Quantum mechanics

"MATHEMATICAL FOUNDATION"

Linear vector spaces

Kets and bras

Operators and their matrix representations

Hermitian

$H = H^+$

real eigenvalues

Unitary

$U^+U = UU^+ = \mathbb{1}$

preserve inner products

The eigenvalue problem

Every hermitian operator can be diagonalized
by a unitary change of basis

$[A, B] = 0 \Rightarrow A, B,$ *"compatible"* $\Rightarrow$ *common set of eigenkets*

Generalization to infinite dimensions $\longrightarrow$ **HILBERT SPACES**

Infinite dimensions, $n \longrightarrow \infty$

Consider a basis $\{|x\rangle\}$ of eigenkets to the position operator X

$$X|x\rangle = x|x\rangle \, ,$$ **defined on $0 < x < L$**

Each point x gets a basis vector $|x\rangle$!

$$\sum \ldots \rightarrow \int \ldots \, dx$$

$$\delta_{ij} \longrightarrow \delta(x-x')$$

Orthogonality $\langle x|x'\rangle = \delta(x-x')$

"Completeness" $\int dx \, |x\rangle\langle x| = \mathbb{1}$

Inner product $\langle f|g\rangle = \int f^*(x)\, g(x)\, dx$

where $f(x) \equiv \langle x|f\rangle$

"wave function" in x-space

$$\Downarrow$$

$$|f\rangle = \int_0^L dx\, |x\rangle\langle x|f\rangle = \int_0^L f(x)\,|x\rangle\, dx$$

Operators

$$\Omega|f\rangle = |\tilde{f}\rangle \Rightarrow \Omega : f(x) \longrightarrow \tilde{f}(x)$$

A particularly important operator:

$\Omega = D$ the **differential operator**

$$D|f\rangle = \left|\frac{df}{dx}\right\rangle$$

ket corresponding to the function $\frac{df}{dx}$ in the x-basis

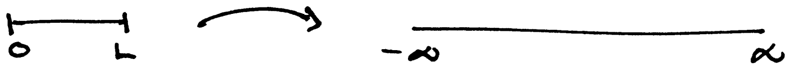
Define $K \equiv -iD$

Hermitian if all functions on 0 < x < L vanish at x = 0 and x = L

HP2!

EIGENVALUE PROBLEM FOR K

$$K|k\rangle = k|k\rangle$$



A nice feature:
The Fourier transform is a "built-in" property of Hilbert spaces

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

$$f(x) = \langle x | f \rangle = \int_{-\infty}^{\infty} \langle x | k \rangle \langle k | f \rangle \, dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} f(k)$$

What's so special with K ?

K and X are conjugate operators !

In the eigenbasis of X, **with** $f(x) = \langle x | f \rangle$:

$$X : f(x) \longrightarrow x f(x)$$

$$K : f(x) \longrightarrow -i \frac{d}{dx} f(x)$$

Notes on Hilbert spaces (course home page)

on

Sakurai, Sec. 1.6

In the eigenbasis of K, **with** $f(k) = \langle k | f \rangle$:

$$K : f(k) \longrightarrow k f(k)$$

$$X : f(k) \longrightarrow -i \frac{d}{dk} f(k)$$

$P = \hbar K$ "momentum operator"

$$[X, P] = i\hbar$$

"CANONICAL COMMUTATION RELATION"

The momentum operator is a *generator of translations*

$$T(\Delta)|x\rangle = |x+\Delta\rangle \quad \Rightarrow \quad T(\Delta) : \psi(x) \to \psi(x-\Delta)$$

$\Delta = \varepsilon \ll 1$. Expand $T(\varepsilon)$!

$$T(\varepsilon) = \mathbb{1} - \frac{i\varepsilon}{\hbar} G + \cancel{O(\varepsilon^2)}$$

What is G ?

$$\langle x | T(\varepsilon) | \psi \rangle = \psi(x-\varepsilon) = \psi(x) - \frac{d\psi(x)}{dx}\varepsilon + \cancel{O(\varepsilon^2)}$$

$$\langle x | \mathbb{1} - \frac{i\varepsilon}{\hbar} G | \psi \rangle = \langle x | \mathbb{1} | \psi \rangle - \frac{i\varepsilon}{\hbar} \langle x | G | \psi \rangle$$

$$= \psi(x) - \frac{i\varepsilon}{\hbar} \langle x | G | \psi \rangle$$

$$\Downarrow$$

$$\langle x | G | \psi \rangle = -i\hbar \frac{d\psi}{dx}$$

$$\Downarrow$$

$$G = P = -i\hbar D$$

$$T(\varepsilon) = \mathbb{1} - \varepsilon P$$

The "postulates" of (non-relativistic) quantum mechanics

Classical mechanics

I.

The state of a particle at any given time is specified by the two variables x(t) and p(t), i.e. as a point in a two-dimensional phase space.

II.

Every dynamical variable ω is a function of x and p: $\omega = \omega(x,p)$.

III.

If the particle is in a state given by x and p, the measurement of the variable ω will yield a value $\omega(x,p)$. The state will remain unaffected.

IV.

CLASSICAL TIME EVOLUTION

Quantum mechanics

I.

The state of the particle is represented by a vector $|\Psi(t)\rangle$ in a Hilbert space.

II.

The independent variables x and p of classical mechanics are represented by Hermitian operators X and P with the following matrix elements in the eigenbasis of X:

$$\langle x|X|x'\rangle = x\,\delta(x-x')$$

$$\langle x|P|x'\rangle = -i\hbar\,\delta'(x-x')$$

The operators corresponding to dependent variables $\omega(x,p)$ are Hermitian operators

$$\Omega(X,P) = \omega(x\to X, p\to P)$$

III.

If the particle is in a state $|\Psi\rangle$, a measurement of the variable (corresponding to) Ω will yield one of the eigenvalues ω, with probability $P(\omega) \sim |\langle\omega|\Psi\rangle|^2$. The state of the system will change from $|\Psi\rangle$ to $|\omega\rangle$ as a result of the measurement.

IV.

QUANTUM TIME EVOLUTION

(LATER)

Possible oucomes of an experiment measuring ω *?*

Classically

Parrticle in a state (x, p) $\longrightarrow \omega(x, p)$

Quantum

Particle in a state $|\psi(t)\rangle$

$$\Big\downarrow$$

four-step program *(← postulates I - III)*

<u>step 1</u>: construct $\Omega = \omega(x \to X, p \to P)$

<u>step 2</u>: find the eigenkets $|\omega_i\rangle$ and eigenvalues ω_i of Ω

<u>step 3</u>: expand $|\psi\rangle$ in this basis :

$$|\psi\rangle = \sum_{i=1}^{n} |\omega_i\rangle\langle\omega_i|\psi\rangle$$

<u>step 4</u>: the probability $P(\omega_i)$ of measuring ω_i :

$$P(\omega_i) \sim |\langle\omega_i|\psi\rangle|^2 = \langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle$$

$$= \langle\psi|\mathbb{P}_{\omega_i}|\psi\rangle$$

Some implications.....

1. Quantum mechanics is a probabilistic theory

...but what about g = $2.0023193048\ldots$ **?**

2. The only possible values of Ω are its eigenvalues

3. $$P(\omega_i) \sim |\langle \omega_i | \psi \rangle|^2 \xRightarrow{\text{NORMALIZE!}} P(\omega_i) = \frac{|\langle \omega_i | \psi \rangle|^2}{\sum_j |\langle \omega_j | \psi \rangle|^2} = \frac{|\langle \omega_i | \psi \rangle|^2}{\langle \psi | \psi \rangle}$$

OK IF $\langle \psi | \psi \rangle$ NORMALIZABLE TO 1

WHAT IF $\langle \psi | \psi \rangle = \delta(0)$?

(LATER...)

MEASUREMENT

4. $$|\psi\rangle = |\omega_i\rangle \longrightarrow \boxed{\Omega} \longrightarrow |\omega_i\rangle$$

MEASUREMENT

5. $$|\psi\rangle = \frac{\alpha|\omega_1\rangle + \beta|\omega_2\rangle}{(|\alpha|^2 + |\beta|^2)^{1/2}} \longrightarrow \boxed{\Omega} \longrightarrow |\omega_1\rangle$$

$$P(\omega_1) = \frac{|\alpha|^2}{|\alpha|^2+|\beta|^2}$$

OR

$$\longrightarrow |\omega_2\rangle$$

$$P(\omega_2) = \frac{|\beta|^2}{|\alpha|^2+|\beta|^2}$$

$$\Omega|\omega_i\rangle = \omega_i|\omega_i\rangle$$

6. $$|\psi\rangle = \sum_i |\omega_i\rangle\langle\omega_i|\psi\rangle$$

$$P(\omega_i) = |\langle\omega_i|\psi\rangle|^2$$

$P(\lambda_j)$? $\quad \Lambda|\lambda_j\rangle = \lambda_j|\lambda_j\rangle$

$$P(\lambda_j) = |\langle\lambda_j|\psi\rangle|^2$$

$$\langle\lambda_j|\psi\rangle = \sum_i \langle\lambda_j|\omega_i\rangle\langle\omega_i|\psi\rangle$$

EXAMPLE

$$|\psi\rangle = \tfrac{1}{2}|\omega_1\rangle + \tfrac{1}{2}|\omega_2\rangle + \tfrac{1}{\sqrt{2}}|\omega_3\rangle$$

Probability to find ω_1 when measuring Ω $= 1/4$

ω_2 $= 1/4$

ω_3 $= 1/2$

Collapse of the state vector

applies to *ideal measurements* (measurements which leave the eigenstates of Ω invariant; cf. classical physics where an ideal measurement leaves *any* state invariant)

$$|\psi\rangle = \sum_i |\omega_i\rangle\langle\omega_i|\psi\rangle$$

in quantum mechanics, a measurement is telling us what a particle is doing right after the measurement

$$|\psi\rangle \longrightarrow \boxed{\Omega} \xrightarrow{|\omega_j\rangle} \boxed{\Lambda} \longrightarrow |\lambda_k\rangle$$

WITH PROBABILITY

$$P(\lambda_k) = |\langle\lambda_k|\omega_j\rangle|^2$$

EX : $|\omega_j\rangle = \frac{1}{\sqrt{3}}|\lambda_1\rangle + \sqrt{\frac{2}{3}}|\lambda_2\rangle + 0 \cdot \text{OTHERS} \Rightarrow P(\lambda_1) = 1/3$

$P(\lambda_2) = 2/3$

To test quantum mechanics:

repeat the experiment many times with the particle in $|\omega_j\rangle$

FILTRATION (selective measurement) $\Omega = |\omega_j\rangle\langle\omega_j|$

QUANTUM ENSEMBLE OF IDENTICALLY PREPARED STATES (pure ensemble)

it is *not* a classical statistical ensemble!

example: throwing a dice...

Caveats :

1. The prescription $\Omega = \omega(x \to X, p \to P)$ is sometimes ambiguous

$$\omega = xp \quad \begin{cases} \Omega = XP \; ? \\ \Omega = PX \; ? \end{cases}$$

Answer: Symmetrize: $\Omega = \frac{1}{2}(PX + XP)$ **, or (in more complicated cases) let experiments decide!**

2. Ω is degenerate

$\omega_1 = \omega_2 = \omega$

$P(\omega)$?

$|\omega,1\rangle, |\omega,2\rangle$ **basis in the degenerate subspace**

$$P(\omega) = |\langle\omega,1|\psi\rangle|^2 + |\langle\omega,2|\psi\rangle|^2$$

$$P(\omega) = \langle\psi|\underbrace{\mathbb{P}_\omega}_{|\omega,1\rangle\langle\omega,1| + |\omega,2\rangle\langle\omega,2|}|\psi\rangle$$

3. What if Ω has no classical counterpart?

Ex. *spin, color, flavor, fractional statistics, "compositeness",...*

NEW PHYSICS !

4. Spectrum of Ω continuous

$$|\psi\rangle = \int |\omega\rangle \underbrace{\langle\omega|\psi\rangle}_{\psi(\omega)} d\omega$$

wave function in ω -space

cf. w = x $\longrightarrow$ "The wave function"

= probability amplitude for finding the particle with the value ω

$P(\omega) = |\langle\omega|\psi\rangle|^2$ **probability density at**

$P(\omega)\,d\omega$ = **probability of obtaining a result between ω and $\omega + d\omega$**

$$\int P(\omega)d\omega = \int |\langle\omega|\psi\rangle|^2 d\omega = \int \langle\psi|\omega\rangle\langle\omega|\psi\rangle d\omega$$

$$= \langle\psi|\mathbb{1}|\psi\rangle = \langle\psi|\psi\rangle = 1$$

if $|\psi\rangle$ a proper vector

what if $\langle\psi|\psi\rangle = \delta(0)$?

(later...)

TWO MORE THINGS...

EXPECTATION VALUES

ENSEMBLE OF N PARTICLES, EACH IN A STATE $|\psi\rangle$

$$\langle\Omega\rangle = \sum_i P(\omega_i)\,\omega_i = \sum_i |\langle\omega_i|\psi\rangle|^2\,\omega_i$$

$$= \sum_i \langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle\,\omega_i$$

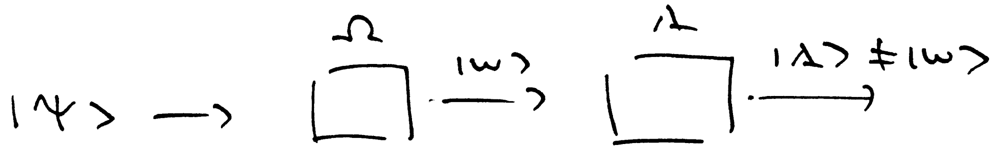
$$= \sum_i \langle\psi|\Omega|\omega_i\rangle\langle\omega_i|\psi\rangle$$

$$= \langle\psi|\Omega|\psi\rangle$$

COMPATIBLE / INCOMPATIBLE OBSERVABLES

$$[\Omega,\Lambda] = 0$$

$$[\Omega,\Lambda] \neq 0$$



Ω AND Λ CANNOT BE MEASURED "SIMULTANEOUSLY"

THE FOURTH POSTULATE : TIME EVOLUTION

$\downarrow$

"QUANTUM DYNAMICS"

Sakurai Chapt. 2

CLASSICAL MECHANICS

The state variables change with time according to Hamilton's equations

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p}$$

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial x}$$

QUANTUM MECHANICS

The state vector $|\psi(t)\rangle$ obeys the Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

where

$$H(X,P) = \mathcal{H}(x \to X, p \to P)$$

is the quantum Hamiltonian operator and $\mathcal{H}$ is the Hamiltonian for the corresponding classical problem.