9/9/2015

Quantum Mechanics

- New way that was developed at the beginning of the 20th century to interpret & predict behaviors of microscopic objects such as atoms, electrons, ...

Purpose of this course : learn to calculate and think in quantum mechanic way.

The conceptual problems will not be discussed in this course but if time is permitted, we will mention a few of them. In fact, this is still a serious problem that a lot of people are still working on.

Two tracks of discoveries

Spectroscopy (discrete) → Bohr's theory of H atom

→ Heisenberg's Matrix Mechanics (orbit is meaningless only frequencies are meaningful)

Einstein's discovery of wave-particle duality of light (photo electric effect) → de Broglie

→ Schrödinger wave equation, wave mechanics

8/10/1995 Q. M.

} ⇒ equivalent, shown by Schrödinger; setting up

by the general formalism of Paul Dirac

Later, Feynman's Path integral formulation; stochastic Q. ..

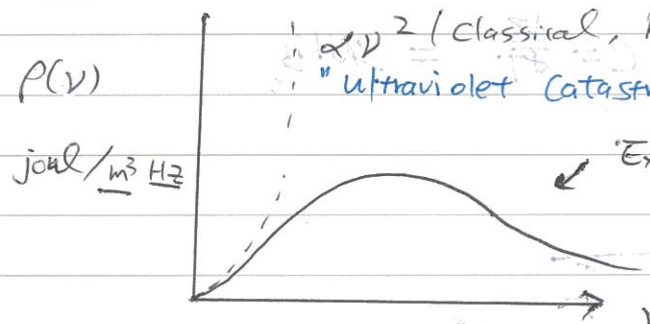
We will follow Schrödinger's path first:

Wave Mechanics

Particle – Wave duality; Complementarity (互補性)

機率詮釋的特性

1. blackbody radiation : Planck (Consideration from statistical mechanics, not dynamics!) ⇒ Charges emit/absorb by $nh\nu$



$\propto \nu^2$ (classical, Rayleigh-Jeans formula)

"ultraviolet catastrophe"

Expt. & Planck: radiating e's energy $= nh\nu$

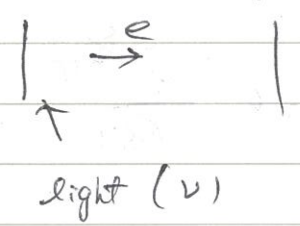
or E.M. waves (viewed as harmonic oscillations) energy $= nh\nu$

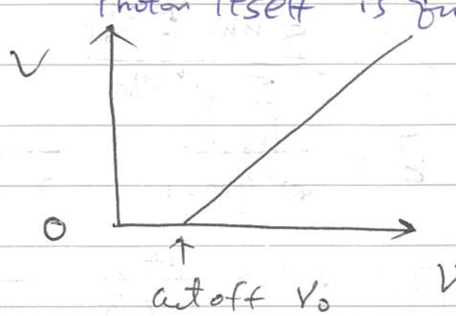
E.M. waves are still waves; continuous!

2. Photoelectric effect : Einstein ($E = nh\nu$ originates dynamically!)

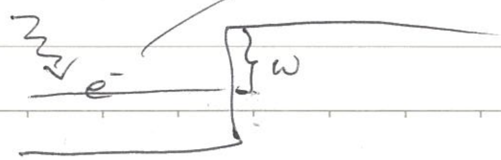
Photon itself is quantized

← V (stopping voltage)





Kinetic energy $= h\nu - w$, $\nu_0 = \frac{w}{h}$



Einstein : photon itself $E = h\nu$

localized packet of energy

Another contribution of Einstein in Q. M. :

Assume $E = nh\nu$ also applies to material oscillators :

Heat capacity :

oscillation

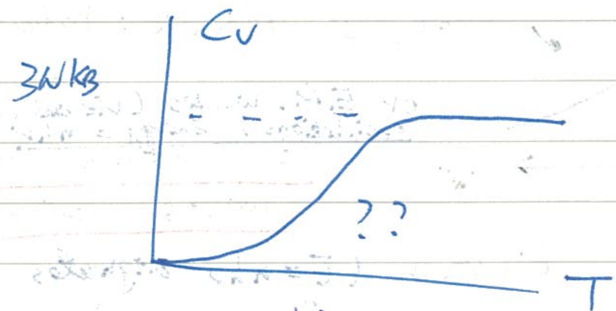
~~classical : N H atoms~~

$\cancel{U = \frac{1}{2}NkT[3+2+2}+1]$

translation

$$U = \frac{1}{2}NkT \times \underset{p_x\,p_y\,p_z}{\underset{\uparrow}{3}} + \frac{1}{2} \times k_BT \times \underset{x^2+y^2+z^2}{\underset{\uparrow}{3}} \times N$$

$$= 3Nk_BT \qquad C = \frac{dU}{dT} = 3Nk_B$$



$$= \frac{\sum nh\nu\, e^{-\frac{nh\nu}{k_BT}}}{\sum e^{-nh\nu/k_BT}}$$

$$\bar{\varepsilon} = \frac{h\nu}{e^{h\nu/k_BT}-1} \xrightarrow[T\to\infty]{} k_BT \qquad \text{classical} \quad \frac{e^{-\varepsilon/k_BT}}{k_BT}$$

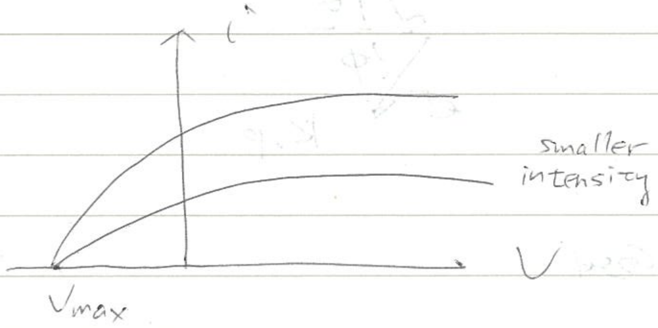
$$\rho(\nu)\,d\nu = \frac{8\pi\nu^2}{c^3}\,\frac{h\nu}{e^{h\nu/k_BT}-1}\,d\nu$$

\# of waves $\propto \nu^2$

each $\propto \bar{\varepsilon}$

classical : K.E. of electron $\propto |\vec{E}|^2$

However, V_{max} is indept. of intensity



fixed ν

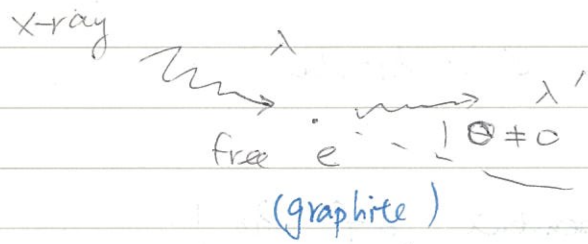
⇐ see the over page of page 2

3. Compton effect : light scatters like particles

⇒ photons

Classical Thomson scattering

⇒ $\lambda = \lambda'$. in all directions

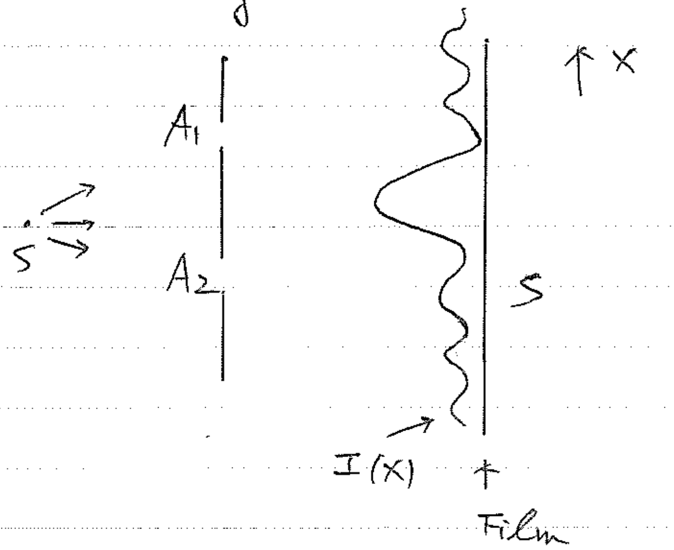


$\lambda \neq \lambda'$ λ' can be found by solving two-particle collision problem!

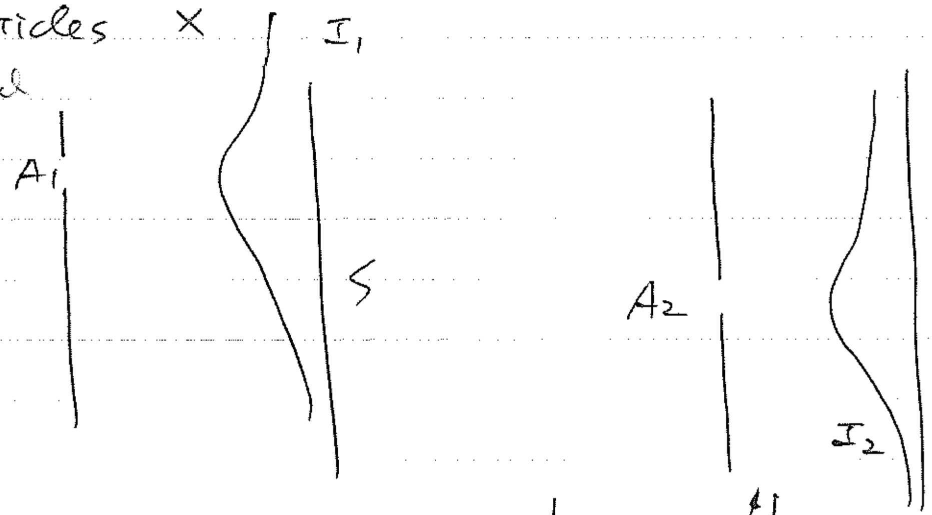
The above show that photons have the properties as particles. On the other hand, we know light propagate as waves.

So, what is it?

Young's double-slit expt.

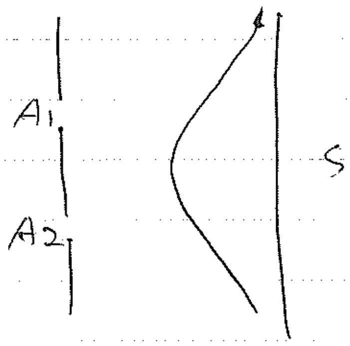


(i) particles
classical



$I = I_1 + I_2$ (classical)

but $I \neq I_1 + I_2$



Question : Could the interference be due to the collisions between particles coming out from A_1 and those from A_2 ?

No, this can be shown by reducing # of particles per sec so that there is only one particle passing through A_1 & A_2 one at a time.

This is an example of "nonlocality" in Q.M.

(ii) pure waves X why?

Put a film on S to record light. We discover if the time of recording is shorten enough, we find light only produces localized impacts on S. These impacts do not represent the "weak" interference pattern. Instead, they are randomly distributed. If we have photon counters to count # of photons arriving at each point and plot the # v.s. x out, they exhibit the interference pattern.

So, each individual photon can not produce the whole pattern and arrives at random spot on S.

So, we arrive at the following picture:

Photons are particle-like because when we detect them, they are localized & corpuscular; ~~of~~ at the same time, they are wave-like because when we accumulate them, their intensity exhibit interference pattern.

Up to now, we have been concentrating ourself on photons. What about other "particles"?

photons: $E = h\nu \underset{=pc}{\rightarrow} p = \hbar k$, $m=0$ (relativistic!)

seems to be particular ($\because m=0$).

But de Broglie proposed that wave-particle duality is true in general, so that those believed to be particles such as electrons should also exhibit wave properties:

$$E = \hbar\omega = \sqrt{p^2c^2 + m^2c^4}$$

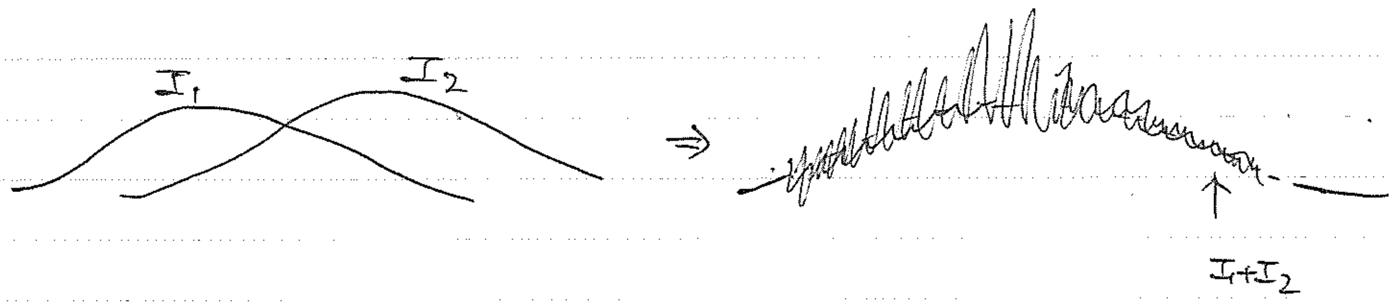
$$p = \hbar k = mv$$

$$\Rightarrow \quad \lambda = \frac{2\pi}{k} = \frac{h}{p} \simeq 10^{-26}\ \text{cm if } v \sim 1\,\text{cm/sec}, \ m \sim 1\text{g}$$

$\Rightarrow$ de Broglie matter wave

λ is so small (10^{-13} times smaller than the radius of a proton)

that in practice, Young's double-slit expt. is an average result, reducing to classical predictions :



Experimental confirmation of matter waves:

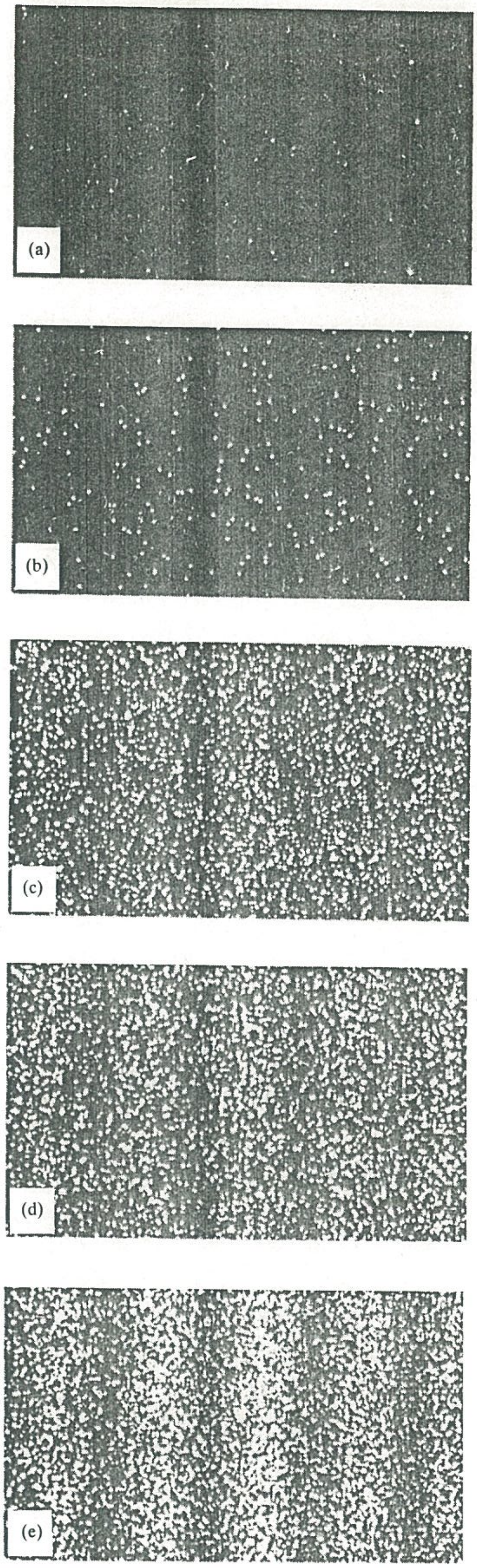
Use microscopic objects such as e'

$\lambda = 1.2 A°$ for K.E. of e = 100 eV.

G. P. Thomson 1927 electron diffraction
Davisson & Germer Bragg reflection

Home work : Review. Eisberg & Resnick 's Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles
Chapter 1-3

Exercise



American Journal
of Physics 57, 117
Tonomura A.

Figure 1.5 The gradual build-up of a two-slit diffraction pattern produced with electrons [16]. The numbers of electron arrival points recorded in sucessive photographs are (a) 10, (b) 100, (c) 3000, (d) 20 000 and (e) 70 000.

What do we learn from Young's expt.?

* First, we need the concept of probability to describe the behavior of particles.

* secondly, probability are not exclusive in classical way!

$$P(x) \neq P_1(x) + P_2(x)$$

Analogy :

Classical E.M. waves

$$I \propto |\vec{E}_1(x) + \vec{E}_2(x)|^2$$

$\Rightarrow$ produce interference

Q.M.

to produce interference $P(x,t)$ needs to be square of something!

$\vec{E}_1(x) \Longleftrightarrow \psi(x,t)$

The whole thing is demystified if one introduces the probability amplitude $\psi(x,t)$ such that

$$p(x,t) = |\psi(x,t)|^2 \text{ is the probability density}$$

(This interpretation is due to Max Born.)

The introduction of $\psi(x,t)$ also demystifies de Broglie's matter wave: $\psi(x,t)$ is simply the mathematical realization of the matter wave!

($\therefore$ $\psi(x,t)$ is also termed wave function.)

Principles for combining amplitudes

(i) "every process" in quantum mechanics is represented by an complex amplitude whose absolute square is the probability associated with that process! (Postulate I)

Why complex? (recall that $\vec{E}(x,t)$ is a real vector!)

Since # of particles must be conserved, accompanid with $\rho(x,t)$, there must exist a continuity equation:

$$\frac{\partial \rho(x,t)}{\partial t} + \nabla \cdot \vec{J}_p = 0$$

Consider a particle with definite momentum (P) and energy (E),

according to de Broglie, $K = \frac{P}{\hbar}$, $\omega = \frac{E}{\hbar}$.

Possible candidates of ψ are $\cos(Kx \pm \omega t)$, $\sin(Kx \pm \omega t)$ or $e^{i(Kx \pm \omega t)}$

For such particles, $\nabla \cdot \vec{J}_p$ must vanish identically!

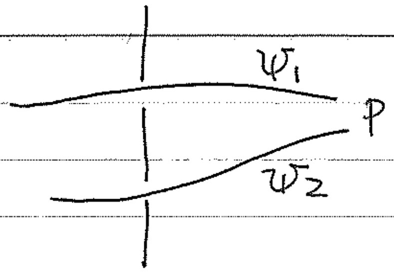
$\therefore \frac{\partial \rho}{\partial t} = 0$ $\therefore$ only when $\psi = e^{i(\vec{K}\cdot\vec{r} \pm \omega t)}$ is acceptable!! This clearly indicates ψ must be complex!

(ii) Superposition: "or" case

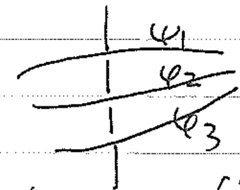
total amplitude = sum of every possible amplitude (route)

("generalized path integral"!)

8/23/96



$p = |\psi_1 + \psi_2|^2 \Rightarrow$ interference



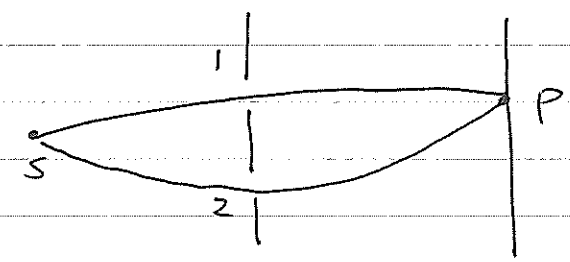
$\Rightarrow \quad p = |\sum_i \psi_i|^2$

(iii) <u>product</u>: total amplitude ("and" case)

= product of sub-amplitudes that are independent from each other.

this follows from $p(a, b) = p(a)\, p(b)$ if a & b are independent

e.g.



$$\psi_{s\to1\to p} = \psi_{s\to1} \cdot \psi_{1\to p}$$
$$\psi_{s\to2\to p} = \psi_{s\to2} \cdot \psi_{2\to p}$$

Combined with (ii) $\psi_{s\to p} = \psi_{s\to1\to p} + \psi_{s\to2\to p}$

$$= \sum_i \psi_{s\to i} \cdot \psi_{i\to p}$$

e.g. particle 1 / particle 2 > no inteaction

$$\psi(1,2) = \psi(1)\, \psi(2)$$

Schrödinger eq. (postulate IV)

Just as that there exist eqs. describing evolution of $\vec{E}$, we need an equation to describe evolution of $\psi(x,t)$

This equation must conform to

(i) linear so that superposition is satisfied!

(ii) consistent with $E = \frac{p^2}{2m} + V$, $E = \hbar\omega$, $p = \hbar k$

In particular, a plane wave $e^{i(kx-\omega t)}$ must be solution when $V=0$.

Condition (i) restricts that eq. can only contain terms such as. ψ, $\frac{\partial \psi}{\partial x}$, $\frac{\partial \psi}{\partial t}$, $\frac{\partial^n \psi}{\partial x^n}$, . . .

An equation that satisfies above is the

Schröding eq. $i\hbar \frac{\partial}{\partial t}\psi = \frac{-\hbar^2 \nabla^2}{2m}\psi + V\psi \equiv \hat{H}\psi$

in which when $V=0$, $\psi = e^{i(kx-\omega t)}$ is a solution just as one replaces $p = \frac{\hbar}{i}\nabla$, $E = i\hbar\frac{\partial}{\partial t}$ in the classical relation $E = \frac{p^2}{2m} + V$

Note that the above is by no means a derivation.
The justification of Schröding eq. fully lies in the support from expt.

8/23/96

Concept of state : collection of all probability amplitude
= state

Above the concept of probability amplitude is the concept of state. (postulate I)

In Q.M., after a careful preparation of a particle, the particle is said to be in a state $\Psi(t)$ or $|\Psi(t)\rangle$ in Dirac's notation.

State — probability amplitude for getting results of ω, p, x . . .

$\Psi(t) \xrightarrow[\text{measurement } \omega]{\text{precise}} \omega, \quad \Psi(\omega, t), \quad \{\Psi_{\omega_0}(t)\} \xrightarrow{\text{second measure}} \omega_0$

$\quad \xrightarrow{\text{" } \vec{p}} p, \quad \Psi(p, t), \quad \{\Psi_{p_0}(t)\} \xrightarrow{\text{"}} p_0$

$\quad \xrightarrow{x} x, \quad \Psi(x, t), \quad \{\Psi_{x_0}(t)\} \longrightarrow x_0$

$\Psi(t) = \{\Psi(x,t)\}$ or $\{\Psi(\omega,t)\}$ $\{\Psi(p,t)\}$

↑ states after ideal measurement!

Copenhagen interpretation: Consider the position measurement, just before the measurement, the particle is in a state of Ψ. One doesn't know where it is.

If, right after the measurement, one performs a second measurement, one gets exactly the same value as the 1st measurent! (postulate III)

Collapse of state : in Copenhagen interpretation, the state of the particle collapses to $\Psi_\omega(t)$ right after the ideal measurement!

$\Leftrightarrow$ This is in sharp contrast to classical idea about measurement: one can leave the system unperturbed (almost) in "ideal" measurement!

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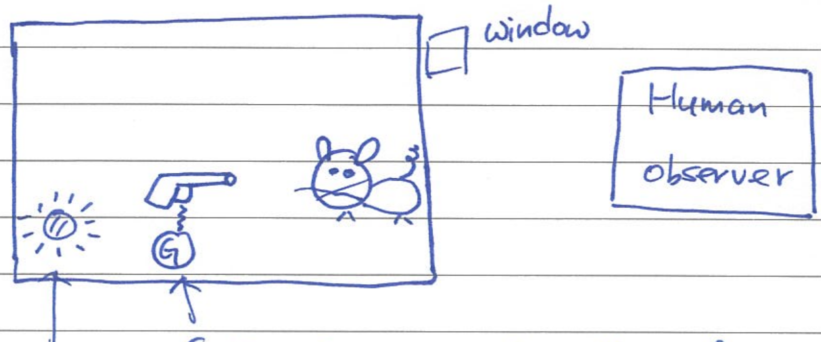
Schrödinger's cat



radioactive half-life time = one hour

Geiger counter, controlling firing the gun

more appropriate, improved version

(Penrose)

· photon's quantum state after the half-silvered mirrored

$= \alpha\,|\xi\rangle + \beta\,|\rightsquigarrow\rangle$ presumably $\alpha = \beta = \frac{1}{\sqrt{2}}$

* The collapse of the wavefunction is the most peculiar feature that appears in the Copenhagen's interpretation, which is not present in Schrödinger eg! This is also the place where probability comes into play. Before that the wavefunction evolves deterministically, only when it comes to the "measurement" point, probability comes in and $|\text{amplitude}|^2$ gives the probability for an outcome to occur.

NO.
DATE 6-2

What is a measurement? Why is it so different from other physical processes?

Why the observer is classical-like?

Is a human observer necessary?

→ Can we use superposition to describe macroscopic objects such as us?

Many people doubt the completeness of quantum mechanics (& the Copenhagen's interpretation) (Such as Gell-mann blamed Bohr "brain-washed" the physics community into thinking the problems were solved), the Schrödinger's cat represents the most serious attack on this! & many above mentioned problems show up in this example!

☆ Because a complete theory should treat things coherently, therefore, the wavefunction of the cat should be $\psi = \frac{1}{\sqrt{2}}(\psi_{alive} + \psi_{dead})$?!

if it can't be described by this, why not?

What is the complete description of our universe?

The Copenhagen's interpretation certainly seems to be correct at microscopic level, can it be ultimate truth about the physical Universe?

* A few widely accepted answers :

the triggering of the Geiger counter is
the measurement !
not the observation of humans !

more precisely : a quantum meaurement occurs
(in Copenhagen's sense) when the quantum mechanical system
interacts with the macroscopic
system (approximately described by
classical mechanics) in such a
way to leave a permanent record

But why don't we describe the macroscopic system quantum mechanically ?

i.e How can we incoorporate classical mechanics
coherently into the Q.M. ?

In facing this problem, physicists' views are
diverse. A good account of this may be
found in the book "The large, the small and
the Human mind" by

Roger Penrose

Statistical analysis & experimental measurements

(i) consider a "process" in which one does measurement on the particle and gets the result ω.

then $\psi(\omega)$ is the associated amplitude

if ω is continuous, $\underline{|\psi(\omega)|^2} d\omega$ = probability of finding the particle with the value of ω between ω & $\omega + d\omega$

probability density

e.g. $\omega = x$. $|\psi(x,t)|^2 dx$ = probability of finding the particle between $(x, x+dx)$ at t

if ω is discrete $|\psi(\omega)|^2$ = probability of getting result ω.

(Postulate III)

e.g. ω = energy of a hydrogen atom.

(ii) <u>normalization</u>

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1 \quad (\because \text{there is only one particle!})$$

or $\int_{-\infty}^{\infty} |\psi(\omega,t)|^2 d\omega = 1$ ω = continuous

such function ⇒ normalizable or L^2 (square integrable)

Functions that are not normalizable must be rejected!

In Q.M., the normalization condition is a bit weaken: in particular, for a plane wave $\psi = e^{i(kx-\omega t)} \cdot N$

We normalized it by $\lim_{L\to\infty} \int_{-L}^{L} |\psi|^2 dx = 1$, $\therefore N = \frac{1}{\sqrt{2L}}$

We shall come back to this point later.

discrete ω, $\sum_{\substack{\text{all}\\ \text{possible}\\ \omega}} |\psi(\omega,t)|^2 = 1$.

* For $\psi(x,t)$, if at $t=0$, $\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$ is done, i.e., $\psi(x,t=0)$ is normalized.

Then the continuity eq. $\nabla\cdot\vec{J}_p + \frac{\partial P}{\partial t} = 0$ implies

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = -\int_{-\infty}^{\infty} \nabla\cdot\vec{J}_p\, dx = 0$$

$\therefore$ the normalization condition is preserved!

For Schrödinger eq. $i\hbar\frac{\partial\psi(x,t)}{\partial t} = \left[\frac{-\hbar^2\nabla^2}{2m} + U(x)\right]\psi(x,t)$,

direct algebra shows $\frac{\partial P(x,t)}{\partial t} = \left[\frac{\partial}{\partial t}\psi^*(x,t)\right]\psi(x,t) + \psi^*(x,t)\frac{\partial\psi(x,t)}{\partial t}$

$$= -\nabla\cdot\left[\frac{\hbar i}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi)\right]$$

$$\therefore \vec{J}_p(x,t) = \frac{\hbar i}{2m}\left[\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right].$$

(iii) expectation values & uncertainty

In a Q.M. measurement, one often calculates

① expectation value (average)

e.g. $\langle x\rangle = \int_{-\infty}^{\infty} x\, P(x,t)\, dx = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx$

discrete ω : $\langle\omega\rangle = \sum_{\omega} \omega\, P(\omega,t) = \sum_{\omega} \psi^*(\omega,t)\, \omega\, \psi(\omega,t)$

② uncertainty (Standard deviation)

$$(\Delta X)^2 \equiv \langle (X - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

$$= \int_{-\infty}^{\infty} \psi^*(x,t)\, x^2\, \psi(x,t)\, dx$$

under certain condition,

$$\Delta f(\hat{A}) = |f'(\langle A \rangle)|\, \Delta A + (\Delta A^3) - \left(\int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx\right)^2$$

* $\Delta E \sim \frac{\langle p \rangle}{m} \Delta p$ not exact, because Δ is not differential

(iv) observables (postulate II)

* operators : many quantities, especially observables, are represented by operators in quantum mechanics (not numbers!)

example : momentum

$$\langle p \rangle = \int_{-\infty}^{\infty} p\, P(p,t)\, dp$$

$$P(p,t) = \Phi^*(p,t)\, \Phi(p,t) \qquad \psi(x,t) = \Phi(p,t)\, e^{\frac{ipx}{\hbar}}$$

$\uparrow$ amplitude for finding particle's momentum = p

Obviously, one has

$$\psi(x,t) = \int \frac{dp}{\sqrt{2\pi\hbar}}\, \Phi(p,t)\, e^{\frac{ip\cdot x}{\hbar}}$$

(see below)

$\sqrt{2\pi\hbar} \Leftarrow$ just a convention, related to normalization of $|p\rangle$

, i.e., just as the ordinary wave, any $\psi(x,t)$ consists of many plane waves — this is essentially what Fourier transformation says!

or equivalently, one has $\Phi(p,t) = \int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{\frac{-ipx}{\hbar}}\, \psi(x,t)$

$$\int_{-\infty}^{\infty} dp \quad \Phi^*(p,t)\, \Phi(p,t)$$

$$= \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi\hbar}} \quad \psi^*(x\,t)\, e^{\frac{ipx}{\hbar}} \quad \psi(x'\,t)\, e^{\frac{-ipx'}{\hbar}}$$

$$= \int_{-\infty}^{\infty} dx \quad \psi^*(x\,t)\, \psi(x\,t) = 1$$

$\therefore$ $P(p,t) = |\Phi(p,t)|^2$ is appropriately normalized

<u>if $P(x,t)$ is</u> !

$$\langle p \rangle = \int_{-\infty}^{\infty} p\, dp \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi\hbar}} \quad \psi^*(x,t)\, \psi(x',t)\, e^{\frac{ip}{\hbar}(x-x')}$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \iint dx\, dx' \quad \psi^*(x\,t)\, \psi(x',t) \left(\frac{-\hbar}{i}\frac{d}{dx'}\right) e^{\frac{ip}{\hbar}(x-x')}$$

$$\underset{\substack{\uparrow \\ \text{integration} \\ \text{by part}}}{=} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \quad e^{\frac{ip}{\hbar}(x-x')} \quad \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \;\psi^*(x\,t)\, \frac{\hbar}{i}\frac{d}{dx'}\, \psi(x',t)$$

$$= \int_{-\infty}^{\infty} dx \quad \psi^*(x,t) \quad \underbrace{\frac{\hbar}{i}\frac{d}{dx}}_{\hat{p}} \psi(x,t)$$

$\hat{p}$, 3D $\Rightarrow$ $\underline{\frac{\hbar}{i}\vec{\nabla}}$

$\therefore$ if we restrict ourselves to $\underbrace{\psi(x,t)}_{\text{be working with}}$, p is represented by $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$

Obviously, in this "representation", $\hat{x} = x$.

In general, given a classical quantity $\omega(x, p)$,

we get an operator representation of ω by replacing p

with $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$, $\Omega(\hat{x}, \hat{p})$

e.g. $T = \frac{p^2}{2m}$. $\langle T \rangle = \int dx\, \psi^*(x,t) \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi(x,t)$

This works well when there is no mixing term such as $x^2 p$ in $\omega(x, p)$. When this occurs,

there is no unique correspondence in quantum mechanics:
because of the ordering problem: $\hat{x}\hat{p} \neq \hat{p}\hat{x}$

$$x^2 p \rightarrow \hat{x}\hat{p}\hat{x}, \quad \frac{1}{2}(\hat{x}^2\hat{p} + \hat{p}\hat{x}^2),$$

$$\frac{1}{3}(\hat{x}^2\hat{p} + \hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2), \ldots$$

(an additional requirement: Hermitian will restrict the possible forms but not down to one!)

An ordering, known as Weyl-ordering, can produce the canonical path integral form. See T.D. Lee's Book page 475. (Particle Physics & Introduction to Field theory)

In general, knowing the classical limit doesn't specify quantum mechanics uniquely. Only expt. can decide which form is correct!

8/24/96

example : energy

$E \rightarrow \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

$$\langle E \rangle = \int dx \; \psi^*(x,t) \left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x,t)$$

$$= \int dx \; \psi^*(x,t) \; i\hbar \frac{\partial}{\partial t} \psi(x,t)$$

$\therefore \hat{H} = i\hbar \frac{\partial}{\partial t}$ too !

* <u>Hermitian</u> : (linear)

From the above discussion, we conclude that observables are represented by operators $\hat{O}$ so that

$\therefore \langle O \rangle = \int dx \; \psi^*(x,t) \; \hat{O} \; \psi(x,t)$

Now, $\because \langle O \rangle$ must be real, $\therefore \langle O \rangle^* = \langle O \rangle$

$$\therefore \int dx \; \psi(x,t) \; \hat{O}^* \; \psi^*(x,t) = \int dx \; \psi^*(x,t) \; \hat{O} \; \psi(x,t) \quad \text{--- (1)}$$

must be satisfied !

Note that $\hat{O}^*$ on the LHS acts on $\psi^*(x,t)$, while $\hat{O}$ on the RHS acts on $\psi(x,t)$

$\therefore$ When (1) is satisfied, the requirement of $\langle O \rangle$ being real is satisfied !

No.

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It is more convenient to talk about this at the level of operators themselves!

For this purpose, we define the Hermitian conjugate operator $\underline{\underline{\hat{O}^+}}$ of $\hat{O}$ by

$$= \left(\int \psi^* O \psi \right)^*$$

$$\int dx \quad \psi^*(x,t) \ \hat{O}^+ \ \psi(x,t) \equiv \int dx \quad \psi(x,t) \ \hat{O}^* \ \psi^*(x,t)$$

⇒ in general $\quad \phi^*(x,t) \quad \psi(x,t) \quad \psi(x,t) \quad \phi^*(x,t)$

Note that $\hat{O}^+$ acts on $\psi(x,t)$ so that ① becomes

$$\int \psi^*(x,t) \ \hat{O}^+ \ \psi(x,t) \ dx = \int dx \ \psi^*(x,t) \ \hat{O} \ \psi(x,t),$$

the requirement of $\langle O \rangle$ being real reduces to

require $\hat{O}^+ = \hat{O}$

When $\hat{O}^+ = \hat{O}$ is satisfied, we term $\hat{O}$ as an Hermitian operator!

Given an operator $\hat{O}$, $\hat{O}^+$ is usually found by integroing by parts to shift $\hat{O}^*$ to act on ψ instead ψ^*:

example $\quad \hat{O} = \hat{P} = \frac{\hbar}{i}\frac{d}{dx}$

$$\int \psi \ \hat{O}^* \ \psi^* = \int \psi \left(-\frac{\hbar}{i}\frac{d}{dx} \psi^* \right)$$

$$= \int \frac{\hbar}{i}\frac{d}{dx} \left(\cancel{-}\psi\psi^* \right) + \int \psi^* \frac{\hbar}{i}\frac{d}{dx} \psi$$

$$0 \qquad \therefore \quad \hat{O}^+ = \frac{\hbar}{i}\frac{d}{dx} = \hat{P},$$

i.e. $\hat{P}^+ = \hat{P}$, $\underline{\hat{P} \text{ is Hermitian}}$! (only in the space when $\psi \to 0$ at ∞)

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As we shall see, Hermitian conjugate defined here is nothing but the Hermitian " for matrices.

When $\hat{O}^* = \hat{O}$, it is simply the transpose of matrices!

* eigenfunctions & eigenvalues

As mentioned, right after a precise measurement of the observable $\hat{O}$, the state Ψ collapses to a state Ψ_α which reproduces the result α if one perform a 2nd measurent. $\therefore \langle O \rangle_\alpha = \frac{\int dx\, \Psi_\alpha^* \hat{O} \Psi_\alpha}{\int dx\, |\Psi_\alpha|^2} = \alpha$

(see over)

So, $\hat{O}\,\Psi_\alpha = \alpha\,\Psi_\alpha$, α = the observed value of $\hat{O}$.

$+\Psi_\beta$ $\quad \int \Psi_\alpha^* \Psi_\beta = 0 >$ $\quad \Psi_\beta$ indept of Ψ_α

$\Rightarrow$ violate linearity

Ψ_α is said to be eigenfunction of $\hat{O}$ with the eigenvalue α. (only eigenvalues can be observed!) (postulate III, including collapse of state)

example 1: $\hat{O} = \hat{P} = \frac{\hbar}{i}\frac{d}{dx}$

$$\hat{P}\,\phi_p(x) = \frac{\hbar}{i}\frac{d}{dx}\phi_p(x) = p\,\phi_p(x)$$

$$\therefore \phi_p(x) = N\, e^{\frac{i}{\hbar}p\cdot x}, \quad N = \text{Normalization factor.}$$

$\boxed{\text{Normalization}}$

$$\int dx\, \phi_{p'}^*(x)\,\phi_p(x) = |N|^2 \underbrace{\int dx\, e^{\frac{i}{\hbar}x(p-p')}}_{2\pi\hbar\,\delta(p-p')} \equiv \underline{\delta(p-p')}$$

(數學上好用之工具)

$$\therefore \text{choose } N = \frac{1}{\sqrt{2\pi\hbar}}$$

real: 用 box-normaliz

$N = \frac{1}{\sqrt{\;\;}}$, $\delta_{p,p'}$

結果是一樣的

example 2. $i\hbar \frac{d\Psi}{dt} = \underbrace{\left(\frac{-\hbar^2}{2m} \nabla^2 + V\right)}_{\hat{H}} \Psi$

if V is time-independent & boundary condition on Ψ is also ", the problem is seperable!

$\Psi = \psi_E(x) e^{\frac{-i}{\hbar}Et}$

$\hat{H} \psi_E(x) = E \underbrace{\psi_E(x)}_{\text{eigenfunction of } \hat{H}}$

Completeness : Note that ψ_α, the state right after collapsing, needs not to be normalized!

Written in terms of normalized ϕ_α, we have $\psi_\alpha = a_\alpha \phi_\alpha$

Just as Young's two-slit expt., we then have the identity $\Psi = \sum_\alpha a_\alpha \phi_\alpha$ ("generalized path integral")

we shall use this Ψ to represent the state $\{\psi_\alpha\}$

$\Leftrightarrow \vec{v} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = x\hat{x} + y\hat{y} + z\hat{z}$

over all possible amplitudes (all possible route!) exhaust all possible α ! → * sum over

$|a_\alpha|^2$ = probability of getting α

(This is actually the spirit of path integral!)

In mathematical language, $\{\phi_\alpha\}$ are complete. From physics picture, this must be true. Otherwise, if there exists a state Ψ which lies outside $\underbrace{\sum_\alpha a_\alpha \phi_\alpha}_{\text{the space spanned}}$, it implies that the particle with $\tilde{\Psi}$ can escape the detection of the measurement operation $\hat{O}$. This would not be acceptable!

This tells us that any state Ψ must be expressible in the form $\sum_\alpha a_\alpha \Phi_\alpha$.

Two things to be noted

(i) suppose $\sum_\alpha a_\alpha \Phi_\alpha = 0$, i.e., we do measurement on nothing. We should get nothing, $\therefore a_\alpha = 0$!

$\therefore$ This implies $\{\Phi_\alpha\}$ are linearly independent!

They form a basis! $\vec{a}\cdot\vec{b} = \delta_{ab}$

(ii) If $\int dx\ \Phi_\alpha^* \Phi_\beta = \delta_{\alpha\beta}$ is further satisfied, (orthogonal if α $\delta_{\alpha\beta}$) they form so-called orthonormal basis.

→ For Hermitian operators, $\hat{O}$, suppose $\{\tilde{\Phi}_\alpha\}$ are eigenfunctions.

$$\hat{O}^* \tilde{\Phi}_\alpha^* = \alpha^* \tilde{\Phi}_\alpha^* \quad \cdots\cdots (2)$$

$$\hat{O} \tilde{\Phi}_\alpha = \alpha \tilde{\Phi}_\alpha \quad \cdots\cdots (3)$$

$$\int dx \left[\tilde{\Phi}_\alpha \cdot (2) - \tilde{\Phi}_\alpha^* \cdot (3)\right] \Rightarrow (\alpha^* - \alpha)\int dx\ |\tilde{\Phi}_\alpha|^2 = \int dx\ \tilde{\Phi}_\alpha(x)\, \hat{O}^* \tilde{\Phi}_\alpha^* - \int dx\ \tilde{\Phi}_\alpha^*\, \hat{O}\, \tilde{\Phi}_\alpha$$

$$= \int \tilde{\Phi}_\alpha^* \left[\hat{O}^+ - \hat{O}\right] \tilde{\Phi}_\alpha = 0$$

$\therefore \alpha^* = \alpha$ $\therefore$ eigenvalues of $\hat{O}$ must be real

Similarly, if we replace α by β in ②, and perform $\int dx\,[-\tilde{\Phi}_\alpha \cdot ② + \tilde{\Phi}^*_\beta \cdot ③]$, we get

$$(\alpha-\beta)\int dx\, \tilde{\Phi}^*_\alpha(x)\tilde{\Phi}_\beta(x) = \int dx\, \tilde{\Phi}^*_\alpha[\hat{O}^+ - \hat{O}]\tilde{\Phi}_\beta = 0$$

$\therefore$ if $\alpha \neq \beta$, then $\int dx\, \tilde{\Phi}^*_\alpha(x)\tilde{\Phi}_\beta = 0$

For $\alpha=\beta$, there are two possibilities:

① non-degenerate : i.e., only one eigenfunction for α

In this case, we obtain an orthonormal basis by defining $\Phi_\alpha = \frac{1}{\sqrt{\int dx|\tilde{\Phi}_\alpha|^2}}\tilde{\Phi}_\alpha$.

② degenerate : there exists more than one eigenfunctions for the eigenvalue α.

Let these eigenfunctions be $\tilde{\Phi}^{(i)}_\alpha$.

They are orthogonal to each other for different α:

$$\int dx\,[\tilde{\Phi}^{(i)}_\alpha]^*\,\tilde{\Phi}^{(j)}_\beta = 0 \qquad \text{if } \alpha\neq\beta.$$

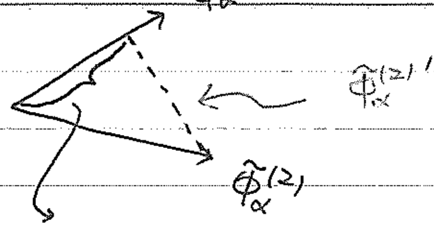
Initially, $\{\tilde{\Phi}^{(i)}_\alpha\}_{i=1,2,\ldots}$ may not be orthogonal to each other, but they can be reorganized via so-called Gram-Schmidt orthogonalization process to become orthogonal:

$$\tilde{\Phi}^{(1)\prime}_\alpha = \tilde{\Phi}^{(1)}_\alpha$$

$$\tilde{\Phi}^{(2)\prime}_\alpha = \tilde{\Phi}^{(2)}_\alpha - \frac{\int dx\,[\tilde{\Phi}^{(2)}_\alpha]^*\,\tilde{\Phi}^{(1)\prime}_\alpha}{\int dx\,|\tilde{\Phi}^{(1)\prime}_\alpha|^2}\,\tilde{\Phi}^{(1)\prime}_\alpha$$

$$\vec{b}' = \vec{b} - \frac{\vec{b}\cdot\hat{a}}{|\hat{a}|}\,\hat{a}$$

$$\tilde{\phi}_\alpha^{(1)'} = \tilde{\phi}_\alpha^{(1)}$$



$$\frac{\int dx\,[\tilde{\phi}_\alpha^{(2)}]^* \tilde{\phi}_\alpha^{(1)'}}{\int dx\,|\tilde{\phi}_\alpha^{(1)'}|^2}\,\tilde{\phi}_\alpha^{(1)'}$$

$$\tilde{\phi}_\alpha^{(3)'} = \tilde{\phi}_\alpha^{3} - \frac{\int dx\,[\tilde{\phi}_\alpha^{(3)}]^* \tilde{\phi}_\alpha^{(2)'}}{\int dx\,|\tilde{\phi}_\alpha^{(2)'}|^2}\,\tilde{\phi}_\alpha^{(2)'} - \frac{\int dx\,[\tilde{\phi}_\alpha^{(3)}]^* \tilde{\phi}_\alpha^{(1)'}}{\int dx\,|\tilde{\phi}_\alpha^{(1)'}|^2}\,\tilde{\phi}_\alpha^{(1)'}$$

$\vdots$

$$\tilde{\phi}_\alpha^{(n)'} = \tilde{\phi}_\alpha^{(n)} - \frac{\int dx\,[\tilde{\phi}_\alpha^{(n)}]^* \tilde{\phi}_\alpha^{(n-1)'}}{\int dx\,|\tilde{\phi}_\alpha^{(n-1)'}|^2}\,\tilde{\phi}_\alpha^{(n-1)'} - \cdots\cdots - \frac{\int dx\,(\tilde{\phi}_\alpha^{n})^* \tilde{\phi}_\alpha^{1'}}{\int dx\,|\tilde{\phi}_\alpha^{1'}|^2}\,\tilde{\phi}_\alpha^{1'}$$

(One notices that the notations we have been using are awkward. We'll see this will be improved by using Dirac's notation!)

Then, by redefining $\phi_\alpha^{(n)} = \dfrac{1}{\sqrt{\int dx\,|\tilde{\phi}_\alpha^{(n)'}|^2}}\,\tilde{\phi}_\alpha^{(n)'}$, we get an orthornormal basis.

In summary, observables are represented as Hermitian operators in Q.M., whose eigenvalues are real and eigenvectors form a complete, orthonormal basis.

* Compatiable & incompatiable variables

Let me emphasize again that observables in Q. M. are represented by operators, not numbers!

This is very important. Associated with it, commutability is now a problem, which of course is not a problem if observables are just numbers as in classical physics.

Consider the following two measurements:

① precise measurement p then followed by an immediate precise measurement of position x

$\xrightarrow{p} e^{\frac{ipx}{\hbar}} \xrightarrow{x}$ all possible x are equally possible

② precise measurement of x followed by precise measurement of p

$\xrightarrow{x} \; x_0 \; \xrightarrow{p}$ all possible p are equally possible

$\delta(x-x_0) = \int \frac{dp}{2\pi\hbar} e^{\frac{ip(x-x_0)}{\hbar}}$

$e^{\frac{ipx}{\hbar}}$

The results of ① & ② are dramatically different:

one is localized at x

the other with definite momentum, is thus delocalized!

This tells us that the "order" of measurements is important. In mathematical language, it tells us

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→ because as we'll see if $[A,B]=0$, they can be simultaneously measured, so can find a common eigenstate

~~that given two observables $\hat{A}$ & $\hat{B}$, $\hat{A}\hat{B}$ is~~ not necessarily the same as $\hat{B}\hat{A}$ (not as numbers), i.e., $\hat{A}$ & $\hat{B}$ may not commute!

Therefore, in Q.M., "simultaneous" measurement becomes tricky since it becomes ambiguous to associate an operator to the simultaneous $\underset{\text{direct-product}}{\wedge}$ measurement of $\hat{A}$ and $\hat{B}$. In fact, if $\hat{A}$ and $\hat{B}$ are not commute, this is impossible!

Compatiable & in compatible observables that can be simutaneously measured to any precision are called compatiable variables; otherwise, they are incompatiable!

Let's consider two observables $\hat{A}$ & $\hat{B}$.

If they are compatiable, they can be measured precisely & simultaneously. This simultaneous measurement is a measurement by itself, so after the measurent, according to what we said, we got $\psi(a,b)$ such that

$$\hat{A}\psi(a,b) = a\psi(a,b)$$
$$\hat{B}\psi(a,b) = b\psi(a,b)$$

i.e. $\psi(a,b)$ is a simultaneous eigenstate of $\hat{A}$ & $\hat{B}$.

Note that $\{\psi(a,b)\}$ is a basis.

Obvioasly, we have $(\hat{A}\hat{B}-\hat{B}\hat{A})\psi(a,b)=0$

$\therefore$ It implies $\underline{[\hat{A}, \hat{B}] = 0}$

On the contrary, if $[\hat{A}, \hat{B}] = 0$, starting from the eigenstates of $\hat{A}$, ψ_a,

$$\because [\hat{A}, \hat{B}]\psi_a = 0$$

$$\Rightarrow \hat{A}(\hat{B}\psi_a) = a(\hat{B}\psi_a)$$

(i) a is non-degenerate, $\hat{B}\psi_a \propto \psi_a$

$$\therefore \hat{B}\psi_a \equiv b\psi_a$$

$\therefore \psi_a$ is a simultaneous eigenfunction of $\hat{A}$ & $\hat{B}$.

Note that, in this case, b is a function of a!

$\underline{\hat{B} = f(\hat{A})}$

(ii) a is degenerate, $\psi_a \to \psi_a^{(i)}$, $i = 1, \ldots, N_a$

The arguement of (i) shows that $\hat{B}\psi_a^{(i)}$ is an eigenstate of $\hat{A}$ with eigenvalue a.

$\therefore \hat{B}\psi_a^{(i)}$ must be a linear combination of $\psi_a^{(j)}$

We have

$$\hat{B}\psi_a^{(i)} = \sum_j \alpha_{ij}\psi_a^{(j)}, \quad \because \int dx\, (\psi_a^{(i)})^* \psi_a^{(j)} = \delta_{ij}$$

$$\Rightarrow \alpha_{ij} = \int dx\, (\psi_a^{(j)})^* \hat{B}\psi_a^{(i)}$$

If we put this in the following form:

$$\hat{B}\begin{pmatrix} \psi_a^{(1)} \\ \psi_a^{(2)} \\ \vdots \\ \psi_a^{(N_a)} \end{pmatrix} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1N_a} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2N_a} \\ \vdots & & & \\ \alpha_{N_a1} & & \cdots & \alpha_{N_aN_a} \end{pmatrix}\begin{pmatrix} \psi_a^{(1)} \\ \vdots \\ \vdots \\ \psi_a^{(N_a)} \end{pmatrix}$$

Or more conveniently, in the form :

$$\psi_a^{(1)} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \psi_a^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \quad \ldots,$$

$$\hat{B} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} \alpha_{11} & \alpha_{21} & \cdots & \\ \alpha_{12} & \alpha_{22} & & \\ \vdots & & \ddots & \\ \alpha_{1N_a} & \cdots & & \alpha_{N_aN_a} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\hat{B} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = \begin{pmatrix} & & \\ & " & \\ & & \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

$$\vdots \qquad\qquad \vdots$$

for a general $\psi_a = \sum_j b_j \psi_a^{(j)}$

$$\hat{B} \begin{pmatrix} b_1 \\ \vdots \\ b_{N_a} \end{pmatrix} = \begin{pmatrix} & & \\ & " & \\ & & \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_{N_a} \end{pmatrix}$$

, the question of whether one can find a linear to be an eigenstate of $\hat{B}$ reduces to diagonalize the matrix $\alpha \equiv \begin{pmatrix} \alpha_{11} & \cdots & \alpha_{N_a1} \\ \vdots & & \\ \alpha_{1N_a} & \cdots & \alpha_{N_aN_a} \end{pmatrix}$.

$$\because \alpha_{ij}^* = \int dx\, \psi_a^{(j)} \hat{B}^* \psi_a^{(i)*} = \int dx\, \psi_a^{(i)*} \hat{B}^\dagger \psi_a^{(j)}$$

$$\underset{\hat{B}^\dagger = \hat{B}}{=} \int dx\, \psi_a^{(i)*} \hat{B} \psi_a^{(j)} = \alpha_{ji},$$

~~α is a Hermitian matrix~~

$\Rightarrow$ such diagonalization is always possible according to Spectral theorem in Linear Algebra.

In summary, if $\hat{A}$ & $\hat{B}$ are compatiable observables,

$[\hat{A}, \hat{B}] = 0 \Leftrightarrow$ one can find simultaneous orthonormal eigenstates!

Complete sets of commuting observables

In the above derivation, one sees that if $\hat{A}$ is degenerate, the introduction of $\hat{B}$ which commutes with $\hat{A}$ tends to help labelling the eigenstates of $\hat{A}$.

The new label (a, b) may not distinguish all base states so we may search for another observable $\hat{C}$, which Commutes with both $\hat{A}$ & $\hat{B}$. . . . until we find the set of observables $\hat{A}, \hat{B}, \hat{C}, \ldots, \hat{L}$ in which any two of them are commuting and they

possess one and only one common basis.

Such set of observables is called complete set of commuting observables! If one carries out simultaneously & precise measurement of these variables, one can be sure that the state after the

measurement is the eigenfunctor $\psi(a, b, c, \ldots, \ell)$!
(This forms a remedy to our simplified picture at beginning 8/24 page 9!)
In particular, if there exists any other observable $\hat{O}$ which commutes with $\hat{A}, \hat{B}, \ldots \hat{L}$, it necessarily has $\{\psi(a,b,c,\ldots,\ell)\}$ as its basis!

$$\therefore \quad \hat{O}\,\psi(a,b,c,\ldots,\ell) = o\,\psi(a,b,\ldots,\ell)$$

in other words, $o = o(a,b,c,\ldots,\ell)$, $\hat{O}$ be a function of $\hat{A}, \hat{B}, \ldots$, and $\hat{L}$!

Incompatible variables

When $[\hat{A}, \hat{B}] \neq 0$, they are incompatible to each other.
There exists no simultaneous eigenbasis to $\hat{A}$ & $\hat{B}$.
Experimentally, they can not be measured precisely at the same time.

This is a new feature!

The most important phenomenon associated with it is the uncertainty principle:

$$(\Delta A)^2 \equiv \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle, \quad (\Delta B)^2 \equiv \langle (\hat{B} - \langle \hat{B} \rangle)^2 \rangle$$

$$\Delta A \, \Delta B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right|$$

Familiar example: $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$ $\quad [\hat{x}, \hat{p}] = -\frac{\hbar}{i}\frac{dx}{dx} = i\hbar$

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

Summary about observables in Q.M.

(i) observables $\Leftrightarrow$ Hermitean operators $(\hat{O})$ that possess a complete, orthonormal set of eigenfunctions (ϕ_α, α) $\int dx\, \phi_\alpha^* \phi_\beta = \delta_{\alpha\beta}$

$\int dx\, \phi_\alpha^{*(i)} \phi_\alpha^{(j)} = \delta_{ij}$ orthogonal Gram-Schm-

* not all Hermitean operators do have this property. to show this is usually a difficult problem.

any $\psi = \sum a_\alpha \phi_\alpha$ $\xrightarrow[\boxed{\text{collapse of state}}]{\text{ideal measure}}$ $a_{\alpha_0} \phi_{\alpha_0}$

$a_\alpha = \int \psi^* \phi_\alpha$

$|a_\alpha|^2 =$ probability of ~~to~~ getting α.

~~For "single" particle" problem~~ $\boxed{\hat{O} = \text{linear.}}$

$$\hat{O}\, \phi_\alpha = \alpha\, \phi_\alpha$$

$$\hat{O}\, (\lambda \phi_\alpha) = \lambda\, \alpha\, \phi_\alpha$$

measure ϕ_α 100 times

$\cong$ measure 100 identical system ϕ_α

Dirac notations & Linear Algebra

* The Ket

As mentioned, on top of probability amplitudes, one has the state :

$$\psi = \sum_{\alpha} a_\alpha \phi_\alpha \quad \cdots \text{①}$$

where α denotes $(a, b, c, \cdots, \ell)$, which are eigenvalues for the complete set of commuting observables.

This is analogous to 3D vectors

$$\vec{v} = \sum_{i=1}^{3} v_i \hat{e}_i$$

where the analogies are

$$\vec{v} \Leftrightarrow \psi$$
$$i \Leftrightarrow \alpha$$
$$\hat{e}_i \Leftrightarrow \phi_\alpha$$
$$v_i \Leftrightarrow a_\alpha$$

For this reason, ψ is also termed "state vector" sometimes.

In Dirac's notations, the state vector is conveniently denoted by $|\psi\rangle$, where $|\ \rangle$ is so-called ket, the symbol ψ inside is just used to distinguish different state.

$\hat{e}_\alpha$也有3個 components!

(a) usually, x is treated as a "parameter" not an observable. So, one writes $\psi(x) = \sum_\alpha a_\alpha \phi_\alpha(x)$ in eq.①, i.e., ψ is not expanded in eigenfunctions of $\hat{X}$.

$\psi(x)$ here is the so-called wave function in the Schrödinger eq.
One can still view $\psi(x)$ as a state vector $|\psi\rangle$
with $x \Leftrightarrow \hat{x}, \hat{y}, \hat{z}$ being component index !

(b) $c|\psi\rangle$: its meaning is just the same as $c\vec{v}$:
defined by the component relation :

$$(c|\psi\rangle)_x = c\,\psi(x)$$

(c) $|\psi\rangle + |\phi\rangle \Leftrightarrow \vec{v}_1 + \vec{v}_2$: defined by the component relation $(|\psi\rangle + |\phi\rangle)_x = \psi(x) + \phi(x)$

* Linear vector space What is a vector?

Given a system, which may be simply a particle, it is convenient to consider the space which includes all possible allowed state vectors.

In Q.M., such space is a linear vector space :
a collection of objects $\{|1\rangle, |2\rangle, \cdots, |\psi\rangle\} \equiv \mathbb{V}$
called vectors (our collections are all possible state vectors for such system.)

with definite rules for
(i) sum , $|1\rangle + |2\rangle$
(ii) multiplication, $\alpha|1\rangle$, $\alpha \in$ specified field, e.g., in Q.M., $\alpha \in$ complex #s.

remark : the sum & multiplication need not to be defined in terms of components of vectors ! They are just mappings to associate another vector in $\mathbb{V}$ to $|1\rangle + |2\rangle$ or $\alpha|1\rangle$.

Since $\mathbb{V}$ has included all possible states, including abstractly $|1\rangle + |2\rangle$, $\alpha|1\rangle$, ..., these mappings are possible!

Under these rules, satisfying

items that sum & multiplication mappings must satisfy

1. $|V\rangle + |W\rangle \in \mathbb{V}$ (linear!)
2. $a(|V\rangle + |W\rangle) = a|V\rangle + a|W\rangle$
3. $(a+b)|V\rangle = a|V\rangle + b|V\rangle$
4. $a(b|V\rangle) = ab|V\rangle$
5. $|V\rangle + |W\rangle = |W\rangle + |V\rangle$
6. $|V\rangle + (|W\rangle + |Z\rangle) = (|V\rangle + |W\rangle) + |Z\rangle$
7. exist $|0\rangle$ such that $|0\rangle + |V\rangle = |V\rangle$
8. exist inverse $|V\rangle + |-V\rangle = \underset{\overset{|||}{0}}{|0\rangle}$ $\Rightarrow$ so that one can define "minus", one often writes $|-V\rangle = -|V\rangle$

$|V\rangle - |V\rangle = 0$!

Example 1. $\mathbb{V} = 2\times 2$ real matrices $= \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \middle| \ a, b, c, d \in \text{Real} \right\}$

define (i) sum (mapping) : $\begin{pmatrix} a & b \\ c & d \end{pmatrix} + \begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix} = \begin{pmatrix} a+a' & b+b' \\ c+c' & d+d' \end{pmatrix}$

$\because$ $a+a'$, $b+b'$, $c+c'$, $d+d' \in$ real

$\therefore \begin{pmatrix} a & b \\ c & d \end{pmatrix} + \begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix} \in \mathbb{V}$

(ii) multiplication (mapping) : $\alpha \in$ real

$$\alpha \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \alpha a & \alpha b \\ \alpha c & \alpha d \end{pmatrix}$$

$1 \sim 8$ are satisfied!

Example 2. $\mathbb{V} = \{ \psi(x,t) \mid \psi(x,t) = \text{solutions to } i\hbar \frac{d\psi(x,t)}{dt} = \hat{H}\psi(x,t) \}$

$\psi(x,t)$ is viewed as components to $|\psi(t)\rangle$

define (i) sum : $[|\psi(t)\rangle + |\phi(t)\rangle]_x = \psi(x,t) + \phi(x,t)$

(ii) multiplication : $\alpha \in$ complex

$$[\alpha |\psi(t)\rangle]_x = \alpha \psi(x,t)$$

1. $\psi(x,t)$, $\phi(x,t)$ are solutions $\Rightarrow$ $\psi + \phi$ is too!
(Schrödinger eq. is linear !)

2 ~ 8 are trivially satisfied !

* Concept of basis ⇐分量之引入

$|1\rangle, |2\rangle, \cdots, |n\rangle, \neq |0\rangle$

if $\sum_{i=1}^{n} a_i |i\rangle = |0\rangle \Rightarrow a_i = 0$ $\quad |1\rangle, |2\rangle, \ldots, |n\rangle$ are said to be linearly independent

otherwise they are linearly dependent.

Given a linear vector space $\mathbb{V}$, if there exists a maximal # of linearly independent vectors $|1\rangle, \cdots, |N\rangle$. N is called the dimension of $\mathbb{V}$.

Consider now a linear combination of $|1\rangle, |2\rangle, \ldots, |N\rangle$ and the $N+1$ th vector $|\psi\rangle$:

$$a_1|1\rangle + a_2|2\rangle + \cdots + a_N|N\rangle + a|\psi\rangle = 0,$$

the existence of N implies $a \neq 0$, $\therefore |\psi\rangle = -\sum_{i=1}^{N} \frac{a_i}{a} |i\rangle$.

Therefore, any vector $|\psi\rangle$ in $\mathbb{V}$ can be expressed as a linear combination of $|1\rangle, |2\rangle, \ldots, |N\rangle$.

$|1\rangle, |2\rangle, \ldots,$ and $|N\rangle$ are thus called basis.

Note that the dimension could be infinite as it often happens for the system we are interested in Q.M.

example. $\mathbb{V} = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \middle| \; a, b, c, d \in \text{Real} \right\}$

basis $|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $|2\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $|3\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$|4\rangle = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

$\Rightarrow$ 4-dimension

elementary definition

* Inner product space & bra (向量有大小、方向)

As one may notice, the wavefunctions we consider have more properties than the vectors in the linear vector space. They have magnitudes $|\psi(x,t)|^2$ which can be compared and have the meaning of being "probability density". What actually has the absolute meaning is the normalization

$$\int dx \; \psi^*(x)\, \psi(x)$$

which gives the total # of particles one can find.

More generally, we consider

$$\int dx\ \phi^*(x)\ \psi(x) .$$

This quantity is to be compared with :

ordinary vector $\vec{a}\cdot\vec{b} = \sum_i a_i b_i = \underbrace{(a_1, a_2, \cdots)\cdot\begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix}}_{\text{matrix product}}$

Complex vector $\vec{a}^*\cdot\vec{b} = \sum_i a_i^* b_i = (a_1^*, a_2^*, \cdots)\begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix}$

$\Leftrightarrow \int dx\ \phi^*(x)\ \psi(x)$, $\quad x \Leftrightarrow i$.

We thus introduce the bra $\langle\phi|$:

$$|\phi\rangle = \begin{pmatrix} 1 \\ 2-i \\ \vdots \\ \vdots \end{pmatrix} \Leftrightarrow \langle\phi| = (1, 2+i, \cdots)$$

$$\therefore \int dx\ \phi^*(x)\ \psi(x) = \langle\phi|\cdot|\psi\rangle \underset{\substack{\uparrow \\ \text{inner product}}}{\equiv} \langle\phi|\psi\rangle$$

The inner product satisfies (抽象化)

(i) $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$

(ii) $\langle\phi|\phi\rangle = \text{real} \geq 0 \quad = 0$ if only if $|\phi\rangle = 0$

(iii) linear in kets

$$\langle\phi|\left(\alpha|\psi\rangle + \beta|\psi'\rangle\right) = \alpha\langle\phi|\psi\rangle + \beta\langle\phi|\psi'\rangle$$

above 3 properties are what we extract and should generally applicable for other inner product too! → see over

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useful terms : ① if $\langle\psi|\phi\rangle = 0$, $\Rightarrow$ $|\psi\rangle, |\phi\rangle$ are orthogonal

② norm of $|\psi\rangle \equiv \sqrt{\langle\psi|\psi\rangle}$

$\equiv |\psi|$

$\cancel{\langle\phi|(\alpha|\psi\rangle + \beta|\psi'\rangle)}$

$= \cancel{\left[(\alpha^*\langle\psi| + \beta^*\langle\psi'|)|\phi\rangle\right]^*}$

$$\underbrace{(\alpha\langle\phi| + \beta\langle\phi'|)}_{\langle\tilde{\phi}|}|\psi\rangle \equiv \langle\tilde{\phi}|\psi\rangle = \langle\psi|\tilde{\phi}\rangle^*$$

$$\because \langle\psi|\tilde{\phi}\rangle = \langle\psi|(\alpha^*|\phi\rangle + \beta^*|\phi'\rangle)$$

$$= \alpha^*\langle\psi|\phi\rangle + \beta^*\langle\psi|\phi'\rangle$$

$$\therefore (\alpha\langle\phi| + \beta\langle\phi'|)|\psi\rangle$$

$$= \alpha\langle\phi|\psi\rangle + \beta\langle\phi'|\psi\rangle$$

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* adjoint operation & dual space

As implied when we define inner product :
given a ket $|\psi\rangle$, one can associate it
with another vector $\langle\psi|$. This is called
adjoint operation

The space that collects $\langle\psi|$ is called dual space
, dual to the linear vector space formed by $|\psi\rangle$.
We have the obvious rules :

$$|\psi\rangle \to \langle\psi| \qquad \langle\psi|\chi\rangle = \langle\chi|\psi\rangle^*$$
$$c|\psi\rangle \to c^*\langle\psi|$$
$$c_1|\psi\rangle + c_2|\phi\rangle \to c_1^*\langle\psi| + c_2^*\langle\phi|$$

* Orthonormal basis

When the basis satisfies : $\langle i|j\rangle = \delta_{ij}$,
it forms an orthonormal basis.

In this case, $|\psi\rangle = \sum_i \psi_i |i\rangle \qquad \langle\psi| = \sum_i \langle i|\psi_i^*$

$$\underline{\psi_i = \langle i|\psi\rangle} \qquad \therefore \langle\psi|i\rangle = \langle i|\psi\rangle^*$$

This is completely analogous to 3D vectors : $\vec{v} = \sum_{i=1}^{3} v_i \hat{e}_i$

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} \iff \langle i|j\rangle = \delta_{ij}$$
$$v_i = \vec{v}\cdot\hat{e}_i \iff \psi_i = \langle i|\psi\rangle$$

* Change basis

3D vectors $\vec{v} = \sum_{i=1}^{3} v_i' \hat{e}_i' = \sum_{i=1}^{3} v_i \hat{e}_i$

$\hat{e}_i'$ are also orthonormal.

$$\therefore v_i' = \hat{e}_i' \cdot \vec{v} = \sum_{j=1}^{3} \hat{e}_i' \cdot \hat{e}_j \, v_j$$

In Q.M., $|\psi\rangle = \sum_i \langle i|\psi\rangle |i\rangle = \sum_i \langle \tilde{i}|\psi\rangle |\tilde{i}\rangle$

$$\langle \tilde{i}|\psi\rangle = \sum_j \underbrace{\langle \tilde{i}|j\rangle}_{\text{"transfer" matrix}} \langle j|\psi\rangle$$

* bases with continuous indices

$|x\rangle$: state of the particle when it is localized at x

$x \Leftrightarrow i$, $\psi(x) \Leftrightarrow v_i$, $\langle x|\psi\rangle \Leftrightarrow \vec{v}\cdot\hat{e}_i$

Recal that $\langle \psi|\phi\rangle = \int dy \, \psi^*(y)\, \phi(y)$

$$\therefore \langle x|x'\rangle = \int dy \, [\langle y|\psi\rangle]^* \langle y|\phi\rangle , \quad \psi = x, \quad \phi = x'$$

$$= \int dy \, \langle \psi|y\rangle \langle y|\phi\rangle$$

Obviously, $\langle y|\phi\rangle = 0$ if $y \neq x'$

$\langle \psi|y\rangle = 0$ if $y \neq x$

$\therefore \langle x|x'\rangle = 0$ if $x \neq x'$ $\Rightarrow$ orthogonal !

What is $\langle x|x\rangle$?

From $\langle \psi|\phi\rangle = \int dy \langle \psi|y\rangle \langle y|\phi\rangle$, if we set $\psi = x$, we get $\phi(x) = \int dy \, \langle x|y\rangle \, \phi(y)$

$\therefore$ obviously $\langle x | y \rangle = \delta(x-y)$ $\rightarrow$ in general

$|\Psi\rangle = \int d\xi \; |\xi\rangle \langle \xi | \Psi \rangle$

$\leftrightarrow \; |\Psi\rangle = \sum |i\rangle\langle i|\Psi\rangle$

When $x=y$, $\langle x | x \rangle = \infty$.

Therefore, for continuous indices, one has:

orthonormal basis : $\langle \xi | \xi' \rangle = \delta(\xi - \xi')$

Another example is $|p\rangle$:

As we have seen, $\langle x | p \rangle = \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}$

$$\int dx \; \phi^*_{p'}(x)\, \phi_p(x) = \delta(p-p')$$

$$\shortparallel$$

$$\int dx \; \langle p' | x \rangle \langle x | p \rangle$$

$$\shortparallel$$

$\langle p' | p \rangle$ $\therefore$ $\langle p' | p \rangle = \delta(p-p')$ is also true.

Once again, if we put $\phi = p$ in the definition

of inner product $\langle \phi | \Psi \rangle = \int dx \; \langle \phi | x \rangle \langle x | \Psi \rangle$, $\xi = x$ $\langle p | \Psi \rangle$

we get

$$\langle p | \Psi \rangle = \int dx \; \langle p | x \rangle \langle x | \Psi \rangle$$

$$= \int dx \; (\langle x | p \rangle)^* \, \Psi(x)$$

$$= \int \frac{dx}{\sqrt{2\pi\hbar}} \; e^{-\frac{i}{\hbar}px} \; \Psi(x)$$

or inverse F.T.

$\xi = p$

$\langle x | \Psi \rangle$

$\therefore$ we get $\Phi(p) = \int \frac{dx}{\sqrt{2\pi\hbar}} \; e^{-\frac{i}{\hbar}px} \; \Psi(x)$

We automatically recover the form of Fourier transformation

轉換[illegible]而已

Here it becomes clearer that $\frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}$ is nothing but the "transfer" matrix for changing basis from $|x\rangle$ to $|p\rangle$! $\Leftrightarrow \hat{e}_i' \cdot \hat{e}_j$

In the discrete case, one has $\vec{v} = \sum_i v_i \hat{e}_i$

$$|\psi\rangle = \sum_i \langle i|\psi\rangle\, |i\rangle .$$

For continuous cases, $\because \langle\xi|\xi'\rangle = \delta(\xi-\xi')$, we get $|\psi\rangle = \int d\xi\, \langle\xi|\psi\rangle\, |\xi\rangle$

* Physical Hilbert space

We shall not give the formal definition of Hilbert space.

Basically, a Hilbert space is a linear vector space + inner product structure + the requirement of square integrable : $\int dx\, |\psi(x)|^2 < \infty$

This last requirement is to assure the norm $\langle\psi|\psi\rangle$ in the inner-product space meaningful and can be normalized to one.

In Q.M., we relax it to be that $|\psi\rangle$ can be normalized to 1 or a Dirac delta function such as $\langle x|x'\rangle = \delta(x-x')$. Such space is called "physical" Hilbert space.

Linear operators

* A reminder : 3 products in vector analysis

Given two vectors $\vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$, $\vec{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$

inner product $\vec{a} \cdot \vec{b} = \vec{a}^T \cdot \vec{b}$

$$= (a_1 \ a_2 \ a_3) \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = a_1 b_1 + a_2 b_2 + a_3 b_3$$

$= \underline{\text{a scalar}}$

outer product $\vec{a} \times \vec{b} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = (a_2 b_3 - a_3 b_2, \ a_3 b_1 - a_1 b_3, \ a_1 b_2 - a_2 b_1) = \underline{\text{a vector}}$

* matrix product $\vec{a}\vec{\mathbf{b}} \equiv \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \cdot (b_1 \ b_2 \ b_3)$ ($a b^T$ is more rigorous!)

$$= \begin{pmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{pmatrix} = \underline{\text{a matrix}}$$

→ can be unified in terms of matrix product → as $a^T b$ & $a b^T$

In particular, one may verify that

$$\hat{x}\hat{x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdots$$

Dirac $\langle a|b\rangle$ $|a\rangle\langle b|$

$$\hat{x}\hat{y} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdots$$

better notation!

∴ in general, one can write

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = a\hat{x}\hat{x} + b\hat{x}\hat{y} + c\hat{x}\hat{z} + d\hat{y}\hat{x} + e\hat{y}\hat{y} + \cdots + i\hat{z}\hat{z}$$

* We have seen some examples of linear operators:

observables $\Rightarrow$ operators ~~(not necessary Linear!)~~

$$\hat{p}\,\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) \leftarrow \text{another state}$$

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

these examples are more restrictive because $\hat{p}$ & $\hat{x}$ are not acting on $|\psi\rangle$. but depend on the special representation $\psi(x)$)

In general, an operator is just a mapping of $|\psi\rangle$ to another vector $|\phi\rangle$ in $\mathbb{V}$:

$$|\psi\rangle \xrightarrow[\text{do something on it}]{} \text{produce a new state} \equiv |\phi\rangle$$

(including observing, measurement such as $\hat{p}$, rotating the system, waiting for a period of time Δt ... performing an operation of $|\psi\rangle$)

Let $\hat{A}$ be the operation, we denote

$$|\phi\rangle = \hat{A}\,|\psi\rangle$$

(Sometimes, one writes it in this way $|\phi\rangle = |A\psi\rangle$).

By linear, we mean that

if $|\phi\rangle = \hat{A}|\psi\rangle$, then $\hat{A}(\alpha|\psi\rangle) = \alpha|\phi\rangle$

i.e. $\hat{A}(\alpha|\psi\rangle) = \alpha(\hat{A}|\psi\rangle)$

and also $\hat{A}(\alpha|\psi_1\rangle + \beta|\psi_2\rangle) = \alpha(\hat{A}|\psi_1\rangle) + \beta(\hat{A}|\psi_2\rangle)$

The nice thing about "linear" is that if we know $\hat{A}|i\rangle$, $i = 1, 2, 3, \ldots$, we know $\hat{A}|\psi\rangle$

since any $|\psi\rangle = \sum_i \psi_i |i\rangle$, (Assume $\{|i\rangle\}$ orthonormal!)

$$|\phi\rangle = \hat{A}|\psi\rangle = \sum_i \psi_i \hat{A}|i\rangle.$$

$$= \sum_i \langle i|\psi\rangle \left(\hat{A}|i\rangle\right)$$

↑ $|i\rangle$ orthonormal

Since $|\phi\rangle$ can be also expanded : $|\phi\rangle = \sum_j \phi_j |j\rangle$

with $\phi_j = \langle j|\phi\rangle$, we can calculate ϕ_j

$$\phi_j = \langle j|\phi\rangle = \sum_i \langle i|\psi\rangle \underbrace{\langle j|\left(\hat{A}|i\rangle\right)}_{\equiv A_{ji}}$$

$$= \sum_i A_{ji} \psi_i$$

Therefore, we completely specify the action of $\hat{A}$ once we know A_{ji}.

In other words, the linear operators are analogous to matrices! The operation of an operator = matrix product. → in terms of component

* linear operators as matrix product ← How do we then represent $\hat{A}$?

As we have shown that in vector analysis, $\vec{a}\,\vec{b}$ means matrix product $\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} (b_1\ b_2\ b_3)$.

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In Dirac notations, matrix product of two states are represented by $|\phi\rangle\langle\psi|$,

while the inner product is $\langle\phi|\psi\rangle$!

Vector analysis $\Longleftrightarrow$ Q.M. (completeness relation)

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z} \qquad I = |1\rangle\langle 1| + |2\rangle\langle 2| + \cdots$$

$$= \sum_i |i\rangle\langle i|$$

example $Iv = v$

$$(\hat{x}\hat{x}+\hat{y}\hat{y}+\hat{z}\hat{z})v = \left[\begin{pmatrix}1\\0\\0\end{pmatrix}(1\,0\,0) + \begin{pmatrix}0\\1\\0\end{pmatrix}(0\,1\,0) + \begin{pmatrix}0\\0\\1\end{pmatrix}(0\,0\,1)\right]\begin{pmatrix}v_x\\v_y\\v_z\end{pmatrix}$$

The simplest linear operator is I: the identity operator.

By definition, we have $I|\psi\rangle = |\psi\rangle$!

Now, $\because$ $|\psi\rangle = \sum_i \psi_i |i\rangle = \sum_i |i\rangle\langle i|\psi\rangle$

$$= \left(\sum_i |i\rangle\langle i|\right)\cdot|\psi\rangle \qquad \left(|\psi\rangle = \int d\xi\, |\xi\rangle\langle\xi|\psi\rangle\right)$$

useful analogy

inner product. = matrix product

$\therefore$ $I = \sum_i |i\rangle\langle i|$ (completeness relation) (see over)

In general, $\because$ $\hat{A}|\psi\rangle = |\phi\rangle = \sum_j \phi_j |j\rangle$

$$= \sum_{i,j} A_{ji}\,\psi_i\,|j\rangle$$

$$= \sum_{i,j} A_{ji}\,|j\rangle\langle i|\psi\rangle$$

可視為 3個 state $|j\rangle$, $\langle i|$, $|\psi\rangle$ 之 matrix product

$$= \left(\sum_{i,j} A_{ji}\,|j\rangle\langle i|\right)\cdot|\psi\rangle$$

$\therefore$ $\hat{A} = \sum_{i,j} A_{ij}\,|i\rangle\langle j|$! $\Longleftrightarrow$ $\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & & \\ & \ddots & \end{pmatrix}$

(matrix representation!)

It becomes clear ~~the~~ that in this representation,

$$A_{ji} \equiv \langle j| (\hat{A}|i\rangle) = (\langle j|\hat{A})\, |i\rangle = \underbrace{\langle j| \cdot \hat{A} \cdot |i\rangle}_{\text{matrix multiplication}}$$

$\therefore$ One simply writes $A_{ji} = \langle j|\hat{A}|i\rangle$.

In matrix representation, $\hat{A}|\psi\rangle$ is the same as $\hat{A} \underset{=}{\cdot} |\psi\rangle$!
inner product!

$\hat{A}\hat{B}|\psi\rangle = \hat{A}\cdot\hat{B}\cdot|\psi\rangle$

* **Adjoint** (Hermitian Conjugate)

As we mentioned, the action of an operator is just to map $|\psi\rangle$ to another state $|\phi\rangle$, denoted by $|\phi\rangle = \hat{A}|\psi\rangle$.

A similar action must also take place in the dual space, we denote the corresponding operator (map) as $\hat{A}^+$ such that

$$\langle\phi| = \langle\psi|\hat{A}^+ = \langle A\psi|$$

$\hat{A}^+$ is the adjoint of $\hat{A}$.
(A dagger!)

Now. $\because$ $|\phi\rangle = \hat{A}|\psi\rangle = \sum_{ij} A_{ij} \langle j|\psi\rangle\, |i\rangle$

$$\therefore \langle\phi| = \sum_{ij} A_{ij}^* \langle j|\psi\rangle^* \langle i|$$

$$= \sum_{ij} \langle\psi|j\rangle A_{ij}^* \langle i|$$

$$= \langle\psi| \cdot \sum_{ij} A_{ij}^* |j\rangle\langle i|$$

$$\therefore \hat{A}^+ = \sum_{ij} A_{ij}^* |j\rangle\langle i| = \begin{pmatrix} A_{11}^* & A_{21}^* & A_{31}^* & \cdots \\ A_{12}^* & A_{22}^* & & \cdots \\ A_{13}^* & \cdots & & \cdots \end{pmatrix}$$

which is exactly the same as $\underbrace{\text{Hermitian conjugate}}_{\substack{\| \\ \text{transpose + complex conjugate}}}$ of a matrix !

There are a few $\overset{\text{useful}}{}$ things to be mentioned here :

(i) A^+ needs not to act on bra only !

$A^+|\psi\rangle$ is also meaningful.

i.e. A^+ itself is an operator.

(ii) in general, $\because \langle\psi|A^+|\chi\rangle = \langle\phi|\chi\rangle = \langle\chi|\phi\rangle^*$

$$\therefore \langle\chi|A|\psi\rangle^* = \langle\psi|A^+|\chi\rangle$$

(iii) $(A^+)^+ = A$: $\langle\chi|(A^+)^+|\psi\rangle = \langle\psi|A^+|\chi\rangle^*$

$$= \left[\langle\chi|A|\psi\rangle^*\right]^* = \langle\chi|A|\psi\rangle$$

(iv) $(AB)^+ = B^+A^+$

$|\phi_{AB}\rangle = AB|\psi\rangle \equiv A(\underbrace{B|\psi\rangle}_{\substack{||| \\ |\phi_B\rangle}})$

$\langle\phi_{AB}| = \langle\phi_B|A^+$, $\quad \because \langle\phi_B| = \langle\psi|B^+$

$$\therefore \langle\phi_{AB}| = (\langle\psi|B^+)A^+$$

But, by definition, $\langle\phi_{AB}| = \langle\psi|(AB)^+$

$$\therefore (AB)^+ = B^+A^+$$

(v) Hermitian (self adjoint) $\quad A^+ = A$

anti-Hermitian $\quad A^+ = -A$

* miscellaneous properties & summary

$\langle a|A|a\rangle = a$
$= \langle a|A^+|a\rangle^*$
$= \langle a|A|a\rangle^*$
$= a^*$

(i) eigenvalue, eigenkets & measurement

$\hat{A}|a\rangle = a|a\rangle$ $\quad \left.\begin{matrix} a = \text{eigenvalue} \\ |a\rangle = \text{eigenket} \end{matrix}\right\}$ of $\hat{A}$

$A^+ = A$ (Hermitian). $\quad a =$ real (observable)

$A^+ = -A$ $\quad a =$ purely imaginary

each $a \Rightarrow$ one $|a\rangle \Rightarrow$ non-degenerate

otherwise $\Rightarrow$ degenerate

△ Suppose the eigenkets $\{|i\rangle\}$ form an orthonormal basis, we have

$$\text{average} = \langle \hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle$$
$$= \langle\psi| I\cdot\hat{A}\cdot I|\psi\rangle$$
$$= \sum_{i,j} \langle\psi|i\rangle \underbrace{\langle i|\hat{A}|j\rangle}_{= a_i\delta_{ij}} \langle j|\psi\rangle$$
$$= \sum_i a_i |\langle i|\psi\rangle|^2$$

$|\langle i|\psi\rangle|^2$ is the weight for a_i!

For $\hat{A}$ being observable, $|\langle i|\psi\rangle|^2$ is the relative probability of measuring $\hat{A}$ to be a_i!

In Q.M., only eigenvalues are seen experimentally!

△ Collapse of state: suppose before measurement $|\psi\rangle = \sum_i \psi_i |i\rangle$

$\xrightarrow[\text{measurement}]{\text{after}}$ $|i\rangle$! the probability of getting $|i\rangle = |\psi_i|^2$.

(ii) unitary $\quad UU^+ = \mathbb{I} = U^+U$

$$|\phi\rangle = U|\psi\rangle$$

$$\langle\phi| = \langle\psi|U^+$$

$$\langle\phi|\phi\rangle = \langle\psi|U^+U|\psi\rangle = \langle\psi|\psi\rangle$$

"length" $\langle\psi|\psi\rangle$ is preserved!

$\Leftrightarrow$ 3D rotations

(iii) trace of $\hat{\Omega}$

orthogonal basis

$$\mathrm{tr}\,\hat{\Omega} \equiv \sum_i \Omega_{ii} = \sum_i \langle i|\hat{\Omega}|i\rangle$$

$\Uparrow$ independent of basis

(iv) Commutators $\Rightarrow$ see over

$$\mathrm{tr}(\hat{A}\hat{B}) = \mathrm{tr}(\hat{B}\hat{A})$$

$$\mathrm{tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{tr}(\hat{B}\hat{C}\hat{A}) = \mathrm{tr}(\hat{C}\hat{A}\hat{B})$$

(Ex 1.7.1)

* more examples of linear operators

(i) discrete : $\mathbb{I} = \sum_i |i\rangle\langle i|$

Continuous : $\langle\phi|\psi\rangle = \int dx\, \langle\phi|x\rangle\langle x|\psi\rangle$

$$= \langle\phi| \cdot \int dx\, |x\rangle\langle x| \cdot |\psi\rangle$$

$$\therefore\ \mathbb{I} = \int dx\, |x\rangle\langle x|$$

in general $\mathbb{I} = \int d\xi\, |\xi\rangle\langle\xi|$

Note that the matrix element of $\mathbb{I} = \sum_i |i\rangle\langle i|$

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(iii) $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

$$\langle x|\hat{H}|\psi\rangle = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi(x) + V(x)\,\psi(x)$$

(iv) Projection operator $\hat{P} = |i\rangle\langle i|$, $\langle i|i\rangle = 1$

$$\hat{P}^2 \equiv \hat{P}\cdot\hat{P} = |i\rangle\langle i|i\rangle\langle i| = |i\rangle\langle i| = \hat{P}$$

$\Leftrightarrow$ 3D vectors $\hat{P}_x = \hat{x}\hat{x}$

$\hat{P}_x \cdot \vec{v} = v_x \hat{x}$ projects $\vec{v}$ to $v_x\hat{x}$!

In general, any operator (Hermitian) $\hat{P}$ satisfies

$$\hat{P}^2 = \hat{P}$$

is a projection operator:

$$|\psi_P\rangle = \hat{P}|\psi\rangle$$

$$\hat{P}|\psi_P\rangle = |\psi_P\rangle \; !$$

$\Rightarrow$ after precise measurement of $\hat{a}$

$|\psi\rangle \to \hat{P}_a|\psi\rangle = |a\rangle\langle a|\psi\rangle$

(Note $\hat{P}$ needs not to be in the form of $|i\rangle\langle i|$ $\langle i|i\rangle = 1$.)

* <u>many degrees of freedom</u> (cartesian coordinates)

$$\psi(x_1, x_2, x_3, \ldots, x_N) = \langle x_1 x_2 \ldots x_N|\psi\rangle$$

$|\psi(x_1, x_2, x_3, \ldots, x_N)|^2 \times dx_1 dx_2 \ldots dx_N$ = probability of finding a particle at (x_1, x_1+dx_1), another at (x_2, x_2+dx_2), . . .

is $\langle i|I|j\rangle = \sum_k \langle i|k\rangle\langle k|j\rangle = \delta_{ij}$, while

for continuous case : $\langle \xi|I|\xi'\rangle = \int d\tilde{\xi}\ \delta(\xi-\tilde{\xi})\,\delta(\tilde{\xi}-\xi')$

$= \delta(\xi-\xi')$

(ii) $\hat{p}$, what is $\langle x|\hat{p}|\psi\rangle$?

First, we know $\langle p|\hat{p}|\psi\rangle = p\langle p|\psi\rangle$

$(\because\ \hat{p}^+ = \hat{p},\quad \langle p|\hat{p} = \langle p|\hat{p}^+ = p\langle p|)$

$$\therefore \langle x|\hat{p}|\psi\rangle = \langle x|I\cdot\hat{p}|\psi\rangle$$

$$= \int dp\ \langle x|p\rangle\langle p|\hat{p}|\psi\rangle$$

$$= \int dp\ \langle x|p\rangle\, p\,\langle p|\psi\rangle$$

$$= \int \frac{dp}{\sqrt{2\pi\hbar}}\ p\, e^{\frac{ipx}{\hbar}}\ \langle p|\psi\rangle$$

$$= \frac{\hbar}{i}\frac{d}{dx}\int \frac{dp}{\sqrt{2\pi\hbar}}\ e^{\frac{ipx}{\hbar}}\ \langle p|\psi\rangle$$

$$= \frac{\hbar}{i}\frac{d}{dx}\int dp\ \langle x|p\rangle\langle p|\psi\rangle$$

$$= \frac{\hbar}{i}\frac{d}{dx}\langle x|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\psi(x)$$

Put $\psi = x'$, we get the matrix element

$$\langle x|\hat{p}|x'\rangle = \frac{\hbar}{i}\frac{d}{dx}\delta(x-x')$$ (postulate II)

(iii) $\hat{x}$, $\langle x\rangle = \langle\psi|\underset{\uparrow I}{}\hat{x}\underset{\uparrow I}{|}\psi\rangle = \int dx\int dx'\ \psi^*(x)\,\langle x|\hat{x}|x'\rangle\,\psi(x')$

since $\langle x\rangle = \int dx\ \psi^*(x)\, x\,\psi(x)$, $\therefore \langle x|\hat{x}|x'\rangle = x\,\delta(x-x')$

i.e. $\hat{x}|x'\rangle = x'|x'\rangle$! (postulate II)

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If one interpretates $(x_1, x_2, \ldots, x_N)$ as the coordinates of one particle (in multi-dimensional space), it = probability of find the particle in the region $(x_1, x_1+dx_1) \times (x_2, dx_2+x_2) \times \ldots \times (x_N, x_N+dx_N)$

$$\langle x_1 x_2 \ldots x_N | x_1' x_2' x_3' \ldots x_N' \rangle = \delta(x_1 - x_1') \ldots \delta(x_N - x_N')$$

$$\langle x_1 x_2 \ldots x_N | \hat{x}_i | \psi \rangle = x_i \langle x_1 x_2 \ldots x_N | \psi \rangle$$

$$\langle x_1 x_2, \ldots x_N | \hat{p}_i | \psi \rangle = \frac{\hbar}{i} \frac{d}{dx_i} \psi(x_1, x_2, \ldots x_N)$$

$$\therefore \langle x y z | \hat{H} | \psi \rangle = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z)$$

$$+ V(x, y, z)\, \psi(x, y, z)$$

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General properties of Schrödinger equation

* **In Dirac notation**

$$\langle x|\hat{H}|\psi(t)\rangle = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi(x,t) + V(x)\,\psi(x,t)$$

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \langle x|\, i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle$$

$$\Leftrightarrow \quad \frac{\partial}{\partial t} v_x(t) = \hat{x}\cdot\frac{\partial}{\partial t}\vec{v}$$

$\because$ Schrödinger eq. $\Rightarrow i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$

$\hat{H}^{+} = \hat{H}$

* **Galilean invariance**

$\Rightarrow$ see page 2 & 3

* time-independant Schrödinger eq.

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

When $\hat{H}$ is time-independant (also boundary conditions), the above eq. is seperable:

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

$$i\hbar\,\frac{T'(t)}{T(t)} = \frac{\hat{H}\,\psi(x)}{\psi(x)} \equiv E$$

$$\therefore T'(t) = e^{-\frac{i}{\hbar}Et} \qquad \hat{H}\psi(x) = E\,\psi(x) \Leftarrow$$ time-independant Schrödinger eq.

$$\psi(x,t) = \psi(x)\,e^{-\frac{i}{\hbar}Et} \qquad \text{or} \quad \hat{H}|\psi\rangle = E|\psi\rangle$$

* evolution operator

One often writes $|E\rangle$ instead of $|\psi\rangle$

to remind us that $\hat{H}|E\rangle = E|E\rangle$.

Complete : $\sum_E |E\rangle\langle E| = \mathbb{I}$

$$\therefore |\psi(t)\rangle = \sum_E \underbrace{\langle E|\psi(t)\rangle}_{\equiv\, a_E(t)}\,|E\rangle$$

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \sum_E i\hbar\,\dot{a}_E(t)\,|E\rangle = \hat{H}|\psi(t)\rangle$$

$$= \sum_E a_E(t)\,E\,|E\rangle$$

$$\therefore \dot{a}_E(t) = -\frac{i}{\hbar}E\,a_E\,, \qquad a_E(t) = \underbrace{a_E(0)}_{=\,\langle E|\psi(0)\rangle}\,e^{-\frac{i E t}{\hbar}}$$

$$\therefore |\psi(t)\rangle = \sum_E |E\rangle\langle E|\psi(0)\rangle e^{-\frac{i}{\hbar}Et}$$

$$= \underbrace{\left(\sum_E e^{-\frac{i}{\hbar}Et}|E\rangle\langle E|\right)}_{\equiv}|\psi(0)\rangle$$

$U(t) \equiv U(t,0)$: evolution operator

$$U(t) = \sum_E e^{-\frac{i}{\hbar}Et}|E\rangle\langle E|$$

$$= \sum_E e^{-\frac{i}{\hbar}\hat{H}t}|E\rangle\langle E| = e^{-\frac{i}{\hbar}\hat{H}t}\underbrace{\sum_E |E\rangle\langle E|}_{I} = e^{-\frac{i}{\hbar}\hat{H}t}$$

☆ It is just as if we integrate the Schrödinger eq. directly!

Note : What do we mean by $e^{\hat{A}}$?

$$e^{\hat{A}} \equiv \mathbb{I} + \frac{\hat{A}}{1!} + \frac{\hat{A}^2}{2!} + \frac{\hat{A}^3}{3!} + \cdots$$

If $\hat{H}^+ = \hat{H}$

(i) ⇒ $\hat{U}$ is unitary, $U^+U = \mathbb{I}$. $\therefore \langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|U^+U|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle$

probability is conserved!

$$(e^{\hat{A}})^+ = \mathbb{I} + \frac{\hat{A}^+}{1!} + \frac{(\hat{A}^+)^2}{2!} + \cdots = e^{\hat{A}^+}$$

$$\therefore \hat{U}^+ = e^{+\frac{i}{\hbar}\hat{H}^+t} = e^{+\frac{i}{\hbar}\hat{H}t} \quad (\hat{H}^+ = \hat{H}\text{, Homework})$$

$$\therefore \hat{U}^+\hat{U} = e^{+\frac{i}{\hbar}\hat{H}t}e^{-\frac{i}{\hbar}\hat{H}t} = \mathbb{I}$$

$$e^A e^B = e^{A+B} \quad \text{if } [A,B] = 0$$

In general, $e^{A+B} \neq e^A e^B$ (Homework)

(ii) When $\hat{H} = \hat{H}(t)$ (time-dependent), the Schrödinger eq is not seperable. The above derivation of $U(t,0)$ fails.

One can still define $\hat{U}(t_1,t_2)$ formally as the operator that connects $|\psi(t_1)\rangle$ & $|\psi(t_2)\rangle$:

$$|\psi(t_1)\rangle = \hat{U}(t_1,t_2)\,|\psi(t_2)\rangle$$

To find $\hat{U}$, we consider $\Delta t = \frac{t_1-t_2}{N}$, for convenience, we take $t_2=0$, $t_1=t$

$$|\psi(\Delta t)\rangle = |\psi(0)\rangle + \Delta t \frac{\partial}{\partial t}|\psi(0)\rangle$$

$$= |\psi(0)\rangle - \frac{i}{\hbar}\Delta t\,\hat{H}(0)\,|\psi(0)\rangle$$

$$\simeq e^{-\frac{i\Delta t}{\hbar}\hat{H}(0)}|\psi(0)\rangle + o(\Delta t^2)$$

$\Delta t = \frac{t}{N}$

$t = N\Delta t$

$t-\Delta t = (N-1)\Delta t$

$$\therefore |\psi(t)\rangle = e^{-i\frac{\Delta t}{\hbar}\hat{H}(t-\Delta t)}|\psi(t-\Delta t)\rangle + o(\Delta t^2)$$

$$= e^{-i\frac{\Delta t}{\hbar}\hat{H}(t-\Delta t)}\,e^{-i\frac{\Delta t}{\hbar}\hat{H}(t-2\Delta t)}|\psi(t-2\Delta t)\rangle + o(\Delta t^2)$$

$$= \cdots = \prod_{k=0}^{N-1} e^{-i\frac{\Delta t}{\hbar}\hat{H}(k\Delta t)}|\psi(0)\rangle + o(\Delta t^2) \quad \cdots ①$$

Note that, in general, $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0$

(a good example: $\hat{H} = \hat{X}^2\cos^2\omega t + \hat{p}^2\sin^2\omega t$), One can't

write $\prod_{k=0}^{N-1} e^{-i\frac{\Delta t}{\hbar}\hat{H}(k\Delta t)}$ as $e^{-\frac{i\Delta t}{\hbar}\sum_{k=0}^{N-1}\hat{H}(k\Delta t)}$

$$\equiv e^{-\frac{i}{\hbar}\int_0^t dt\,\hat{H}(t)}$$

In the special case when $\hat{H}$ is indept. of t, we can do it! we get $e^{-\frac{i}{\hbar}\int_0^t dt\,\hat{H}(t)} = e^{-\frac{i}{\hbar}\hat{H}t}$

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, recovering the previous result.

We introduce a new notation :

$$T\left[e^{\frac{-i}{\hbar}\int_0^t dt\, \hat{H}(t)} \right] = \lim_{N\to\infty} \prod_{k=0}^{N-1} \exp\left[\frac{-i}{\hbar} H(k\Delta t)\Delta t\right]$$

$\uparrow$

time-ordered product : <u>later times are at left</u> !

$$\therefore \quad U(t_1, t_2) = T\left[e^{\frac{-i}{\hbar}\int_{t_2}^{t_1} dt\, \hat{H}(t)} \right] \Rightarrow \text{important note! (see over)}$$

Useful properties of $\hat{U}$

(i) $U(t,t) = \mathbb{1}$

(ii) $\because \hat{U}(t,0)|\psi(0)\rangle = |\psi(t)\rangle$

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

$$\therefore \left[i\hbar \frac{d}{dt}\hat{U}(t,0)\right]|\psi(0)\rangle = \hat{H}(t)\hat{U}(t,0)|\psi(0)\rangle$$

$$\therefore i\hbar \frac{d}{dt}\hat{U}(t,0) = \hat{H}(t)\hat{U}(t,0) \quad \text{--- ①}$$

Unlike ordinary differential eq. :

$$\frac{dy}{dx} = \alpha(x)\, y(x) \Rightarrow \frac{dy}{y} = \alpha\, dx$$

$$y(x) = y_0\, e^{\int_{x_0}^{x} \alpha(t)dt}$$

Here, $\hat{U}$ & $\hat{H}$ are operators. We can't integrate it as we do for ODE. because

$$\int d\hat{U}(t,0)\,\hat{U}^{-1}(t,0) \neq \ln \hat{U}(t,0)$$

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It turns out $\hat{U}(t,0) \equiv T\left[e^{-\frac{i}{\hbar}\int_0^t dt\, \hat{H}(t)}\right]$

satisfies ①. (exercise)

(iii) $U(0,t)\,U(t,0)\,|\psi(0)\rangle = U(0,t)\,|\psi(t)\rangle$

$= |\psi(0)\rangle$

$\therefore U(0,t)\,U(t,0) = \mathbb{I}$ similarly $U(t,0)\,U(0,t) = \mathbb{I}$

$\therefore U(t_1,t_2) = U^{-1}(t_2,t_1)$

(iv) $\hat{U}^{+}(t,0) = \left(e^{-\frac{i}{\hbar}\Delta t\,\hat{H}(t-\Delta t)}\, e^{-\frac{i}{\hbar}\Delta t\,\hat{H}(t-2\Delta t)} \cdots \right.$

$\left. \cdots e^{-\frac{i}{\hbar}\Delta t\,\hat{H}(\Delta t)}\right)^{+}$

$= e^{\frac{i}{\hbar}\Delta t\,\hat{H}(\Delta t)}\, e^{\frac{i}{\hbar}\Delta t\,\hat{H}(2\Delta t)} \cdots e^{\frac{i}{\hbar}\Delta t\,\hat{H}(t-\Delta t)}$

$\hat{H}^{+} = \hat{H}$

$|\psi(0)\rangle = |\psi(\Delta t)\rangle - \Delta t \frac{d}{dt}|\psi(\Delta t)\rangle + O(\Delta t^2)$

$= e^{\frac{i}{\hbar}\Delta t\,\hat{H}(\Delta t)}\,|\psi(\Delta t)\rangle + O(\Delta t^2)$

$= \hat{U}(0,t) = \hat{U}^{-1}(t,0)$

$\therefore \hat{U}^{+}(t,0)\,\hat{U}(t,0) = \mathbb{I}$

Note that $U^{+}(t,0) \neq T\left[e^{\frac{i}{\hbar}\int_0^t dt'\,\hat{H}(t')}\right]$

$\tilde{T}\left[e^{\frac{i}{\hbar}\int_0^t dt'\,\hat{H}(t')}\right]$

i.e. + & T can't commute with each other.

(v) $\hat{U}(t_1,t_2)\,\hat{U}(t_2,t_3) = \hat{U}(t_1,t_3)$

$\because \hat{U}(t_1,t_2)\,\hat{U}(t_2,t_3)\,|\psi(t_3)\rangle$

$= |\psi(t_1)\rangle$

$\hat{U}(t_1,t_3)\,|\psi(t_3)\rangle = |\psi(t_1)\rangle$

* Conservation of probability

$$\vec{j} = \frac{\hbar}{2mi}(\psi^* \nabla\psi - \psi\nabla\psi^*)$$

$\downarrow$ $\psi = Ae^{ikx}$, $\quad \vec{j} = \frac{\hbar k}{m}|A|^2 = v|A|^2$

local conservation : $\frac{\partial \rho(r,t)}{\partial t} + \nabla\cdot\vec{j}(r,t) = 0$

global conservation : $\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\psi(0)\rangle$

if $U^\dagger(t,0)\,U(t,0) = \mathbb{I}$

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\,U^\dagger(t,0)\,U(t,0)\,|\psi(0)\rangle$$
$$= \langle\psi(0)|\psi(0)\rangle$$

As we have seen $U^\dagger U = \mathbb{I}$ is guaranteed by $\hat{H}^\dagger = \hat{H}$.

Occasionally, one needs to model the situations when particles are not conserved, e.g., photons being absorbed, decay of particles to other particles, ...

In this case, we relax $\hat{H}^\dagger = \hat{H}$ and phenomenologically model it by $\quad H = \frac{p^2}{2m} + V_R - iV_I \quad . \quad V_I = \text{Const}.$

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}_R t - \frac{1}{\hbar}V_I t}$$
$$\hat{U}^\dagger(t) = e^{+\frac{i}{\hbar}\hat{H}_R t - \frac{1}{\hbar}V_I t}$$
$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|\,e^{(\frac{i}{\hbar}\hat{H}_R - \frac{V_I}{\hbar})t}\,e^{(\frac{-i}{\hbar}\hat{H}_R - \frac{1}{\hbar}V_I)t}\,|\psi(0)\rangle$$
$$= e^{-\frac{2}{\hbar}V_I t}\,\langle\psi(0)|\psi(0)\rangle$$

Total Probability decays!

This also happens locally : $\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = -\frac{2V_I}{\hbar}\psi^*\psi = -\frac{2V_I}{\hbar}\rho$

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Statistical Mechanics & Quantum Mechanics

— Density matrix

In an ideal measurement, the state one prepares is a pure state $|\psi\rangle$ so that

$$\hat{O}|\psi\rangle = \alpha|\psi\rangle$$

$\hat{O}$ = the observable that is measured.

In real measurements, however, it may not be always possible to control the prepared state to be identical.

Therefore, suppose one prepares 1000 states to do 1000 measurements, one may end up with 400 states in $|\psi\rangle$, 100 state in $|\psi_1\rangle$, 200 states in $|\psi_2\rangle$, ...

Clearly, in this case, the obtained average of $\hat{O} \equiv \bar{O} = \frac{1}{1000}[400\langle\psi|\hat{O}|\psi\rangle$
$+100\langle\psi_1|\hat{O}|\psi_1\rangle + 200\langle\psi_2|\hat{O}|\psi_2\rangle$
$+\cdots]$

In general, for any measurement $\hat{A}$, the ensemble of prepared systems is characterized by

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probability $p_i = \frac{n_i}{N}$ for ith state $|\psi_i\rangle$

with N = total # of systems in the ensemble

n_i = # of systems in $|\psi_i\rangle$

then $\bar{A} = \sum_i p_i \langle\psi_i| A |\psi_i\rangle$.

The ensemble is termed mixed ensemble.

* Remark: the mixed ensemble involves probability p_i that is statistically originated.

and is hence very different from quantum probability.

One may wonder how it is to be different from the pure state

$$|\psi_0\rangle = \sum_i \sqrt{p_i}\, |\psi_i\rangle$$

(if $|\psi_i\rangle$s is orthonormal, $\langle\psi|\psi\rangle = \sum_i p_i = 1$)

then $|\psi_0\rangle$ is coherent superposition of $|\psi_i\rangle$

In $|\psi\rangle$, one also gets probability p_i

to be in $|\psi_i\rangle$!

The point of difference is that if all N systems are in $|\psi_0\rangle$, for some measurements one should be able to see (cross) interference terms:

$$\langle B \rangle = \sum_{ij} \sqrt{P_i P_j} \langle \psi_i | B | \psi_j \rangle$$

Cross terms are present so that

the average of measure $B \neq \sum_i P_i \langle i | B | i \rangle$

Density matrix

$Tr\, |\psi\rangle\langle\psi| \hat{A}$ complete basis

$= \sum_i \langle i|\psi\rangle\langle\psi|\hat{A}|i\rangle$

$\bar{A}$ can be rewritten as

$= \sum_i \langle\psi|\hat{A}|i\rangle\langle i|\psi\rangle$

$$\bar{A} = Tr \sum_i \left[P_i |\psi_i\rangle\langle\psi_i| \hat{A} \right]$$

$= \langle\psi|\hat{A}\, \mathbb{I}\, \psi\rangle$

$= \langle\psi|\hat{A}\psi\rangle$

if one defines
$$\hat{\rho} = \sum_i P_i |\psi_i\rangle\langle\psi_i|$$

$$\bar{A} = Tr\, \hat{\rho}\hat{A} = \sum_{ij} \rho_{ij} A_{ji} = \sum_i P_i \langle i|A|i\rangle$$

$\hat{\rho}$ is the so-called density (operator) matrix that characterizes the situation with statistical distributions. It has the following properties

(i) $\{|\psi_i\rangle\}$ needs not to be orthogonal!
but $\langle\psi_i|\psi_i\rangle = 1$

(ii) $Tr\rho = \sum_i P_i = 1$

(iii) $\rho^{+} = \rho$ ($\hat{\rho}$ = Hermitian operator)

$\langle\psi|\rho|\psi\rangle \geq 0$ real positive definite

More about density matrix

Caution on density matrix

① $\langle\psi|\rho|\psi\rangle \geq 0$ $\begin{cases} \text{real} \\ \text{positive definite} \end{cases}$

$\because \rho = A + Bi$ $A = A^\dagger$ $A = \frac{\rho+\rho^\dagger}{2}$

$B = B^\dagger$ $Bi = \frac{\rho-\rho^\dagger}{2}$

$\langle\psi|C|\psi\rangle \overset{?}{=} 0$ for any Hermitian matrix C

$\therefore$ B must be zero

$\therefore \rho = A =$ Hermitian $\Rightarrow$ Can be diagonalized

$\rho = \sum \lambda_i |\lambda_i\rangle\langle\lambda_i|$ $\sum \lambda_i = 1$

$\lambda_i \geq 0$ $\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$

② ρ can be represented

by a matrix

& can be diagonalized!

but it doesn't mean the ensemble

it describes must be $\sum_i \lambda_i |\lambda_i\rangle\langle i|$!

$\because \rho \longrightarrow \sum \lambda_i |\lambda_i\rangle\langle\lambda_i|$ is via

some $\underbrace{\text{linear superposition of } \{\lambda_i\}}_{\Downarrow}$ to diagonalized ρ

its 's superposition of different systems has no physical meaning!

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(iv) $\hat{\rho}$ is a ~~positive~~ definite positive operator.

i.e. for any $|\phi\rangle$

$$\langle\phi|\hat{\rho}|\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle$$

$$= \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0$$

(v) Since $\hat{\rho}$ is Hermitian, one can always diagonalize it with some orthonormal basis $|i\rangle$

$$\therefore \hat{\rho} = \sum_i \lambda_i |i\rangle\langle i|.$$

(iv) & (ii) imply $\lambda_i \geq 0$. $\sum_i \lambda_i = 1$. $\therefore \lambda_i \leq 1$

$$\therefore \hat{\rho}^2 = \sum_{ij} \lambda_i |i\rangle\langle i|j\rangle\langle j| \lambda_j$$

$$= \sum_i \lambda_i^2 |i\rangle\langle i|$$

$$\therefore \mathrm{Tr}\rho^2 = \sum_i \lambda_i^2 \leq \sum_i \lambda_i \leq 1$$

For pure states $|\psi\rangle$, $\hat{\rho} = |\psi\rangle\langle\psi|$

$$\mathrm{Tr}\hat{\rho}^2 = \mathrm{Tr}|\psi\rangle\langle\psi| = 1$$

$\therefore$ " $=$ " $1 \iff$ pure state

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

$$-i\hbar \frac{d\langle\psi|}{dt} = \langle\psi| H^{+} = \langle\psi| H$$

$$\therefore\ i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}] + \underbrace{i\hbar \sum_i \frac{dp_i}{dt} |\psi_i\rangle\langle\psi_i|}_{\begin{array}{c}|||\\ i\hbar \frac{\partial \rho}{\partial t}\end{array}}$$

Some useful ensembles

* uniformly distribution

$$\rho = \frac{1}{N} I$$

* Quantum statistics

$$Z = \sum_k e^{-\beta E_k} = \mathrm{Tr}\, e^{-\beta \hat{H}} \quad . \quad \beta = \frac{1}{k_B T}$$

$$\hat{\rho} = \frac{1}{Z} \sum_k e^{-\beta E_k} |k\rangle\langle k|$$

$$= \sum_k \frac{1}{Z} e^{-\beta \hat{H}} |k\rangle\langle k|$$

$$= \frac{1}{Z} e^{-\beta \hat{H}}\, \mathbb{I} = \frac{1}{Z} e^{-\beta \hat{H}}$$

One can check $\hat{\rho}$ is a solution to the equation that $\hat{\rho}$ satisfies.

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The most important characterization of the density matrix $\hat{\rho}$ is

(i) $\mathrm{Tr}\,\hat{\rho} = 1$

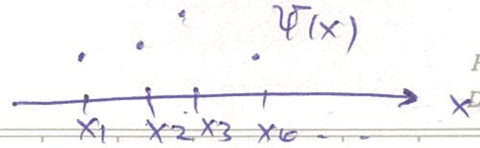
(ii) $\langle\phi|\hat{\rho}|\phi\rangle \geq 0$ for any ϕ.

One thus has the following theorem:

An Hermitian operator $\hat{\rho}$ is the density operator associated with some ensemble $\{p_i, |\psi_i\rangle\}$ if any only if it satisfies

(i) $\mathrm{Tr}\,\rho = 1$

(ii) $\langle\phi|\rho|\phi\rangle \geq 0$ for any ϕ



Summary

Vector	Dirac Notation
choose $\hat{e}_1, \hat{e}_2, \hat{e}_3$	choose $x_1, x_2, \dots x_n \dots$
$\vec{v} \Rightarrow \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$	$\vert\psi\rangle \Rightarrow \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}$
	(ψ_i usually written as $\psi(x_i)$)
$\hat{e}_i$	$\vert x\rangle$
$v_i = \hat{e}_i \cdot \vec{v}$	$\psi(x) = \langle x \vert \cdot \vert \psi\rangle \equiv \langle x \vert \psi\rangle$
$\vec{v} = \sum_i v_i \hat{e}_i$	$\vert\psi\rangle = \int dx\, \vert x\rangle \langle x \vert \psi\rangle$
$\vec{A} \cdot \vec{B}$	$\langle\phi\vert \cdot \vert\psi\rangle \equiv \langle\phi\vert\psi\rangle$
$\sum_i A_i B_i$	$\int dx\, \phi^*(x)\, \psi(x)$
$\vec{v}^{\,t} \Rightarrow (v_1 \, v_2 \, v_3)$	$\langle\psi\vert \Rightarrow (\psi_1^*, \psi_2^*, \dots)$
$(\vec{v}^{\,t})_i$	$\langle\psi\vert x\rangle$
$(\vec{u}+\vec{v})_i = u_i + v_i$	$\langle x\vert\, (\vert\phi\rangle + \vert\psi\rangle)$
	$= \langle x\vert\phi\rangle + \langle x\vert\psi\rangle$

Useful result $\quad \langle\phi\vert\psi\rangle = \int dx\, \phi^*(x)\, \psi(x)$

$$= \langle\psi\vert\phi\rangle^*$$

$$\therefore \langle\phi\vert x\rangle = \langle x\vert\phi\rangle^* = \phi^*(x)$$

$$\therefore \langle\phi\vert\psi\rangle = \int dx\, \langle\phi\vert x\rangle\langle x\vert\psi\rangle$$

bases : (The above ~~picture~~ notations apply well to other basis such as $\vert p\rangle$)

$\phi = x$, $\langle x|\psi\rangle = \int dx' \langle x|x'\rangle \langle x'|\psi\rangle$

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

Similarly $\langle p|p'\rangle = \delta(p-p')$

other discrete basis which can expand ψ

say $|i\rangle$ $\langle i|i'\rangle = \delta_{ii'}$

Operators

<u>vector</u>	Dirac notation
$A\cdot\vec{v}$ $\uparrow$ matrix $(n\times n)$	$\hat{A}|\psi\rangle$
$(A\vec{v})^T = \vec{v}^T\cdot A^T$	$\langle\psi| A^+$
$\vec{u}^t\cdot(A\vec{v})$	$\langle\phi|\cdot(\hat{A}|\psi\rangle)$
$=$	$=$
$(\vec{u}^t\cdot A)\cdot\vec{v}$	$(\langle\phi|\hat{A})\cdot|\psi\rangle$
written as $\vec{u}^t\cdot A\cdot\vec{v}$	$= \langle\phi|\hat{A}|\psi\rangle$
diadic form	...

useful result. $(\hat{A}\hat{B})^+ = \hat{B}^+\hat{A}^+$

$\Leftrightarrow (AB)^T = B^T A^T$

$(A^+)^+ = A. \Leftrightarrow (A^T)^T = A$

$(\lambda A)^+ = \lambda^* A^+$

pf: $|\phi\rangle = \hat{A}\hat{B}|\varphi\rangle = \hat{A}|\lambda\rangle$ $(|\lambda\rangle = \hat{B}|\varphi\rangle)$

$\langle\phi| = \langle\varphi|(\hat{A}\hat{B})^+ = \langle\lambda|A^+ = \langle\varphi|B^+A^+$

$(|u\rangle\langle v|)^+ = |v\rangle\langle u|$

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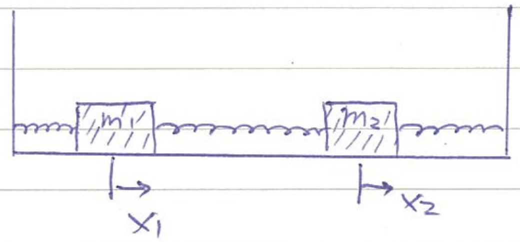
An example



$$m\ddot{x}_1 = -k(x_1 - x_2) - kx_1$$

$$m\ddot{x}_2 = +k(x_1 - x_2) - kx_2$$

$$\therefore \ \ddot{x}_1 = -\frac{2k}{m}x_1 + \frac{k}{m}x_2 \qquad \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix} = \begin{pmatrix} \frac{-2k}{m} & \frac{k}{m} \\ \frac{k}{m} & \frac{-2k}{m} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\ddot{x}_2 = \frac{k}{m}x_1 - \frac{2k}{m}x_2$$

$$|\psi\rangle = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad (\vec{r})$$

$$\Rightarrow \ \frac{d^2}{dt^2}|\psi\rangle = \hat{\Omega}|\psi\rangle, \qquad \hat{\Omega} = \begin{pmatrix} \frac{-2k}{m} & \frac{k}{m} \\ \frac{k}{m} & \frac{-2k}{m} \end{pmatrix}$$

$$\Leftrightarrow \ i\hbar\frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle$$

Note that we have implicitly taken the basis vectors as $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |1\rangle$ $\quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |2\rangle$

$$\therefore \ |\psi\rangle = x_1|1\rangle + x_2|2\rangle$$

$$x_1 = (1\ 0)\cdot\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \langle 1| \cdot |\psi\rangle \equiv \langle 1|\psi\rangle = \psi_1$$

$$x_2 = \langle 2|\psi\rangle \equiv \psi_2$$

$$\therefore \ |\psi\rangle = \sum_i |i\rangle\langle i||\psi\rangle = \langle 1|\psi\rangle|1\rangle + \langle 2|\psi\rangle|2\rangle$$

$$\Leftarrow \ \vec{r}\cdot\vec{r} = x_1^2 + x_2^2 = (x_1, x_2)\cdot\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \langle\psi|\psi\rangle$$

$$\langle\psi| = (x_1\ x_2) = \langle 1|\psi\rangle^* \langle 1| + \langle 2|\psi\rangle^* \langle 2|$$

$$= \langle 1|\psi\rangle\langle 1| + \langle 2|\psi\rangle\langle 2|$$

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$$|\phi\rangle = \begin{pmatrix} x_1' \\ x_2' \end{pmatrix} \begin{matrix} \Leftarrow \langle 1|\phi\rangle \\ \Leftarrow \langle 2|\phi\rangle \end{matrix}$$

$$\langle\phi|\psi\rangle = (x_1' \ x_2') \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = x_1' x_1 + x_2' x_2$$

$$= \sum_i \langle\phi|i\rangle\langle i|\psi\rangle$$

<u>Operator</u> : $\hat{\Omega}$

linear : $\hat{\Omega}(|\psi\rangle + |\phi\rangle)$

$$= \begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -2k/m \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} & \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \end{pmatrix}$$

$$= \hat{\Omega}|\psi\rangle + \hat{\Omega}|\phi\rangle$$

$$\hat{\Omega}|\psi\rangle = \begin{pmatrix} -2k/m & k/m \\ k/m & -2k/m \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \frac{k}{m}x_2 - \frac{2k}{m}x_1 \\ \frac{k}{m}x_1 - \frac{2k}{m}x_2 \end{pmatrix}$$

$$\Leftrightarrow \left(-\frac{2k}{m}|1\rangle\langle 1| + \frac{k}{m}|1\rangle\langle 2| + \frac{k}{m}|2\rangle\langle 1| - \frac{2k}{m}|2\rangle\langle 2|\right) \cdot (x_1|1\rangle + x_2|2\rangle)$$

$$= \left(\frac{k}{m}x_2 - \frac{2k}{m}x_1\right)|1\rangle + \left(\frac{k}{m}x_1 - \frac{2k}{m}x_2\right)|2\rangle$$

$$\langle\psi|\hat{\Omega}^+ = (x_1 \ x_2) \begin{pmatrix} -2k/m & k/m \\ k/m & -2k/m \end{pmatrix} = \left(\frac{k}{m}x_2 - \frac{2k}{m}x_1, \ \frac{k}{m}x_1 - \frac{2k}{m}x_2\right) = (\hat{\Omega}|\psi\rangle)^+$$

$$\Leftrightarrow (x_1\langle 1| + x_2\langle 2|) \cdot \left(-\frac{2k}{m}|1\rangle\langle 1| + \frac{k}{m}|1\rangle\langle 2| + \frac{k}{m}|2\rangle\langle 1| - \frac{2k}{m}|2\rangle\langle 2|\right)$$

$$= \left(\frac{k}{m}x_2 - \frac{2k}{m}x_1\right)\langle 1| + \left(\frac{k}{m}x_1 - \frac{2k}{m}x_2\right)\langle 2|$$

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matrix form $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ v.s. $a|1\rangle\langle 1| + b|2\rangle\langle 2| + c|2\rangle\langle 1| + d|2\rangle\langle 2|$

$\Downarrow$ not writing out basis vectors explictly

$\Downarrow$ ~~[illegible]~~ explictly writing basis vectors as $|1\rangle$ & $|2\rangle$ even though we have not specify $|1\rangle$ & $|2\rangle$

$$\langle\phi| \cdot (\hat{\Omega}|\psi\rangle)$$

$$= (x_1', x_2') \cdot \begin{pmatrix} \frac{k}{m}x_2 - \frac{2k}{m}x_1 \\ \frac{k}{m}x_1 - \frac{2k}{m}x_2 \end{pmatrix}$$

$$= \frac{k}{m}x_1'x_2 - \frac{2k}{m}x_1x_1' + \frac{k}{m}x_2'x_1 - \frac{2k}{m}x_2'x_2$$

$$(\langle\phi|\hat{\Omega}) \cdot |\psi\rangle$$

$$= \left[(x_1'\ x_2') \begin{pmatrix} \frac{-2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix} \right] \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$= \left(\frac{k}{m}x_2' - \frac{2k}{m}x_1', \frac{k}{m}x_1' - \frac{2k}{m}x_2' \right) \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$\therefore \langle\phi|(\hat{\Omega}|\psi\rangle) = (\langle\phi|\hat{\Omega})|\psi\rangle \equiv \langle\phi|\hat{\Omega}|\psi\rangle$$

Eigenstates (written as kets, $\Rightarrow$ eigenkets)

~~$\hat{\Omega}|\psi\rangle = \lambda I|\psi\rangle$~~ $\hat{\Omega}|\lambda\rangle = \lambda|\lambda\rangle$

Suppose $|\lambda\rangle = \alpha|1\rangle + \beta|2\rangle$

$$\Rightarrow \begin{pmatrix} \frac{-2k}{m}, & k/m \\ k/m & \frac{-2k}{m} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\det \begin{pmatrix} \frac{-2k}{m} - \lambda & k/m \\ k/m & \frac{-2k}{m} - \lambda \end{pmatrix} = 0$$

$$\Rightarrow \quad \left(\lambda + \frac{2k}{m}\right)^2 = (k/m)^2 \quad \therefore \quad \lambda = \underbrace{-k/m}_{= -\omega_1^2} \text{ or } \underbrace{-3k/m}_{= -\omega_2^2}$$

$\lambda = -\omega_1^2 \qquad |I\rangle = \frac{1}{\sqrt{2}} |1\rangle + \frac{1}{\sqrt{2}} |2\rangle$ — ①

(normal modes)

$\lambda = -\omega_2^2 \qquad |II\rangle = \frac{-1}{\sqrt{2}} |1\rangle + \frac{1}{\sqrt{2}} |2\rangle$ — ②

$$\Omega |I\rangle = -\omega_1^2 |I\rangle$$
$$\Omega |II\rangle = -\omega_2^2 |II\rangle$$

Use $|I\rangle$ & $|II\rangle$ as basis:

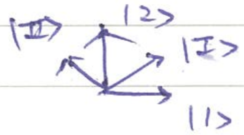
$|I\rangle, |II\rangle$ complete (spectral theorem, $\Omega = \Omega^+$ $\Rightarrow$ basis complete)

$\langle I|I\rangle = 1 \quad , \langle II|II\rangle = 1$

$\langle I|II\rangle = 0$ orthonormal !

We now view ① & ② as some operations:

$$|I\rangle = \hat{R} |1\rangle$$
$$|II\rangle = \hat{R} |2\rangle$$



$\hat{R}$ = rotation $\underline{45°}$

What is $\hat{R}$? use $|1\rangle, |2\rangle$ as basis to express.

$$\hat{R} = \begin{pmatrix} \cos 45° & -\sin 45° \\ +\sin 45° & \cos 45° \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ +1 & 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \left(|1\rangle\langle 1| - |1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 2| \right)$$

$\therefore \quad |1\rangle = \hat{R}^{-1} |I\rangle$

$\quad\; |2\rangle = \hat{R}^{-1} |II\rangle$

meaning $\underline{\hat{R}^{-1}\hat{R} = \mathbb{I}}$. $\quad \hat{R}^{-1}$ = inverse of $\hat{R}$

$\mathbb{I} \cdot |\psi\rangle = |\psi\rangle$ for any $\underline{|\psi\rangle}$ $\quad \mathbb{I} \equiv$ unit operator

What is $\hat{R}^{-1}$? $\because \hat{R}^{-1}$ operates on $|I\rangle$, $|II\rangle$, we must use $|I\rangle$ & $|II\rangle$ to express $\hat{R}^{-1}$.

Obvious, if we rotate $(-45°)$, $|II\rangle \to |2\rangle$, $|2\rangle \to |I\rangle$

$$\therefore \hat{R}^{-1} = \begin{pmatrix} \cos(-45°), & -\sin(-45°) \\ +\sin(-45°), & \cos(-45°) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & +1 \\ -1 & 1 \end{pmatrix}$$

note : this is in terms of $|I\rangle$ & $|II\rangle$, i.e.,

$$\hat{R}^{-1} = \frac{1}{\sqrt{2}} \left(|I\rangle\langle I| + |I\rangle\langle II| - |II\rangle\langle I| + |II\rangle\langle II| \right)$$

$$\therefore \quad |1\rangle = \hat{R}^{-1} |I\rangle = \frac{1}{\sqrt{2}} |I\rangle - \frac{1}{\sqrt{2}} |II\rangle \quad — ③$$

$$|2\rangle = \hat{R}^{-1} |II\rangle = \frac{1}{\sqrt{2}} |I\rangle + \frac{1}{\sqrt{2}} |II\rangle \quad — ④$$

<u>The other way</u> to get ③ & ④

①, ② $\Rightarrow$ $\left.\begin{array}{ll} \langle 1|I\rangle = \frac{1}{\sqrt{2}}, & \langle 2|I\rangle = \frac{1}{\sqrt{2}} \\ \langle 1|II\rangle = -\frac{1}{\sqrt{2}}, & \langle 2|II\rangle = \frac{1}{\sqrt{2}} \end{array}\right\}$ real

$\therefore \quad \langle I|1\rangle = \frac{1}{\sqrt{2}}, \; \langle II|1\rangle = \frac{-1}{\sqrt{2}} \Rightarrow |1\rangle = \frac{1}{\sqrt{2}} |I\rangle - \frac{1}{\sqrt{2}} |II\rangle$

$\quad\; \langle I|2\rangle = \frac{1}{\sqrt{2}}, \; \langle II|2\rangle = \frac{1}{\sqrt{2}} \Rightarrow |2\rangle = \frac{1}{\sqrt{2}} |I\rangle + \frac{1}{\sqrt{2}} |II\rangle$

Ex verify $\hat{R}\cdot\hat{R}^{-1} = I = |1\rangle\langle 1| + |2\rangle\langle 2|$

or $= |I\rangle\langle I| + |II\rangle\langle II|$

~~$\hat{R}\hat{R}^{-1} = \frac{1}{2}$~~

$\hat{R}|I\rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} \times 2|2\rangle = |2\rangle$

$\hat{R}|II\rangle = -|1\rangle$

$\therefore \hat{R}\cdot\hat{R}^{-1} = \hat{R}\frac{1}{\sqrt{2}}\left(|I\rangle\langle I| + |I\rangle\langle II| - |II\rangle\langle I| + |II\rangle\langle II|\right)$

$= \frac{1}{\sqrt{2}}\left[|2\rangle\left(\langle I| + \langle II|\right) + |1\rangle\left(\langle I| - \langle II|\right)\right]$

$= |2\rangle\langle 2| + |1\rangle\langle 1|$

Write $\hat{\Omega}$ in terms $|I\rangle$ & $|II\rangle$:

Originally, $\hat{\Omega} = \begin{pmatrix} \frac{-2k}{m} & \frac{k}{m} \\ \frac{k}{m} & \frac{-2k}{m} \end{pmatrix}$ is referring to

basis $|1\rangle$ & $|2\rangle$, so $\underbrace{\hat{\Omega}}_{\begin{pmatrix} \frac{-2k}{m} & \frac{k}{m} \\ \frac{k}{m} & \frac{-2k}{m} \end{pmatrix}}$ must acting on $|1\rangle$ & $|2\rangle$, or vectors expressed in term of $|1\rangle$ & $|2\rangle$

~~Using ③ & ④, we have~~

~~$|1\rangle = \hat{\Omega}\hat{R}^{-1}|I\rangle$~~

~~$\hat{\Omega}|\psi\rangle = x\hat{\Omega}|1\rangle + y\hat{\Omega}|2\rangle$~~

~~$= x\hat{\Omega}\hat{R}^{-1}|I\rangle + y\hat{\Omega}\hat{R}^{-1}|II\rangle$~~

To express $\hat{\Omega}$ in terms of $|I\rangle$ & $|II\rangle$, i.e., to find the matrix form of $\hat{\Omega}$ that can operate on $|\psi\rangle = \begin{pmatrix} x \\ y \end{pmatrix} = x|I\rangle + y|II\rangle$, we need to trace & unitary

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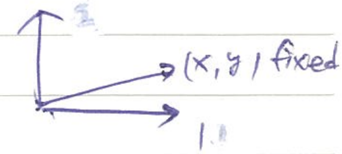
how $|\psi\rangle = x|1\rangle + y|2\rangle$ is expressed in terms of $|I\rangle$ & $|II\rangle$:



$$\begin{pmatrix} x' \\ y' \end{pmatrix}_{I,II} = \begin{pmatrix} \cos 45^\circ & \sin 45^\circ \\ -\sin 45^\circ & \cos 45^\circ \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}_{1,2}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \hat{R}^{-1} \begin{pmatrix} x \\ y \end{pmatrix}_{1,2}$$

in terms of $|I\rangle$ & $|II\rangle$

$$\therefore \begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix}_{1,2} = \begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}_{1,2}$$

$$\begin{pmatrix} \ddot{x}' \\ \ddot{y}' \end{pmatrix}_{I,II} = \hat{R}^{-1} \begin{pmatrix} \ddot{x} \\ \ddot{y} \end{pmatrix}_{1,2} = \underbrace{\hat{R}^{-1} \begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix} \hat{R}}_{} \begin{pmatrix} x' \\ y' \end{pmatrix}_{I,II}$$

$\hat{\Omega}'$ connects vectors in the basis $|I\rangle$ & $|II\rangle$

$$\hat{\Omega}' = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} -\frac{2k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{k}{m} & 0 \\ 0 & -\frac{3k}{m} \end{pmatrix}_{I,II}$$

eigenvalues

diagonal !!

We see the advantage of using $|I\rangle$ & $|II\rangle$ as basis:

if we write $\underbrace{|\psi(t)\rangle}_{\text{the solution}} = x_I(t)|I\rangle + x_{II}(t)|II\rangle$

SEASON

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Since $\frac{d^2}{dt^2}|\Psi\rangle = \hat{\Omega}|\Psi\rangle$

$$\Rightarrow \begin{pmatrix} \ddot{X}_I(t) \\ \ddot{X}_{II}(t) \end{pmatrix} = \begin{pmatrix} -\omega_1^2 & 0 \\ 0 & -\omega_2^2 \end{pmatrix} \begin{pmatrix} X_I \\ X_{II} \end{pmatrix}$$

$$\therefore \ddot{X}_I(t) = -\omega_1^2 X_I$$
$$\ddot{X}_{II}(t) = -\omega_2^2 X_{II}$$

If initial velocity $=0$, i.e., $\frac{d}{dt}|\Psi(t)\rangle\big|_{t=0} = 0$,

$$\Rightarrow X_I(t) = X_I(0)\cos\omega_1 t$$
$$X_{II}(t) = X_{II}(0)\cos\omega_2 t$$

$$|\Psi(t)\rangle = |I\rangle X_I(0)\cos\omega_1 t + |II\rangle X_{II}(0)\cos\omega_2 t$$
$$|\Psi(0)\rangle = |I\rangle X_I(0) + |II\rangle X_{II}(0)$$
$$X_I(0) = \langle I|\Psi(0)\rangle, \quad X_{II}(0) = \langle II|\Psi(0)\rangle$$

$$|\Psi(t)\rangle = |I\rangle\langle I|\Psi(0)\rangle\cos\omega_1 t + |II\rangle\langle II|\Psi(0)\rangle\cos\omega_2 t$$

$$= \Big[\cos\omega_1 t\,|I\rangle\langle I| + \cos\omega_2 t\,|II\rangle\langle II|\Big]|\Psi(0)\rangle$$

$$\equiv \hat{U}(t)|\Psi(0)\rangle$$

↑ evolution operator or propagator

which brings $|\Psi\rangle$ from $t=0$ to t!

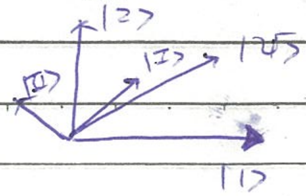
In general, given $\frac{d^2}{dt^2}|\Psi\rangle = \hat{\Omega}|\Psi\rangle$

or Schröding eq. $i\hbar\frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle$

we can find an operator $\hat{U}(t)$ which brings $|\Psi\rangle$ from 0 to t. $|\Psi(t)\rangle = \hat{U}(t)|\Psi(0)\rangle$

↑ evolution operator!!

Summarize eigenvectors & matrices



$$\frac{d^2}{dt^2}|\Psi\rangle = \hat{\Omega}\,|\Psi\rangle$$

以 $|1\rangle, |2\rangle$ 為 basis $\quad \hat{\Omega} = \begin{pmatrix} \frac{-2K}{m} & \frac{K}{m} \\ \frac{K}{m} & \frac{-2K}{m} \end{pmatrix}$

$$|I\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle$$

$$|II\rangle = \frac{-1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \qquad \hat{\Omega} = \begin{pmatrix} \frac{-K}{m} & 0 \\ 0 & -\frac{3K}{m} \end{pmatrix} \text{ diagonal}$$

not specify to any basis

$$\hat{R} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \qquad \hat{R}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$-\frac{K}{m}$ eigenvector $\qquad -3K/m$ eigenvector

$$\begin{pmatrix} \frac{-K}{m} & 0 \\ 0 & \frac{-3K}{m} \end{pmatrix} = \hat{R}^{-1} \begin{pmatrix} \frac{-2K}{m} & \frac{K}{m} \\ \frac{K}{m} & \frac{-2K}{m} \end{pmatrix} \hat{R}$$

Specify to $|1\rangle, |2\rangle$

$$\frac{d^2}{dt^2}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} \frac{-2K}{m} & \frac{K}{m} \\ \frac{K}{m} & \frac{-2K}{m} \end{pmatrix}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$$

Specify to $|I\rangle, |II\rangle$

$$\frac{d^2}{dt^2}\begin{pmatrix} X_I \\ X_{II} \end{pmatrix} = \begin{pmatrix} -\frac{K}{m} & 0 \\ 0 & -\frac{3K}{m} \end{pmatrix}\begin{pmatrix} X_I \\ X_{II} \end{pmatrix}$$