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 operators, the orthogonality of different eigenkets were proved on the basis of non-degeneracy.

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

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

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

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

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

$$[\because \hat{A}|a'\rangle = a'|a'\rangle]$$

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~~ 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 $\sum_{a'} |C_{a'}|^2 = 1$.

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

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

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

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

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

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

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

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

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

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

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

Therefore,

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

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 $\left.\begin{aligned} U|1\rangle &= |+\rangle \\ U|0\rangle &= |-\rangle \end{aligned}\right\}$ (check).

Therefore this operator takes ~~$|+\rangle$~~ $|1\rangle$ 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

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

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

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

U is ~~a~~ unitary operator.

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

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

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 $\hat{X}$.

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

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

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

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

$$\begin{aligned}
Tr(\hat{X}) &= \sum_{a'} \langle a'|\hat{X}|a'\rangle \\
&= \sum_{a' b' b''} \langle a'|b'\rangle \langle b'|\hat{X}|b''\rangle \langle b''|a'\rangle \\
&= \sum_{b', b''} \langle b''|\Big(\sum_{a'} |a'\rangle\langle a'|\Big)|b'\rangle \langle b'|\hat{X}|b''\rangle \\
&= \sum_{b' b''} \langle b''|b'\rangle \langle b'|\hat{X}|b''\rangle \\
&= \sum_{b'} \langle b'|\hat{X}|b'\rangle .
\end{aligned}$$

(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):

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

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

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

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

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

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

Diagonalization:

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

This problem is the equivalent 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.

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

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

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