

# II. Fundamentals of quantum optics

Various optical quantum properties originate from the fact that the light energy is discrete and there is the minimum unit of the energy, which is called “photon.”

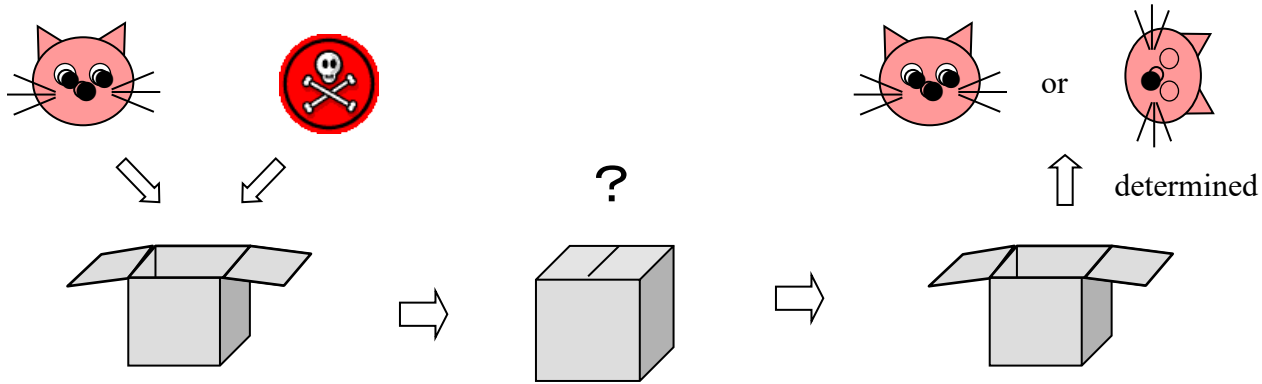
This chapter introduces the fundamentals of quantum mechanics for the following chapters.

## Schrödinger’s cat

Suppose that we put a cat into a box with a poison food and then seal the box. The poison is so strong that one bite instantly kills the cat. The sealing is perfect, and we cannot observe the cat’s state from the outside at all.

When we open the box to observe the cat’s state, we get to know whether the cat is dead or alive.

Then, here is a question; what is the cat’s state in the sealed box before opening ?



Answer #1: The cat is *either* alive *or* dead. It is determinative though not observed.

Answer #2: The cat may be alive *and* dead.

We do not know which, thus it can be alive *and* dead. Both is possible.

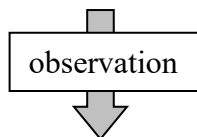
Quantum mechanics adopts A2; the cat in the box is alive *and* dead, which is expressed as

$$\text{Cat in the box} = a \times \text{alive} + b \times \text{dead} \quad \boxed{\text{Quantum mechanical superposition state}}$$

where, *a* and *b* are coefficients representing the probabilities (not directly, as described later).

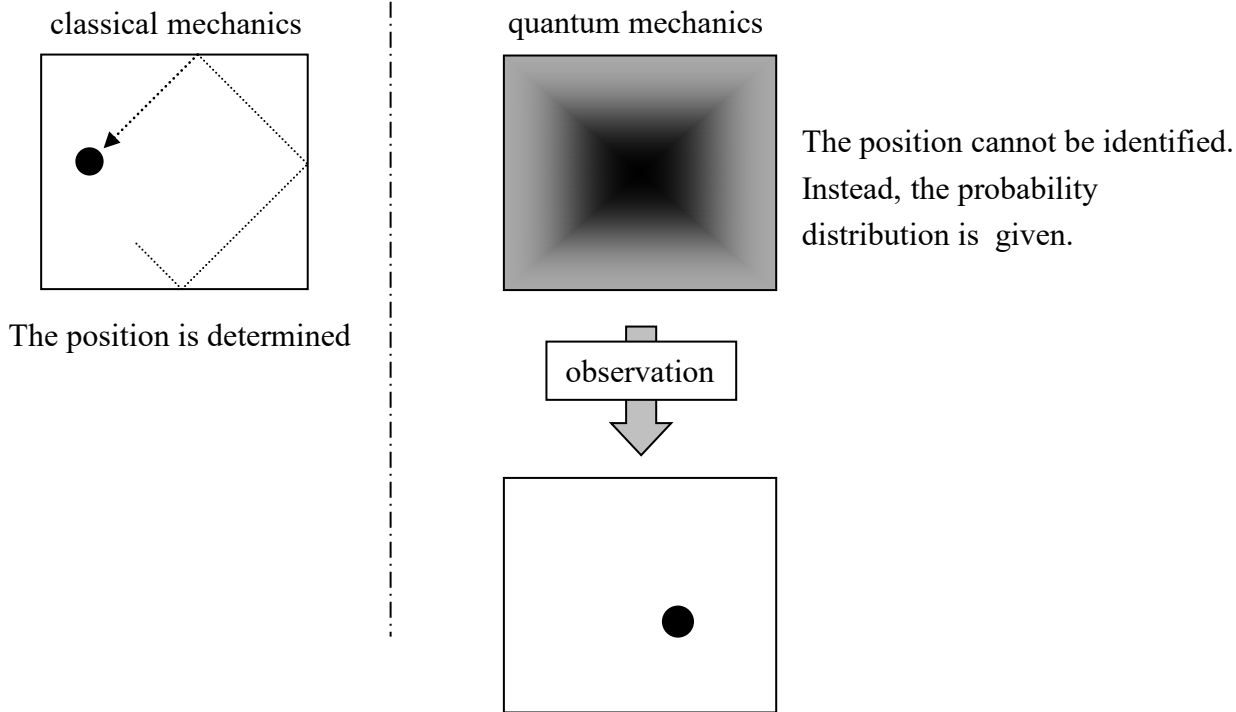
When we open the box and look at the cat, we find that the cat is dead *or* alive (either one of them).

$$\text{Cat in the box} = a \times \text{alive} + b \times \text{dead} \quad (\text{probabilistic})$$



$$\text{Cat in the box} = \text{alive} \quad \text{or} \quad \text{dead} \quad (\text{deterministic})$$

The point in the above story is; “a physical state is probabilistic.”  
For example, an electron confined in a small area is;

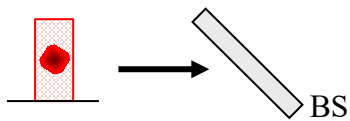


In quantum mechanics,

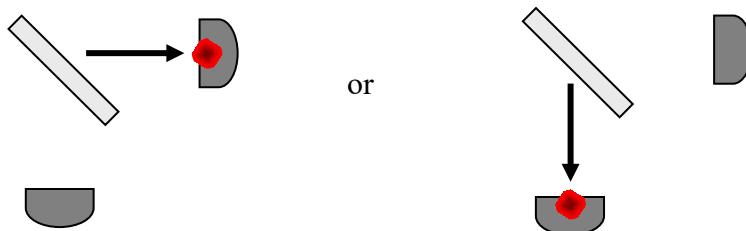
- A physical state is probabilistic; a state can be plural conditions simultaneously.
- A probabilistic state changes to be deterministic when observed.

### Single-photon state through a beam splitter

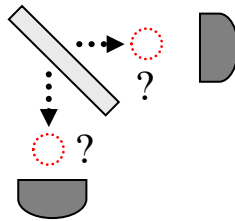
Suppose that an optical pulse of one-photon energy is incident onto a beam splitter (BS).



When we measure the light energy at the BS outputs, one photon is detected at either one of the two output ports, not both because a photon is the minimum unit of the light energy.



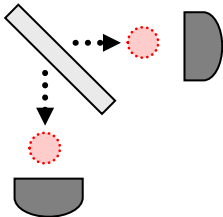
Here is a question: “What is the photon state just after the beam splitter (before detection) ?”



This situation is similar to the cat in the box in the previous section.

The quantum mechanical answer is

“the photon is a superposition of a photon at the transmission port and that at the reflection port”.

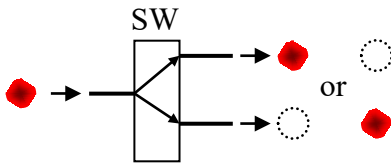


$$\text{The photon after the beam splitter} = a \times (\text{trans.}) + b \times (\text{ref.})$$

Note

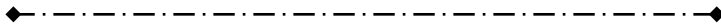
A state should not be deterministic *in principle* for being “superposition state”.

For example, a photon that is randomly switched according to random numbers is not super-positioned.

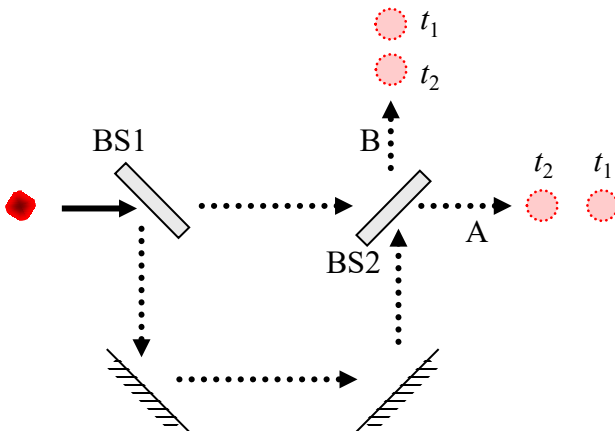


The photon position looks random, but it is deterministic in principle.

⇓  
not superposition state.



Next, let us extend the beam splitting system as below.



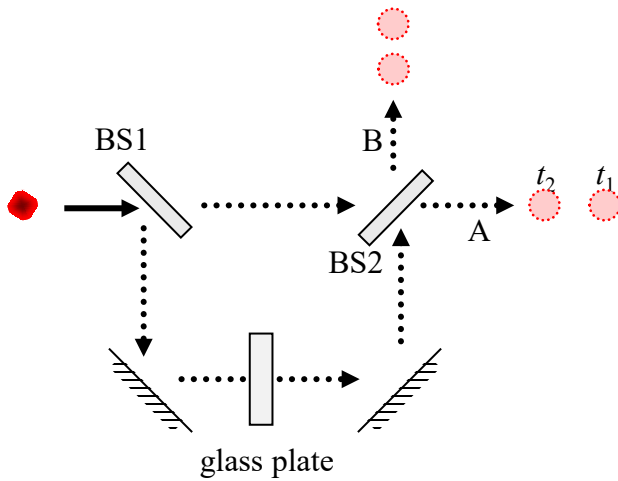
A photon possibly goes through

- 1) BS1 → short path → BS2 → port A
- 2) BS1 → short path → BS2 → port B
- 3) BS1 → long path → BS2 → port A
- 4) BS1 → long path → BS2 → port B



$$\begin{aligned} \text{Output state} = & a \times (\text{photon @ } \{A, t_1\}) \\ & + b \times (\text{photon @ } \{B, t_1\}) \\ & + c \times (\text{photon @ } \{A, t_2\}) \\ & + d \times (\text{photon @ } \{B, t_2\}) \end{aligned}$$

Here, we place a glass plate in the longer path.



The photon's routes are the same as the above. However, the output state must be different because of the glass plate.

We want to express this difference.

Therefore, we assume that coefficients as complex numbers.

$$\begin{aligned} \text{Output state} = & a \times (\text{photon @ } \{A, t_1\}) \\ & + b \times (\text{photon @ } \{B, t_1\}) \\ & + ce^{i\theta} \times (\text{photon @ } \{A, t_2\}) \\ & + de^{i\theta} \times (\text{photon @ } \{B, t_2\}) \end{aligned}$$

↑  
phase shift due to the glass plate

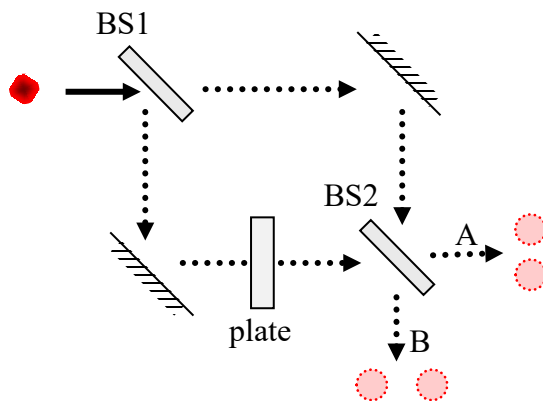
Then, the probability of each state is given by the absolute square of its complex coefficient.

$$\begin{aligned} \text{probability of (photon@}\{A, t_1\}) &= |a|^2 & \text{probability of (photon@}\{B, t_1\}) &= |b|^2 \\ \text{probability of (photon@}\{A, t_2\}) &= |c|^2 & \text{probability of (photon@}\{B, t_2\}) &= |d|^2 \end{aligned}$$

$$\left[ \text{Note: } |a|^2 + |b|^2 + |c|^2 + |d|^2 = 1 \right]$$

- Coefficients of a superposition state are complex numbers.
- The probability of each sub-state is given by the absolute square of its coefficient.

Next, we reconstruct the above system as below.



A photon possibly goes through

- 1) BS1 → upper path → BS2 → port A
- 2) BS1 → upper path → BS2 → port B
- 3) BS1 → lower path → BS2 → port A
- 4) BS1 → lower path → BS2 → port B



$$\begin{aligned} \text{Output state @A} &= c_1 \times (\text{photon via route 1}) \\ &+ c_3 \times (\text{photon via route 3}) \end{aligned}$$

At port A, the states of (photon via route 1) and (photon via route 3) are indistinguishable.

We do not know whether a photon at port A passed through route 1 or route 3.

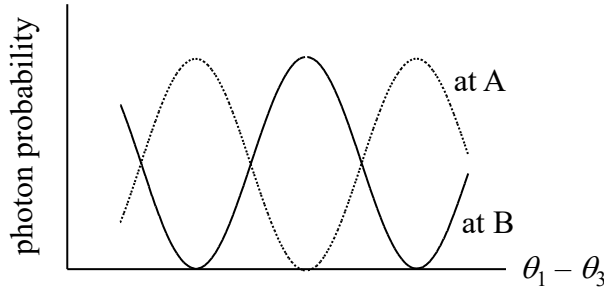
Thus, they are merged to one state as

$$\begin{aligned} \text{Output state @A} &= c_1 \times (\text{photon via route 1}) + c_3 \times (\text{photon via route 3}) \\ &= (c_1 + c_3) \times (\text{photon @A}) \end{aligned}$$

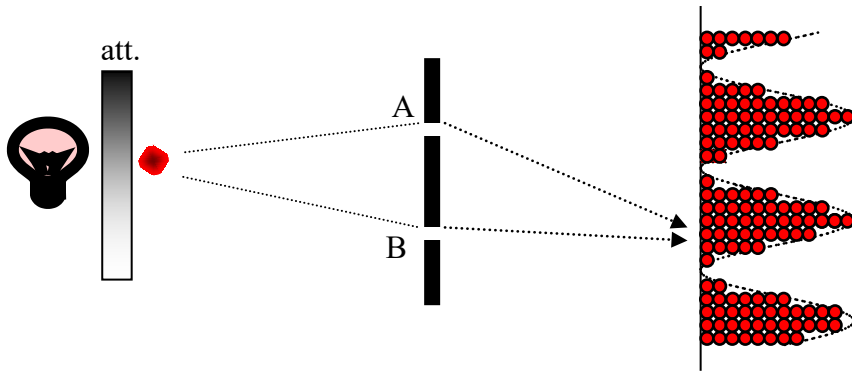
Then, the probability of a photon being at port A is given by

$$\begin{aligned}
 |c_1 + c_3|^2 &= |c_1|^2 + |c_3|^2 + 2\text{Re}[c_1c_3^*] \\
 &= |c_1|^2 + |c_3|^2 + 2|c_1||c_3|\cos(\theta_1 - \theta_3)
 \end{aligned}
 \quad \left( \begin{array}{l} c_1 \equiv |c_1| e^{i\theta_1} \\ c_3 \equiv |c_3| e^{i\theta_3} \end{array} \right)$$

This probability is dependent on the relative phase between the upper and lower paths.

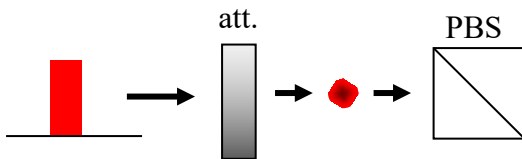


The above situation is equivalent to one-photon Young's interference.



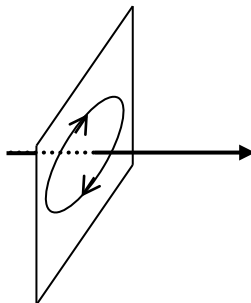
Polarization state of a photon (another example of superposition state)

Suppose that light with one-photon energy is incident onto a polarization beam splitter (PBS).



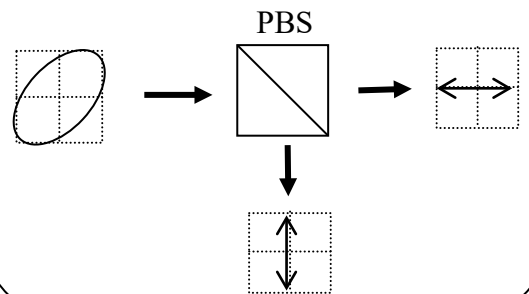
[Polarization state of light]

The electrical field of lightwave oscillates in a plane perpendicular to the propagation direction. The manner of the electrical field oscillation in the perpendicular plane is called "polarization".

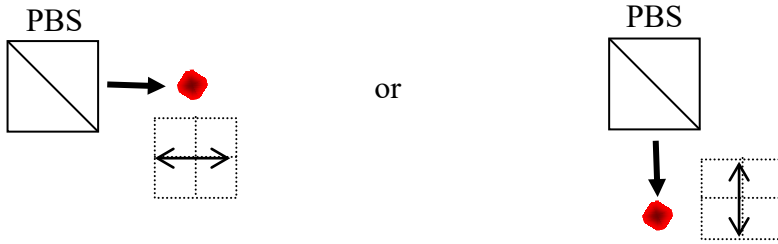


[Polarization beam splitter (PBS)]

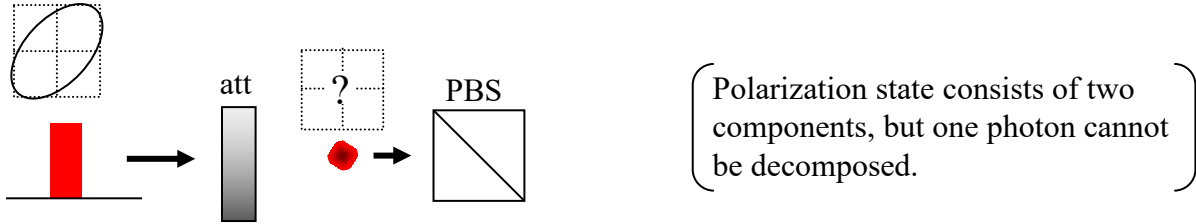
An optical device that splits incident light into horizontally and vertically oscillating components



Through the PBS, a photon goes to *either* one of the two output ports.  
 In accordance with the function of a PBS, it is reasonable to regard a photon at the transmission/reflection ports as a photon in the horizontal/vertical polarization states, respectively.



Here is a question; “What is the polarization state of a photon just before the PBS ?”



Answer: a superposition of the horizontally polarized photon and the vertically polarized photon.

$$\text{photon state before PBS} = c_H \times (\text{horizontal photon}) + c_V \times (\text{vertical photon})$$

Coefficient  $\{c_H, c_V\}$  should be consistent with the polarization state before the attenuator.

+45 diagonal

$$E_0 e^{i\omega t} (1, 1) \rightarrow \text{att} \rightarrow \text{photon} \quad \frac{1}{\sqrt{2}} \times (\text{H state}) + \frac{1}{\sqrt{2}} \times (\text{V state})$$

$$\left[ \frac{1}{\sqrt{2}} \text{ is attached for the total probability to be unity.} \right]$$

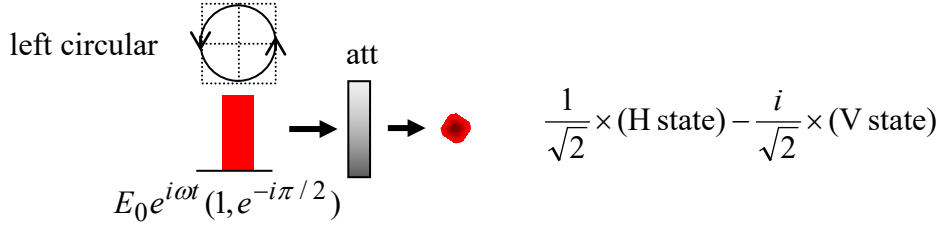
*normalization constant*

-45 diagonal

$$E_0 e^{i\omega t} (1, e^{i\pi}) \rightarrow \text{att} \rightarrow \text{photon} \quad \frac{1}{\sqrt{2}} \times (\text{H state}) - \frac{1}{\sqrt{2}} \times (\text{V state})$$

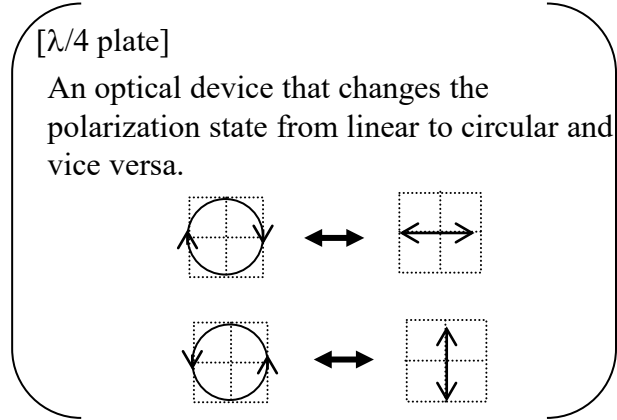
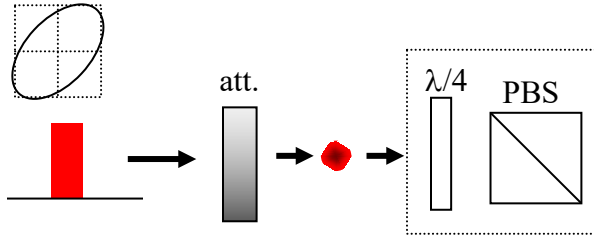
right circular

$$E_0 e^{i\omega t} (1, e^{i\pi/2}) \rightarrow \text{att} \rightarrow \text{photon} \quad \frac{1}{\sqrt{2}} \times (\text{H state}) + \frac{i}{\sqrt{2}} \times (\text{V state})$$

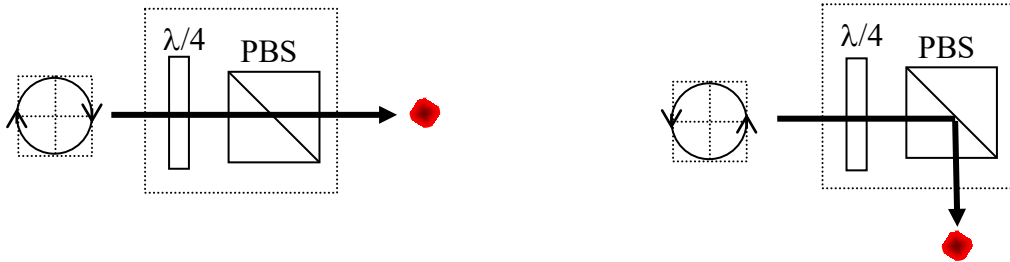


Note that the way of expressing the photon polarization state is not unique, as shown below.

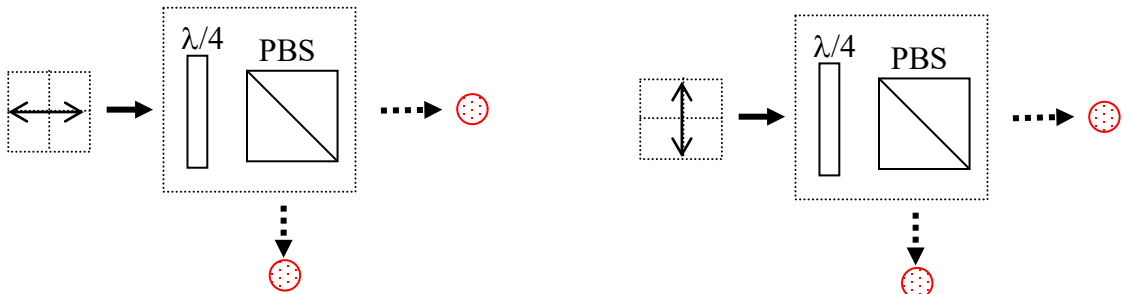
Suppose that a  $\lambda/4$  plate is placed before a PBS, and regard  $\{\lambda/4 + \text{PBS}\}$  as one measurement system.



Because of the  $\lambda/4$  plate, the right circular state definitely goes to one output port, and the left circular state definitely goes to the other output port.



On the other hand, to which port the photon goes is probabilistic for linearly polarized states.



In this measurement system,  $\{\text{right circular state, left circular state}\}$  work as the same way as  $\{\text{horizontal linear state, vertical linear state}\}$  in the PBS system.



The photon polarization state can be regarded as a superpositioned state of the right and left circular states.

$$\text{photon before } \{\lambda/4 + \text{PBS}\} = c_R \times (\text{right circular state}) + c_L \times (\text{left circular state})$$

$$\left\{ \begin{array}{l} \text{(right-circular state)} = \frac{1}{\sqrt{2}} \times (\text{horizontal photon}) + \frac{i}{\sqrt{2}} \times (\text{vertical photon}) \\ \text{(right-circular state)} = \frac{1}{\sqrt{2}} \times (\text{horizontal photon}) - \frac{i}{\sqrt{2}} \times (\text{vertical photon}) \end{array} \right.$$



$$\left\{ \begin{array}{l} \text{(horizontal state)} = \frac{1}{\sqrt{2}} \times (\text{right-circular photon}) + \frac{1}{\sqrt{2}} \times (\text{left-circular photon}) \\ \text{(vertical state)} = -i \left\{ \frac{1}{\sqrt{2}} \times (\text{right-circular photon}) - \frac{1}{\sqrt{2}} \times (\text{left-circular photon}) \right\} \\ \qquad \qquad \qquad = \frac{1}{\sqrt{2}} \times (\text{right-circular photon}) - \frac{1}{\sqrt{2}} \times (\text{left-circular photon}) \end{array} \right.$$

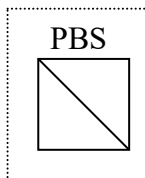
Quantum states are evaluated by probabilities, and the probabilities are given by the absolute square of coefficients, and thus  $(-i)$  multiplexed onto the whole state does not matter.

Using these relationships,

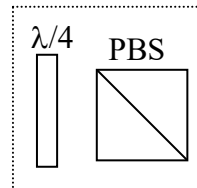
$$\begin{aligned} \text{(photon polarization state)} &= c_H \times (\text{horizontal photon}) + c_V \times (\text{vertical photon}) \\ &= c_H \left\{ \frac{1}{\sqrt{2}} \times (\text{right-circular photon}) + \frac{1}{\sqrt{2}} \times (\text{left-circular photon}) \right\} \\ &\quad + c_V \left\{ \frac{1}{\sqrt{2}} \times (\text{right-circular photon}) - \frac{1}{\sqrt{2}} \times (\text{left-circular photon}) \right\} \\ &= \underbrace{\frac{c_H + c_V}{\sqrt{2}}}_{c_R} \times (\text{right-circular photon}) + \underbrace{\frac{c_H - c_V}{\sqrt{2}}}_{c_L} \times (\text{left-circular photon}) \end{aligned}$$

Whether the photon polarization state is regarded as a superposition of {horizontal photon & vertical photon} or {right-circular photon & left-circular photon} depends on the measurement system.

By the way, a measurement system is used for evaluating a physical quantity, generally speaking.



a measurement system  
for {horizontal or vertical}



a measurement system  
for {right circular or left circular}





How to express a superpositioned state is dependent on a concerned physical quantity.

||

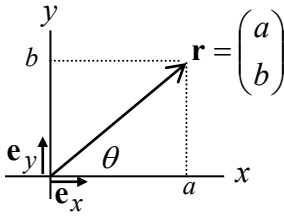
How to express a quantum state is dependent on a concerned physical quantity.

## Complex Hilbert space

The previous sections qualitatively explains what is a quantum state and how to express it. For quantitatively (or analytically) describing a quantum state, we need some mathematical frameworks, which are introduced in this section.

The mathematical stage for quantum states is (complex) Hilbert space, which is a generalized version of the Euclid space.

First, we review the Euclid space.



$$\begin{aligned} \text{Inner product: } (\mathbf{r}_1 \cdot \mathbf{r}_2) &= |\mathbf{r}_1||\mathbf{r}_2|\cos\theta \\ &= a_1a_2 + b_1b_2 \end{aligned}$$

$$\left( \mathbf{r}_1 = \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \quad \mathbf{r}_2 = \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \right)$$

$$\text{Length of a vector: } |\mathbf{r}| = \sqrt{a^2 + b^2} = \sqrt{(\mathbf{r} \cdot \mathbf{r})}$$

Orthogonality of vectors:

$$(\mathbf{r}_1 \cdot \mathbf{r}_2) = 0 \iff \theta = 90^\circ \iff \mathbf{r}_1 \text{ and } \mathbf{r}_2 \text{ are orthogonal}$$

There exist unit vectors defined as

$$\mathbf{e}_x \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \mathbf{e}_y \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\left( \begin{array}{l} \mathbf{e}_x: \text{unit vector along the } x\text{-direction} \\ \mathbf{e}_y: \text{unit vector along the } y\text{-direction} \end{array} \right)$$

- Its length is unity:  $|\mathbf{e}_x| = |\mathbf{e}_y| = 1$

- They are orthogonal to each other:  $(\mathbf{e}_x \cdot \mathbf{e}_y) = 0$

- An arbitrary vector can be expressed by a linear combination of the unit vectors:

$$\mathbf{r} = a\mathbf{e}_x + b\mathbf{e}_y$$

- A component of a vector is given by the inner product with the corresponding unit vector:

$$\left\{ \begin{array}{l} (\mathbf{e}_x \cdot \mathbf{r}) = |\mathbf{r}| \cos\theta = a \\ (\mathbf{e}_y \cdot \mathbf{r}) = |\mathbf{r}| \sin\theta = b \end{array} \right. \quad \text{or} \quad \left\{ \begin{array}{l} (\mathbf{e}_x \cdot \mathbf{r}) = \mathbf{e}_x \cdot \{a\mathbf{e}_x + b\mathbf{e}_y\} \\ \quad \quad \quad = a(\mathbf{e}_x \cdot \mathbf{e}_x) + b(\mathbf{e}_x \cdot \mathbf{e}_y) = a \\ (\mathbf{e}_y \cdot \mathbf{r}) = \mathbf{e}_y \cdot \{a\mathbf{e}_x + b\mathbf{e}_y\} = b \end{array} \right.$$

The Euclid space is a concrete space in the real world.

The Hilbert space is a conceptual space whose framework is similar to that of Euclid space, in which, however, components of vectors are complex numbers.

- A vector is expressed as;

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \quad \begin{array}{l} (|\psi\rangle: \text{'ket'}) \\ (c_i: \text{complex number}) \end{array}$$

- The inner product is defined as below:

The inner product of  $|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$  and  $|\varphi\rangle = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{pmatrix}$  is  $\langle\varphi|\psi\rangle = d_1^*c_1 + d_2^*c_2 + \dots + d_N^*c_N$

Components multiplexed from the left side are complex conjugate. With this definition,  $\langle\psi|\psi\rangle = |c_1|^2 + |c_2|^2$  is a positive real number, which is consistent with the concept that the inner product of a vector and itself is the square of the length of the vector.

- The norm, that corresponds to the vector length, is defined as  $\|\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle}$

- The orthogonality is defined as:  $\langle\varphi|\psi\rangle = 0 \iff |\psi\rangle$  and  $|\varphi\rangle$  are orthogonal

Similarly to the Euclid space, unit vectors  $\phi_i$  are defined, which are called "basis".

- Its norm is unity:  $\|\phi_i\rangle\| = 1$   
 - They are orthogonal to each other:  $\langle\phi_i|\phi_j\rangle = 0$

}  $\langle\phi_i|\phi_j\rangle = \delta_{ij}$  (Kronecher's delta)

- An arbitrary vector is expressed by a linear combination of the basis vectors

$$|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + \dots + c_N|\phi_N\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

- A coefficient of a linear combination is given by the inner product with its basis vector.

$$\langle\phi_i|\psi\rangle = \langle\phi_i|\{c_1|\phi_1\rangle + c_2|\phi_2\rangle + \dots + c_N|\phi_N\rangle\} = c_i \quad \left[ \langle\phi_i|\phi_j\rangle = \delta_{ij} \right]$$

In other words, a space is formed by basis vectors.

Quantum mechanics utilizes the Hilbert space for expressing a quantum state (superposition state) as;

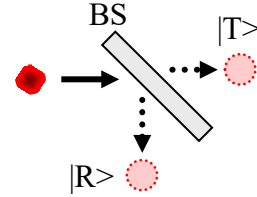
- A state is expressed by a vector in a Hilbert space, which is called "ket vector" or "ket state" or simply "ket"
- Possible states for a state to take are expressed by basis vectors, which are called "basis states".
- Coefficients in a linear combination of basis vectors = components of a vector

For example;

- A photon state after BS:

$$|\psi\rangle = a|T\rangle + b|R\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

where the basis is  $\left\{ \begin{array}{l} |T\rangle: \text{transmitted photon state} \\ |R\rangle: \text{reflected photon state} \end{array} \right\}$



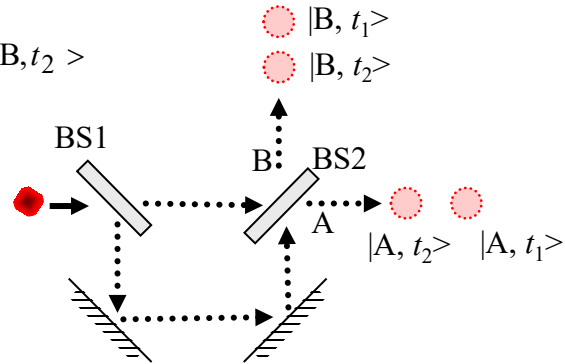
- A photon after split and combined:

$$|\psi\rangle = a|A, t_1\rangle + b|B, t_1\rangle + c|A, t_2\rangle + d|B, t_2\rangle$$

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

where the basis is

$\left\{ \begin{array}{l} |A, t_1\rangle: \text{photon at A via the short path} \\ |B, t_1\rangle: \text{photon at B via the short path} \\ |A, t_2\rangle: \text{photon at A via the long path} \\ |B, t_2\rangle: \text{photon at B via the long path} \end{array} \right\}$

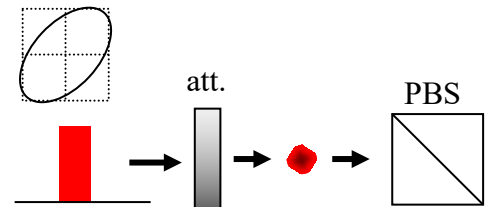


- A photon polarization before PBS:

$$|\psi\rangle = c_H|H\rangle + c_V|V\rangle = \begin{pmatrix} c_H \\ c_V \end{pmatrix}$$

where the basis is

$\left\{ \begin{array}{l} |H\rangle: \text{horizontally polarized photon} \\ |V\rangle: \text{vertically polarized photon} \end{array} \right\}$



Similarly to mathematical Hilbert spaces, the inner product of two kets is defined for physical states.

$$\langle \varphi | \psi \rangle = d_1^* c_1 + d_2^* c_2 + \dots + d_N^* c_N$$

This expression of the inner product is rewritten in a matrix form as

$$\langle \psi | \varphi \rangle = \underbrace{c_1^* d_1 + c_2^* d_2 + \dots + c_N^* d_N}_{\text{matrix form}} = \underbrace{(c_1^* \quad c_2^* \quad \dots \quad c_N^*)}_{\text{bra vector}} \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{pmatrix} \quad \left( \begin{array}{l} |\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \\ |\varphi\rangle = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{pmatrix} \end{array} \right)$$

The above equation indicates

$$\langle \psi | = (c_1^* \quad c_2^*)$$

This  $\langle \psi |$ , which is written in the left side in inner products, is called “bra vector” or “bra state” or simply “bra”.

Concretely, a bra is a  $1 \times N$  matrix that originates from a  $N$ -dimensional ket with complex conjugating.

The inner product quantitatively indicates the similarity (or overlap) of two physical states.

### Summary

- A quantum state is a probabilistic superposition state.
- A quantum state is expressed by a ket vector in a Hilbert space.
- Basis vectors of a quantum mechanical Hilbert space are states for an observed subject possibly to take.
- A ket vector of a quantum state is expressed by a linear combination of basis vectors.
- Coefficients in the linear combination are components of a ket vector.
- The absolute square of a coefficient in the linear combination gives the probability that the subject takes the corresponding the basis state.

In the above, basis vectors forming a Hilbert space are phenomenologically introduced, assuming a concrete measurement system.

As physics, however, a general (or conceptual) theoretical framework is desired, which will be presented in the following sections.

A Hilbert space is formed by basis vectors.

Here is a question; how to mathematically define basis vectors in general ?

The answer is; a physical quantity is expressed by an operator, whose eigenvectors turn to be basis vectors that form a quantum-mechanical Hilbert space.

The above postulate is explained step-by-step in the following.

As the first step, the theoretical framework of mathematical Hilbert spaces is introduced.

- Generally, there is a matrix that changes a ket vector to another ket vector as

$$\mathbf{A}|\psi\rangle = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} a_{11}c_1 + a_{12}c_2 \\ a_{21}c_1 + a_{22}c_2 \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = |\varphi\rangle \quad (\text{in case of a two-dimensional space})$$

- Such a matrix is called “operators”, and denoted as  $\hat{A}$  ("A hat").

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

- A matrix (operator) has eigenvectors and eigenvalues.

$$\hat{A}|\phi_i\rangle = \alpha_i|\phi_i\rangle$$

$|\phi_i\rangle$ : eigenvector  
 $\alpha_i$ : eigenvalue

- Generally, an operator  $\hat{A}$  has its Hermitian conjugate operator, which is expressed as  $\hat{A}^\dagger$ .

Suppose that  $\hat{A}$  operates on ket  $|\psi\rangle$  and create another ket state as:

$$\hat{A}|\psi\rangle = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} a_{11}c_1 + a_{12}c_2 \\ a_{21}c_1 + a_{22}c_2 \end{pmatrix}$$

the bra of which is written as:

$$\begin{pmatrix} a_{11}c_1 + a_{12}c_2 \\ a_{21}c_1 + a_{22}c_2 \end{pmatrix} \xrightarrow{\text{bra}} \begin{pmatrix} a_{11}^*c_1^* + a_{12}^*c_2^* & a_{21}^*c_1^* + a_{22}^*c_2^* \end{pmatrix} = \begin{pmatrix} c_1^* & c_2^* \end{pmatrix} \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix}$$

|||  
 Hermitian conjugate of  $\hat{A}$ ,  
 which is denoted by  $\hat{A}^\dagger$

In General, an Hermitian conjugate of  $\hat{A}$  is an operator satisfying the following relationship

$$\langle \text{bra of } \hat{A}|\psi\rangle = \langle \psi | \hat{A}^\dagger$$

In a matrix expression, an Hermitian conjugate is a transposed matrix with complex conjugate.

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \xrightarrow{\text{Hermitian conjugate}} \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix}$$

(Intuitively speaking, Hermitian conjugate is complex conjugate of a matrix or an operator)

Hermitian operator:  $\hat{A}^\dagger = \hat{A}$

- Eigenvalues of an Hermitian operator are real numbers.

$$\hat{A}|\phi_i\rangle = a_i|\phi_i\rangle$$

$\uparrow$  (Hermitian operator)       $\uparrow$  (real number)

proof

Suppose that  $\hat{A}$  has eigenvalue/eigenvector of  $\{a, |\phi\rangle\}$

$$\hat{A}|\phi\rangle = a|\phi\rangle \tag{1}$$

Inner product with  $|\phi\rangle$

$$\langle\phi|\hat{A}|\phi\rangle = a\langle\phi|\phi\rangle$$

On the other hand, bra of Eq. (1) is

$$\langle\phi|\hat{A}^\dagger = a^*\langle\phi|$$

Inner product with  $|\phi\rangle$

$$\langle\phi|\hat{A}^\dagger|\phi\rangle = a^*\langle\phi|\phi\rangle$$

$\downarrow$  (Hermitian)

$$\langle\phi|\hat{A}|\phi\rangle = a^*\langle\phi|\phi\rangle$$

$\rightarrow a\langle\phi|\phi\rangle = a^*\langle\phi|\phi\rangle$   
 $\downarrow$   
 $a = a^*$   
 $\downarrow$   
 $a \text{ is a real number}$

- Eigen vectors of an Hermitian operator are orthogonal to each other.

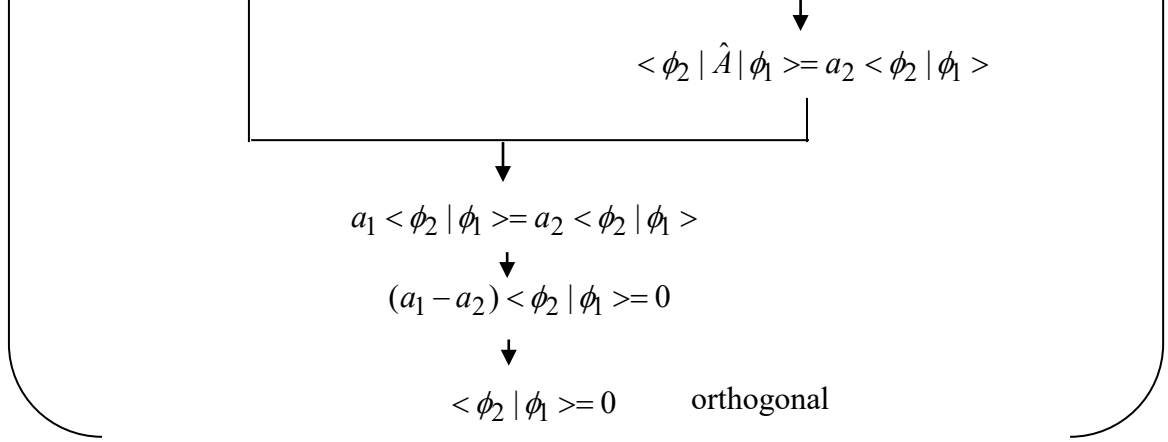
$$\left. \begin{array}{l} \hat{A}|\phi_1\rangle = a_1|\phi_1\rangle \\ \hat{A}|\phi_2\rangle = a_2|\phi_2\rangle \\ \left( \begin{array}{l} \hat{A} : \text{Hermitian operator} \\ a_1 \neq a_2 \end{array} \right) \end{array} \right\} \rightarrow \langle\phi_1|\phi_2\rangle = 0$$

proof

Suppose there are two sets of eigenvalue/eigenvector

$\hat{A}|\phi_1\rangle = a_1|\phi_1\rangle$ 
 $\downarrow$  inner product with  $\langle\phi_2|$ 
 $\langle\phi_2|\hat{A}|\phi_1\rangle = a_1\langle\phi_2|\phi_1\rangle$

$\hat{A}|\phi_2\rangle = a_2|\phi_2\rangle \tag{a_1 \neq a_2}$ 
 $\downarrow$  bra
  $\langle\phi_2|\hat{A}^\dagger = a_2^*\langle\phi_2|$ 
 $\downarrow$   $\hat{A}$  is an Hermitian operator  
 $a_2$  is a real number
  $\langle\phi_2|\hat{A} = a_2\langle\phi_2|$ 
 $\downarrow$  inner product with  $|\phi_1\rangle$



- An arbitrary ket vector is represented by a linear combination of eigenvectors.

$$|\Psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle + \dots = \sum_i c_i |\phi_i\rangle \quad \left[ |\phi_i\rangle: \text{eigenvector} \right]$$

- A set of eigenvectors whose norm is unity is called “complete orthogonal system”.

$$|\Psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle + \dots = \sum_i c_i |\phi_i\rangle \quad \left[ \hat{A}|\phi_i\rangle = \alpha_i |\phi_i\rangle \right]$$

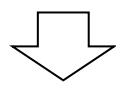
where  $\langle \phi_i | \phi_i \rangle = 1$

On the other hand,  $\langle \phi_i | \phi_j \rangle = 0$  for  $i \neq j$

$$\left. \begin{array}{l} \text{where } \langle \phi_i | \phi_i \rangle = 1 \\ \text{On the other hand, } \langle \phi_i | \phi_j \rangle = 0 \text{ for } i \neq j \end{array} \right\} \Rightarrow \boxed{\langle \phi_i | \phi_j \rangle = \delta_{ij}} \quad \left( \begin{array}{l} \text{Kronecker delta} \\ \delta_{ij} = \begin{cases} 1 & \text{for } i=j \\ 0 & \text{otherwise} \end{cases} \end{array} \right)$$

- A coefficient in a linear combination of a complete orthogonal system representing a ket vector is given by the inner product of the ket vector and the corresponding unit eigenvector.

$$\begin{aligned}
 \langle \phi_i | \Psi \rangle &= \langle \phi_i | \{c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle + \dots\} \\
 &= c_1 \langle \phi_i | \phi_1 \rangle + c_2 \langle \phi_i | \phi_2 \rangle + c_3 \langle \phi_i | \phi_3 \rangle + \dots \\
 &= c_i
 \end{aligned}$$



The above postulates or properties indicate that unit eigenvectors of an Hermitian operator are nothing else but basis vectors.

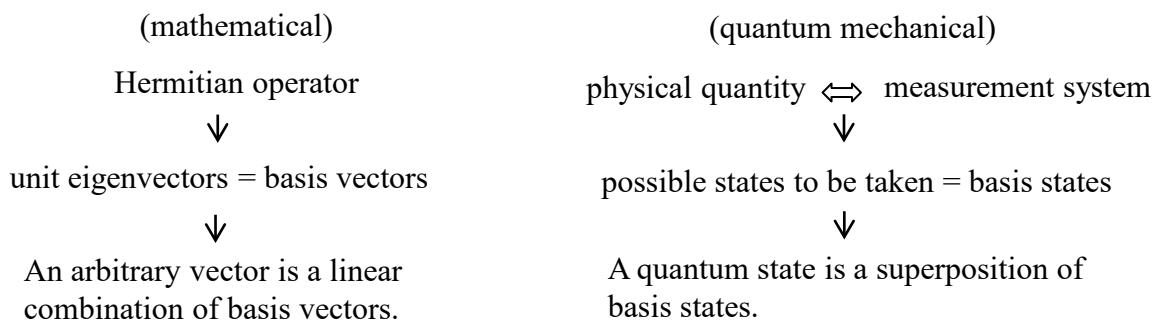
Then, a Hilbert space is formed by such basis vectors.

Components of a ket vector in a Hilbert space = Coefficients in a linear combination of basis vectors.

### Quantum mechanical Hilbert space

The theoretical framework of the above mathematical Hilbert space is utilized to describe quantum states.

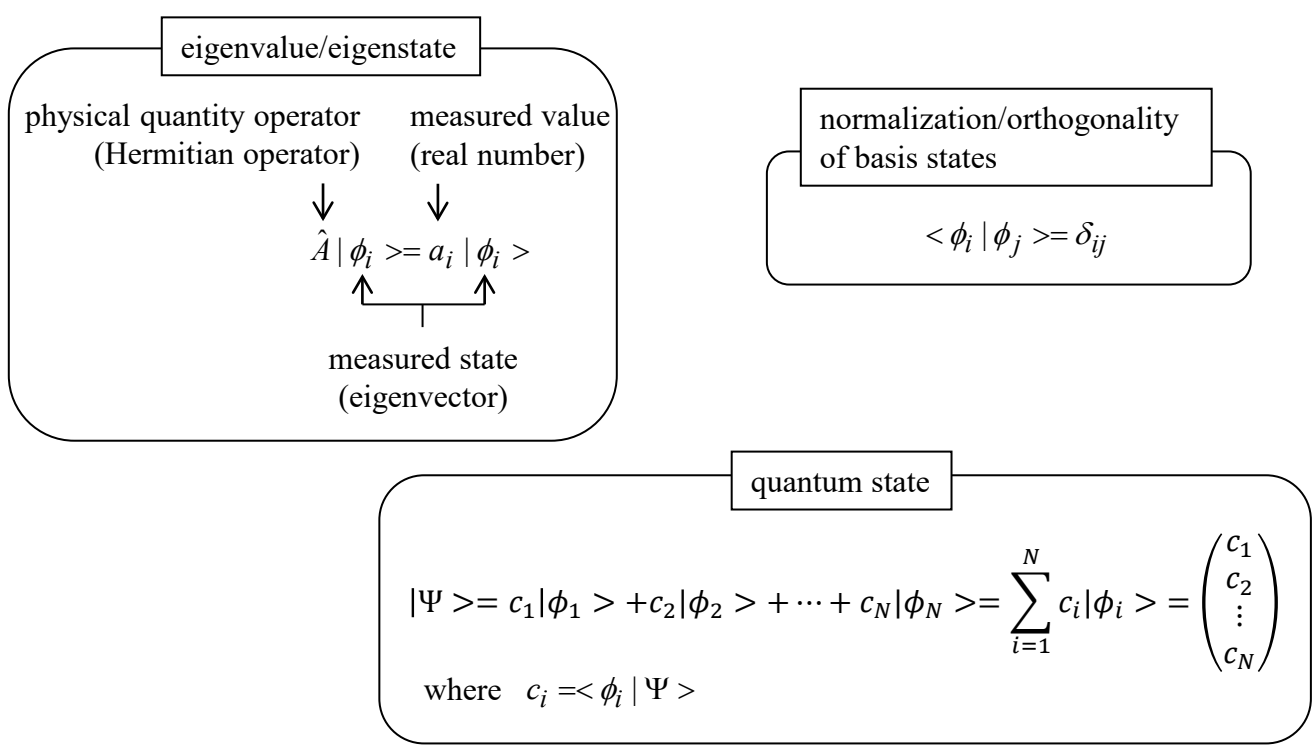
A mathematical Hilbert space is formed by unit eigenvectors of an Hermitian operator. On the other hand, basis states forming a superpositioned state are candidates states, these states are determined by a measurement system, and the measurement system is determined by a physical quantity to be measured.



From the above similarity, here are postulates:

- “a physical quantity is expressed by an Hermitian operator,”
- “a quantum state is a superpositioned state of eigenstates of a physical quantity operator, and is expressed by a ket vector in a Hilbert space formed by basis vectors of eigenstates.”

In addition,  
 “eigenvalues of a physical quantity operator are measured values of the physical quantity,”  
 which corresponds to the fact that eigenvalues of an Hermitian operator are also real numbers.





In the previous section where quantum states are qualitatively explained, we see that the absolute square of coefficients of basis states represents their probabilities. This postulate is also applied to the ket vector representation in Hilbert spaces; When a quantum state expressed by  $|\Psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + \dots + c_N|\phi_N\rangle$  is measured, The probability of the state being  $|\phi_i\rangle$  is given by  $|c_i|^2$ .

Consequently, the following condition is satisfied, because the total probability should be unity.

$$\sum_i |c_i|^2 = 1 \quad \boxed{\text{normalization condition}}$$

Consequently, the norm of a ket vector representing a quantum state is;

$$\begin{aligned} \langle \Psi | \Psi \rangle &= \{c_1^* \langle \phi_1 | + c_2^* \langle \phi_1 | + \dots + c_N^* \langle \phi_N | \} \{c_1 | \phi_1 \rangle + c_2 | \phi_2 \rangle + \dots + c_N | \phi_N \rangle\} \\ &= \sum_{i,j} c_i^* c_j \langle \phi_i | \phi_j \rangle = \sum_{i,j} c_i^* c_j \delta_{ij} = \sum_i |c_i|^2 = 1 \end{aligned}$$

◆-----◆

A quantum state is a superposition state (= probabilistic state) in general, and thus the result of measurement on a quantum state is different for each time, which means that a measured value of a physical quantity is stochastic.

By the way, a static variable is generally characterized by the average and the variance (or the standard deviation).

Thus, we would like to theoretically express the average (or the expected value) of measured values of a physical quantity.

Utilizing the postulates of “the absolute square of a coefficient in a linear combination represents probability” and “eigenvalues of a physical quantity operator represent measured values,” the mean value of a physical quantity can be expressed as:

$$\boxed{\text{the mean value of a physical quantity of a quantum state } |\Psi\rangle: \langle \Psi | \hat{A} | \Psi \rangle}$$

$|\Psi\rangle$  is expressed by a linear combination of eigenstates of a physical quantity operator  $\hat{A}$ .

$$|\Psi\rangle = \sum_j c_j |\phi_j\rangle$$

↓ (operate  $\hat{A}$ )

$$\hat{A} |\Psi\rangle = \sum_i c_i \hat{A} |\phi_i\rangle = \sum_i c_i a_i |\phi_i\rangle$$

$$\left[ \hat{A} |\phi_j\rangle = a_j |\phi_j\rangle \right]$$

↓ (inner product with  $|\Psi\rangle$ )

$$\left[ \langle \phi_i | \phi_j \rangle = \delta_{ij} \right]$$

$$\langle \Psi | \hat{A} | \Psi \rangle = \left( \sum_j c_j^* \langle \phi_j | \right) \left( \sum_i c_i a_i |\phi_i\rangle \right) = \sum_{i,j} c_j^* c_i a_i \langle \phi_j | \phi_i \rangle = \sum_i |c_i|^2 a_i$$

This is nothing else but the average of measured values.  
( $a_j$  : measured value,  $|c_j|^2$  : probability)

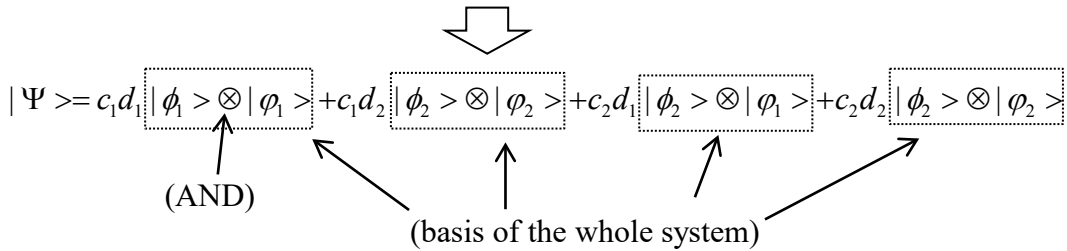
Here is a terminology; coefficient  $c_i$  in a linear combination is called “probability amplitude”.

In the previous sections, a system of one quantum (e.g., one photon) is considered. We can also regard a system including multiple quanta as one quantum state, which is called “product state.”

Each quantum is a superposition state, i.e., a linear combination of the bases that are eigenstates of a physical quantity operator of interest. Accordingly, the whole system consisting of multiple quanta is also a superposition of all combinations of the bases of each quantum.

Ex.) A system consisting two quanta of two-dimensional superposition

$$\{|\psi_a\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle, |\psi_b\rangle = d_1|\varphi_1\rangle + d_2|\varphi_2\rangle\}$$



A product state is expressed as

$$|\Psi\rangle = |\psi_1\rangle_a \otimes |\psi_2\rangle_b \otimes |\psi_3\rangle_c \otimes \dots$$

↑  
quantum *b* is in state  $|\psi_2\rangle$

or

$$|\Psi\rangle = |\psi_1\rangle_a |\psi_2\rangle_b |\psi_3\rangle_c \dots \quad (\text{similar to “}xy\text{” instead of “}x \times y\text{”})$$

$$= |\psi_1, \psi_2, \psi_3, \dots\rangle \quad (\text{The order indicates quanta } a, b, c, \dots)$$

### Theoretical framework for continuous physical quantities

In the previous sections, physical quantities whose measured values are discrete are considered. However, there are many physical quantities that have continuous values (e.g., position of a photon). This section extends the formula for discrete physical quantities to continuous ones.

A quantum mechanical superposition state is expressed by a linear combination of basis states, where the absolute square of a coefficient represents the probability of the state being the corresponding basis state.

This postulate is extended to continuous quantities as;

Quantum state for a discrete quantity:  $|\Psi\rangle = \sum_i c_i |\phi_i\rangle$

↓  
(summation  $\rightarrow$  integral)

Quantum state for a continuous quantity:  $|\Psi\rangle = \int da \cdot \psi(a) |\phi_a\rangle$

$$\left( \begin{array}{l} |\phi_a\rangle: \text{state giving a measured value of } a \text{ (basis state)} \\ \psi(a): \text{probability amplitude of a basis state giving a measured value of } a \end{array} \right)$$

$$\hat{A}|\phi_a\rangle = a|\phi_a\rangle$$

These basis states are orthogonal to each other and their norms are unity.

Here, the “inner product” must be introduced for defining “orthogonality,” because two states are “orthogonal” when their “inner product” is zero.

For discrete systems, the inner product is given by

$$\langle \Psi' | \Psi \rangle = \sum_i c_i^* c_i$$

which comes from normal and orthogonal properties of basis states;  $\langle \phi_i | \phi_j \rangle = \delta_{ij}$

$$\left( \langle \Psi' | \Psi \rangle = \left( \sum_j \langle \phi_j | c_j^* \right) \left( \sum_i c_i | \phi_i \rangle \right) = \sum_{i,j} c_j^* c_i \langle \phi_j | \phi_i \rangle = \sum_{i,j} c_j^* c_i \delta_{ij} = \sum_i c_i^* c_i \right)$$

The above framework is extended to continuous systems as follows.

First, the inner product for continuous variables is defined as

$$\langle \Psi' | \Psi \rangle = \int_{-\infty}^{\infty} da \cdot \psi'(a)^* \psi(a)$$

In order to have the above expression of the inner product, the following equation should be satisfied.

$$\int_{-\infty}^{\infty} da' \cdot \psi'(a')^* \langle \phi_{a'} | \phi_a \rangle = \psi'(a)^*$$

because

$$\langle \Psi' | \Psi \rangle = \left( \int_{-\infty}^{\infty} da' \cdot \psi'(a')^* \langle \phi_{a'} | \right) \left( \int_{-\infty}^{\infty} da \cdot \psi(a) | \phi_a \rangle \right) = \iint da' da \cdot \psi'(a')^* \psi(a) \langle \phi_{a'} | \phi_a \rangle$$

The above equation is made by introducing “Dirac delta,” which is a hyper-function satisfying the following equation for an arbitrary function  $f(x)$ .

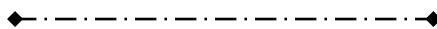
$$\int_{-\infty}^{\infty} f(x') \underbrace{\delta(x'-x)}_{\text{Dirac delta}} dx' = f(x) \quad \left( \begin{array}{l} \delta(x'-x) = 0 \quad \text{for } x' \neq x \\ \delta(0) \text{ itself is not defined.} \end{array} \right)$$

Expressing the inner product of basis states with this function  $\delta(x)$  as  $\langle \phi_a | \phi_{a'} \rangle = \delta(a-a')$

we have

$$\langle \Psi' | \Psi \rangle = \iint da' da \cdot \psi'(a')^* \psi(a) \langle \phi_{a'} | \phi_a \rangle = \iint da' da \cdot \psi'(a')^* \psi(a) \delta(a'-a) = \int da \cdot \psi'(a)^* \psi(a)$$

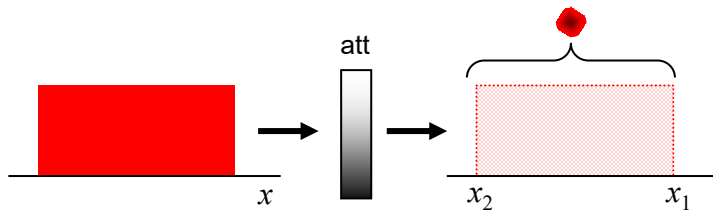
Then, the extension from discrete systems to continuous ones is accomplished.



With the above expressions, the mean value of a physical quantity  $\hat{A}$  in a quantum state  $|\Psi\rangle$  is written as

$$\begin{aligned} \langle \Psi | \hat{A} | \Psi \rangle &= \left( \int da' \cdot \psi'(a')^* \langle \phi_{a'} | \right) \hat{A} \left( \int da \cdot \psi(a) | \phi_a \rangle \right) = \iint da' da \cdot \psi'(a')^* \psi(a) \langle \phi_{a'} | \hat{A} | \phi_a \rangle \\ &= \iint da' da \cdot \psi'(a')^* \psi(a) \langle \phi_{a'} | \phi_a \rangle = \iint da' da \cdot \psi'(a')^* \psi(a) a \delta(a'-a) \\ &= \int a |\psi(a)|^2 da \quad \left( \text{discrete system : } \langle \Psi | \hat{A} | \Psi \rangle = \sum_i |c_i|^2 a_i \right) \end{aligned}$$

A long rectangular pulse is attenuated to be one-photon energy, and the spatial position of a photon in the pulse is measured after the attenuation.



The basis state is a state that a photon is at  $x$ :  $|\phi_x\rangle$

The photon state is super-positioned of the basis:  $|\Psi\rangle = \int_{x_1}^{x_2} dx \cdot \psi(x) |\phi_x\rangle$

The probability amplitude is quoted from a classical plane wave:  $\psi(x) = Ae^{i(kx-\omega t)}$

$$\left( \begin{array}{l} k: \text{propagation const. } \omega: \text{angular freq. } A: \text{normalization const.} \\ \langle \Psi | \Psi \rangle = \int_{x_1}^{x_2} |\psi(x)|^2 dx = \int_{x_1}^{x_2} |A|^2 dx = |A|^2 (x_2 - x_1) = 1 \rightarrow |A|^2 = 1/(x_2 - x_1) \end{array} \right)$$

This example of a photon state suggests a concrete expression of the physical quantity operator of energy or momentum as follows.

As mentioned in Chap. 1, one photon energy is

$$E = hf = \hbar\omega$$

$$\left( \begin{array}{l} k = \frac{2\pi}{\lambda} = \frac{2\pi f}{c} \\ \hbar = \frac{h}{2\omega} : \text{Planck const. for angular freq.} \end{array} \right)$$

Let us multiply this to probability amplitude  $\psi$ .

$$E\psi = \hbar\omega Ae^{i(kx-\omega t)} = i\hbar \frac{\partial}{\partial t} Ae^{i(kx-\omega t)} = i\hbar \frac{\partial}{\partial t} \psi$$

suggesting that an operator representing energy is written as

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

Similarly, the momentum of a photon is  $p = \frac{hf}{c} = \frac{h}{2\pi} k = \hbar k$

Let us multiply this to probability amplitude  $\psi$ .

$$p\psi = \hbar k Ae^{i(kx-\omega t)} = \frac{\hbar}{i} \frac{\partial}{\partial x} Ae^{i(kx-\omega t)} = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi$$

suggesting that an operator representing momentum is written as

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

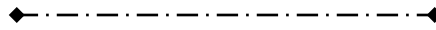
On the other hand, position  $x$  does not have such a particular expression as an operator, and its operator form is simply

$$\hat{x} = x$$

Uncertainty principle:

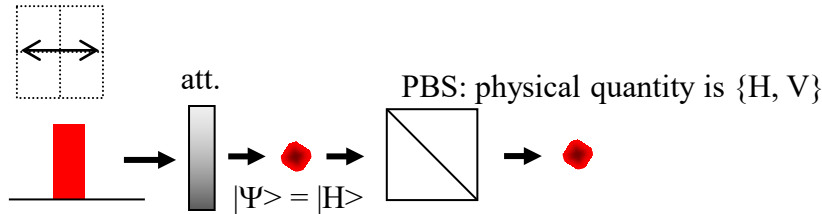
“Some physical quantities cannot be simultaneously and precisely determined or measured.”

This famous principle can be described in terms of the theoretical framework presented so far.

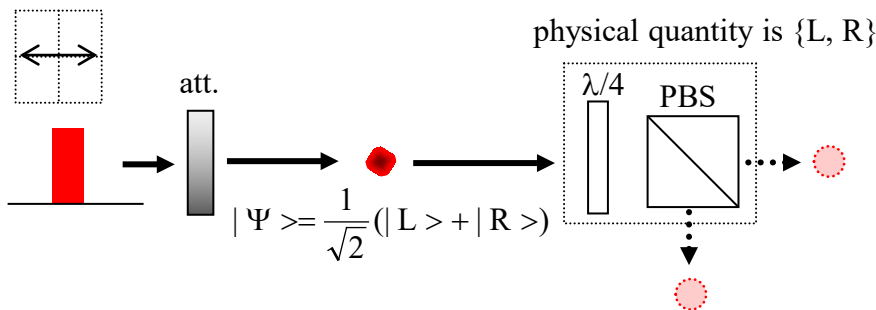


A quantum state is generally a superposition state (or probabilistic).

However, in a particular case such that a given state is in an eigenstate of a physical quantity operator, the measurement result is deterministic.



On the other hand, when another physical quantity is measured for the same state, the measurement result becomes probabilistic.

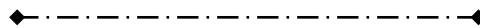


The above considerations indicate that the physical quantity of {H, V} and that of {L, R} cannot be simultaneously deterministic.

*Uncertainty principle*

Here, we can say that

the physical quantity of {H or V} and that of {R or L} are in an uncertainty relationship.



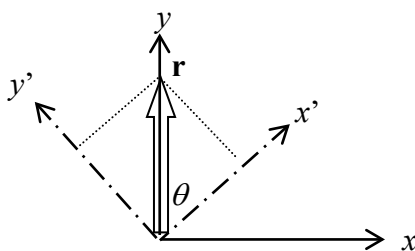
More generally,

when two physical quantity operators have different sets of eigenstates,

they are in an uncertainty relationship, that is,

these physical quantities are not deterministic simultaneously.

(intuitive image)



$(x, y)$ : Hilbert space of  $\hat{A}$   
 $(x', y')$ : Hilbert space of  $\hat{B}$

$\mathbf{r} = c\mathbf{e}_y$  ← deterministic for  $\hat{A}$   
 $= c \cos \theta \cdot \mathbf{e}_{x'} + c \sin \theta \cdot \mathbf{e}_{y'}$  ← probabilistic for  $\hat{B}$

The above criteria of the uncertainty principle, i.e., “whether two physical operators have identical eigenstates or not,” can be mathematically described by “commutator,” which is defined as

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \quad \boxed{\text{commutator}}$$

$$\left( \begin{array}{l} [\hat{A}, \hat{B}] = 0 \quad \longleftrightarrow \quad \hat{A}\hat{B} = \hat{B}\hat{A} \quad \longleftrightarrow \quad \hat{A} \text{ and } \hat{B} \text{ are commutative.} \\ [\hat{A}, \hat{B}] \neq 0 \quad \longleftrightarrow \quad \hat{A}\hat{B} \neq \hat{B}\hat{A} \quad \longleftrightarrow \quad \hat{A} \text{ and } \hat{B} \text{ are noncommutative.} \end{array} \right)$$

Using this notation, the following postulate is given.

“Physical quantity operators satisfying  $[\hat{A}, \hat{B}] \neq 0$  have different sets of eigenstates.”.

**proof**

Suppose that  $\hat{A}$  and  $\hat{B}$  satisfying  $[\hat{A}, \hat{B}] \neq 0$  have an identical eigenstate.

$$\hat{A}|\phi\rangle = a|\phi\rangle \quad \hat{B}|\phi\rangle = b|\phi\rangle$$

Suppose  $\hat{B}$  operates on the left equation.

$$\hat{B}\hat{A}|\phi\rangle = a\hat{B}|\phi\rangle = ab|\phi\rangle$$

Suppose  $\hat{A}$  operates on the right equation.

$$\hat{A}\hat{B}|\phi\rangle = b\hat{A}|\phi\rangle = ba|\phi\rangle$$

$$\hat{B}\hat{A}|\phi\rangle = \hat{A}\hat{B}|\phi\rangle$$

$$\hat{B}\hat{A} - \hat{A}\hat{B} = 0$$

contradict to  $[\hat{A}, \hat{B}] \neq 0$

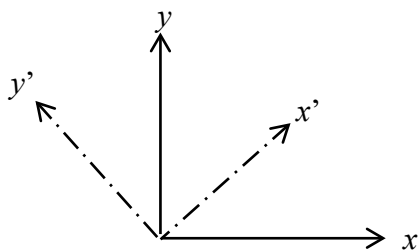
An identical eigenstate does not exist.

Therefore,

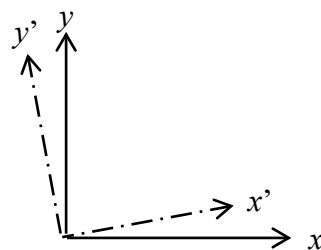
“Physical quantity operators satisfying  $[\hat{A}, \hat{B}] \neq 0$  cannot be deterministic simultaneously.”

**Uncertainty principle**

Then, a next question will be “how uncertain two physical quantities are”.



The difference is large.  
||  
large uncertainty



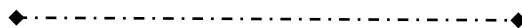
The difference is small.  
||  
small uncertainty

The degree of the uncertainty is expressed also by the commutator as follows.

Denoting the averages of variances of physical quantities  $\hat{A}$  and  $\hat{B}$  as  $\langle (\Delta\hat{A})^2 \rangle$  and  $\langle (\Delta\hat{B})^2 \rangle$ , we have

$$\langle (\Delta\hat{A})^2 \rangle \langle (\Delta\hat{B})^2 \rangle \geq \frac{|\langle [\hat{A}, \hat{B}] \rangle|^2}{4}$$

( The minimum of the product of fluctuations of  $\hat{A}$  and  $\hat{B}$  is given by  $[\hat{A}, \hat{B}]$ . )



proof

We first introduce operators  $\Delta\hat{A}$  and  $\Delta\hat{B}$  that represent fluctuations of physical quantities  $\hat{A}$  and  $\hat{B}$  being noncommutative each other as  $[\hat{A}, \hat{B}] \neq 0$

$$\Delta\hat{A} \equiv \hat{A} - \langle \hat{A} \rangle \quad \Delta\hat{B} \equiv \hat{B} - \langle \hat{B} \rangle$$

By the way, fluctuation of a stochastic variable  $x$  is generally evaluated by variance ( $\langle x^2 \rangle - \langle x \rangle^2$ ). Following this criterion, we consider  $\langle (\Delta\hat{A})^2 \rangle$  and  $\langle (\Delta\hat{B})^2 \rangle$ , defined as below, as indexes representing fluctuations (or uncertainties) of  $\hat{A}$  and  $\hat{B}$ .

$$\left[ \begin{array}{l} \langle (\Delta\hat{A})^2 \rangle = \langle \Delta\hat{A}^2 \rangle = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle \\ \langle (\Delta\hat{B})^2 \rangle = \langle \Delta\hat{B}^2 \rangle = \langle (\hat{B} - \langle \hat{B} \rangle)^2 \rangle \end{array} \right. \quad \left[ \begin{array}{l} \langle \Delta\hat{A} \rangle = \langle \hat{A} - \langle \hat{A} \rangle \rangle = \langle \hat{A} \rangle - \langle \hat{A} \rangle = 0 \\ \langle \Delta\hat{B} \rangle = \langle \hat{B} - \langle \hat{B} \rangle \rangle = \langle \hat{B} \rangle - \langle \hat{B} \rangle = 0 \end{array} \right]$$

Here, in order to evaluate  $\langle (\Delta\hat{A})^2 \rangle \langle (\Delta\hat{B})^2 \rangle$ , we introduce operator  $\hat{D} = t\Delta\hat{A} - i\Delta\hat{B}$ , and evaluate the average of  $\hat{D}^\dagger \hat{D}$ .

$$\begin{aligned} \langle \hat{D}^\dagger \hat{D} \rangle &= \langle (t\Delta\hat{A} + i\Delta\hat{B})(t\Delta\hat{A} - i\Delta\hat{B}) \rangle && \left[ \Delta\hat{A}, \Delta\hat{B} : \text{Hermitian operator} \right] \\ &= \langle t^2 (\Delta\hat{A})^2 + it(\Delta\hat{B}\Delta\hat{A} - \Delta\hat{A}\Delta\hat{B}) + (\Delta\hat{B})^2 \rangle \\ &= t^2 \langle (\Delta\hat{A})^2 \rangle + it \langle (\hat{B} - \langle \hat{B} \rangle)(\hat{A} - \langle \hat{A} \rangle) \rangle - it \langle (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) \rangle + \langle (\Delta\hat{B})^2 \rangle \\ &= t^2 \langle (\Delta\hat{A})^2 \rangle + it(\langle \hat{B}\hat{A} \rangle - \langle \hat{B} \rangle \langle \hat{A} \rangle - \langle \hat{B} \rangle \langle \hat{A} \rangle - \langle \hat{B} \rangle \langle \hat{A} \rangle) \\ &\quad - it(\langle \hat{A}\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle \langle \hat{B} \rangle) + \langle (\Delta\hat{B})^2 \rangle \\ &= t^2 \langle (\Delta\hat{A})^2 \rangle + it(\langle \hat{B}\hat{A} \rangle - \langle \hat{B} \rangle \langle \hat{A} \rangle) - it(\langle \hat{A}\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle) + \langle (\Delta\hat{B})^2 \rangle \\ &= t^2 \langle (\Delta\hat{A})^2 \rangle - it \langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle + \langle (\Delta\hat{B})^2 \rangle \\ &= t^2 \langle (\Delta\hat{A})^2 \rangle - it \langle [\hat{A}, \hat{B}] \rangle + \langle (\Delta\hat{B})^2 \rangle \end{aligned}$$

By the way, the following inequality is made in general.

$$\langle \hat{X}^\dagger \hat{X} \rangle = \langle \Psi | \hat{X}^\dagger \hat{X} | \Psi \rangle = \| \hat{X} | \Psi \rangle \|^2 \geq 0$$

$$\text{Thus, } \langle \hat{D}^\dagger \hat{D} \rangle \geq 0 \quad \longrightarrow \quad \langle \hat{D}^\dagger \hat{D} \rangle = t^2 \langle (\Delta\hat{A})^2 \rangle - it \langle [\hat{A}, \hat{B}] \rangle + \langle (\Delta\hat{B})^2 \rangle \geq 0$$



$$\langle \Delta \hat{A} \rangle^2 \left\{ \left( t - \frac{i \langle [\hat{A}, \hat{B}] \rangle}{2 \langle \Delta \hat{A} \rangle^2} \right)^2 + \frac{\langle [\hat{A}, \hat{B}] \rangle^2 + 4 \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle}{4 \langle (\Delta \hat{A})^2 \rangle^2} \right\} \geq 0$$

$$\downarrow \left[ \langle (\Delta \hat{A})^2 \rangle \geq 0 \right]$$

$$\left( t - \frac{i \langle [\hat{A}, \hat{B}] \rangle}{2 \langle \Delta \hat{A} \rangle^2} \right)^2 + \frac{\langle [\hat{A}, \hat{B}] \rangle^2 + 4 \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle}{4 \langle (\Delta \hat{A})^2 \rangle^2} \geq 0$$

$$\left( t - \frac{i \langle [\hat{A}, \hat{B}] \rangle}{2 \langle \Delta \hat{A} \rangle^2} \right)^2 \geq - \frac{\langle [\hat{A}, \hat{B}] \rangle^2 + 4 \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle}{4 \langle (\Delta \hat{A})^2 \rangle^2}$$

$\downarrow$  (The minimum of the left side is 0)

$$- \frac{\langle [\hat{A}, \hat{B}] \rangle^2 + 4 \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle}{4 \langle (\Delta \hat{A})^2 \rangle^2} \leq 0$$

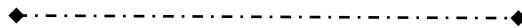
$$\langle [\hat{A}, \hat{B}] \rangle^2 + 4 \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq 0$$

$$\langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq - \frac{\langle [\hat{A}, \hat{B}] \rangle^2}{4}$$

$\downarrow$  { In inequality of  $\langle \hat{D}^\dagger \hat{D} \rangle \geq 0$ ,  $\langle (\Delta \hat{A})^2 \rangle$  and  $\langle (\Delta \hat{B})^2 \rangle$  are real,  
thus  $\langle [\hat{A}, \hat{B}] \rangle$  is a imaginary. }

$$\langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq \frac{|\langle [\hat{A}, \hat{B}] \rangle|^2}{4}$$

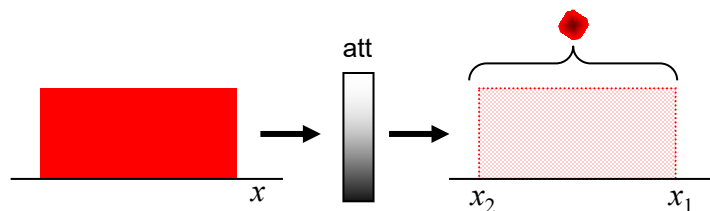
or simply  $\Delta A \Delta B \geq \frac{|\langle [\hat{A}, \hat{B}] \rangle|}{2}$



The minimum fluctuation condition is  $\Delta A \Delta B = \frac{|\langle [\hat{A}, \hat{B}] \rangle|}{2}$

which is called “minimum uncertainty state”.

ex) Position and momentum of a photon in a plane-wave pulse



$$|\Psi \rangle = \int_{x_1}^{x_2} \psi(x) |\phi_x \rangle dx$$

with  $\psi(x) = A e^{i(kx - \omega t)}$



$$\left\{ \begin{array}{l} \text{position operator: } \hat{x} = x \\ \text{momentum operator: } \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \end{array} \right.$$

Suppose that  $(\hat{x}\hat{p} - \hat{p}\hat{x})$  is acted on an arbitrary function  $f(x)$

$$(\hat{x}\hat{p} - \hat{p}\hat{x})f(x) = \hat{x} \frac{\hbar}{i} \frac{\partial f(x)}{\partial x} - \frac{\hbar}{i} \frac{\partial}{\partial x} (xf) = \frac{\hbar}{i} \left[ x \frac{df}{dx} - \left( x \frac{df}{dx} + f \right) \right] = i\hbar f$$

$$\begin{aligned} \hat{x}\hat{p} - \hat{p}\hat{x} &= i\hbar \\ [\hat{x}, \hat{p}] &= i\hbar \longrightarrow \Delta x \Delta p \geq \frac{\hbar}{2} \end{aligned}$$

## Schrödinger equation

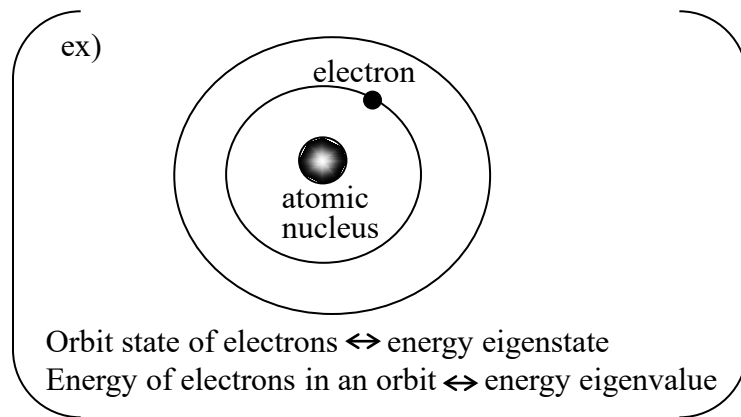
Up to now, we have seen what is a quantum state and how to express it mathematically. Subsequently, how quantum states evolve in time, i.e., the motion equation of a quantum state, is described in this section.

The time evolution of a quantum state in a closed system follows the Schrödinger equation given by

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \quad \boxed{\text{Schrödinger equation}}$$

where  $\hat{H}$  is an operator representing the energy of a quantum system, called “Hamiltonian,” and has energy eigenvalues and energy eigenstates.

$$\begin{array}{ccc} \text{Hamiltonian} & & \text{energy eigenvalue} \\ \downarrow & & \downarrow \\ \hat{H} |\phi_n\rangle & = & E_n |\phi_n\rangle \\ \uparrow & & \uparrow \\ & \text{energy eigenstate} & \end{array}$$



Let us see the time evolution in some particular cases.

In case when a quantum state initially in one of energy eigenstates;

$$|\Psi(0)\rangle = |\phi_n\rangle \longrightarrow |\Psi(t)\rangle = e^{-iE_n t/\hbar} |\phi_n\rangle$$

Substitute  $\Psi(t)$  into the left side of Schrödinger eq.

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = i\hbar \frac{\partial}{\partial t} e^{-iE_n t/\hbar} |\phi_n\rangle = -i\hbar \frac{iE_n}{\hbar} e^{-iE_n t/\hbar} |\phi_n\rangle = E_n e^{-iE_n t/\hbar} |\phi_n\rangle$$

Substitute  $\Psi(t)$  into the right side.

$$\hat{H} |\Psi(t)\rangle = e^{-iE_n t/\hbar} \hat{H} |\phi_n\rangle = e^{-iE_n t/\hbar} E_n |\phi_n\rangle$$

(left) = (right), thus  $\Psi(t)$  is a solution of Schrödinger eq.

The state at time  $t$  is equal to the initial state with some phase.  
 Because the overall phase does not matter for the state condition, we can say the quantum system holds the initial state.

A next situation is that the initial state is super-positioned over several energy eigenstates.

$$|\Psi(0)\rangle = \sum_n c_n |\phi_n\rangle$$

Each eigenstate evolves in time as  $|\phi_n\rangle \rightarrow e^{-iE_n t/\hbar} |\phi_n\rangle$

Therefore,  $|\Psi(t)\rangle = \sum_n e^{-iE_n t/\hbar} c_n |\phi_n\rangle$       A quantum state temporally changes.

Substitute  $\Psi(t)$  into the left side of Schrödinger eq.

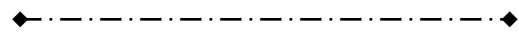
$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = i\hbar \frac{\partial}{\partial t} \sum_n e^{-iE_n t/\hbar} |\phi_n\rangle = -i\hbar \sum_n \frac{iE_n}{\hbar} e^{-iE_n t/\hbar} |\phi_n\rangle = \sum_n E_n e^{-iE_n t/\hbar} |\phi_n\rangle$$

Substitute  $\Psi(t)$  into the right side.

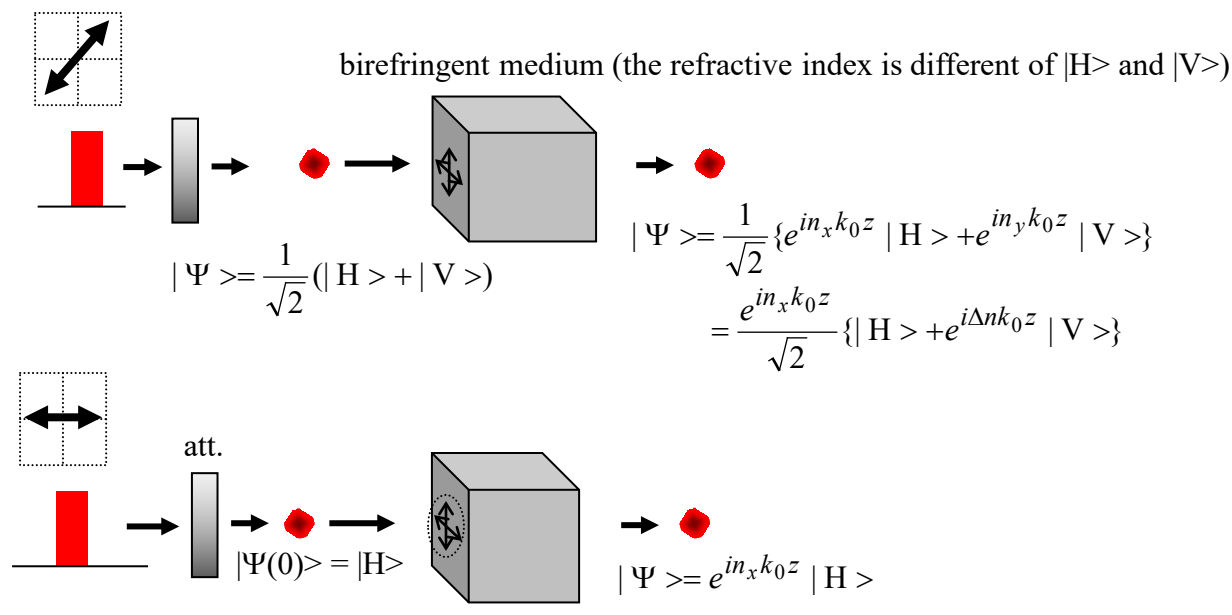
$$\hat{H} |\Psi(t)\rangle = \hat{H} \sum_n e^{-iE_n t/\hbar} |\phi_n\rangle = \sum_n e^{-iE_n t/\hbar} E_n |\phi_n\rangle$$

$\left( \hat{H} \text{ is invariant of } t. \right)$   
 energy conservation

(left) = (right)



Ex)



There is another way to describe the state evolution, which is called “Heisenberg picture.”

Schrödinger equation can be formally solved as

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \longrightarrow |\Psi(t)\rangle = \exp[-(i/\hbar)\hat{H}t] |\Psi(0)\rangle$$

On the other hand, the expectation value of a physical quantity  $\hat{A}$  is given by

$$\langle \Psi(t) | \hat{A} | \Psi(t) \rangle = \langle \Psi(0) | \exp[(i/\hbar)\hat{H}^\dagger t] \hat{A} \exp[-(i/\hbar)\hat{H}t] | \Psi(0) \rangle$$

Here, we introduce the following time-dependent operator:

$$\hat{A}_H(t) \equiv \exp[(i/\hbar)\hat{H}^\dagger t] \hat{A} \exp[-(i/\hbar)\hat{H}t] \quad (\text{note: } \hat{H}^\dagger = \hat{H} \text{ )}$$

(sometimes called “Heisenberg operator”)

Subsequently, the expectation value is expressed as

$$\langle \Psi(t) | \hat{A} | \Psi(t) \rangle = \langle \Psi(0) | \hat{A}_H(t) | \Psi(0) \rangle$$

This expression suggests that an expectation value can be obtained by

- (i) evaluating a time-dependent physical quantity operator  $\hat{A}_H(t)$ , then
- (ii) evaluating the expectation value of  $\hat{A}_H(t)$  with respect to the initial state  $|\Psi(0)\rangle$ .

For calculating  $\hat{A}_H(t)$ , the following differential equation is available.

$$\begin{aligned} \frac{d}{dt} \hat{A}_H(t) &= \frac{d}{dt} \{ e^{i(\hat{H}/\hbar)t} \hat{A} e^{-i(\hat{H}/\hbar)t} \} \\ &= \frac{i}{\hbar} \hat{H} e^{i(\hat{H}/\hbar)t} \hat{A} e^{-i(\hat{H}/\hbar)t} - \frac{i}{\hbar} e^{i(\hat{H}/\hbar)t} \hat{A} \hat{H} e^{-i(\hat{H}/\hbar)t} \\ &= \frac{i}{\hbar} \hat{H} \hat{A}_H - \frac{i}{\hbar} \hat{A}_H \hat{H} \\ &= \frac{i}{\hbar} [\hat{H}, \hat{A}_H(t)] \end{aligned}$$

Heisenberg equation (of motion)

In the Chapter discussing optical amplifier noise, we will fully utilize this Heisenberg equation.