathbb{H}$ and delivers another one.

$$\hat{Q}|\alpha\rangle = |\beta\rangle$$

Operations:

Sum of 2 operators: $(\hat{Q}+\hat{R})|\alpha\rangle = \hat{Q}|\alpha\rangle + \hat{R}|\alpha\rangle$

Product of 2 operators: $\hat{Q}\hat{R}|\alpha\rangle = \hat{Q}(\hat{R}|\alpha\rangle)$

Functions of operators: typically defined by the power series expansion:

$$e^{\hat{Q}} \equiv 1 + \hat{Q} + \frac{1}{2}\hat{Q}^2 + \frac{1}{3!}\hat{Q}^3 + \cdots\cdots$$

$$\frac{1}{1-\hat{Q}} \equiv 1 + \hat{Q} + \hat{Q}^2 + \hat{Q}^3 + \hat{Q}^4 + \cdots\cdots$$

$$\ln(1+\hat{Q}) \equiv \hat{Q} - \frac{1}{2}\hat{Q}^2 + \frac{1}{3}\hat{Q}^3 - \frac{1}{4}\hat{Q}^4 + \cdots\cdots$$

Change of basis in Dirac notation

Dirac notation { frees us from working in any particular basis.
makes changing basis coherent.

Let's take: $|x\rangle \equiv$ position eigenstates $\Rightarrow 1 = \int dx\, |x\rangle\langle x|$

$|p\rangle \equiv$ mometum eigenstates $\Rightarrow 1 = \int dp\, |p\rangle\langle p|$

$|n\rangle \equiv$ energy eigenstates $\Rightarrow 1 = \sum |n\rangle\langle n|$

Acting on $S(t)$ (state vector):

$$\Rightarrow \begin{cases} |S(t)\rangle = \int dx\, |x\rangle\langle x|S(t)\rangle = \int \Psi(x,t)\, |x\rangle\, dx \\ |S(t)\rangle = \int dp\, |p\rangle\langle p|S(t)\rangle = \int \phi(p,t)\, |p\rangle\, dp \\ |S(t)\rangle = \sum_n |n\rangle\langle n|S(t)\rangle = \sum_n c_n(t)\, |n\rangle \end{cases}$$

Change of basis in Dirac notation

Position-space, momentum-space & energy-space wavefunctions are the components of $|S(t)\rangle$ in the respective bases.

Operators also take different forms in different bases:

$\hat{x} \to x$ in the position basis

$\hat{x} \to i\hbar \frac{\partial}{\partial p}$ in the momentum basis

Operators act on kets; eg $\hat{x}|S(t)\rangle$:

$\langle x|\hat{x}|S(t)\rangle$ = action of $\hat{x}$ operator in x basis $= x\Psi(x,t)$

$\langle p|\hat{x}|S(t)\rangle$ = action of $\hat{x}$ operator in p basis $= i\hbar \frac{\partial}{\partial p}\phi$

This notation allows us to transform operators between bases.