Functional space :

$$\Psi(x) = \sum C_E u_E(x)$$

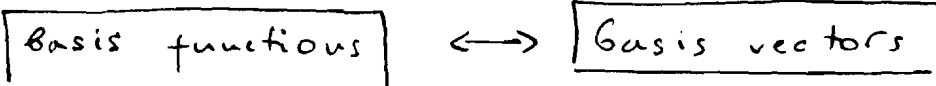expansion ↗   basis functions ↑
coefficients

3D space

$$\vec{A} = a_x \vec{i} + a_y \vec{j} + a_z \vec{k}$$

expansion ↗   ↖ basis vectors
coefficients

__Analogy__ : | Basis functions | ⟷ | Basis vectors |

One can consider the wave function as a point in the functional space of basis functions

$u_n(x)$

$u_1(x)$ $u_5(x)$ ← point in the Hilbert space

$\Psi(x)$

$u_2(x)$ $u_3(x)$ $u_4(x)$
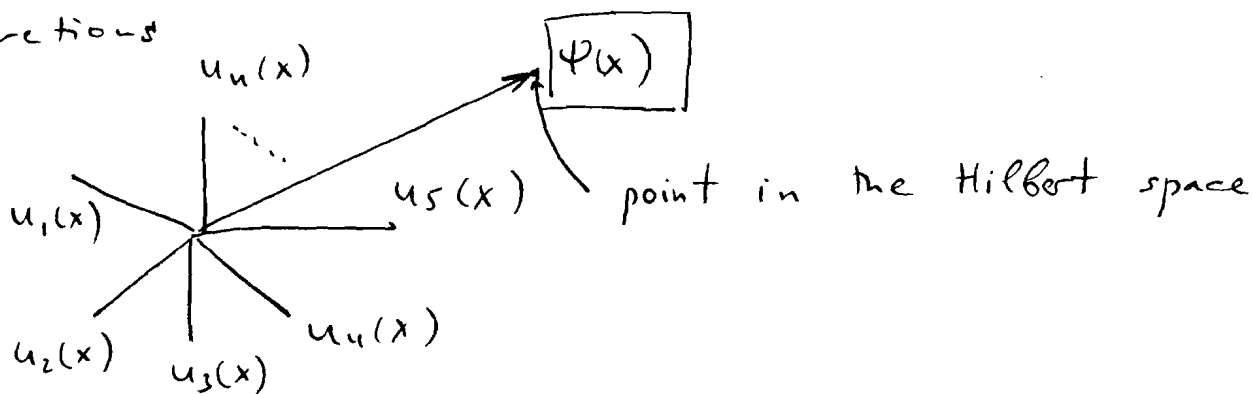
| Each quantum state is a point in Hilbert space |

Scalar product :

$$\vec{A} \cdot \vec{B} = a_x b_x + a_y b_y + a_z b_z$$

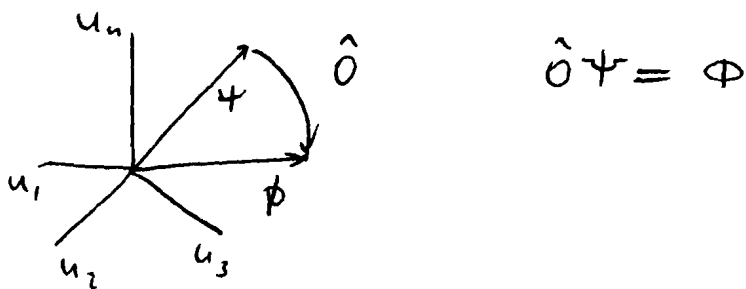$$\Psi(x) \cdot \Phi(x) = \int_{-\infty}^{\infty} \Psi^*(x) \Phi(x) \, dx$$

if $\quad \Psi(x) = \sum A_n u_n(x), \quad \Phi(x) = \sum B_n u_n(x), \quad$ then

$$\Psi(x) \cdot \Phi(x) = \sum A_n^* B_n$$

$$\downarrow \left(\underline{\text{similar to}} \right.$$

$$a_x b_x + a_y b_y + a_z b_z$$

Operators transform one vector to another in the Hilbert space

$$\hat{O} \qquad \hat{O}\Psi = \Phi$$

Linear operators : $\qquad \hat{O}(\alpha_1 \Psi_1 + \alpha_2 \Psi_2) = \alpha_1 \hat{O}\Psi_1 + \alpha_2 \hat{O}\Psi_2$

Hermitian conjugate operator : $\qquad \hat{O}^+$

$$\int_{-\infty}^{\infty} dx\, \Psi^* \hat{O}^+ \psi \quad = \quad \overline{\int_{-\infty}^{\infty} dx\, (\hat{O}\Psi)^* \psi} \quad = \quad \int_{-\infty}^{\infty} dx\, \psi(x) (\hat{O}\Psi)^*$$

① Real expectation value $\qquad \langle A \rangle = \langle A \rangle^* \longrightarrow \boxed{A = A^+}$

$\qquad\qquad\qquad\qquad\qquad\qquad$ Hermitian operator

If $\quad \hat{A} = \hat{A}^+, \quad$ then

$$\int dx\, \Phi^*(x)\, \hat{A}\, \Psi(x) = \int dx\, \Psi(x) \left(\hat{A}\, \Phi(x) \right)^*$$

② Eigenfunctions corresponding to different eigenvalues are orthogonal

$$\hat{A} u_1 = a_1 u_1 (x)$$

$$\hat{A} u_2 = a_2 u_2 \qquad \longrightarrow \qquad (\hat{A} u_2)^* = a_2^* u_2^*$$

$$\underbrace{\int dx \, u_2^* \hat{A} u_1 - \int dx \, u_1 (\hat{A} u_2)^*}_{= 0} = (a_1 - a_2^*) \int u_2^* u_1 \, dx$$

$$\int dx \, u_2^* \hat{A} u_1 = \int dx \, (\hat{A} u_2)^* u_1$$
$$\underset{\text{since } \hat{A} \text{ hermitian}}{\uparrow}$$

since $a_1 \neq a_2^*$, $\quad \int u_2^* u_1 \, dx = 0 \leftarrow$ orthogonality

③. The product of two hermitian operators is not necessarily hermitian

$$(AB)^+ = B^+ A^+ = BA = AB - [A, B]$$

The condition for the product to be hermitian is that the operators commute

$$[A, B] = 0$$

This is the reason why here is no terms like $p^n f(x)$ in the Hamiltonian, the Hamiltonian operator would not be hermitian in that case.

If $[\hat{A}, \hat{B}] = 0$, an eigenfunction of $\hat{A}$ is simultaneously an eigenfunction of $\hat{B}$.

Degeneracy: Assume there are several eigenfunctions for $\hat{A}$ with the same eigenvalue a:

$$\hat{A} \, u_a^{(1)}(x) = a \, u_a^{(1)}(x)$$

$$\hat{A} \, u_a^{(2)}(x) = a \, u_a^{(2)}(x)$$

We can always find a linear combination of $u_a^{(1)}$ and $u_a^{(2)}$ that satisfies the condition

$$\begin{cases} B \, U_a^{(1)} = b_1 \, U_a^{(1)} \\ B \, U_a^{(2)} = b_2 \, U_a^{(2)} \end{cases} \rightarrow \begin{cases} \text{since} \quad b_1 \neq b_2, \\ U_a^{(1)} \text{ is orthogonal to} \\ U_a^{(2)} \end{cases}$$

It turns out that it is sufficient to choose two eigenfunctions of $\hat{A}$ that are orthogonal to each other to make them simultaneously the eigenfunctions of $\hat{B}$.

A set of mutually commuting operators is called <u>the complete set of commuting observables</u> → it gives the maximum information that can be learned about a system in a single measurement.

Commutation of operators is related to uncertainty in measurements:

$$(\Delta A)^2 (\Delta B)^2 \geq \tfrac{1}{4} \langle i[A,B] \rangle^2$$

5-5 Time dependence and the classical limit

Time dependence of the expectation value:

$$\langle A \rangle_t = \int \psi^*(x,t) \, \hat{A} \, \psi(x,t) \, dx$$

operator standing for
the observable variable

$$\frac{d \langle A \rangle_t}{dt} = \int \psi^* \frac{\partial \hat{A}}{\partial t} \psi \, dx + \int \frac{\partial \psi^*}{\partial t} \hat{A} \psi \, dx +$$

$$+ \int \psi^* \hat{A} \frac{\partial \psi}{\partial t} \, dx =$$

$$= \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{-i\hbar} \int (\hat{H}\psi)^* A \psi \, dx + \int \psi^* \hat{A} \frac{1}{i\hbar} \hat{H} \psi \, dx$$

$$= \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i\hbar} \int \psi^* [\hat{A}, \hat{H}] \psi \, dx$$

H is a Hermitian operator

$$\int (\hat{H}\psi)^* \hat{A} \psi \, dx = \int \psi^* \hat{H} \hat{A} \psi \, dx$$

$$\boxed{\frac{\partial \langle A \rangle}{\partial t} = \frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle}$$

If $\hat{A}$ commute with $\hat{H}$, then $[\hat{H}, \hat{A}] = 0$

and $\qquad \frac{\partial \langle A \rangle}{\partial t} = 0$

The observable A is then a __constant__

__of motion__, $\qquad \langle A \rangle = Const.$

__Special cases__:

① $\hat{A} = x$

$$\frac{d \langle x \rangle}{dt} = \underset{\underset{velocity}{\nearrow}}{v} = \frac{i}{\hbar} \langle [H, x] \rangle = \frac{i}{\hbar} \langle [\frac{p^2}{2m} + v, x] \rangle$$

$$[p^2, x] = p^2 x - x p^2 = p(-i\hbar + xp) - x p^2 =$$

$$= -2 i \hbar p$$

$$\frac{d \langle x \rangle}{dt} = \frac{\langle p \rangle}{m} = v \quad \leftarrow \text{ definition of classical velocity as a result of quantum observations of the momentum}$$

②. $A = p$

$$\frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} + V, p\right]\right\rangle =$$

$$= \left\langle\frac{i}{\hbar}Vp - \frac{i}{\hbar}pV\right\rangle = -\frac{\partial\langle V\rangle}{\partial x}$$

The quantum equation of motion:

$$\frac{d\langle p\rangle}{dt} = -\left\langle\frac{dV}{dx}\right\rangle$$

Combining with $\dfrac{d\langle x\rangle}{dt} = \dfrac{\langle p\rangle}{m}$, one gets the extension of the Newton's law to quantum particles

$$\boxed{m\frac{d^2}{dt^2}\langle x\rangle = -\left\langle\frac{dV}{dx}\right\rangle}$$

What is the difference to classical equations?

In the classical case,

$$F = -\frac{\partial V(\langle x\rangle)}{\partial\langle x\rangle}$$

↗ force

↑ quantum averaged coordinate,
classical observable

Harmonic oscillator:

$$V(x) = +\frac{1}{2}kx^2$$

$$\left\langle\frac{\partial V}{\partial x}\right\rangle = k\langle x\rangle, \qquad \frac{\partial V}{\partial\langle x\rangle} = k\langle x\rangle$$

Since $\left\langle\frac{\partial V}{\partial x}\right\rangle = \frac{\partial V}{\partial\langle x\rangle}$, equations of motion are the same for quantum and classical harmonic oscillator.

Coulomb potential

$$V(x) = -\frac{c}{x}$$

$$\left\langle\frac{\partial V}{\partial x}\right\rangle = \left\langle\frac{c}{x^2}\right\rangle$$

$$\frac{\partial V}{\partial\langle x\rangle} = \frac{c}{\langle x\rangle^2}$$

Quasiclassical limit (small quantum uncertainties).

$$\frac{c}{x^2} = \frac{c}{(\langle x\rangle + \delta x)^2} \approx \frac{c}{\langle x\rangle^2} - \frac{2c\langle\delta x\rangle}{\langle x\rangle^3} - \frac{c\langle\delta x^2\rangle}{\langle x\rangle^4} + \cdots$$

quantum uncertainty of coordinate measurements

5-17. Calculate $\langle x(t) \rangle$, $\langle p(t) \rangle$ when

$$H = \frac{p^2}{2m} - eE_0 x \cos \omega t$$

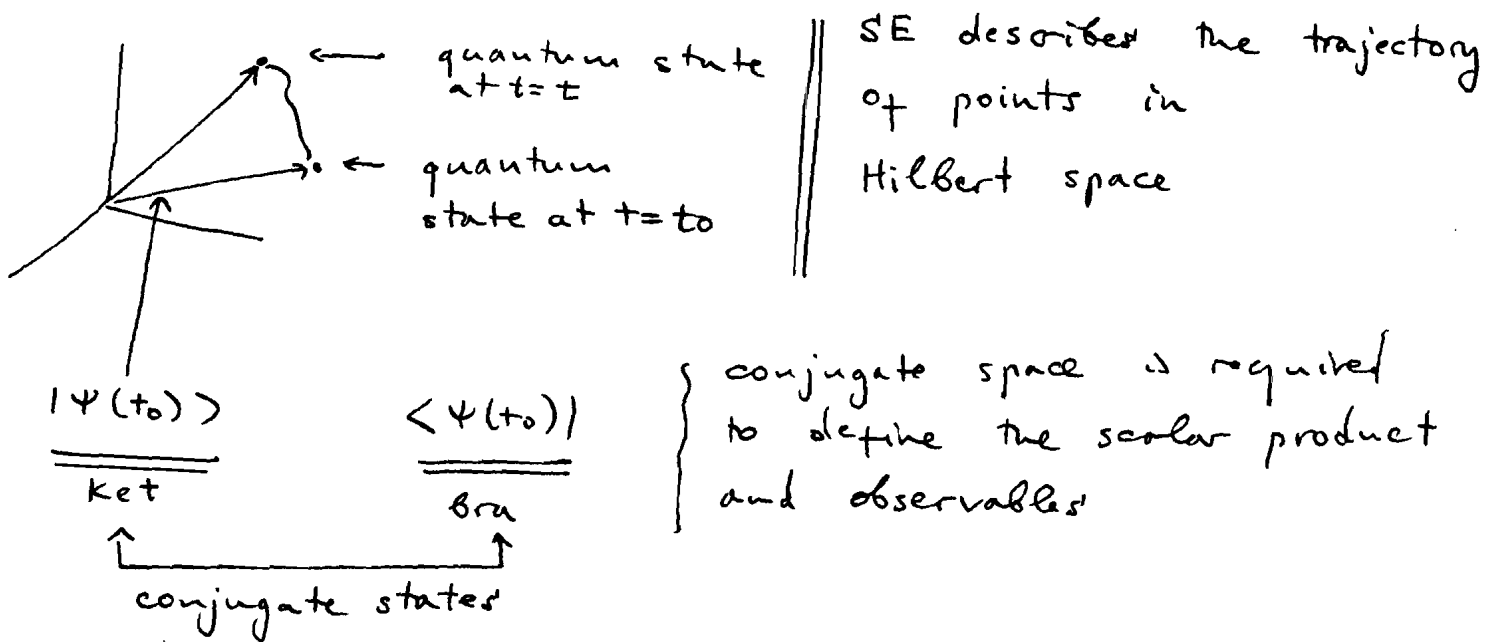$$\frac{d\langle x \rangle}{dt} = \frac{\langle p \rangle}{m}$$

$$\frac{d\langle p \rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} \right\rangle = -\left\langle \frac{\partial H}{\partial x} \right\rangle = eE_0 \cos \omega t$$

$$\langle p(t) \rangle = p_0 + \frac{eE_0}{\omega} \sin \omega t$$

$$\frac{d\langle x \rangle}{dt} = \frac{p_0}{m} + \frac{eE_0}{\omega m} \sin \omega t$$

$$\langle x \rangle_t = x_0 + \frac{p_0 t}{m} + \frac{eE_0}{m\omega^2}\left(1 - \cos \omega t\right)$$

Hilbert space

quantum state
at t = t

quantum
state at t = to

SE describes the trajectory
of points in
Hilbert space

$| \Psi(t_0) \rangle$ — ket

$\langle \Psi(t_0) |$ — Bra

conjugate states

conjugate space is required
to define the scalar product
and observables'

Scalar product in Hilbert space is defined by an infinite integral, it is defined as a combination of two conjugate vectors,

Bra - ket , in Dirac notation

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

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

$$\langle \Phi | \alpha \Psi_1 + \beta \Psi_2 \rangle = \alpha \langle \Phi | \Psi_1 \rangle + \beta \langle \Phi | \Psi_2 \rangle$$

Operator : changes the state ⟶ moves a point
in Hilbert space

$$A | \Psi \rangle = | A \Psi \rangle$$

equivalent representations

$$\langle \Phi | A \Psi \rangle = \langle \Phi | A | \Psi \rangle$$

Hermitian conjugate:

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

$$\langle \phi | A^+ | \psi \rangle^* = \langle A\phi | \psi \rangle^* = \langle \psi | A | \phi \rangle$$

if $\phi = \psi$, $\langle \psi | A^+ | \psi \rangle^* = \langle \psi | A | \psi \rangle$ and

$$A^+ = A \leftarrow \text{expectation values are real for Hermitian operators}$$

Expansion of wavefunctions:

$$|\psi\rangle = \sum_n c_n |n\rangle, \qquad \langle n | m \rangle = \delta_{nm}$$

$$\searrow \text{orthonormality condition}$$

$$c_n = \langle n | \psi \rangle$$

$$|\psi\rangle = \sum_n |n\rangle \langle n | \psi \rangle \rightarrow \boxed{\sum_n |n\rangle\langle n| = 1 \quad \text{completeness relation}}$$

Example 6-1: show that eigenstates corresponding to different eigenvalues are orthogonal

$$H|a\rangle = a|a\rangle \qquad \langle \beta | H | a \rangle = a \langle \beta | a \rangle$$
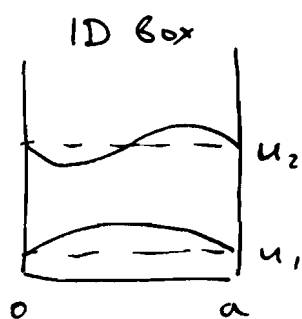$$H|\beta\rangle = \beta|\beta\rangle \qquad \langle a | H | \beta \rangle = \beta \langle a | \beta \rangle$$

$$\langle a | H | \beta \rangle = \langle a | H^+ | \beta \rangle = \langle Ha | \beta \rangle = \langle \beta | Ha \rangle^* =$$
$$= \langle \beta | H | a \rangle^*$$

$$\langle \beta | H | a \rangle = \beta \langle \beta | a \rangle \rightarrow (a - \beta)\langle \beta | a \rangle = \underset{0}{\underline{\underline{0}}}$$

Example of how to use the completeness relation :

ID Box

How to calculate

$$\langle m | x^2 | n \rangle = \int u_m^*(x) \, x^2 \, u_n(x) \, dx \quad ?$$

$$\langle m | x^2 | n \rangle =$$

$$= \langle m | x \cdot x | n \rangle =$$

$$= \langle m | x \sum_k | k \rangle \langle k | x | n \rangle = \sum_k \langle m | x | k \rangle \langle k | x | n \rangle$$

For instance, $\quad \langle m | x^2 | m \rangle = \sum_k | \langle m | x | k \rangle |^2$

X - representation of quantum states

According to quantum mechanics, if we make measurements of positions, it should provide us with a complete set of states.

Let $| x \rangle$ be an <u>eigenket</u> of coordinates' measurement:

$$\hat{x} | x \rangle = x | x \rangle$$

Therefore any quantum state $| \psi \rangle$ can be expanded in terms of $| x \rangle$

$$| \psi \rangle = \int_{-\infty}^{\infty} dx \, c(x) \, | x \rangle$$

Since x is a continuous variable, $\langle x' | x \rangle = \delta(x - x')$

$$c(x) = \langle x | \Psi \rangle = \Psi(x)$$

this is the ordinary wave function that comes to the Schrödinger equation

$$\underline{|c(x)|^2 = |\Psi(x)|^2} \leftarrow$$ the probability of finding a particle at point x

p-representation of quantum states

We can now "project" our state $|\Psi\rangle$ on the momentum variable

$$\hat{p}|p\rangle = p|p\rangle$$

eigenket of the momentum operator

$$|\Psi\rangle = \int_{-\infty}^{\infty} dp \, c(p) |p\rangle, \qquad c(p) = \Phi(p) = \langle p | \Psi \rangle$$

$$\underline{|c(p)|^2 = |\Phi(p)|^2} \leftarrow$$ probability that measuring momentum on state $|\Psi\rangle$ will give the value of p.

Connecting two representations
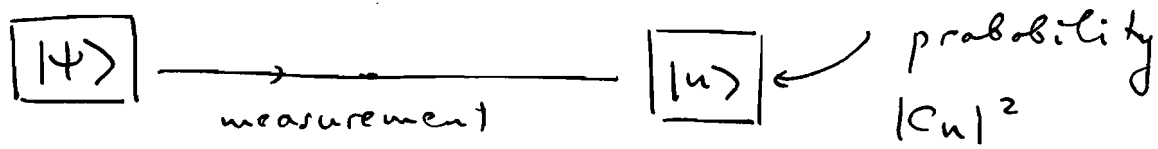
Use the completeness relation

$$\Psi(x) = \langle x | \Psi \rangle = \langle x | \underbrace{\sum_p |p\rangle\langle p|}_{\equiv 1} |\Psi\rangle =$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$$= \int_{-\infty}^{\infty} dp \, \langle x|p\rangle \langle p|\Psi\rangle = \int_{-\infty}^{\infty} dp \, \langle x|p\rangle \Phi(p) \qquad \text{standard Fourier transform}$$

Projection operators

Measurement of a quantum property amounts to projecting a given quantum state to the eigenstate of that property

$$\boxed{|\psi\rangle} \xrightarrow[\text{measurement}]{} \boxed{|n\rangle} \longleftarrow \text{probability } |c_n|^2$$

$$\boxed{|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle}$$

$\longrightarrow$ expansion in all possible results of the measurements

$$P_n \equiv |n\rangle\langle n| \longleftarrow \text{projection operator}$$

$$P_m P_n = |m\rangle\langle m|n\rangle\langle n| = \delta_{mn} |n\rangle\langle n| = \delta_{mn} P_n$$

$$P_n^2 = P_n, \qquad \sum_n P_n = 1$$

$$P_n |\psi\rangle = \langle\psi|n\rangle |n\rangle \longleftarrow \text{gives a formal description of a laboratory measurement}$$

The system Hamiltonian can be expanded in terms of possible measurements of the energy

$$H = \sum_n E_n P_n$$

$\longleftarrow$ measured eigenvalues

Expectation value:

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \int \psi^*(x) H \psi(x) \, dx =$$

$$= \sum E_n \underbrace{|\langle \psi | n \rangle|^2}_{\text{probabilities}}$$

The interesting result of this is that the knowledge of the wave function $\psi(x)$ central to Schrödinger's formulation can be completely bypassed.