Density matrix theory.

Till now, we have seen that a quantum mechanic state can be described by a vector in the Hilbert space, known as the ket vector. $|\psi\rangle$.

Here we are going to generalize this concept by introducing Density matrices.

To do so, first we are going to replace the state vector $|\psi\rangle$ by a matrix in the following way.

$$|\psi\rangle \longrightarrow |\psi\rangle\langle\psi| := \rho_\psi .$$

Both these representations are physically same, though mathematically a little different.

Consider now a state is changed by an unitary evolution $U : \rightarrow |\psi(t)\rangle = U(t,0)|\psi\rangle$.

In the matrix representation, the same evolution is given by

$$|\psi\rangle \xrightarrow{U(t,0)} |\psi(t)\rangle$$

$$|\psi\rangle\langle\psi| \xrightarrow{U(t,0)} |\psi(t)\rangle\langle\psi(t)|$$

$$= U|\psi\rangle\langle\psi|U^\dagger .$$

$$= U\rho_\psi U^\dagger .$$

Let us now consider Hermitian operators and expectation values.

$$\hat{O}|\psi\rangle = |\phi\rangle.$$

Expectation value :- $\langle \hat{O} \rangle_\psi = \langle \psi | \hat{O} | \psi \rangle.$

$$= \langle \psi | \hat{O} | \psi \rangle \langle \psi | \psi \rangle.$$

$$= \langle \psi | \hat{O} (|\psi\rangle\langle\psi|) | \psi \rangle.$$

Generally speaking, say $\{|\psi_i\rangle\}$ forms a ortho-normal set of ket vectors.

Then $\langle \hat{O} \rangle = \sum_{ij} \langle \psi_j | \hat{O} | \psi_i \rangle \langle \psi_i | \psi_j \rangle.$

$$= \mathrm{Tr}(\hat{O} \rho_{\psi_i}).$$

Mixed and pure states :

Pure state : $\rightarrow |\psi\rangle\langle\psi|$ (projection operators).

$$\rho_\psi = |\psi\rangle\langle\psi|.$$

Properties : $\rho_\psi^2 = \rho_\psi . \rho_\psi = |\psi\rangle\langle\psi||\psi\rangle\langle\psi|$

$$= \rho_\psi. \text{ (Idempotent).}$$

Alternatively we can say, pure states are rank 1 positive matrices (Explain later).

Mixed states :- probabilistic combination of pure states.

Example : Lets say $\{|\psi_i\rangle\}$ forms an orthonormal set of ~~ket~~ complete ket vectors.

Each of those $|\psi_i\rangle$ s are individual pure states. $|\psi_i\rangle\langle\psi_i|$

Now consider the following matrix.

$$\rho = p|\psi_1\rangle\langle\psi_1| + (1-p)|\psi_2\rangle\langle\psi_2|.$$

$p \to$ probability $(0 \leq p \leq 1)$.

Now we have.

$$\rho^2 = \rho.\rho = \left(p|\psi_1\rangle\langle\psi_1| + (1-p)|\psi_2\rangle\langle\psi_2|\right).\left(p|\psi_1\rangle\langle\psi_1| + (1-p)|\psi_2\rangle\langle\psi_2|\right).$$

$$= p^2|\psi_1\rangle\langle\psi_1| + (1-p)^2|\psi_2\rangle\langle\psi_2|$$

$$\neq \rho.$$

Observe that : $\mathrm{Tr}\,\rho = p + (1-p) = 1.$

But $\mathrm{Tr}\,\rho^2 = p^2 + (1-p)^2 < 1.$

It can only be 1, when $p = 0, 1$. when the ~~densi~~ mixed state reduces to a pure state $|\psi_1\rangle\langle\psi_1|$ or $|\psi_2\rangle\langle\psi_2|$.

What is the point ?

Mixed state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ incorporates the probabilistic mixture of different pure states.

For a pure state $|\psi_i\rangle\langle\psi_i|$, we are certain that the the particle is in a particular state $|\psi_i\rangle$.

For a mixed state $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, we are not certain anymore.

The paritiicle ~~bed~~ can be in a certain eigen state $|\psi_i\rangle$ with a probability p_i.

This is a considerable reduction of knowledge. (or loss of information).

This can be understood as incorporation of noise.

It is like a frequency represented by $|\psi_1\rangle\langle\psi_1|$ is intercepted by other frequencies $|\psi_2\rangle\langle\psi_2|$, $|\psi_3\rangle\langle\psi_3|$ etc.

Since in a practical situation, a quantum system is alway subjected to external influences and noise, a mixed state is much more realistic representation of the very state.

Understanding expectation values.

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We have seen that expectation value on

$$\langle \hat{O} \rangle_\psi = \langle \psi_i | \hat{O} | \psi_i \rangle ,$$

where $|\psi_i\rangle$ is a pure state.

Now for a mixed state, the expectation value should also be a probabilistic mixture of different eigenstates:

$$\langle \hat{O} \rangle_\rho = \sum_i P_i \langle \psi_i | \hat{O} | \psi_i \rangle .$$

where $\rho = \sum P_i |\psi_i\rangle\langle\psi_i|$.

Therefore $\langle \hat{O} \rangle_\rho = \sum_{i,j} \langle \psi_j | \hat{O} | (P_i |\psi_i\rangle\langle\psi_i|) | \psi_j \rangle$

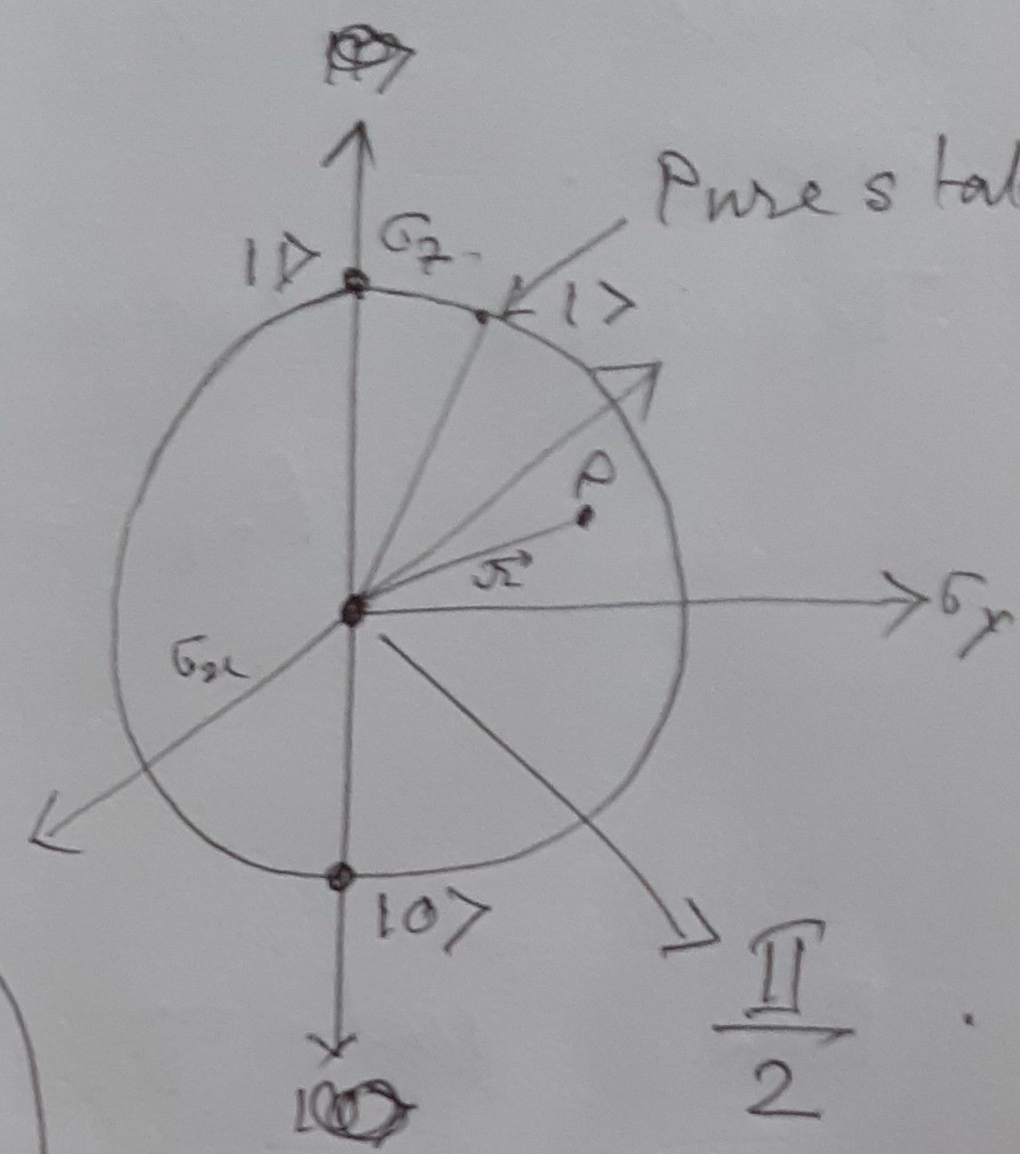
$$= Tr(\hat{O}\rho) = \sum_i P_i \langle \psi_i | \hat{O} | \psi_i \rangle$$

As we know that, trace is independent of basis, we can choose any other orthonormal basis also.

(Prove it).

Bloch sphere representation: (of a qubit)

A general two qubit state:



$$\rho = \frac{1}{2}\left(\mathbb{I} + \vec{\Omega}\cdot\vec{\sigma}\right).$$

$$\vec{\Omega}\cdot\vec{\sigma} = \Omega_1\sigma_1 + \Omega_2\sigma_2 + \Omega_3\sigma_3.$$

$$= \begin{pmatrix} 0 & \Omega_1 \\ \Omega_1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i\Omega_2 \\ i\Omega_2 & 0 \end{pmatrix} + \begin{pmatrix} \Omega_3 & 0 \\ 0 & -\Omega_3 \end{pmatrix}.$$

$$= \begin{pmatrix} \Omega_3 & \Omega_1 - i\Omega_2 \\ \Omega_1 + i\Omega_2 & -\Omega_3 \end{pmatrix}$$

$$\rho = \begin{pmatrix} \frac{1+\Omega_3}{2} & \frac{\Omega_1 - i\Omega_2}{2} \\ \frac{\Omega_1 + i\Omega_2}{2} & \frac{1-\Omega_3}{2} \end{pmatrix}.$$

$0 \leq |\vec{\Omega}| \leq 1$

↳ Radius of the bloch sphere when equal to unity.

$|\vec{\Omega}| = 0 \Rightarrow \rho = \mathbb{I}/2$ → Maximally Mixed state.

Maximally mixed state means even probability distribution of of complete basis ~~vect~~ states.

We know $\mathbb{I} = \sum_i |v_i\rangle\langle v_i|$

where $\{|v_i\rangle\} \rightarrow$ Complete orthonormal basis.

Therefore Maximally mixed state.

$$\rho_M = \frac{1}{d}\sum_i |v_i\rangle\langle v_i|$$

$\hookrightarrow$ dimension of the Hilbert space.

For qubit

$$\rho_M = \frac{\mathbb{I}}{2} = \frac{1}{2}|1\rangle\langle 1| + \frac{1}{2}|0\rangle\langle 0|.$$

$$= \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -|.$$

$$= \frac{1}{2}|\psi^+\rangle\langle\psi| + \frac{1}{2}|\psi^-\rangle\langle\psi^-|.$$

Now when $|\vec{r}| = 1 \rightarrow$ the corresponding state is over the surface of the Bloch sphere, i.e. a pure state.

Proof :

For a pure state $\quad \mathrm{Tr}\,\rho^2 = 1 = \mathrm{Tr}(\rho)$.

$$\rho = \frac{1}{2}\begin{pmatrix} 1+r_3 & r_1 - ir_2 \\ r_1 + ir_2 & 1-r_3 \end{pmatrix}$$

$$\rho^2 = \frac{1}{4}\begin{pmatrix} 1+r_3 & r_1 - ir_2 \\ r_1 + ir_2 & 1-r_3 \end{pmatrix}\begin{pmatrix} 1+r_3 & r_1 - ir_2 \\ r_1 + ir_2 & 1-r_3 \end{pmatrix}$$

$$= \frac{1}{4}\begin{pmatrix} (1+r_3)^2 + r_1^2 + r_2^2 & 0 \cdots \\ 1 \cdots & (1-r_3)^2 + r_1^2 + r_2^2 \end{pmatrix}$$

$$\mathrm{Tr}\,\rho^2 = \frac{(1+r_3)^2 + (1-r_3)^2 + 2(r_1^2 + r_2^2)}{4} = 1$$

$$\Rightarrow \quad 2 + 2r_3^2 + 2r_1^2 + 2r_2^2 = 4$$

$$\Rightarrow \quad \boxed{r_1^2 + r_2^2 + r_3^2 = 1}$$

$$\Rightarrow \quad |\vec{r}| = 1.$$

Why $|\vec{r}| \not> 1$?

For a matrix to be a valid density matrix, it has to be positive semidefinite

Therefore $\rho = \frac{1}{2}\begin{pmatrix} 1+r_3 & r_1 - ir_2 \\ r_1 + ir_2 & 1-r_3 \end{pmatrix} \geq 0$

For that, diagonal elements has to be positive and determinant has to be positive for 2×2 matrix (Sylvester criteria).

Diagonal element positive $\Rightarrow 0 \leq r_3 \leq 1$

Determinant positive $\Rightarrow$

$$(1+r_3)(1-r_3) - (r_1+ir_2)(r_1-ir_2) \geq 0$$

$$\Rightarrow \quad 1 - r_3^2 - r_1^2 - r_2^2 \geq 0$$

$$\Rightarrow \quad r_1^2 + r_2^2 + r_3^2 \leq 1$$

$$\Rightarrow \quad |\vec{r}| \leq 1 .$$

Rotation operators about the Bloch sphere:

$$R_{\vec{\Omega}}(\theta) = \exp\left(-\theta\,\hat{\Omega}\cdot\vec{\sigma}/2\right).$$

$$\hat{\Omega} = \frac{\vec{\Omega}}{|\vec{\Omega}|}.$$

Rotation about z-axis $\rightarrow$.

$$R_z(\theta) = \exp\left(-\frac{i\theta\,\sigma_z}{2}\right).$$

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

$$= \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}.$$

Rotation about x axis $\rightarrow$.

$$R_x(\theta) = \exp\left(-\frac{i\theta\,\sigma_x}{2}\right).$$

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

$$\left(|\pm\rangle = \frac{|1\rangle \pm |0\rangle}{\sqrt{2}}\right).$$

$$= \begin{pmatrix} \cos\theta/2 & -i\sin\theta/2 \\ i\sin\theta/2 & \cos\theta/2 \end{pmatrix}.$$

Tensor product:

Tensor product of two matrices with example :-

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}.$$

$$A \otimes B = \begin{pmatrix} a_{11} B & a_{12} B \\ a_{21} B & a_{22} B \end{pmatrix}.$$

$$= \begin{pmatrix} a_{11}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{12}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ a_{21}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} & a_{22}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \end{pmatrix}.$$

$$= \begin{pmatrix} a_{11} b_{11} & a_{11} b_{12} & a_{12} b_{11} & a_{12} b_{12} \\ a_{11} b_{21} & a_{11} b_{22} & a_{12} b_{21} & a_{12} b_{22} \\ a_{21} b_{11} & a_{21} b_{12} & a_{22} b_{11} & a_{22} b_{12} \\ a_{21} b_{21} & a_{22} b_{22} & a_{22} b_{21} & a_{22} b_{22} \end{pmatrix}$$

Show that $A \otimes B \neq B \otimes A$

Tensor product of two vectors:

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} ; \quad |b\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$$

$$|a\rangle \otimes |b\rangle = \begin{pmatrix} a_1 \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \\ a_2 \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{pmatrix}.$$

What does tensor product structure signifies for quantum systems?

Tensor product structure is needed in quantum mechanics, when we consider two or more different quantum systems at a time.

This total system ~~sys~~ consisting of two or more individual quantum systems is called a composite quantum system.

The most simple of any composite quantum system is called a bi-partite quantum systems, consisting of two separate quantum systems.

We will restrict ourselves in the bi-partite scenario only

Let us consider two separate quantum system represented by density matrices ρ_A and ρ_B.

Then the composite quantum system

$$\rho_{AB} = \rho_A \otimes \rho_B$$ will be called a product state. A product state is called completely uncorrelated, because there is no connection between them whatsoever. They are completely independent of each other.

Separable state.

Now consider the following bi-partite quantum state

$$\rho_{AB} = p\, \rho_A^{(1)} \otimes \rho_B^{(1)} + (1-p)\, \rho_A^{(2)} \otimes \rho_B^{(2)}$$

It is nothing but a convex combination (probabilistic combination) of two product states. But they are not completely uncorrelated any more. There is a correlation present between A and B systems via the probabilis combination.

Separable states: When a composite quantum state can be represented by a probabilistic combination of product states, it is called a separable state.

$$\rho_{AB} = \sum_i p_i\, \rho_A^{(i)} \otimes \rho_B^{(i)}.$$

But still the state is not "entangled".

Entanglement is a special type of correlation, which cannot be realised by any local representation.

Definition: A composite quantum system will be called entangled, when it cannot be presented by the separable representation $\rho_{AB} = \sum_i p_i \rho_A^{(i)} \otimes \rho_B^{(i)}$.

Example from two qubit pure states:

The state $|a\rangle = |0\rangle \otimes |0\rangle = |00\rangle$

is product.

The state $|b\rangle = \frac{1}{2}(|00\rangle + |11\rangle + |01\rangle + |10\rangle)$

$$= \frac{1}{2}(|0\rangle \otimes (|0\rangle + |1\rangle) + |1\rangle \otimes (|0\rangle + |1\rangle)$$

$$= \frac{(|0\rangle + |1\rangle)}{\sqrt{2}} \otimes \frac{(|0\rangle + |1\rangle)}{\sqrt{2}}$$

is also product.

But the following states:

$$\left.\begin{array}{l} \dfrac{|00\rangle \pm |11\rangle}{\sqrt{2}} \\[2ex] \dfrac{|01\rangle \pm |10\rangle}{\sqrt{2}} \end{array}\right\} \text{Bell states}$$

are entangled.

Note: There are no separable states in pure states only product and entangled

Partial trace and Partial measurements:

When we consider a composite quantum system, the parts of which are possibly separated by a great distance, we need to understand the concept of local and global.

We know that two things can be done with a quantum system → a) unitary evolution, b) measurements.

Partial trace:

We know $Tr(\hat{A}) = \sum_i \langle v_i | \hat{A} | v_i \rangle$;

where $\{|v_i\rangle\}$ forms a complete orthonormal basis vectors.

Here $\hat{A}$ is an operator corresponding to the Hilbert space where $\{|v_i\rangle\}$ is contained.

i.e. $\{|v_i\rangle\}$ is contained in d dimensional Hilbert space, then $\hat{A}$ is a $d \times d$ dimensional square matrix.

Now consider an operator $\hat{O}_{AB}$ corresponding to the tensor product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. Here A and B are two parties of the bipartite system AB.

Then partial trace over B part is

$$Tr_B(\hat{O}_{AB}) = \sum_i I \otimes {}_B\langle v_i | \hat{O}_{AB} | I \otimes | v_i \rangle_B .$$

Example for 2×2 system.

Consider a 2×2 dimensional quantum system with density matrix

$$\rho_{AB} = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{12} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix}.$$

Partial trace over B system the reduced density matrix of A part.

$$\rho_A = Tr_B(\rho_{AB})$$

$$= \mathbb{I} \otimes \langle 1| \rho_{AB} \mathbb{I} \otimes |1\rangle + \mathbb{I} \otimes \langle 0| \rho_{AB} | \mathbb{I} \otimes |0\rangle.$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{bmatrix} \rho_{AB} \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$+ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{bmatrix} \quad \end{bmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$+ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \rho_{11} & \rho_{13} \\ \rho_{21} & \rho_{23} \\ \rho_{31} & \rho_{33} \\ \rho_{41} & \rho_{43} \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \rho_{12} & \rho_{14} \\ \rho_{22} & \rho_{24} \\ \rho_{32} & \rho_{34} \\ \rho_{42} & \rho_{44} \end{pmatrix}$$

$$= \begin{pmatrix} \rho_{11} & \rho_{13} \\ \rho_{31} & \rho_{33} \end{pmatrix} + \begin{pmatrix} \rho_{22} & \rho_{24} \\ \rho_{42} & \rho_{44} \end{pmatrix}$$

$$= \begin{pmatrix} \rho_{11}+\rho_{22} & \rho_{13}+\rho_{24} \\ \rho_{31}+\rho_{42} & \rho_{33}+\rho_{44} \end{pmatrix}.$$

$$\mathrm{Tr}\,\rho_A = \rho_{11}+\rho_{22}+\rho_{33}+\rho_{44} = \mathrm{Tr}\,\rho_{AB}.$$

Similarly

$$\mathrm{Tr}_A\,\rho_{AB} = \rho_B = \sum_i \langle v_i | \otimes \mathbb{I}\, \rho_{AB}\, | v_i \rangle \otimes \mathbb{I}.$$

Partial trace of product state

=

$$\rho_{AB} = \rho_A \otimes \rho_B.$$

$$\mathrm{Tr}_B\,\rho_{AB} = \rho_A \times \mathrm{Tr}\,\rho_B = \rho_A \quad [\because \mathrm{Tr}\,\rho_B = 1].$$

$$\mathrm{Tr}_A\,\rho_{AB} = \mathrm{Tr}\,\rho_A \times \rho_B = \rho_B.$$

Partial trace of separable states:

$$\rho_{AB} = p\,\rho_A^{(1)} \otimes \rho_B^{(1)} + (1-p)\,\rho_A^{(2)} \otimes \rho_B^{(2)}.$$

$$\mathrm{Tr}_B\,\rho_{AB} = p\,\rho_A^{(1)} \times \mathrm{Tr}(\rho_B^{(1)}) + (1-p)\,\rho_A^{(2)} \times \mathrm{Tr}\,\rho_B^{(2)}$$

$$= p\,\rho_A^{(1)} + (1-p)\,\rho_B^{(2)}.$$

Partial measurement:

Consider POVM $M_i^B \geq 0$

$$\sum_i M_i^B = \mathbb{I}$$

Partial measurement.

$$\left(\mathbb{I} \otimes M_i\,\rho_{AB}\right).$$

Post measurement state.

$$\rho'_{AB} = \frac{\mathbb{I} \otimes A_i\,\rho_{AB}\,\mathbb{I} \otimes A_i^{\dagger}}{\mathrm{Tr}\left(\mathbb{I} \otimes A_i\,\rho_{AB}\,\mathbb{I} \otimes A_i^{\dagger}\right)}.$$

where $M_i = A_i^{\dagger} A_i$.