Bra-Ket and Matrix representation:

Let us consider the eigenkets and eigenvalues of a Hermitian operator A.

We begin with an important theorem.

Theorem: The eigenvalues of a Hermitian operator A are real; the eigenkets of A corresponding to different eigenvalues are orthogonal.

(Proof already discussed).

Eigenkets as base kets:

We have seen that the normalized eigenkets of A form a complete orthonormal set.

Given an arbitrary ket $|\alpha\rangle$ in the ket space spanned by the eigenkets of A, we expand it as

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle .$$

We have seen that $c_{a'} = \langle a'|\alpha\rangle$.

Therefore we have $|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle$

This is analogous to an expansion of a vector $\vec{V}$ in (real) Euclidean space.

$$\vec{V} = \sum_i \hat{e}_i (\hat{e}_i \cdot \vec{V})$$

with $\{\hat{e}_i\}$ form an orthonormal basis.

We have already learned that

$$\sum_{a'} |a'\rangle\langle a'| = \mathbb{I} .$$

This relation is known as ~~a~~ the "completeness relation".

This product $|\cdot\rangle\langle\cdot|$ is called the "Outer product".

Usefullness of completeness relation can never be overestimated. For example:

$$\langle\alpha|\alpha\rangle = \langle\alpha|\left(\sum_{a'} |a'\rangle\langle a'|\right)|\alpha\rangle$$

$$= \sum_{a'} |\langle a'|\alpha\rangle|^2$$

Incidentally if $|\alpha\rangle$ is normalized,

$$\sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 = \sum_{a'} |C_{a'}|^2$$

Therefore $C_{a'} = \langle a'|\alpha\rangle$ can be understood as probability amplitude.

Let us consider an element of $|\alpha\rangle = \sum_{a'} C_{a'}|a'\rangle$ as

$$C_{a'}|a'\rangle = |a'\rangle\langle a'|\alpha\rangle .$$

We see that $|a'\rangle\langle a'|$ selects a portion of $|\alpha\rangle$, parallel to $|a'\rangle$.

Therefore "$|a'\rangle\langle a'|$" operator is known as projection operator, denoted by

$$\Lambda_{a'} = |a'\rangle\langle a'| .$$

The completeness relation can therefore be written as

$$\sum_{a'} \Lambda_{a'} = \mathbb{I}$$

Matrix representation.

Having specified the base kets, we now show how to represent an operator 'X' by a square matrix.

Before that, let us understand that since $|\,\rangle$ - ket represents a vector, it can be represented as a column vector:

$$|\cdot\rangle = \begin{pmatrix} a \\ b \\ \vdots \\ \vdots \end{pmatrix}$$

It's conjugate bra:

$$\langle\cdot| = (a^*, b^*, \cdots)$$

The complex number inner product:

$$\langle\cdot|\cdot\rangle = (a^*, b^* \cdots) \begin{pmatrix} a \\ b \\ \vdots \\ \vdots \end{pmatrix}.$$

The matrix outer product

$$|\cdot\rangle\langle\cdot| = \begin{pmatrix} a \\ b \\ \vdots \\ \vdots \end{pmatrix} (a^* \; b^* \cdots).$$

Now let us consider operator X, which can be written as

$$X = \left(\sum_{a''} |a''\rangle\langle a''|\right) X \left(\sum_{a'} |a'\rangle\langle a'|\right).$$

$$= \sum_{a',a''} |a''\rangle\langle a''|X|a'\rangle\langle a'|.$$

There are altogether N^2 numbers of form $\langle a''|X|a'\rangle$, where N is the dimension of the ket space.

We can arrange them as a $N \times N$ square matrix such that, the elements of the matrix can be understood as

$$\langle a''|X|a'\rangle.$$

Row Column.

Explicits written form.

$$X = \begin{pmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \cdots \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \cdots \\ \vdots & & \end{pmatrix}$$

where $\langle a''|X|a'\rangle = \langle a'|X^{\dagger}|a''\rangle^*$

Then for X hermitian, we have

$$\langle a''|X|a'\rangle = \langle a'|X|a''\rangle^*$$

Let us consider a more specific example from 2 dimension.

Let $|a_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|a_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

$$\langle a_1|a_1\rangle = \langle a_2|a_2\rangle = 1 \quad \text{(check)}.$$

$$\langle a_1|a_2\rangle = \langle a_2|a_1\rangle = 0 \quad \text{(check)}.$$

$$|a_1\rangle\langle a_1| + |a_2\rangle\langle a_2| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{(check)}.$$

Now consider an operator

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{(One of the Pauli operators)}.$$

$$\langle a_1|\sigma_z|a_1\rangle = 1 \quad \text{(check)}.$$

$$\langle a_2|\sigma_z|a_2\rangle = -1 \quad \text{(check)}.$$

$$\langle a_1|\sigma_z|a_2\rangle = \langle a_2|\sigma_z|a_2\rangle = 0.$$

Therefore, $\sigma_z = \sum_{i,j=1,2} |a_i\rangle\langle a_i|\sigma_z|a_j\rangle\langle a_j|$.

with the elements $\langle a_i|\sigma_z|a_j\rangle$ ~~specif~~ specified earlier.

The previous example is a bit easy, because $|a_1\rangle, |a_2\rangle$ are the normalized eigenvectors of σ_z operator. $\sigma_z|a_1\rangle = |a_1\rangle$; $\sigma_z|a_2\rangle = -|a_2\rangle$

Let us therefore consider a different example.

Consider another Pauli matrix $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

For ~~In~~ the expansion in the basis $|a_1\rangle, |a_2\rangle$.

we have

$$\langle a_1|\sigma_x|a_1\rangle = (1 \quad 0)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= (1 \quad 0)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

$$\langle a_2|\sigma_x|a_2\rangle = 0$$

$$\langle a_1|\sigma_x|a_2\rangle = \langle a_2|\sigma_x|a_1\rangle = 1.$$

Now consider a different basis.

$$|+\rangle = \frac{|a_1\rangle + |a_2\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

$$|-\rangle = \frac{|a_1\rangle - |a_2\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Check

$$\langle +|+\rangle = \langle -|-\rangle = 1$$

$$\langle +|-\rangle = \langle -|+\rangle = 0.$$

$$|+\rangle\langle +| + |-\rangle\langle -| = \mathbb{I}.$$

$$\langle +|\sigma_x|+\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 1/\sqrt{2} \end{pmatrix}.$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = 1.$$

$$\langle -|\sigma_x|-\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}.$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = -1.$$

$$\langle +|\sigma_x|-\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}.$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = 0.$$

$$\langle -|\sigma_x|+\rangle = 0 \quad \text{(similarly)}.$$

Therefore in the basis $(|+\rangle, |-\rangle)$ the matrix

$$\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$|+\rangle$ and $|-\rangle$ are the eigenbasis of σ_x.

$$\sigma_x |+\rangle = |+\rangle.$$

$$\sigma_x |-\rangle = -|-\rangle.$$

The way we arrange $\langle a''|X|a'\rangle$ into a square matrix is in conformity with the usual rule of matrix multiplication. To see this just note that the matrix representation of the operator relation

$$Z = XY$$

reads $\langle a''|Z|a'\rangle = \langle a''|XY|a'\rangle$.

$$= \sum_{a'''} \langle a''|X|a'''\rangle\langle a'''|Y|a'\rangle .$$

Here we have inserted the identity operator.

Let us now examine how the ket relation

$$|\gamma\rangle = X|\alpha\rangle$$

can be represented in our base ket representation.

$$|\gamma\rangle = X|\alpha\rangle.$$

$$\langle a'|\gamma\rangle = \langle a'|X|\alpha\rangle$$

$$= \sum_{a''} \langle a'|X|a''\rangle\langle a''|\alpha\rangle$$

These are just the rules of matrix multiplication.

$$|\alpha\rangle = \begin{pmatrix} \langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots \\ \vdots \end{pmatrix} \qquad |\gamma\rangle = \begin{pmatrix} \langle a^{(1)}|\gamma\rangle \\ \langle a^{(2)}|\gamma\rangle \\ \vdots \\ \vdots \end{pmatrix}$$

The inner product :

$$\langle \beta | \alpha \rangle = \sum_{a'} \langle \beta | a' \rangle \langle a' | \alpha \rangle$$

$$= \left(\langle a^{(1)} | \beta \rangle^*, \langle a^{(2)} | \beta \rangle^* \cdots \right) \begin{pmatrix} \langle a^{(1)} | \alpha \rangle \\ \langle a^{(2)} | \alpha \rangle \\ \vdots \\ \vdots \end{pmatrix}$$

The outer product :

$$|\beta\rangle\langle\alpha| = \sum_{a', a''} |a'\rangle\langle a' | \beta\rangle\langle\alpha | a''\rangle\langle a''| .$$

$$\therefore \quad |\beta\rangle\langle\alpha| = \begin{pmatrix} \langle a^{(1)} | \beta \rangle \langle a^{(1)} | \alpha \rangle^* & \langle a^{(1)} | \beta \rangle \langle a^{(2)} | \alpha \rangle^* \cdots \\ \langle a^{(2)} | \beta \rangle \langle a^{(1)} | \alpha \rangle^* & \langle a^{(2)} | \beta \rangle \langle a^{(2)} | \alpha \rangle^* \cdots \\ \vdots & \end{pmatrix}$$

Spin-1/2 Systems.

We are now going to consider one of the most important and elementary systems in quantum mechanics.
The smallest possible system that can be considered in QM is the spin-1/2 system, which can be represented by a 2-dimensional Hilbert space.

The base kets are denoted as $|1\rangle$ and $|0\rangle$.

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

In the language of Physics, they are also called energy eigen basis.
In the language of Quantum information Science, they are called computational basis.
The identity operator can be written by the completeness relation

$$\mathbb{I} = \sum_{\alpha} |\alpha\rangle\langle\alpha| = |0\rangle\langle 0| + |1\rangle\langle 1|.$$

The Pauli matrix σ_z can be written as

$$\sigma_z = \hbar/2 \left(|1\rangle\langle 1| - |0\rangle\langle 0| \right).$$

$$= \hbar/2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The eigenket - eigenvalue relation.

$$\cancel{\sigma_z |\pm\rangle = \pm \frac{\hbar}{2} |}$$

$$\sigma_z |1\rangle = \frac{\hbar}{2} |1\rangle$$

$$\sigma_z |0\rangle = -\frac{\hbar}{2} |0\rangle .$$

It is instructive to look at two other operators,

$$\sigma_+ = \hbar |1\rangle\langle 0| \quad , \quad \sigma_- = \hbar |0\rangle\langle 1| .$$

which are both non-hermitian.

The operator σ_+ acting on $|0\rangle$, turns $|0\rangle$ into $|1\rangle$ and σ_- does the vice-versa

The spin-$1/2$ system in a nut-shell can be represented as.

The Pauli operators : σ_x , σ_y , σ_z

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} ; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

$$\cancel{\sigma_+ = (1}$$

$$\sigma_+ = \sigma_x + i\sigma_y$$

$$\sigma_- = \sigma_x - i\sigma_y .$$

$$(\sigma_+)^\dagger = \sigma_- .$$

Measurements:

Having developed the mathematics of ket space, we are now in a position to discuss the quantum theory of measurement process.

To ~~start~~ begin, we start with the description of measurement in the words of great P. A. M. Dirac —

" A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured

Let us elaborate this statement.

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle .$$

be a quantum state.

When the measurement is performed, the system is "thrown into" one of the eigenstates. $|a'\rangle$ of an observable $\hat{A}$.

In other words

$$|\alpha\rangle \xrightarrow{\hat{A}\text{ measurement}} |a'\rangle$$

Example :

Let us consider a projection operator $\hat{P} = |a_1\rangle\langle a_1|$ and a quantum state

$$|\psi\rangle = \sum_i c_{a_i} |a_i\rangle$$

Therefore $\hat{P}|\psi\rangle = \sum_i c_{a_i} |a_1\rangle\langle a_1|a_i\rangle$.

$$= c_{a_1} |a_1\rangle .$$

i.e. the operator $\hat{P}$ projects $|\psi\rangle$ into the eigen ket $|a_1\rangle$, discarding all the others components.

Now consider a general one.

$$\sigma_z = \frac{\hbar}{2}\left(|1\rangle\langle 1| - |0\rangle\langle 0|\right).$$

$$|\psi\rangle = \alpha|1\rangle + \beta|0\rangle .$$

Therefore $\sigma_z|\psi\rangle = \frac{\hbar}{2}\left(|1\rangle\langle 1| - |0\rangle\langle 0|\right)\left(\alpha|1\rangle + \beta|0\rangle\right)$

$$= \frac{\hbar}{2}\left(\alpha|1\rangle - \beta|0\rangle\right).$$

We donot know in advance, that into which state it will be thrown into, as a result of measurement. We do know, however, the probability of jumping into a particular state $|a_i\rangle$ as

$$P_{a_i} = |\langle a_i|\psi\rangle|^2 .$$

$|\psi\rangle \rightarrow$ normalized.

The probability interpretation of the squared inner product $|\langle a_i|\alpha\rangle|^2$ is one of the most fundamental postulates of QM. Therefore it cannot be proven.

Expectation value :

We define the expectation value of an operator $\hat{A}$ with respect to state $|\alpha\rangle$ as

$$\langle \hat{A} \rangle_\alpha = \langle \alpha | \hat{A} | \alpha \rangle ,$$

providing $|\alpha\rangle$ is normalized.

However, if $|\alpha\rangle$ is not normalized, then

$$\langle \hat{A} \rangle_\alpha = \frac{\langle \alpha | \hat{A} | \alpha \rangle}{\langle \alpha | \alpha \rangle} .$$

Donot confuse expectation values with eigenvalues.

We will show the difference by considering an example in spin-1/2 system.

Example:

$$\sigma_z = \frac{\hbar}{2}\left(|1\rangle\langle 1| - |0\rangle\langle 0|\right).$$

Let us consider $|\psi\rangle = \alpha|1\rangle + \beta|0\rangle$.

$$\langle\psi|\psi\rangle = |\alpha|^2 + |\beta|^2 = 1.$$

Eigenvalues: $\sigma_z|1\rangle = \frac{\hbar}{2}|1\rangle$

Eigenvalues.

$\sigma_z|0\rangle = -\frac{\hbar}{2}|0\rangle$

Expectation value:

$$\langle\sigma_z\rangle_\psi = \langle\psi|\sigma_z|\psi\rangle.$$

$$= \left(\alpha^*\langle 1| + \beta^*\langle 0|\right)\left[\frac{\hbar}{2}\left(|1\rangle\langle 1| - |0\rangle\langle 0|\right)\right]\left(\alpha|1\rangle + \beta|0\rangle\right)$$

$$= \left(\alpha^*\langle 1| + \beta^*\langle 0|\right)\left(\frac{\hbar}{2}\alpha|1\rangle - \frac{\hbar}{2}\beta|0\rangle\right).$$

$$= |\alpha|^2\frac{\hbar}{2} + |\beta|^2\hbar/2.$$

$$= \frac{\hbar}{2}\left(|\alpha|^2 + |\beta|^2\right) = \hbar/2.$$

General expression:

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle.$$

$$\langle\hat{A}\rangle_\alpha = \langle\alpha|\hat{A}|\alpha\rangle = \sum_{a'a''}\langle\alpha|a'\rangle\langle a'|\hat{A}|a''\rangle\langle a''|\alpha\rangle.$$

$$= \sum_{a'a''} c^*_{a'} c_{a''}\langle a'|\hat{A}|a''\rangle.$$

Spin-1/2 system once again:

Before proceeding into a general discussion of observables, we again consider a spin-1/2 system.

$|1\rangle$ and $|0\rangle$ are the eigenkets of the Pauli operator σ_z.

Let us now consider a quantum state $|+\rangle_x$, such that

$$|\langle 1|+\rangle_x| = |\langle 0|+\rangle_x| = \frac{1}{\sqrt{2}}.$$

i.e. $|+\rangle$ state contains $|1\rangle$ and $|0\rangle$ with equal probabilities of $1/2$.

Let us expan $|+\rangle$ in the basis of $\{|1\rangle, |0\rangle\}$

$$|+\rangle_x = \mathbb{I}.|+\rangle_x = (|0\rangle\langle 0| + |1\rangle\langle 1|)|+\rangle_x.$$

$$= \langle 0|+\rangle_x |0\rangle + \langle 1|+\rangle_x |1\rangle.$$

Now since, $|\langle 0|+\rangle_x| = |\langle 1|+\rangle_x| = \frac{1}{\sqrt{2}}$,

we can consider $\langle 1|+\rangle_x = \frac{1}{\sqrt{2}}$ and

$\langle 0|+\rangle_x = \frac{1}{\sqrt{2}} e^{i\delta_1}$.

with $\delta_1 \to$ real.

Therefore $|+\rangle_x = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}} e^{i\delta_1}|0\rangle$.

$\delta_1 \to$ is called the phase.

Similarly we can construct another state vector

$$|-\rangle_x = \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}e^{i\delta_1}|0\rangle .$$

It is easy to check that $\{|+\rangle_x, |-\rangle_x\}$ form an orthonormal basis. (check).

Let us construct the operator $\hat{S}_x$ using the orthonormal basis $\{|+\rangle, |-\rangle\}$ as.

$$\hat{S}_x = \frac{\hbar}{2}\left[|+\rangle_{x\,x}\langle +| - |-\rangle_x\langle -|\right].$$

$$= \frac{\hbar}{2}\left[e^{-i\delta_1}|1\rangle\langle 0| + e^{i\delta_1}|0\rangle\langle 1|\right]$$

(check).

Notice that $\hat{S}_x$ we have constructed is hermitian.

Similarly we can construct another orthonormal set

$$|\pm\rangle_y = \frac{1}{\sqrt{2}}|1\rangle \pm e^{i\delta_2}|0\rangle .$$

and Hermitian operator

$$\hat{S}_y = \frac{\hbar}{2}\left[e^{-i\delta_2}|1\rangle\langle 0| + e^{i\delta_2}|0\rangle\langle 1|\right].$$

Is there any way to determine δ_1, δ_2 ?

Let us consider a particular situation.

As we have considered.

$$\cancel{|\langle +|+\rangle| =}$$

$$|\langle 1|+\rangle_x| = |\langle 0|+\rangle_x| = \frac{1}{\sqrt{2}}.$$

and $$|\langle 1|-\rangle_x| = |\langle 0|-\rangle_x| = \frac{1}{\sqrt{2}}.$$

Similarly, we have

$$|{}_y\langle \pm|+\rangle_x| = |{}_y\langle \pm|-\rangle_x| = \frac{1}{\sqrt{2}}.$$

The interpretation of this consideration is the same as before.

Inserting $|\pm\rangle_x$ and $|\pm\rangle_y$, we have

$$\frac{1}{2}|1 \pm e^{i(\delta_1-\delta_2)}| = \frac{1}{\sqrt{2}} \quad \text{(check)}.$$

which is satisfied only if

$$\delta_2 - \delta_1 = \pi/2 \text{ or } -\pi/2.$$

We can therefore consider $\delta_1 = 0$ and $\delta_2 = \pi/2$.

To summerize, we have

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}|1\rangle \pm \frac{1}{\sqrt{2}}|0\rangle.$$

$$|\pm\rangle_y = \frac{1}{\sqrt{2}}|1\rangle \pm \frac{i}{\sqrt{2}}|0\rangle.$$

$S_x \neq \frac{\hbar}{2}$

and $\hat{S}_x = \frac{\hbar}{2}\left(|1\rangle\langle 0| + |0\rangle\langle 1|\right)$.

$\hat{S}_y = \frac{\hbar}{2}\left(-i|1\rangle\langle 0| + i|0\rangle\langle 1|\right)$.

These are nothing but the Pauli operators, we discussed before.

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y .$$

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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

Anti commutator $\rightarrow$ $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$.

Relations:

i) $[\hat{S}_i, \hat{S}_j] = i\varepsilon_{ijk}\hbar\hat{S}_k$.

ii) $\{\hat{S}_i, \hat{S}_j\} = \frac{\hbar^2}{2}\delta_{ij}\mathbb{I}$.

If $\hat{S}^2 = \hat{S}\cdot\hat{S} = S_x^2 + S_y^2 + S_z^2$, then

iii) $[\hat{S}^2, S_i] = 0$.

ε_{ijk} → Levi-Civita symbol.

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (x,y,z), (y,z,x) \ (z,x,y). \\ -1 & \text{if } (z,y,x), (x,z,y) \ (y,x,z) \\ 0 & \text{if repitition occurs.} \end{cases}$$

δ_{ij} → Kronecker Delta.

$$\delta_{ij} = \begin{cases} 1 & \text{if } i=j. \\ 0 & \text{if } i \neq j. \end{cases}$$

Example Levi Civita →

$$\varepsilon_{xyz} = \varepsilon_{yzx} = \varepsilon_{zxy} = 1.$$

$$\varepsilon_{yxz} = -1 = \varepsilon_{yzx}$$

$$\varepsilon_{yyz} = 0.$$

Compatible observables:

Returning again to the general observables formalism, we will discuss compatible vs incompatible observables.

Two observables given by the operators $\hat{A}$ and $\hat{B}$ are compatible when the corresponding operators commute,

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

and incompatible when

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

For example $\hat{S}^2$ and S_z are compatible, but S_x, S_y, S_z are not.

Degeneracy: Suppose there are two or more linearly independent eigenkets of $\hat{A}$ having the same eigenvalue. Then the eigenvalue of the two eigenkets will be called degenerate. In such a case, the eigenket $|a'\rangle$ ascribed to eigenvalue a' is not a complete description.

Furthermore, recall that in the theorem on Hermitian ~~of~~ operators, the orthogonality of different eigenkets were proved on the basis of non-degeneracy.

Theorem: Suppose $\hat{A}$ and $\hat{B}$ are compatibe observables and eigenvalues of $\hat{A}$ are non-degenerate. Then the matrix elements $\langle a''|\hat{B}|a'\rangle$ are all diagonal.

Proof:
$$[\hat{A}, \hat{B}] = 0$$

$$\Rightarrow \quad \langle a''|[\hat{A};\hat{B}]|a'\rangle = 0$$

$$\Rightarrow \quad \langle a''|\hat{A}\hat{B}|a'\rangle - \langle a''|\hat{B}\hat{A}|a'\rangle = 0$$

$$\Rightarrow \quad (a''-a')\langle a''|\hat{B}|a'\rangle = 0$$

$$\left[\because \quad \hat{A}|a'\rangle = a'|a'\rangle\right].$$

For off diagonal elements, $a' \neq a''$, and hence $\langle a''|\hat{B}|a'\rangle$ must vanish for $a' \neq a''$. Only the diagonal elements $\langle a'|\hat{B}|a'\rangle$ will survive, ~~sim~~ proving our assertion. (Proved).

We can therefore write
$$\langle a''|\hat{B}|a'\rangle = \delta_{a'a''}\langle a'|\hat{B}|a'\rangle.$$

The consequence of this theorem is that ~~of~~ both $\hat{A}$ and $\hat{B}$ can be expressed by the same set of eigenkets $\{|a'\rangle\}$.

The ket is therefore a simultaneous eigenket of both $\hat{A}$ and $\hat{B}$. Just to be impartial, we may use the modified notation $|a'b'\rangle$ to represent the base kets.

$$\hat{A}|a',b'\rangle = a'|a',b'\rangle$$
$$\hat{B}|a',b'\rangle = b'|a',b'\rangle$$

Incompatibe observables:

We now turn to the case of incompatible observables, which are more non-trivial. The first point to be noted that, incompatible observables do not have simultaneous eigenkets. To make the point more clear, let us consider the contrary and state that $\hat{A}$, $\hat{B}$ operators with $[\hat{A},\hat{B}] \neq 0$, have same set of base kets $\{|a',b'\rangle\}$.

Therefore
$$\hat{A}\hat{B}|a'.b'\rangle = b'\hat{A}|a',b'\rangle = a'b'|a'b'\rangle$$
$$\hat{B}\hat{A}|a'b'\rangle = a'\hat{B}|a'b'\rangle = a'b'|a'b'\rangle$$

which produces $[\hat{A},\hat{B}] = 0$.

This contradicts the initial assumption. Therefore we get that incompatible observables cannot have simultaneous eigenkets.

The uncertainty relation:

Given an observable $\hat{A}$, Let us define an operator $\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$,
where the expectation value is to be taken for a certain physical state under consideration. The expectation value of $(\Delta A)^2$ is is known as the dispersion of $\hat{A}$

$$\langle(\Delta A)^2\rangle = \langle A^2 - 2A\langle A\rangle + \langle A\rangle^2\rangle$$
$$= \langle A^2\rangle - 2\langle A\rangle^2 + \langle A\rangle^2$$
$$= \langle A^2\rangle - \langle A\rangle^2.$$

Sometimes the term variance or mean square deviation are used for the same quantity.
The dispersion of an observable is considered as "fuzziness" or "uncertainty" of measurement for an observable.
For example, for a spin-half system,

$$\langle\hat{S}_x^2\rangle - \langle\hat{S}_x\rangle^2 = \hbar^2/4.$$

for the system to be in the eigenket of S_z. $\{|0\rangle, |1\rangle\}$. (Check).
For the same eigenkets the dispersion of $\hat{S}_z$ will be zero.
Therefore for base kets $\{|0\rangle, |1\rangle\}$ $\hat{S}_z$ is "sharp" and $\hat{S}_x$ is "fuzzy".

Therefore, for two observables $\hat{A}$ and $\hat{B}$, we now state the uncertainty relation

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2 .$$

To prove this, we first need to state three Lemmas.

Lemma 1: The Schwarz inequality:

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2 .$$

Proof: First note:

$$(\langle \alpha | + \lambda^* \langle \beta |) \cdot (|\alpha\rangle + \lambda |\beta\rangle) \geq 0 .$$

where λ is any complex number.

Therefore we have.

$$\langle \alpha | \alpha \rangle + \lambda^* \langle \beta | \alpha \rangle + \lambda \langle \alpha | \beta \rangle + |\lambda|^2 \langle \beta | \beta \rangle \geq 0 .$$

Set $\lambda = - \dfrac{\langle \beta | \alpha \rangle}{\langle \beta | \beta \rangle}$.

Therefore we have,

$$\langle \alpha | \alpha \rangle + \frac{|\langle \alpha | \beta \rangle|^2}{\langle \beta | \beta \rangle} - \frac{|\langle \alpha | \beta \rangle|^2}{\langle \beta | \beta \rangle} + \frac{|\langle \alpha | \beta \rangle|^2}{\langle \beta | \beta \rangle} \geq 0$$

$$\Rightarrow \quad \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2 .$$

(Proved).

Lemma 2: The expectation value of a Hermitian operator is real.

Proof: Consider a hermitian operator $\hat{A}$ with base kets $\{|a'\rangle\}$:

Therefore we have $\hat{A}|a'\rangle = a'|a'\rangle$

$\hookrightarrow$ real.

Consider $|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle$ with $\sum_{a'} |c_{a'}|^2 = 1$.

$$\therefore \quad \langle \hat{A} \rangle_\alpha = \langle \alpha | \hat{A} | \alpha \rangle.$$

$$= \sum_{a' a''} c_{a''} c_{a'}^* \langle a' | A' | a'' \rangle.$$

$$= \sum_{a'} a' |c_{a'}|^2 \longrightarrow \text{real}.$$

(Proved).

Lemma 3: The expectation value of an anti-hermitian operator is purely imaginary.

Proof: It is similar to that of hermitian case. Anti hermitian op. $C = -C^\dagger$.

First prove that the eigenvalues of an anti-hermitian operator is purely imaginary.

Then ~~the~~ (Check).

Armed with these three Lemmas, we are in a position to prove the Uncertainty relation

Let us consider.

$$|\alpha\rangle = \Delta A|\ \rangle.$$

$$|\beta\rangle = \Delta B|\ \rangle.$$

where the blank ket signifies that our consideration may be applied to any kets.

Therefore $\langle\alpha|\alpha\rangle = \langle|(\Delta A)^2|\rangle = \langle(\Delta A)^2\rangle$

$$\langle\beta|\beta\rangle = \langle|(\Delta B)^2|\rangle = \langle(\Delta B)^2\rangle$$

$$\langle\alpha|\beta\rangle = \langle|\Delta A\,\Delta B|\rangle \quad \langle\Delta A\,\Delta B\rangle$$

Using Lemma 1, we have.

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle\Delta A\,\Delta B\rangle|^2$$

here hermiticity of ΔA and ΔB has been used. To evaluate the RHS, we note.

$$\Delta A\,\Delta B = \frac{\Delta A\,\Delta B - \Delta B\,\Delta A}{2} + \frac{\Delta A\,\Delta B + \Delta B\,\Delta A}{2}$$

$$= \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\}.$$

Now. $[\Delta A, \Delta B] = [\hat{A} - \langle\hat{A}\rangle, \hat{B} - \langle\hat{B}\rangle]$.

$$= [\hat{A}, \hat{B}] \quad \text{(check)}.$$

$$[\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}] \rightarrow \text{antihermitian}.$$

$$\{\Delta\hat{A}, \Delta\hat{B}\}^\dagger = \{\hat{A}, \hat{B}\} \rightarrow \text{hermitian}.$$

$$\therefore \langle\Delta A\,\Delta B\rangle = \underbrace{\frac{1}{2}\langle[A, B]\rangle}_{\text{Purely imaginary}} + \underbrace{\frac{1}{2}\langle\{\Delta A, \Delta B\}\rangle}_{\text{purely real}}.$$

Therefore,

$$|\langle \Delta A \, \Delta B \rangle|^2 = \frac{1}{4} |\langle [A, B] \rangle|^2 + \frac{1}{4} |\langle \{\Delta A, \Delta B\} \rangle$$

Therefore.

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2 .$$

(Proved).

Change of basis:

Transformation operator:

Suppose we have two incompatible operators $\hat{A}$ and $\hat{B}$. The ket space in question, can be viewed as $\{|a'\rangle\}$ or $\{|b'\rangle\}$. For example, the base kets of $\hat{S}_z$ operator $\{|0\rangle, |1\rangle\}$ or alternatively the base kets of $\hat{S}_x$ operator $\{|+\rangle, |-\rangle\}$. We are interested to find out, how the two ket spaces are related. Changing the set of base kets is referred to as change of basis.

Our basic task is to construct an operator which connects one basis set to other.

Let us consider the case of spin-$1/2$ system. We want to find a transformation operator U, which will give us

$$\{|1\rangle, |0\rangle\} \xrightarrow{U} \{|+\rangle, |-\rangle\}.$$

where $|\pm\rangle = \dfrac{|1\rangle \pm |0\rangle}{\sqrt{2}}$.

Let us construct the following matrix

$$U = |+\rangle\langle 1| + |-\rangle\langle 0|.$$

Such that
$$\left.\begin{aligned} U|+\rangle &= |+\rangle \\ U|0\rangle &= |-\rangle \end{aligned}\right\} \text{(check)}.$$

Therefore this operator takes ~~|+, 0⟩~~ $|1\rangle$ to $|+\rangle$ and $|0\rangle$ to $|-\rangle$.

Now consider $U^\dagger = |1\rangle\langle +| + |0\rangle\langle -|$.

This $U^\dagger$ will do the reverse operation. i.e. it will take $|+\rangle$ to $|1\rangle$ and $|-\rangle$ to $|0\rangle$.

Now
$$UU^\dagger = (|+\rangle\langle 1| + |-\rangle\langle 0|)(|1\rangle\langle +| + |0\rangle\langle -|)$$
$$= |+\rangle\langle +| + |-\rangle\langle -| = \mathbb{I}.$$

$$U^\dagger U = (|1\rangle\langle +| + |0\rangle\langle -|)(|+\rangle\langle 1| + |-\rangle\langle 0|)$$
$$= |1\rangle\langle 1| + |0\rangle\langle 0| = \mathbb{I}.$$

Therefore, we have $\boxed{UU^\dagger = U^\dagger U = \mathbb{I}}$

U is an unitary operator.

Theorem: Given two set of base kets, both satisfying orthonormality and completeness, there exists an unitary operator, such that

$$|b^{(1)}\rangle = U|a^{(1)}\rangle, \quad |b^{(2)}\rangle = U|a^{(2)}\rangle \cdots, \quad |b^{(n)}\rangle = U|a^{(n)}\rangle.$$

By unitary operator, we mean an operator U, fulfilling the condition $UU^{\dagger} = U^{\dagger}U = \mathbb{I}$.

Proof: We prove this by explicit construction. ~~We~~ Let us consider a transformation of basis $\{|a^{(i)}\rangle\} \longrightarrow \{|b^{(i)}\rangle\}$ where both the sets are complete and orthonormal.

Consider an operator $U = \sum_k |b^{(k)}\rangle\langle a^{(k)}|$.

It is clear that U gives the required transformation.

Now see that $UU^{\dagger} = \left(\sum_k |b^{(k)}\rangle\langle a^{(k)}|\right)\left(\sum_l |a^{(l)}\rangle\langle b^{(l)}|\right)$.

$$= \sum_k |b^{(k)}\rangle\langle b^{(k)}| = \mathbb{I}.$$

Similarly $U^{\dagger}U = \sum_l |a^{(l)}\rangle\langle a^{(l)}| = \mathbb{I}$.

This proves the theorem.

Transformation matrix:

It is instructive to study the matrix representation of unitary operators in the old basis.

The matrix element of U can be given by

$$\langle a^{(k)} | U | a^{(l)} \rangle = \langle a^{(k)} | b^{(l)} \rangle .$$

In other words, the matrix elements of U operator, are build up of the inner products of old and new base bra and ket vectors respectively.

For example, let us consider a transformation in real vector space (Euclidian).

$$(\hat{x}, \hat{y}, \hat{z}) \longrightarrow (\hat{x}', \hat{y}', \hat{z}') .$$

The unitary operator corresponding to this transformation

$$R = \begin{pmatrix} \hat{x}.\hat{x}' & \hat{x}.\hat{y}' & \hat{x}.\hat{z}' \\ \hat{y}.\hat{x}' & \hat{y}.\hat{y}' & \hat{y}.\hat{z}' \\ \hat{z}.\hat{x}' & \hat{z}.\hat{y}' & \hat{z}.\hat{z}' \end{pmatrix}$$

The square matrix made up of $\langle a^{(k)} | U | a^{(l)} \rangle$ is reffered to as transformation matrix from $\{|a'\rangle\}$ basis to $\{|b'\rangle\}$ basis.

Physically unitary operation can be understood as rotation in the Hilbert space.

Now we will consider a situation, where a ket vector $|\alpha\rangle$ ~~is transformed by~~ which given in the old basis $\{|a'\rangle\}$ as

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle,$$ with $\langle a'|\alpha\rangle$ are the coefficient in the old basis.

Our question is what will be the coefficients of $|\alpha\rangle$, $\langle b'|\alpha\rangle$ in the new basis $\{|b'\rangle\}$.

$$\{|a'\rangle\} \xrightarrow{U} \{|b'\rangle\}.$$

$$\langle b^{(k)}|\alpha\rangle = \sum_{l} \langle b^{(k)}|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle.$$

$$\langle b^{(k)}|a^{(l)}\rangle = \langle a^{(k)}|U^{+}|a^{(l)}\rangle.$$

Therefore, we have.

$$\langle b^{(k)}|\alpha\rangle = \sum_{l} \langle a^{(k)}|U^{+}|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle.$$

$$(\text{New}) = (U^{+})(\text{old}).$$

Relation between the old matrix elements and the new one, for an operator $\hat{X}$.

$$\langle b^{(k)}|\hat{X}|b^{(l)}\rangle = \sum_{m,n} \langle b^{(k)}|a^{(m)}\rangle\langle a^{(m)}|\hat{X}|a^{(n)}\rangle\langle a^{(n)}|b^{(l)}\rangle.$$

$$= \sum_{mn} \langle a^{(k)}|U^{-1}|a^{(m)}\rangle\langle a^{(m)}|\hat{X}|a^{(n)}\rangle\langle a^{(n)}|U|a^{(l)}\rangle.$$

$$\therefore \quad \hat{X}' \longrightarrow U^{+}\hat{X}U.$$

Therefore, if a state vector is transformed in the way $|\beta\rangle = U|\alpha\rangle$,

the operator will transform like

$$\hat{X}' = U^{+} X U$$

The trace of an operator $\hat{X}$ is defined as the sum of all diagonal elements.

$$Tr(\hat{X}) = \sum_{a'} \langle a'|\hat{X}|a'\rangle .$$

$Tr(\hat{X})$ is turned out to be independent of the description.

Proof: Let $\{|b'\rangle\} = \{U|a'\rangle\}$.

$$Tr(\hat{X}) = \sum_{a'} \langle a'|\hat{X}|a'\rangle .$$

$$= \sum_{a'b'b''} \langle a'|b'\rangle\langle b'|\hat{X}|b''\rangle\langle b''|a'\rangle .$$

$$= \sum_{b',b''} \langle b''|\left(\sum_{a'} |a'\rangle\langle a'|\right)|b'\rangle \langle b'|\hat{X}|b''\rangle .$$

$$= \sum_{b'b''} \langle b''|b'\rangle \langle b'|\hat{X}|b''\rangle$$

$$= \sum_{b'} \langle b'|\hat{X}|b'\rangle .$$

(Proved).

We can also prove

i) $Tr(\hat{X}\hat{Y}) = Tr(\hat{Y}\hat{X})$.

ii) $Tr(U^{\dagger}\hat{X}U) = Tr(\hat{X})$.

iii) $Tr(|a'\rangle\langle a''|) = \delta_{a'a''}$

iv) $Tr(|b'\rangle\langle a'|) = \langle a'|b'\rangle$.

Proof of (i) :

$$Tr(\hat{X}\hat{Y}) = \sum_{a'} \langle a'|\hat{X}\hat{Y}|a'\rangle.$$

$$= \sum_{a'a''} \langle a'|\hat{X}|a''\rangle\langle a''|\hat{Y}|a'\rangle.$$

$$= \sum_{a'a''} \langle a''|\hat{Y}|a'\rangle\langle a'|\hat{X}|a''\rangle.$$

$$= \sum_{a''} \langle a''|\hat{Y}\hat{X}|a''\rangle = Tr(\hat{Y}\hat{X})$$

Proof of (ii) :

$$Tr(U^{\dagger}XU) = \sum_{a'} \langle a'|U^{\dagger}\hat{X}U|a'\rangle.$$

$$= \sum_{a'a''a'''} \langle a'|U^{\dagger}|a''\rangle\langle a''|\hat{X}|a'''\rangle\langle a'''|U|a'\rangle.$$

$$= \sum_{a'a''a'''} \cancel{\langle a'''|a'\rangle\langle a'|}\ \langle a'''|U|a'\rangle\langle a'|U^{\dagger}|a''\rangle\langle a''|\hat{X}|a'''\rangle$$

$$= \sum_{a''a'''} \langle a'''|UU^{\dagger}|a''\rangle\langle a''|\hat{X}|a'''\rangle.$$

$$= \sum_{a''a'''} \langle a'''|a''\rangle\langle a''|\hat{X}|a'''\rangle.$$

$$= \sum_{a''} \langle a''|\hat{X}|a''\rangle = Tr(\hat{X}).$$

Diagonalization:

We will now discuss, how to find the eigenvalues and eigenkets of an operator $\hat{B}$, whose matrix elements in the ~~ot~~ old $\{|a'\rangle\}$ basis are known

This problem is the equivalant of finding the unitary matrix that diagonalizes $\hat{B}$.

We are interested in obtaining the eigenvalue b' and eigenket $|b'\rangle$ with the property

$$\hat{B}|b'\rangle = b'|b'\rangle$$

First we rewrite this as

$$\sum_{a'} \langle a''|\hat{B}|a'\rangle\langle a'|b'\rangle = b'\langle a''|b'\rangle$$

When $|b'\rangle$ is the l-th eigenket of operator $\hat{B}$, we can write this in the following notation.

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} & \cdots \\ B_{21} & B_{22} & B_{23} & \cdots \\ \vdots & & & \end{pmatrix}\begin{pmatrix} c_1^{(l)} \\ c_2^{(l)} \\ \vdots \\ \vdots \end{pmatrix} = b^{(l)}\begin{pmatrix} c_1^{(l)} \\ c_2^{(l)} \\ \vdots \\ \vdots \end{pmatrix}$$

with

$$B_{ij} = \langle a^{(i)}|B|a^{(j)}\rangle$$

$$c_k^{(l)} = \langle a^{(k)}|b^{(l)}\rangle$$

where i, j, k run upto N, the dimensionality of the ket space.

Nontrivial solution of $c_k^{(l)}$ is only possible when we have $\mathrm{Det}(\hat{B} - \lambda \mathbb{I}) = 0$

This is called the characteristic equation.

It is to be noted that all matrices cannot be diagonalized. Hermitian, anti-hermitian, unitary matrices are some of the matrices which can be diagonalized.

In general a "normal matrix" obeying the property $AA^{\dagger} = A^{\dagger}A$ is diagonalized. You can check that hermitian matrices, anti-hermitian matrices, or unitary matrices all obey this property.

Unitary equivalent observable:

We conclude this chapter by discussing a remarkable theorem on the unitary transformation of an observable.

Theorem: Consider two sets of orthonormal basis $\{|a'\rangle\}$ and $\{|b'\rangle\}$ connected by the unitary operator U. Knowing U, we may construct a unitary transformation of $\hat{A}$, as $U\hat{A}U^{\dagger}$; then $\hat{A}$ and $U\hat{A}U^{\dagger}$ are said to be unitarily equivalent observables.

$$\hat{A}|a^{(i)}\rangle = a^{(i)}|a^{(i)}\rangle$$

clearly implies $U\hat{A}U^{\dagger}U|a^{(i)}\rangle = a^{(i)}U|a^{(i)}\rangle$.

$$\Rightarrow (U\hat{A}U^{\dagger})|b^{(i)}\rangle = a^{(i)}|b^{(i)}\rangle$$

Quantum Dynamics:

Now we are going to discuss how a quantum state evolves in time. In otherwords we are now concerned with the quantum mechanical analouge of Newton's equation (or Lagrange's or Hamilton's) ~~equation~~ of motion.

Time evolution and Schrödinger equation:

The first important point we should keep in mind, that time is just a parameter in quantum mechanics, not an operator.

The time evolution operator:

Our basic concern in this section is, how does a state ket change in time.

Let us consider a quatum state evolving in time from t_0 to t. as

$$|\alpha, t_0; t\rangle \quad \text{for } (t > t_0).$$

Because time is assumed to be a continuous parameter, we have.

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle = |\alpha, t_0\rangle.$$

Let us consider the time evolution operator to be $U(t, t_0)$. Therefore

$$|\alpha, t_0; t\rangle = U(t, t_0)\,|\alpha, t_0\rangle$$

The first requirement is that of probability conservation.

Let us consider $|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0)\, |a'\rangle$.

Similarly we have $|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t)\, |a'\rangle$.

In general $|c_{a'}(t_0)| \neq |c_a(t)|$.

But for conservation of probability requires $\sum_{a'} |c_{a'}(t)|^2 = \sum_{a'} |c_{a'}(t_0)|^2 = 1$.

which is followed by:

$$\langle \alpha, t_0; t | \alpha, t_0; t\rangle = \langle \alpha, t_0 | \alpha, t_0\rangle$$

$$\Rightarrow \quad \langle \alpha, t_0 | U^\dagger(t, t_0)\, U(t, t_0) | \alpha, t_0\rangle = \langle \alpha, t_0 | \alpha, t_0\rangle$$

$$\Rightarrow \quad U^\dagger(t, t_0)\, U(t, t_0) = \mathbb{I}.$$

i.e. $U(t, t_0)$ is a unitary operator.

It is one of the most fundamental property of $U(t, t_0)$.

(Later in this course we will learn that there is a more general operation in quantum processes, which includes dissipation and other losses).

The second important property is that of composition:

$$U(t_2, t_0) = U(t_2, t_1)\, U(t_1, t_0) \quad (t_2 > t_1 > t_0)$$

This equation says that if we are interested in obtaining time evolution from t_0 to t_2, then we can obtain the same result by dividing it from t_0 to t_1 and then t_1 to t_2, where t_1 is any arbitrary intermediate time. This process can be repeated arbitrary number of times.

In a more general quantum process, this property is referred to as divisibility property.

It turns out ~~that~~ to be advantageous to consider an infinitisimal time evolution $U(t_0 + dt, t_0)$:

$$|\alpha, t_0; t_0 + dt\rangle = U(t_0 + dt, t_0)\, |\alpha, t\rangle$$

where $\lim_{dt \to 0} U(t_0 + dt, t_0) = \mathbb{I}$.

These requirements are satisfied by

$$U(t_0 + dt, t_0) = \mathbb{I} - i\Omega\, dt,$$

where Ω is a hermitian operator, and $dt \to 0$, such that higher order of dt can be safely ignored.

Unitarity :

$$U^{\dagger}(t_0+dt, t_0)\, U(t_0+dt, t_0)$$

$$= (\mathbb{I} + i\Omega\, dt)(\mathbb{I} - i\Omega\, dt)$$

$$= \mathbb{I} + i\Omega\, dt - i\Omega\, dt - \cancel{\Omega^2 dt^2} \rightarrow \text{ignore}$$

$$= \mathbb{I}.$$

Composition :

$$U(t_0+dt_1+dt_2, t_0) = U(t_0+dt_1+dt_2, t_0+dt_1) \cdot U(t_0+dt_1, t_0).$$

Proof :

$$U(t_0+dt_1+dt_2, t_0) = \mathbb{I} - i\Omega(t_0+dt_1+dt_2 - t_0).$$

$$= \mathbb{I} - i\Omega(t_0+dt_1+dt_2 - dt_1 - t_0) - i\Omega(dt_1 + t_0 - t_0).$$

$$= U(t_0+dt_1+dt_2, t_0+dt_1)\, U(t_0+dt_1, t_0).$$

(Proved).

To sum up, the infinitisimal time evolution operator can be written as

$$U(t_0+dt, t_0) = \mathbb{I} - \frac{iH\,dt}{\hbar}$$

where the hermitian operator H is called the Hamiltonian.

The Schrödinger equation:

We are now in a position to derive the fundamental differential equation for the time evolution operator $U(t, t_0)$.

Using the composition property we have

$$U(t+dt, t_0) = U(t+dt, t)\,U(t, t_0)$$

$$= \left(\mathbb{I} - \frac{iH\,dt}{\hbar}\right) U(t, t_0).$$

$$\Rightarrow \quad U(t+dt, t_0) - U(t, t_0) = -\frac{iH\,dt}{\hbar} U(t, t_0).$$

$$\Rightarrow \quad \lim_{dt \to 0} \frac{U(t+dt, t_0) - U(t, t_0)}{dt} = -\frac{iH}{\hbar} U(t, t_0).$$

$$\Rightarrow \quad i\hbar \frac{\partial}{\partial t} U(t, t_0) = H\,U(t, t_0)$$

Multiplying $|\alpha, t_0\rangle$ on the right side:

$$i\hbar \frac{\partial}{\partial t} U(t, t_0)|\alpha, t_0\rangle = H\,U(t, t_0)|\alpha, t_0\rangle$$

$$\Rightarrow \quad \boxed{i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H\,|\alpha, t_0; t\rangle}$$

Energy eigenkets:

To be able to evaluate the effect of the time evolution operator on a general initial ket $|\alpha\rangle$, we must know how it acts on the base kets used in expanding $|\alpha\rangle$.

This is particularly straightforward if the base kets used are eigenkets of A such that

$$[A, H] = 0.$$

Then the eigenkets of A are also the eigenkets of H, called "energy eigenkets", whose eigenvalues are $E_{a'}$:

$$H|a'\rangle = E_{a'}|a'\rangle$$

We can now expand $\exp\left(-\frac{iHt}{\hbar}\right)$ in terms of $|a'\rangle\langle a'|$.

$$\exp\left(-\frac{iHt}{\hbar}\right) = \exp\left[-\frac{i}{\hbar}\sum_{a'} E_{a'}|a'\rangle\langle a'|\right].$$

$$= \mathbb{I} - \frac{i}{\hbar}\sum_{a'} E_{a'}|a'\rangle\langle a'| + \left(-\frac{i}{\hbar}\right)^2\sum_{a'} E_{a'}^2|a'\rangle\langle a'| + \cdots$$

$$= \sum_{a'}|a'\rangle\langle a'| - \frac{i}{\hbar}\sum_{a'} E_{a'}|a'\rangle\langle a'| + \left(-\frac{i}{\hbar}\right)^2\sum_{a'} E_{a'}^2|a'\rangle\langle a'| + \cdots$$

$$= \sum_{a'} \exp\left(-\frac{iE_{a'}t}{\hbar}\right)|a'\rangle\langle a'|.$$

Therefore

$$|\alpha, t_0=0; t\rangle = \exp\left(-\frac{iHt}{\hbar}\right)|\alpha\rangle$$

$$= \exp\left(-\frac{iHt}{\hbar}\right)\sum_{a'}|a'\rangle\langle a'|\alpha\rangle$$

$$|\alpha, t\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle \exp\left(-\frac{iE_{a'}t}{\hbar}\right).$$

In other words, the expansion coefficients.

$$\langle a'|\alpha, t\rangle = \langle a'|\alpha\rangle \exp\left(-\frac{iE_{a'}t}{\hbar}\right).$$

$$C_{a'}(t) = C_{a'}(0)\exp\left(-\frac{iE_{a'}t}{\hbar}\right).$$

Time dependence of expectation values:

Let us consider $|a, t\rangle = U(t,0)|a\rangle$.

Therefore $\langle B\rangle_{|\alpha,t\rangle} = \langle a,t|B|a,t\rangle$

$$= \langle a|U^{\dagger}(t,0)|B|U(t,0)|a\rangle.$$

$$= \langle a|e^{iE_at/\hbar}\, B\, e^{-iE_at/\hbar}|a\rangle.$$

$$= \langle a|B|a\rangle$$

So the expectation value of an observable taken with respect to an energy eigenket does not change in time.

Case I: Hamiltonian independent of time.

$$U(t, t_0) = \mathbb{I} - \frac{iH}{\hbar}(t - t_0)$$; when $t - t_0 = \Delta t$ to be very small.

When $t - t_0 = N\Delta t$, we have

$$U(t, t_0) = U(t, t_0 - \Delta t) \cdot U(t_0 - \Delta t, t_0 - 2\Delta t) \cdots U(t - (N-1)\Delta t, t_0 - (N-1)\Delta t)$$

$$= \lim_{N \to \infty} \left[\mathbb{I} - (iH/\hbar)\frac{(t - t_0)}{N} \right]^N$$

$$U(t, t_0) = \exp\left(-\frac{iH(t - t_0)}{\hbar}\right).$$

It can be checked that the given function satisfies all the properties of unitary operators.

Case II: Hamiltonian dependent on time

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')\right].$$

The situation is more interesting, when the expectation value is taken with respect to a superposition of energy eigenkets.

$$|\alpha\rangle = \sum_{a'} C_{a'} |a'\rangle .$$

$$\langle \hat{B} \rangle = \left[\sum_{a'} C_{a'}^{*} \langle a' | \exp\left(\frac{iE_{a'}t}{\hbar}\right) \right] \cdot \hat{B} \cdot$$

$$\left[\sum_{a''} C_{a''} \exp\left(\frac{iE_{a''}t}{\hbar}\right) |a''\rangle \right] .$$

$$= \sum_{a',a''} C_{a'}^{*} C_{a''} \langle a' | \hat{B} | a'' \rangle \exp\left[\frac{-i(E_{a''} - E_{a'})t}{\hbar} \right]$$

So this time the expectation value consists of oscillating terms with angular frequency

$$\omega_{a''a'} = \frac{E_{a''} - E_{a'}}{\hbar} .$$

Spin precession:

It is appropriate to consider an example in this situation.

We start with a Hamiltonean of a spin 1/2 system with moment $e\hbar/2m_e c$ (magnetic) subjected to an external magnetic field $\hat{B}$.

$$\hat{H} = -\left(\frac{e}{m_e c}\right)\hat{S}\cdot\hat{B}. \qquad (e < 0 \text{ for electron})$$

where
$$\hat{S} = \hat{S}_x\hat{x} + \hat{S}_y\hat{y} + \hat{S}_z\hat{z}$$
$$\hat{B} = \hat{B}_x\hat{x} + \hat{B}_y\hat{y} + B_z\hat{z}.$$

Furthermore consider $\hat{B} = B_z\hat{z}$ and B_z is independent of time and uniform along z-direction.

$$\therefore \quad \hat{H} = -\left(\frac{eB}{m_e c}\right)\hat{S}_z \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

$$\hat{H} = \mp\frac{e\hbar B}{2m_e c}.$$

It is convenient to define ω in such a way that the difference between two energy eigenvalues is $\hbar\omega$.

~~Then~~ with $\omega = \dfrac{|e|B}{m_e c}$.

Therefore $H = \omega S_z$

and $\quad U(t,0) = \exp\left(\frac{-i\omega S_z t}{\hbar}\right)$

we apply this to the initial ket vector

$$|\alpha\rangle = c_+ |1\rangle + c_- |0\rangle$$

We have, $\quad H|1\rangle = \frac{\hbar\omega}{2}|1\rangle$

$$H|0\rangle = -\frac{\hbar\omega}{2}|0\rangle$$

Therefore

$$|\alpha, t\rangle = U(t,0)|\alpha\rangle$$

$$= c_+ \exp\left(-\frac{i\omega t}{2}\right)|1\rangle + c_- \exp\left(\frac{i\omega t}{2}\right)|0\rangle$$

Consider $\quad c_+ = c_- = \frac{1}{\sqrt{2}}$.

The probabities of finding the state in

$$|S_x, \pm\rangle = \frac{|1\rangle \pm |0\rangle}{\sqrt{2}}.$$

$$P_\pm = |\langle S_x, \pm | \alpha, t\rangle|^2$$

$$= \left|\left[\frac{\langle 1| \pm \langle 0|}{\sqrt{2}}\right]\left[\frac{1}{\sqrt{2}} e^{-i\omega t/2}|1\rangle + \frac{1}{\sqrt{2}} e^{i\omega t/2}|0\rangle\right]\right|^2$$

$$= \left|\frac{e^{-\frac{i\omega t}{2}} \pm e^{\frac{i\omega t}{2}}}{2}\right|^2$$

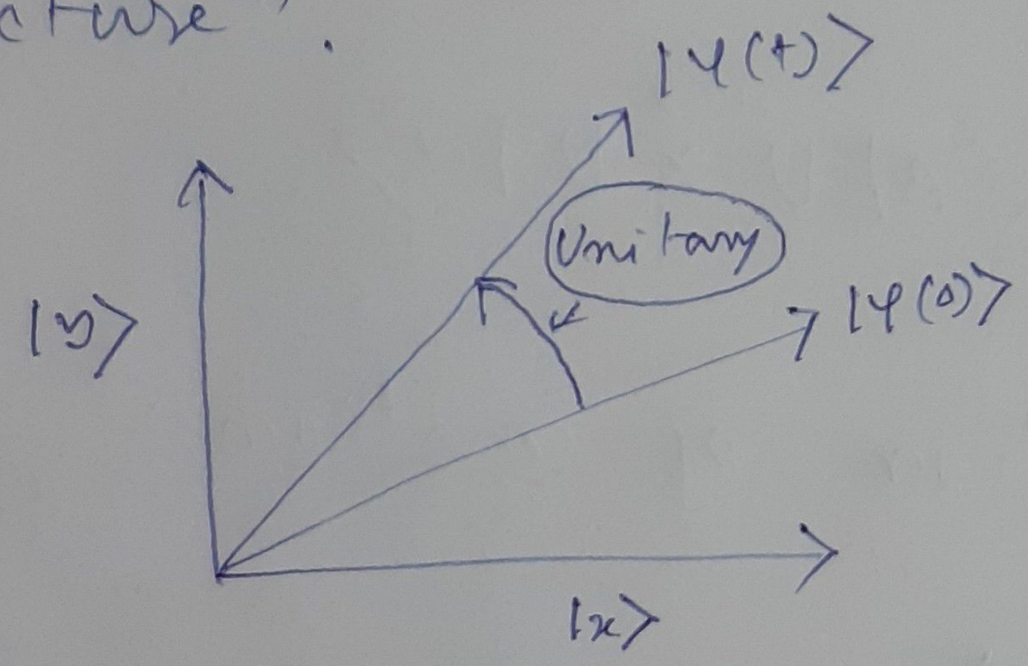
$$= \begin{cases} \cos^2 \omega t/2, & \text{for } |S_x +\rangle \\ \sin^2 \omega t/2 & \text{for } |S_x -\rangle \end{cases}$$

The Schrödinger vs the Heisenberg picture:

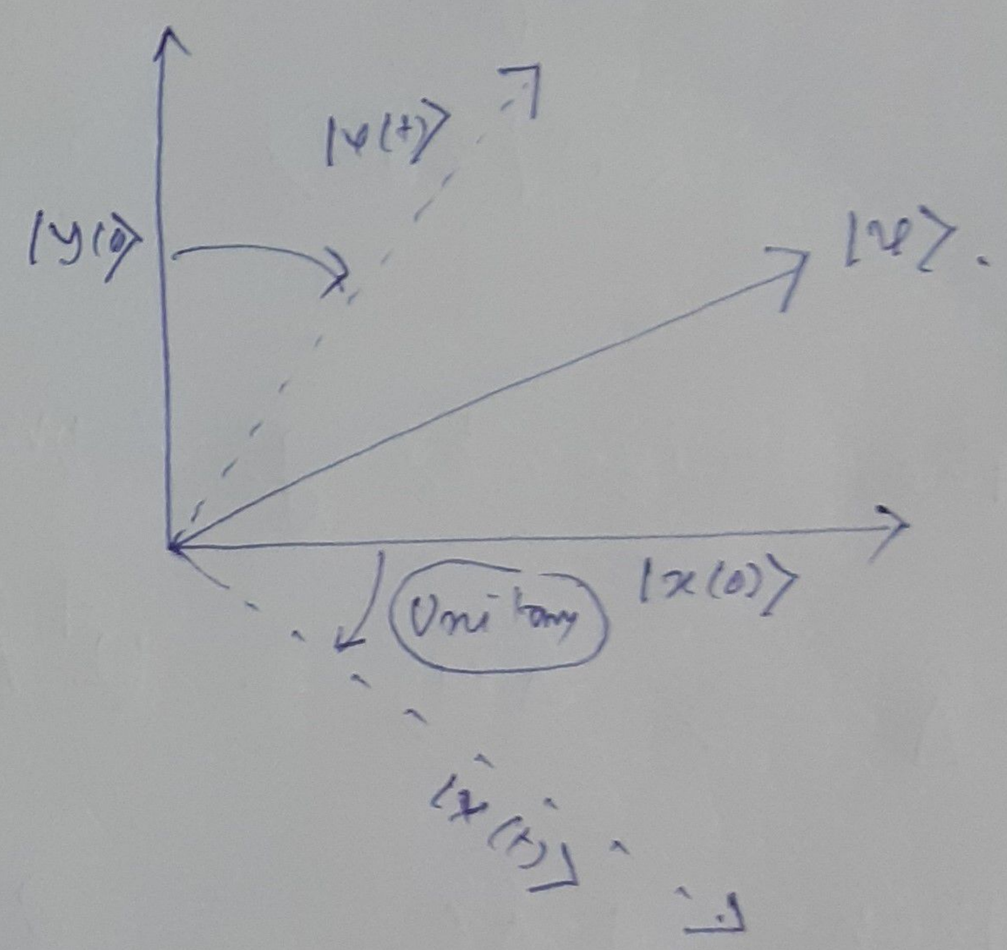
In the previous lecture, we have introduced the concept of time development, by introducing an operator which affects the state kets.

This approach is called "Schrödinger picture"

There is another fundamental formulation of Quantum Mechanics, where the observables, rather than the state ket vectors, evolve in time. This approach is called "Heisenberg picture".



Schrödinger picture.



Heisenberg picture.

Both the representations are equivalent, since they corresponds to same physical changes; i.e. the expectation value remains unchanged.

Schrödinger $\rightarrow$ $|\alpha\rangle \rightarrow U|\alpha\rangle$ (operator unchanged)

Heisenberg $\rightarrow$ $\hat{X} \rightarrow U^{\dagger}\hat{X}U$ (state kets unchanged)

Expectation value

Schrödinger :

$$\langle \beta | \alpha \rangle = \langle \beta | U^{\dagger} U | \alpha \rangle = \langle \beta | \alpha \rangle .$$

Heisenberg :

$$\langle \beta | \alpha \rangle = \langle \beta | \alpha \rangle .$$

Schrödinger :

$$\langle \beta | \hat{x} | \alpha \rangle \rightarrow \langle \beta | U^{\dagger} \hat{x} U | \alpha \rangle .$$

Heisenberg :

$$\langle \beta | \hat{x} | \alpha \rangle \rightarrow \langle \beta | U^{\dagger} \hat{x} U | \alpha \rangle .$$

The Heisenberg equation of motion :

$$\hat{A} \longrightarrow \hat{A}(t) = U^{\dagger} \hat{A} U .$$

Then $$\frac{d \hat{A}(t)}{dt} = \frac{\partial U^{\dagger}}{\partial t} \hat{A} U + U^{\dagger} \hat{A} \frac{\partial U}{\partial t} .$$

Now $$\hat{U} = \exp.\left(-\frac{i \hat{H} t}{\hbar}\right)$$

$$\therefore \frac{\partial \hat{U}}{\partial t} = -\frac{i \hat{H}}{\hbar} \hat{U} ; \quad \frac{\partial U^{\dagger}}{\partial t} = \frac{i \hat{H}}{\hbar} \hat{U} .$$

Therefore $$\cancel{\frac{d \hat{A}(t)}{dt}} =$$

Therefore

$$\frac{d\hat{A}(t)}{dt} = \frac{i\hat{H}}{\hbar}\hat{U}^{\dagger}\hat{A}\hat{U} - \frac{i}{\hbar}\hat{U}^{\dagger}\hat{A}\hat{H}\hat{U}.$$

$$= \frac{i}{\hbar}\underbrace{\hat{U}^{\dagger}\hat{H}\hat{U}}\,\underbrace{\hat{U}^{\dagger}\hat{A}\hat{U}} - \frac{i}{\hbar}\underbrace{\hat{U}^{\dagger}\hat{A}\hat{U}}\,\underbrace{\hat{U}^{\dagger}\hat{H}\hat{U}}.$$

$$= \frac{i}{\hbar}\hat{H}(t)\hat{A}(t) - \frac{i}{\hbar}\hat{A}(t)\hat{H}(t).$$

$$= -\frac{i}{\hbar}\left[\hat{A}(t), \hat{H}(t)\right].$$

$$\Rightarrow \boxed{i\hbar\frac{d\hat{A}(t)}{dt} = \left[\hat{A}(t), \hat{H}(t)\right].}$$

Now, since $[\hat{H}, \hat{U}] = 0$.

$$\hat{H}(t) = \hat{U}^{\dagger}\hat{H}\hat{U} = \hat{H}\hat{U}^{\dagger}\hat{U} = \hat{H}.$$

This equation is known Heisenberg equation of motion.

Ehrenfest's Theorem :

Whether we work in Schrödinger picture, or Heisenberg picture, to be able to use the equations of motion, we must first learn how to construct the appropriate Hamiltonian operator. For a physical systems with classical analogues, we assume the Hamiltonian's to be of the same form as in Classical physics; we merely replace the classical x_i and P_i s by the corresponding QM operators. With this assumption, we can reproduce correct classical equations in the classical limit.

In practical application the following formulas are useful.

$$[\hat{x}_i, \hat{F}(\hat{p})] = i\hbar \frac{\partial \hat{F}}{\partial p_i}.$$

$$[\hat{p}_i, G(x)] = -i\hbar \frac{\partial \hat{G}}{\partial x_i}.$$

$\hat{F}$, $\hat{G}$ are functions that can be expanded in powers of $\hat{p}_i$ and $\hat{x}_i$ respectively.

Simple Harmonic Oscillator :

The simple Harmonic Oscillator is one of the most important problems in Quantum mechanics. From a pedagogical point of view, it is used to illustrate the basic concepts and methods in Quantum Mechanics. From a practical point of view it has applications in a variety of branches of modern physics - molecular spectroscopy, solid state physics, nuclear structure, quantum field theory, quantum optics etc.

Energy eigenkets and eigenvalues :

The basic Hamiltonian of SHO is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$$

ω is the angular frequency given by $\sqrt{K/m}$, where K is the spring constant.

Let us define two operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)$$

$$\hat{a}^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)$$

They are called annihilation and creation operators.

The commutation relation

$$[\hat{a}, \hat{a}^\dagger] = \left[\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right), \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\right]$$

$$= \frac{i}{2\hbar}[\hat{p}, \hat{x}] - \frac{i}{2\hbar}[\hat{x}, \hat{p}]$$

$$= \frac{i}{2\hbar}(-i\hbar) - \frac{i}{2\hbar} i\hbar = 1 .$$

We also define the number operator

$$\hat{N} = \hat{a}^\dagger a = \frac{m\omega}{2\hbar}\left(\hat{x} - \frac{i\hat{p}}{m\omega}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right).$$

$$= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) + \left(\frac{i}{2\hbar}\right)[\hat{x}, \hat{p}]$$

$$= \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} .$$

So we have an important relation

$$\hat{H} = \left(\hbar\omega + \frac{1}{2}\right)\hat{N} .$$

Because $\hat{H}$ is just a linear function of $\hat{N}$, they have the same eigenvectors.
Let us denote the eigenvectors as $|n\rangle$ such that

$$\hat{N}|n\rangle = n|n\rangle .$$

and $$\hat{H}|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle .$$

We will later show that n is a non-negative integer.

The energy eigenvalues are thus given by

$$E_n = (n+\tfrac{1}{2})\hbar\omega .$$

To appriciate the physical significance of $\hat{a}$ and $\hat{a}^\dagger$ and $\hat{N}$, let us first note that

$$[\hat{N}, \hat{a}] = [\hat{a}^\dagger \hat{a}, \hat{a}] = a^\dagger [\hat{a}, \hat{a}] + [a^\dagger, \hat{a}]\hat{a}$$

$$= -\hat{a}$$

Similarly $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$.

Therefore, we have

$$\hat{N}\hat{a}^\dagger|n\rangle = (\hat{N}a^\dagger - a^\dagger\hat{N} + \hat{a}^\dagger\hat{N})|n\rangle .$$

$$= ([\hat{N}, a^\dagger] + \hat{a}^\dagger\hat{N})|n\rangle .$$

$$= (a^\dagger + a^\dagger\hat{N})|n\rangle .$$

$$\Rightarrow \hat{N}(\hat{a}^\dagger|n\rangle) = (n+1)(\hat{a}^\dagger|n\rangle) .$$

Similarly $\hat{N}(\hat{a}|n\rangle) = ([\hat{N}, \hat{a}] + \hat{a}\hat{N})|n\rangle .$

$$= (-\hat{a} + \hat{a}\hat{N})|n\rangle$$

$$= (n-1)(\hat{a}|n\rangle)$$

This relations imply that $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$ are also eigenkets of $\hat{N}$ with eigenvalues increased (decreased) by 1.

This implies $\hat{a}|n\rangle \rightarrow |n-1\rangle$

$$a^\dagger|n\rangle \rightarrow |n+1\rangle .$$

Let us say $\hat{a}|n\rangle = c|n-1\rangle$

$\longrightarrow$ constant.

Therefore

$$\langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = |c|^2$$

$$\Rightarrow \langle n|\hat{N}|n\rangle = |c|^2$$

$$\Rightarrow |c|^2 = n$$

$$\Rightarrow c = \sqrt{n}.$$

$$\therefore \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle.$$

Similarly $a^{\dagger}|n\rangle = d|n+1\rangle.$

$$\Rightarrow \langle n|aa^{\dagger}|n\rangle = |d|^2$$

$$\Rightarrow \langle n|aa^{\dagger} - a^{\dagger}a + a^{\dagger}a|n\rangle = |d|^2$$

$$\Rightarrow \langle n|[a, a^{\dagger}] + \hat{N}|n\rangle = |d|^2$$

$$\Rightarrow \langle n|(1+\hat{N})|n\rangle = |d|^2$$

$$\Rightarrow d = \sqrt{n+1}$$

$$\therefore a^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle.$$

$$a^2|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle$$

$$a^3|n\rangle = \sqrt{n(n-1)(n-2)}\,|n-3\rangle$$

$\vdots$

$$a^{\dagger 2}|n\rangle = \sqrt{(n+1)(n+2)}\,|n+2\rangle$$

$$a^{\dagger 3}|n\rangle = \sqrt{(n+1)(n+2)(n+3)}\,|n+3\rangle$$

$\vdots$

Now, $\hat{N}|n\rangle = n|n\rangle$.

$$\Rightarrow \quad n = \langle n|\hat{N}|n\rangle$$
$$= \langle n|a^{\dagger}a|n\rangle$$
$$= (\langle n|a^{\dagger})(a|n\rangle) \geq 0.$$

which implies $n \rightarrow$ non-negative

Now if we start with an integer n and reduce by 1, we will end up to 0, which is the smallest.
But if we start with a non-integer and reduce by 1, we can get to negative n and the sequence will continue. But the positivity of n does not allow that.
Thereby the conclusion is n is a non-negative integer.

Ground state $\rightarrow$ Least energy eigenstate $|0\rangle$ with $n=0$.

$$\hat{H}|0\rangle = \frac{1}{2}\hbar\omega|0\rangle \; ; \; E_0 = \frac{1}{2}\hbar\omega.$$

$$|1\rangle = a^{\dagger}|0\rangle.$$
$$|2\rangle = \frac{a^{\dagger}}{\sqrt{2}}|1\rangle = \frac{(a^{\dagger})^2}{\sqrt{2}}|0\rangle.$$
$$|3\rangle = \frac{(a^{\dagger})^3}{\sqrt{3!}}|0\rangle.$$
$$\vdots$$
$$|n\rangle = \frac{(a^{\dagger})^n}{\sqrt{n!}}|0\rangle \rightarrow E_n = (n+\tfrac{1}{2})\hbar\omega.$$

$$\langle n' | a | n \rangle = \sqrt{n}\, \delta_{n', n-1}$$

$$\langle n' | a^{\dagger} | n \rangle = \sqrt{n+1}\, \delta_{n', n+1} .$$

Now $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a} + \hat{a}^{\dagger} \right)$.

$$\hat{P} = i \sqrt{\frac{m\hbar\omega}{2}} \left(-\hat{a} + \hat{a}^{\dagger} \right) .$$

$$\therefore \langle n' | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n}\, \delta_{n', n-1} + \sqrt{n+1}\, \delta_{n', n+1} \right) .$$

$$\langle n' | \hat{P} | n \rangle = i \sqrt{\frac{m\hbar\omega}{2}} \left(-\sqrt{n}\, \delta_{n', n-1} + \sqrt{n+1}\, \delta_{n', n+1} \right)$$

Notice that either $\hat{x}$ or $\hat{P}$ are not diagonal in the $\hat{N}$-representation.

The reason you all know !!!

The operator method can also be used to obtain the energy eigen functions in position space.

Let us start with the ground state

$$\hat{a}|0\rangle = 0$$

Which in x-representation reads as

$$\langle x'|\hat{a}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\,\langle x'|\hat{x} + \frac{i\hat{p}}{m\omega}|0\rangle = 0.$$

$$\Rightarrow \left(x' + x_0^2 \frac{d}{dx'}\right)\langle x'|0\rangle = 0$$

$$\left[\langle x'|\hat{p}|\alpha\rangle = -i\hbar \frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right]$$

with $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

The solution of this equation:

$$\langle x'|0\rangle = \frac{1}{\pi^{1/4}\sqrt{x_0}} \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

1st excited state:

$$\langle x'|1\rangle = \langle x'|a^\dagger|0\rangle$$

$$= \left(\frac{1}{\sqrt{2}x_0}\right)\left(x' - x_0^2 \frac{d}{dx'}\right)\langle x'|0\rangle.$$

$$\langle x'|2\rangle = \frac{1}{\sqrt{2}}\langle x'|a^{\dagger 2}|0\rangle = \left(\frac{1}{\sqrt{2!}}\right)\left(\frac{1}{\sqrt{2}x_0}\right)^2 \left(x' - x_0^2 \frac{d}{dx}\right)^2 \langle x'|0\rangle$$

$$\langle x'|n\rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}}\left(\frac{1}{x_0^{n+1/2}}\right)\left(x' - x_0^2 \frac{d}{dx}\right)^n \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

It is instructive to look at the expectation values of $\hat{x}^2$ and $\hat{p}^2$ for the ground state.

$$\hat{x}^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}^{+2} + \hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+}\right).$$

$$\langle 0|\hat{x}^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|\left(\hat{a}^2 + \hat{a}^{+2} + \hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+}\right)|0\rangle.$$

$$= \frac{\hbar}{2m\omega}\langle 0|\hat{a}\hat{a}^{+}|0\rangle.$$

$$= \frac{\hbar}{2m\omega}\langle 0|(a^{+}a + 1)|0\rangle = \frac{\hbar}{2m\omega_0}$$

Similarly we find.

$$\langle 0|\hat{p}^2|0\rangle = \frac{\hbar m\omega}{2}. \text{ (check)}.$$

It follows that the kinetic and potential energies are.

$$\left\langle \frac{\hat{p}^2}{2m} \right\rangle = \frac{\hbar\omega}{4} = \frac{\langle H\rangle}{2}$$

$$\left\langle \frac{m\omega^2 x^2}{2} \right\rangle = \frac{\hbar\omega}{4} = \frac{\langle H\rangle}{2}$$

It can be ~~easi~~ easily shown $\langle x\rangle = \langle p\rangle = 0$ (check).

Therefore $\langle(\Delta x)^2\rangle = \langle x^2\rangle = \frac{\hbar}{2m\omega}$.

$$\langle(\Delta p)^2\rangle = \langle p^2\rangle = \frac{\hbar m\omega}{2}$$

$$\Rightarrow \quad \langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{\hbar^2}{4} \text{ (Uncertainty relation)}$$

Spin-half systems and finite rotation:

We are now going to discuss another very important basic quantum mechanical system; i.e. the spin-$1/2$ system. It is the lowest possible dimensional system in quantum theory (2-dim).

The Pauli operators:

$$\hat{S}_x = \frac{\hbar}{2}\left(|1\rangle\langle 0| + |0\rangle\langle 1|\right).$$

$$\hat{S}_y = \frac{i\hbar}{2}\left(|0\rangle\langle 1| - |1\rangle\langle 0|\right).$$

$$\hat{S}_z = \frac{\hbar}{2}\left(|1\rangle\langle 1| - |0\rangle\langle 0|\right).$$

$|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}$; $|0\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ are the energy eigenkets

They are also the eigenvectors of $\hat{S}_z$ operator.

Sometimes (or more often) the Pauli operators are denoted without the $\hbar/2$ factor.

Important thing is to notice that the Pauli operators are not only Hermitian but also unitary. This is a unique example which can be found in dimension two. In this course, we will find that the two dimensional systems has many such unique attributes, which are absent in higher dimensions.

Consider a rotation by a finite angle ϕ about z direction. The rotated ket vector can then be given by

$$|\alpha\rangle_R = D_z(\phi)\,|\alpha\rangle$$

with $$D_z(\phi) = \exp\left(-\frac{i\hat{S}_z\phi}{\hbar}\right).$$

To see that this operator really rotates the physical system, let us look at its effect on $\langle\hat{S}_x\rangle$.

$$\langle\hat{S}_x\rangle = {}_R\langle\alpha|\hat{S}_x|\alpha\rangle_R = \langle\alpha|D_z^\dagger(\phi)\,\hat{S}_x\,D_z(\phi)|\alpha\rangle$$

We must therefore compute $D_z^\dagger(\phi)\,\hat{S}_x\,D_z(\phi)$.

For understanding, we evaluate this in two different ways.

Derivation 1:

$$D_z^\dagger(\phi)\,\hat{S}_x\,D_z(\phi) = \frac{\hbar}{2}\,e^{\frac{i\hat{S}_z\phi}{\hbar}}\left(|+\rangle\langle-| + |-\rangle\langle+|\right)e^{-\frac{i\hat{S}_z\phi}{\hbar}}$$

Now $$e^{\frac{i\hat{S}_z\phi}{\hbar}} = \cancel{\mathbb{1} + \frac{i\hat{S}_z}{\hbar} + \left(\frac{i}{\hbar}\right)^2\frac{\hat{S}_z^2}{2!} + \left(\frac{i}{\hbar}\right)^3\frac{\hat{S}_z^3}{3!} + \cdots}$$

$$= e^{i\phi/2}|1\rangle\langle 1| + e^{-i\phi/2}|0\rangle\langle 0|.$$

$$e^{-i\hat{S}_z\phi/\hbar} = e^{-i\phi/2}|1\rangle\langle 1| + e^{+i\phi/2}|0\rangle\langle 0|.$$

$$\therefore \cancel{D_z^\dagger\,\hat{S}_x\,D_z = \frac{\hbar}{2}}.$$

Therefore $D_z^{\dagger}(\phi)\, S_x\, D_z(\phi)$

$$= \frac{\hbar}{2}\left(e^{i\phi/2}|1\rangle\langle 1| + e^{-i\phi/2}|0\rangle\langle 0|\right).$$

$$\left(|1\rangle\langle 0| + |0\rangle\langle 1|\right)\left(e^{-i\phi/2}|1\rangle\langle 1| + e^{i\phi/2}|0\rangle\langle 0|\right).$$

$$= \frac{\hbar}{2}\left(e^{i\phi/2}|1\rangle\langle 0| + e^{-i\phi/2}|0\rangle\langle 1|\right).\left(e^{-i\phi/2}|1\rangle\langle 1| + e^{i\phi/2}|0\rangle\langle 0|\right)$$

$$= \frac{\hbar}{2}\left(e^{-i\phi}|0\rangle\langle 1| + e^{i\phi}|1\rangle\langle 0|\right).$$

$$= \frac{\hbar}{2}\left((\cos\phi - i\sin\phi)|0\rangle\langle 1| + (\cos\phi + i\sin\phi)|1\rangle\langle 0|\right).$$

$$= \frac{\hbar}{2}\left(\cos\phi\left(|1\rangle\langle 0| + |0\rangle\langle 1|\right) + \sin\phi\; i\left(|1\rangle\langle 0| - |0\rangle\langle 1|\right)\right)$$

$$= \cos\phi\,\hat{S}_x - \sin\phi\,\hat{S}_y.$$

Derivation 2 :

$$\exp\left(\frac{i\hat{S}_z\phi}{\hbar}\right)\hat{S}_x\exp\left(\frac{-i\hat{S}_z\phi}{\hbar}\right)$$

$$= \hat{S}_x + \left(\frac{i\phi}{\hbar}\right)\left[\hat{S}_z, \hat{S}_x\right] + \left(\frac{1}{2!}\right)\left(\frac{i\phi}{\hbar}\right)^2\left[S_z, [S_z, S_x]\right].$$

$$+ \left(\frac{1}{3!}\right)\left(\frac{i\phi}{\hbar}\right)^3\left[S_z, [S_z, [S_z, S_x]]\right] + \cdots$$

$$= \hat{S}_x\left[1 - \frac{\phi^2}{2!} + \cdots\right] - \hat{S}_y\left[\phi - \frac{\phi^3}{3!} + \cdots\right].$$

$$= \hat{S}_x\cos\phi - \hat{S}_y\sin\phi.$$

$$\langle \hat{S}_x \rangle \rightarrow \langle \hat{S}_x \rangle \cos\phi + \langle \hat{S}_y \rangle \sin\phi$$
$$\langle \hat{S}_y \rangle \rightarrow \langle \hat{S}_y \rangle \cos\phi + \langle \hat{S}_x \rangle \sin\phi$$
$$\langle \hat{S}_z \rangle \rightarrow \langle \hat{S}_z \rangle$$

→ under $\hat{S}_z$ rotation

Spin precession Revisited :

We recall the basic Hamiltonian of the problem is given by

$$\hat{H} = -\left(\frac{e}{m_e c}\right) \vec{S}.\vec{B} = \omega S_z ,$$

with $\omega = \dfrac{|e| B}{m_e c}$.

The time evolution operator based on this Hamiltonian is given by

$$\hat{U}(t,0) = \exp\left(-\frac{i\hat{H}t}{\hbar}\right) = \exp\left(-\frac{i S_z \omega t}{\hbar}\right).$$

Comparing with the previous rotation, we see.

$$\langle S_x \rangle_t = \langle S_x \rangle_0 \cos\omega t - \langle S_y \rangle_0 \sin\omega t$$
$$\langle S_y \rangle_t = \langle S_y \rangle_0 \cos\omega t + \langle S_x \rangle_0 \sin\omega t$$
$$\langle S_z \rangle_t = \langle S_z \rangle_0 .$$

after $t = \frac{2\pi}{\omega}$, spin returns to its original direction.

Let us now look at the time evolution of the state ket itself.

$$\hat{U}(t,0) = \exp\left(-\frac{i S_z \omega t}{\hbar}\right)$$

$$= \exp\left(-\frac{i\omega t}{2}\sigma_z\right) \qquad \text{with } \frac{\hbar}{2}\sigma_z = S_z .$$

$$= e^{-i\omega t/2}|1\rangle\langle 1| - e^{i\omega t/2}|0\rangle\langle 0| .$$

Now $|\alpha\rangle = |1\rangle\langle 1|\alpha\rangle + |0\rangle\langle 0|\alpha\rangle$.

$$\therefore |\alpha, t\rangle = e^{-i\omega t/2}|1\rangle\langle 1|\alpha\rangle + e^{i\omega t/2}|0\rangle\langle 0|\alpha\rangle ,$$

Expression acquires a minus sign at $t = 2\pi/\omega$ and returns to initial state at $t = 4\pi/\omega$.

Spin precission $\tau_p = 2\pi/\omega$.

Complete revolution $\tau_c = 4\pi/\omega$.

Pauli two component formalism:

Manipulations with the state kets of spin-1/2 systems can be conveniently carried out by two component spinor formalism introduced by W. Pauli in 1926.

The base kets (energy eigen kets)

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \chi_+ \; ; \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \chi_-$$

$$\langle 1| = (1, 0) = \chi_+^\dagger \; ; \quad \langle 0| = (0 \; 1) = \chi_-^\dagger$$

General state

$$|\alpha\rangle = |+\rangle\langle +|\alpha\rangle + |-\rangle\langle -|\alpha\rangle$$

$$= \begin{pmatrix} \langle +|\alpha\rangle \\ \langle -|\alpha\rangle \end{pmatrix} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

$$\langle \alpha| = \langle \alpha|+\rangle\langle +| + \langle \alpha|-\rangle\langle -|.$$

$$= (\langle \alpha|+\rangle, \langle \alpha|-\rangle) = (c_+^*, c_-^*).$$

The matrix elements $\langle 1,0|S_k|1,0\rangle$, apart from $\hbar/2$ are to be set equal to those of 2×2 matrices σ_k, known as Pauli matrices.

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; ; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; ; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$\sigma_i^2 = \mathbb{I} \; , \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij} \quad \cancel{i \neq j}$$

$$[\sigma_i, \sigma_j] = 2i\,\varepsilon_{ijk}\,\sigma_k \; .$$

Also notice that $\sigma_i^\dagger = \sigma_i$

$$\det(\sigma_i) = -1$$

$$\mathrm{Tr}(\sigma_i) = 0$$

We now consider $\vec{\sigma}.\vec{a}$ with $\vec{\sigma}$ be a 3 dimensional vector.

$$\vec{\sigma}.\vec{a} = \sum_k \sigma_k a_k = \begin{pmatrix} a_3 & a_1 - ia_2 \\ a_1 + ia_2 & -a_3 \end{pmatrix}.$$

There is also very important identity

$$(\vec{\sigma}.\vec{a})(\vec{\sigma}.\vec{b}) = \vec{a}.\vec{b} + i\,\vec{\sigma}.(\vec{a}\times\vec{b}).$$

Proof: $\sum_j \sigma_j a_j \sum_k \sigma_k b_k$

$$= \sum_{jk} (\sigma_j \sigma_k a_j b_k) = \frac{1}{2}\sum_{jk} (\sigma_j \sigma_k a_j b_k + \sigma_k \sigma_j a_j b_k + \sigma_j \sigma_k a_j b_k - \sigma_k \sigma_j a_j b_k).$$

$$= \sum_{jk} \left(\frac{1}{2}\{\sigma_j, \sigma_k\} + \frac{1}{2}[\sigma_j, \sigma_k]\right) a_j b_k$$

$$= \sum_{jk} (\delta_{jk} a_j b_k + i\varepsilon_{jkl}\sigma_l a_j b_k).$$

$$= \vec{a}.\vec{b} + i\,\vec{\sigma}.(\vec{a}\times\vec{b}).$$

(Proved).

Rotation in two component formalism

The rotation matrix.

$$D(\hat{n}, \phi) = \exp\left(-\frac{i\,\hat{S}.\hat{n}\,\phi}{\hbar}\right).$$

$$= \exp\left(-\frac{i\,\vec{\sigma}.\hat{n}\,\phi}{2}\right).$$

using $(\vec{\sigma}.\hat{n})^n = \begin{cases} 1 & \text{for } n \text{ even} \\ \vec{\sigma}.\hat{n} & \text{for } n \text{ odd} \end{cases}$.

Therefore

$$\exp\left(-i\frac{\vec{\sigma}.\hat{n}\,\phi}{2}\right) = \left[1 - \frac{(\vec{\sigma}.\hat{n})^2}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{(\vec{\sigma}.\hat{n})^4}{4!}\left(\frac{\phi}{2}\right)^4 - \cdots\right]$$

$$- i\left[(\vec{\sigma}.\hat{n})\frac{\phi}{2} - \frac{(\vec{\sigma}.\hat{n})^3}{3!}\left(\frac{\phi}{2}\right)^3 + \cdots\right].$$

$$= \cos\frac{\phi}{2}\,\mathbb{I} - i\,\vec{\sigma}.\hat{n}\,\sin\left(\frac{\phi}{2}\right).$$

$$= \begin{pmatrix} \cos\phi/2 - i n_z \sin\phi/2 & -(n_x + n_y)\sin\phi/2 \\ -(i n_x - n_y)\sin\phi/2 & \cos\phi/2 + i n_z \sin\phi/2 \end{pmatrix}$$

Postulates of Quantum mechanics :

1. A physically isolated system is associated with a Hilbert space called the state space. The system, at a particular time is completely described by a unit vector in this Hilbert space.

2. The evolution, described by a Hamiltonean $\hat{H}$, which is a hermitian operator, is governed by the Schrödinger equation.

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

2a. A closed quantum system evolves unitarily.

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

3. A state can be measured by measurement operators $\{M_i\}$, where M_is are the projection operators with the idempotent property $M_i^2 = I$ and $M_i M_j = 0 \ \forall i \neq j$

specifically $M_i = |i\rangle\langle i|$.

4. Observables are identified as the Hermitian operators acting on the Hilbert space.

5. The average value of any observable is given by the expectation value

$$\frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle}$$

6. The set of eigenvectors of an observable $\hat{O}$ will form a complete set of linear eigenvectors.

7. The probability of finding a particle in a given state $|\psi\rangle$ is given by the inner product $\langle \psi | \psi \rangle$.