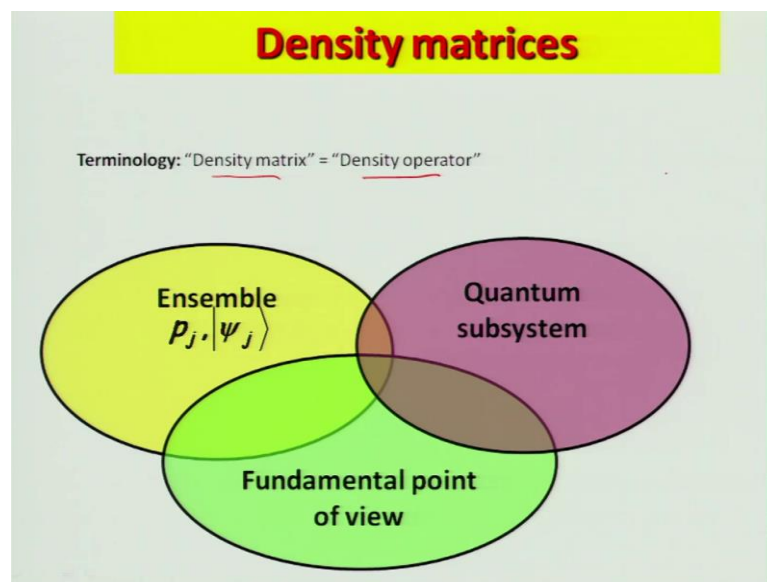


**Implementation Aspects of Quantum Computing**  
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**Lecture – 35**  
**Understanding the Ensemble of Qubits from Density Matrix**

We have been looking at density matrices, as it is 1 of the most important aspects that helps us in implementing quantum computing and quantum information processing. And in the first lecture of this week we have looked at some of the basic fundamentals of density matrices which have been implicitly use by us, but it was important for us to start off on this area to make sure that the understanding is complete in this field.

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So, on going forward we want to just ensure that we are in this topic of density matrix where we are using reversibly the terminology of density operator as the same as density matrix. And we are looking at statistical ensemble where the quantum sub system these being treated with some probability of the way functions that essentially create the subsystem quantum sub system. And this is a very fundamental point of view as it enables us to understand the system even though we have we have difficulty in gaining information about it.

So, in some sense for pure states, we know that we can find out the expectation value of the system by applying; it helps us to know about the system even though we have very little knowledge about the system.

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**More examples of density matrices**

The *density matrix* of the mixed state  $(|\psi_1\rangle, p_1), (|\psi_2\rangle, p_2), \dots, (|\psi_d\rangle, p_d)$  is:

$$\rho = \sum_{k=1}^d p_k |\psi_k\rangle\langle\psi_k|$$

**Examples (from previous lecture):**

1. & 2.  $|0\rangle + |1\rangle$  and  $-|0\rangle - |1\rangle$  both have

3.  $\begin{cases} |0\rangle \text{ with prob. } \frac{1}{2} \\ |1\rangle \text{ with prob. } \frac{1}{2} \end{cases}$

4.  $\begin{cases} |0\rangle + |1\rangle \text{ with prob. } \frac{1}{2} \\ |0\rangle - |1\rangle \text{ with prob. } \frac{1}{2} \end{cases}$

6.  $\begin{cases} |0\rangle \text{ with prob. } \frac{1}{4} \\ |1\rangle \text{ with prob. } \frac{1}{4} \\ |0\rangle + |1\rangle \text{ with prob. } \frac{1}{4} \\ |0\rangle - |1\rangle \text{ with prob. } \frac{1}{4} \end{cases}$

$$\rho = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\rho = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

So, going ahead with this principle of the density matrices; here are some of the examples that we have been starting to look at. The density matrix of mixed state can be written as a sum total of the in a product and the probability of observing that particular state.

From previous lecture we have few examples that we had looked at; a super position of 2 states whether they have a face factor would give rise to the same way density matrix. So, whether it is ket 0 plus ket 1 or ket minus 0 minus ket 1 both of them will have the same density matrix. Similarly with ket 0 and ket 1 with probability half, ket 0 and ket 1 with probability half super position of ket 0 and 1 with probability half, super position when the in mutual sin is minus with probability half versus a super position of ket 0 ket 1 0 plus 1 and 0 minus 1 each of probability quarter will all have the same density matrix half 1 0.

So, given this definition when we look at these different density matrices we realise that the properties of these 2 are indistinguishable as per as the density matrix is concerned. Similarly, the properties of all these sets combinations where all of them could occur having a total density matrix which can be given rise as a result of any of these 3

combinations 3 4 and 6 will all have the same density matrix. However, when they all have the same density matrices they cannot be having distinguishable property in terms of density matrices. So, all the properties (Refer Time: 04:15) density matrices would only work on the rho and as such all the 3 cases; 3, 4 and 6 will behave similarly.

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**More examples of density matrices**

Examples (continued):

5.  $\begin{cases} |0\rangle & \text{with prob. } \frac{1}{2} \\ |0\rangle + |1\rangle & \text{with prob. } \frac{1}{2} \end{cases}$

has:  $\rho = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} = \begin{bmatrix} 3/4 & 1/2 \\ 1/2 & 1/4 \end{bmatrix}$

7. The first qubit of  $|01\rangle - |10\rangle$

Again a case where we have ket 0 with probability half and ket 0 and 1 with probability half would have a density matrix, which would be given by rho half this plus rho half of each of them half of which give rise to a total density matrix of this kind. Now these all these individual density matrices say and this particular density matrix, they are all distinct and they will all be possibility be distinguished. And similarly taken all be looked at a independently and they will have different values.

We can also have another way of looking at density matrices. For example, if we have a combination where we have a state which is mix of 2 different super positions states, and in that case if we are measuring one of the qubits say we measure the first qubit of this combination, then the first qubit probabilities which will be 0 will be will becoming only form here and first qubit of this which will be having a probability of 1 will only come from this contribution.

So, they will have distinct contribution. We have actually dealt with these kinds of cases earlier, when we were discussing the aspects of implementation and developing the principle of quantum information and computing. So, they all very relevant and it is

important to note that in most cases the information of anything which is not pure can only be determined when we are looking at the density matrices.

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**To Remember:** Three Properties of Density Matrices

$$\rho = \sum_{k=1}^d p_k |\psi_k\rangle\langle\psi_k|$$

**Three properties of  $\rho$ :**

- $\text{Tr}\rho = 1$  ( $\text{Tr}M = M_{11} + M_{22} + \dots + M_{dd}$ )
- $\rho = \rho^\dagger$  (i.e.  $\rho$  is Hermitian) —
- $\langle\phi|\rho|\phi\rangle \geq 0$ , for all states  $|\phi\rangle$

Moreover, for **any** matrix  $\rho$  satisfying the above properties, there **exists a probabilistic mixture** whose density matrix is  $\rho$ .

So, there are 3 properties of density matrix which are important; which is that trace of rho is going to be 1 always, which means that it is a normalized case and that is because the trace of the density matrices essentially the total probability of the system. So, it is a sum total of the diagonal elements, it is the density matrices going to be Hermitian always.

The projection of the density matrix along any of the composite states will always be either 0 or more than 0. Essentially stating that the projection of the density operator any of the states that constitute the density matrix is either going to be 0 or more than 0 as that they represent the probability of the occurrence of or the weight age factor of the contributing state. Moreover for any density matrix rho satisfying the ever properties there exist a probabilistic mixture whose density matrix is rho.

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**Use of Density Matrix and Trace to Calculate the probability of obtaining state in measurement**

If we perform a **Von Neumann measurement** of the state  $\rho = |\psi\rangle\langle\psi|$  with respect to a basis containing  $|\phi\rangle$ , the probability of obtaining  $|\phi\rangle$  is

$$|\langle\psi|\phi\rangle|^2 = \text{Tr}(\rho|\phi\rangle\langle\phi|)$$

This is for a pure state.  
How it would be for a mixed state?

So, we can use density matrices and trace to calculate the probability of obtaining state in measurement. So, if we perform a Von Neumann measurement of the state rho with respect to a basis containing get phi.

The probability of obtaining get phi is given by bracket of psi rho square, which is the probability and that happens to be the trace of rho times in a product of phi. Now this is for a pure state, this is the definition for a pure state question could be how it would be for a mixed state and as we have discussed in the last class it will be the same.

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**Use of Density Matrix and Trace to Calculate the probability of obtaining state in measurement (now for measuring a mixed state)**

If we perform a **Von Neumann measurement** of the state  $\{(q_k, |\psi_k\rangle)\}$  wrt a basis containing  $|\phi\rangle$  the probability of obtaining  $|\phi\rangle$  is

$$\sum_k q_k |\langle\psi_k|\phi\rangle|^2 = \sum_k q_k \text{Tr}(|\psi_k\rangle\langle\psi_k| |\phi\rangle\langle\phi|)$$
$$= \text{Tr}\left(\sum_k q_k |\psi_k\rangle\langle\psi_k| |\phi\rangle\langle\phi|\right)$$
$$= \text{Tr}(\rho|\phi\rangle\langle\phi|)$$

The same state

So, this we have looked at in the last class this is just to remind you that essentially it is the same thing. So, if we use the density matrix and trace to calculate the probability of obtaining the state in the measurement, we basically for measuring the making the measurement for a mixed state, it will be the same he will always get the same state. So, if you perform a Von Neumann measurement of the state with respect to the basis containing  $\phi$  get, the probability obtaining the  $\phi$  get is going to be given by same probability which is the outer products square time it is a weightage and we can get the trace reduce to the same function same form as we had for the pure state.

Which means that this is a is one of the biggest achievements of density matrix is that it enables us to look at mixed state in the same mixed state and provide information which is otherwise so difficult to get.

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### **Conclusion: Density Matrix Has Complete Information**

In other words, the density matrix contains all the information necessary to compute the probability of any outcome in any future measurement.

Conclusions that we have achieved as a result of discussions that we did in the last lecture and now is that the density matrix has the complete information and otherwise the density matrix contains the information necessary to compute the probability of any outcome in any future experiments.

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### Spectral decomposition can be used to represent a useful form of density matrix

- Often it is convenient to **rewrite** the density matrix as a **mixture of its eigenvectors**
- Recall that **eigenvectors with distinct eigenvalues are orthogonal**;
  - for the **subspace of eigenvectors with a common eigenvalue ("degeneracies")**, we can **select an orthonormal basis**

So, spectral decomposition can be used to representing useful form of the density matrix; often it is convenient to rewrite the density matrix as a mixture of eigenvectors. Eigenvectors with distinct eigenvalues are orthonormal that is one of the fundamental requirements of quantum mechanics.

For the subspace of eigenvectors with a common eigenvalue, which are degeneracies we can select an orthonormal cases.

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### Continue - Spectral decomposition used to diagonalize the density matrix

- In other words, **we can always "diagonalize"** a density matrix so that it is written as

$$\rho = \sum_k p_k |\varphi_k\rangle\langle\varphi_k|$$

where  $|\varphi_k\rangle$  is an **eigenvector** with **eigenvalue**  $p_k$  and  $\{|\varphi_k\rangle\}$  forms an orthonormal basis

In other words we can always diagonalize a density matrix. So, that it is written in terms of this form where  $\phi_k$  get is the eigenvector with eigenvalues of  $P_k$  and  $\phi_k$  set forms an orthonormal basis. So, this is basically the definition of density matrix which we have been following. It is a very useful definition because this is one of the ways to get information of states which I have otherwise not possible as we have been discussing.

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**Review: Outer product notation**

Let  $|\psi\rangle$  and  $|\phi\rangle$  be vectors.

Define a linear operation (matrix)  $|\psi\rangle\langle\phi|$  by  
 $|\psi\rangle\langle\phi|(|\gamma\rangle) = |\psi\rangle\langle\phi|\gamma\rangle$

**Example:**  $|1\rangle\langle 0|(\alpha|0\rangle + \beta|1\rangle) = |1\rangle\alpha = \alpha|1\rangle$

**Connection to matrices:**  
 If  $|a\rangle = \sum_j a_j |j\rangle$ , and  $|b\rangle = \sum_j b_j |j\rangle$  then  $|a\rangle\langle b| = b_k^* |a\rangle$ .

But  $\begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} \begin{bmatrix} b_1^* & b_2^* & \dots \end{bmatrix} \begin{bmatrix} \vdots \\ 1 \\ \vdots \end{bmatrix} = b_k^* |a\rangle$ .

Thus  $|a\rangle\langle b| = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} \begin{bmatrix} b_1^* & b_2^* & b_3^* \end{bmatrix}$ .

As we remember, this is a matrix, we showed how to calculate it

So, we have been using the notation of the matrix notation as well as the vector notations interchangeably. So, it is important to have a small review of the product notations here. So, this is an outer product notation where we show how the wave function  $\psi$  get and  $\phi$  get which have vectors, and if we define a linear operation matrix by this form which is more commonly also known as the outer product notation, then we get his particular form where you can write it out, and in the simplest form we can essentially get a projection or get the contribution of the particular state in the super position.

And this can be connected to the matrices by utilizing the fact that these are connected by using their coefficients and that can be written in this kind of a form in bra versus the ket forming the rho versus the column matrices; so the rho is the ket and the bra is the column and by utilizing these principles we can actually write out that the outer product of 2 vectors a and b is simply the multiplication of a column matrix with a rho matrix. The bra being the rho matrix which is the, and get being the column matrix and the bra being the one which is complex conjugate notation.



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**Outer product notation**

**Example:**  $|0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$

**Example:**  $|1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$

**Example:**  $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$

**Example:**  $|0\rangle\langle 1| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

**Example:**  $|1\rangle\langle 0| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$

**Example:**  $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0|$

So, when we use this outer product notation we are able to get these different examples where we can see that the 0 0 is a diagonal matrix of 1 0 versus 1 1 is a diagonal matrix of 0 1, and we can have operations which would essentially mean the gate.

So for instances, Z gate is nothing but in operation where we have the outer product 0 0 of and minus of outer product 1 1 would give rise to the j ket; the outer product of 0 and 1 would give rise to the half diagonal element and similarly the one with 1 and 0 would give the other of diagonal element and that way we can also have the X ket which can be the super position of the 0 1 and 1 0. So, the X ket could be the super position of 0 1 and 1 0 inner products.

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## Outer product notation

One of the advantages of the outer product notation is that it provides a convenient tool with which to describe projectors, and thus quantum measurements.

**Recall:** The projector  $P$  onto  $\text{sp}(|e_1\rangle, |e_2\rangle)$  acts as

$$P(\alpha|e_1\rangle + \beta|e_2\rangle + \gamma|e_3\rangle) = \alpha|e_1\rangle + \beta|e_2\rangle$$

This gives us a simple explicit formula for  $P$ , since

$$(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|)(\alpha|e_1\rangle + \beta|e_2\rangle + \gamma|e_3\rangle) = \alpha|e_1\rangle + \beta|e_2\rangle$$

More generally, the projector onto a subspace spanned by orthonormal vectors  $|e_1\rangle, \dots, |e_m\rangle$  is given by

$$P = \sum_j |e_j\rangle\langle e_j|.$$

One of the advantages of the auto product notation is that it provides a convenient tool with which to describe the projectors, and thus the quantum measurements.

So, if we recall that the projector  $P$  on to space  $e_1 e_2$  acts as the  $P$  applied on to  $\alpha e_1 + \beta e_2 + \gamma e_3$ , it will be essentially  $\alpha e_1 + \beta e_2$ . This gives a simple exhibit it formula for  $P$ , since we know that an outer product form of the 2 would give rise to  $e_1 e_1$  and  $e_2 e_2$  coming together in the outer product from a super position of that would give rise to the projection operator. More generally the projector on to a sub space span by the orthonormal vectors is given by this projector, where which is generally they outer product of the 2 vectors  $e_j$  and  $e_j$  summed over all of them.

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**REMINDER: Ensemble point of view**

Imagine that a quantum system is in the state  $|\psi_j\rangle$  with probability  $p_j$ .

We do a measurement described by projectors  $P_k$ .

Probability of outcome  $k = \sum_k \Pr(k | \text{state } \psi_j) p_j$   
 $= \sum_k \langle \psi_j | P_k | \psi_j \rangle p_j$   
 $= \sum_k p_j \text{tr}(|\psi_j\rangle \langle \psi_j | P_k)$

Probability of outcome  $k = \text{tr}(\rho P_k)$

where  $\rho \equiv \sum_j p_j |\psi_j\rangle \langle \psi_j|$  is the density matrix.  
 $\rho$  completely determines all measurement statistics.

We should also revise the ensemble point of view in this particular context which can be looked at in this way.

Once we imagine a quantum system in the state  $|\psi_j\rangle$  with probability  $P$  of  $j$ ; we can do a measurement which is described by projectors  $P$  of  $k$ . The probability of the outcome of  $k$  being in state  $|\psi_j\rangle$  can be written in terms of this particular form probability of  $k$  times state  $|\psi_j\rangle$   $P_j$  with probability of being in that states with  $P_j$  can be written in this particular form, so this is in the in terms of the projectors. So that can be rewritten in terms of the trace of the property and then we have the very important aspect where we have the trace  $\rho$  times the projector  $P_k$ , where  $\rho$  is again  $P_j |\psi_j\rangle \langle \psi_j|$  and this is the density matrix. So,  $\rho$  completely determines all measurement statistics.

So, that is one of the reasons once again the measurement statistics so important and so understanding when we do ensemble measurements, because  $\rho$  basically gives rise to all the results that we are interested. So, this is a high lighting result and so this is something which should be remembered.

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**Qubit example REMINDER: calculate the density matrix**

Suppose  $|\psi\rangle = |0\rangle$  with probability 1.  
 Then  $\rho = |0\rangle\langle 0| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ .

Suppose  $|\psi\rangle = |1\rangle$  with probability 1.  
 Then  $\rho = |1\rangle\langle 1| = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ .

Suppose  $|\psi\rangle = \frac{|0\rangle + i|1\rangle}{\sqrt{2}}$  with probability 1.  
 Then  $\rho = \left( \frac{|0\rangle + i|1\rangle}{\sqrt{2}} \right) \left( \frac{\langle 0| - i\langle 1|}{\sqrt{2}} \right) = \frac{1}{2} \begin{bmatrix} 1 \\ i \end{bmatrix} \begin{bmatrix} 1 & -i \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}$ .

where  $\rho = \sum_j p_j |\psi_j\rangle\langle \psi_j|$  is the density matrix.

Conjugate and change kets to bras

Density matrix is a generalization of state

Density matrix

So, let us now connect it to the qubit case. So, we can calculate the density matrix in this form; suppose we say that the pure state of psi 0 with the full probability, then our probability density matrix is outer product of zeros which give rise to this particular density matrix; if we have the wave function representing the pure state 1 then we have the other case where it is rho 1. So, if we have the wave function which is a combination of say 0 and i of i, i of 1 with root 2 with probability 1 then the rho would be a conjugate of these 2 times where we change the bras and the kets we get the negative sin

Then we will be having a density matrix which we look like this. So, density matrix is generalization of state and it can be looked at for any particular state that we are looking at. So, we can calculate density matrix respective of how the particular state looks like: pure states as well as states which have different contributions all give rise to values which can be represented by density matrices.

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**Qubit example: a measurement using density matrix**

Suppose  $|\psi\rangle = |0\rangle$  with probability  $p$ , and  $|\psi\rangle = |1\rangle$  with probability  $1-p$ .

Then  $\rho = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|$

$$= p \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + (1-p) \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix}.$$

Measurement in the  $|0\rangle, |1\rangle$  basis yields

$$\Pr(0) = \text{tr}(\rho |0\rangle\langle 0|) = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = p.$$

Similarly,  $\Pr(1) = 1-p$ .

Now, if we let the probability of measuring the pure states 0 with P and pure state 1 with probability 1 minus P, then we can find that the density matrix would be represented in terms of the probabilities of these 2 and that trace has to be 1 so the probability of state 0 is along the diagonals with P and 1 minus P.

So, the measurement in the 0 1 basis leads to the probability which can be looked at with respect to this and so the probability of 0 simply is the trace of rho with respect to the outer product of 0 states and we get the correctly the value is P as our probability and similarly when we do the same with for 1 we get 1 minus P as expected.

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**Why work with density matrices?**

Answer: *Simplicity!*

The quantum (mixed) state is:

- $|0\rangle$  with probability 0.1
- $|1\rangle$  with probability 0.1
- $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$  with probability 0.15
- $\frac{|0\rangle - |1\rangle}{\sqrt{2}}$  with probability 0.15
- $\frac{|0\rangle + i|1\rangle}{\sqrt{2}}$  with probability 0.25
- $\frac{|0\rangle - i|1\rangle}{\sqrt{2}}$  with probability 0.25

?

$\rho = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$

Sum of these probabilities must be equal one

We know the probabilities of states and we want to find or check the density matrix

So, the advantages I have been mentioning is the simplicity of the overall process the quantum states which are mixed that can be looked at as a result of density matrix notation. If we have an arbitrary some of states which are with all these probabilities as long as the sum of these probabilities has to be one as we know.

We can have a condition where we can sum them up and you can write them out the density matrix; we know that the probabilities of the states have been one to find out check the density matrix, we can always write it down with each of the probabilities for each of them to find out the density matrix and as long as it is only 2 states involved it will be a 2 by 2 density matrix and so on and so forth.

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### Dynamics and the density matrix

Suppose we have a quantum system in the state  $|\psi_j\rangle$  with probability  $p_j$ .

The quantum system undergoes a dynamics described by the unitary matrix  $U$ .

The quantum system is now in the state  $U|\psi_j\rangle$  with probability  $p_j$ .

The **initial density matrix** is  $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ .

The **final density matrix** is  $\rho' = \sum_j p_j U|\psi_j\rangle\langle\psi_j|U^\dagger$ .

$$= U\left(\sum_j p_j |\psi_j\rangle\langle\psi_j|\right)U^\dagger.$$

$\rho' = U\rho U^\dagger$ .

Initial density matrix

So, we can also look at the dynamics of the density matrix, if we have a quantum state in state  $\psi_j$  with probability  $P_j$  the quantum system under goes the dynamics described by the unitary matrix  $U$ . The quantum system is now in the state  $U\psi_j$  with probability  $P_j$ . The initial density matrix is as we have discussed  $P_j \psi_j$  outer product. The final density matrix is  $\rho$ 's prime with an unitary operator applying on both sides and since the unitary operation is commutative it will come out and will we can get back to this form which gives rise to the operator; the unitary operator acting on the  $\rho$  to give rise to the final result.

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### Dynamics and the density matrix

$$\rho' = U\rho U^\dagger.$$

This way, we can **calculate a new density matrix** from old density matrix and unitary evolution matrix  $U$

This is analogous to calculate a new state from old state and unitary evolution matrix  $U$ .

The new formalism is **more powerful** since it refers also to mixed states.

$S_1 = U * S_0$

So, the dynamics of the density matrix can be calculated a new density matrix from the old density matrix and unitary evolution of the matrix. This is analogous to calculating a new state from an old state and unitary evolution matrix  $U$  this new formalism is more powerful since  $\rho$  also refers to mixed states, and that is the biggest advantage of the density matrix. And so whenever this particular operation is being done, it can be looked at for any particular state.

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Single-qubit example: **calculating new density matrix by operating with an inverter on old density matrix**

Suppose  $|\psi\rangle = |0\rangle$  with probability  $p$ , and  $|\psi\rangle = |1\rangle$  with probability  $1-p$ .

Then  $\rho = \begin{bmatrix} p & 0 \\ 0 & 1-p \end{bmatrix}$ .

Suppose an  $X$  gate is applied. Then  $\rho' = X\rho X^\dagger = \begin{bmatrix} 1-p & 0 \\ 0 & p \end{bmatrix}$ .

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Suppose  $|\psi\rangle = |0\rangle$  and  $|\psi\rangle = |1\rangle$  with equal probabilities  $\frac{1}{2}$ .

Then  $\rho = \frac{I}{2}$ . ← "Completely mixed state"

Suppose any unitary gate  $U$  is applied.

Then  $\rho' = U \frac{I}{2} U^\dagger = \frac{I}{2}$ .

Let us take a single qubit example, where we calculate new density matrix by operating with an inverter on old density matrix. Say you have the pure state 0 with probability  $P$  and state 1 with probability  $1 - P$ , then our density matrix will be  $\begin{bmatrix} P & 0 \\ 0 & 1 - P \end{bmatrix}$  as we have discussed. If there is an  $X$  gate is applied then  $\rho'$  will be  $X\rho X^\dagger$  essentially and that will be equivalent to this.

Now if wave function is 0 and 1 with equal probabilities. Then  $\rho$  is equal to  $\frac{I}{2}$  which is the completely mixed state and if we have any unitary operation  $U$  is mixed, unitary gate  $U$  is applied then  $\rho'$  will again give rise to the  $\frac{I}{2}$  (Refer Time: 23:22).



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**Characterizing the density matrix**

What class of matrices correspond to possible density matrices?

Suppose  $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$  is a density matrix.

Then  $\text{tr}(\rho) = \sum_j p_j \text{tr}(|\psi_j\rangle\langle\psi_j|) = \sum_j p_j = 1$  ←

Trace of a density matrix is one

For any vector  $|a\rangle$ ,

$$\langle a|\rho|a\rangle = \sum_j p_j \langle a|\psi_j\rangle\langle\psi_j|a\rangle = \sum_j p_j |\langle a|\psi_j\rangle|^2 > 0$$

**Summary :  $\text{tr}(\rho)=1$  and  $\rho$  is a positive matrix.**

So, what class of matrices correspond to possible density matrix? Suppose we have rho equal to probability times the outer product of psi j and psi j is a density matrix, then the trace of the density matrix should be equivalent to equal to 1, the trace of the density matrix is one. So, for any vector a as long as we can write the density matrix in such a way that this trace is 1, and any projection of that is going to be greater than 0 then it will be occurrence.

Summary is that the trace is going to be 1 and rho is a positive matrix then we can consider that to be a density matrix. So, to consider any matrix to be a density matrix this is the first 2 properties that and necessary to be seen.

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**Summary of the ensemble point of view**

**Definition:** The density matrix for a system in state  $|\psi_j\rangle$  with probability  $p_j$  is  $\rho \equiv \sum_j p_j |\psi_j\rangle\langle\psi_j|$ .

**Dynamics:**  $\rho \rightarrow \rho' = U\rho U^\dagger$ .

**Measurement:** A measurement described by projectors  $P_k$  gives result  $k$  with probability  $\text{tr}(P_k\rho)$ , and the post-measurement density matrix is  $\rho'_k = \frac{P_k\rho P_k}{\text{tr}(P_k\rho P_k)}$ .

**Characterization:**  $\text{tr}(\rho)=1$ , and  $\rho$  is a positive matrix. Conversely, given any matrix satisfying these properties, there exists a set of states  $|\psi_j\rangle$  and probabilities  $p_j$  such that  $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ .

So, in summary the ensemble point of view that we are looking at it has the definition of density matrix for a subsystem, for a system with state  $|\psi_j\rangle$  with probability  $p_j$  which is given by density matrix which is the outer product of the  $|\psi_j\rangle$  states with probability  $p_j$ . The dynamics can be seen as any unitary operation can be utilized to see the new state. A measurement can be described by projectors  $P_k$  which give result  $k$  with probability  $\text{tr}(P_k\rho)$ , and the post measurement density is  $\rho'_k$  which is  $\frac{P_k\rho P_k}{\text{tr}(P_k\rho P_k)}$ .

And it can be characterized with the fact that  $\text{tr}(\rho) = 1$  and  $\rho$  is a positive matrix. Conversely given any matrix satisfying these properties there exists a set of states  $|\psi_j\rangle$  and probabilities  $p_j$  such that  $\rho$  is equal to summation over  $j$  of  $p_j$  outer product of  $|\psi_j\rangle$ 's.

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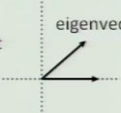
## Normal matrices

**Definition:** A matrix  $M$  is normal if  $M^\dagger M = M M^\dagger$

**Theorem:**  $M$  is normal iff there exists a unitary  $U$  such that  $M = U^\dagger D U$ , where  $D$  is diagonal (i.e. unitarily diagonalizable)

$$D = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_d \end{bmatrix}$$

Examples of abnormal matrices:

$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$ is not even diagonalizable	$\begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}$ is diagonalizable, but not unitarily	eigenvectors: 
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So, in this regard what we have been discussing is a very important property of these normal matrices also which have been implicit; which is that in matrix is normal if it is commutative. So, the concept is if there exist a unitary  $U$  such that the diagonal such that there is a matrix  $M$  which can be reached by using a unitary operator through a diagonal matrix, that is a unitary diagonalizable then the matrix  $m$  is normal. So, examples of abnormal matrices is for example, this particular simple matrix  $\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$  which is not even diagonalizable, and the other which is  $\begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}$  which is diagonalizable, but not unitary.

So, these are the kinds of abnormal matrices, but generally matrices are normal which is what we use if this is satisfied and if they are unitarily diagonalizable. So, these two properties are to be satisfied for having normal matrices; eigenvectors and eigenfunctions always utilized normal matrices.

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### Unitary and Hermitian matrices

**Normal:**  $M = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_d \end{bmatrix}$  with respect to some orthonormal basis

**Unitary:**  $M^\dagger M = I$  which implies  $|\lambda_k|^2 = 1$ , for all  $k$

**Hermitian:**  $M = M^\dagger$  which implies  $\lambda_k \in \mathbf{R}$ , for all  $k$

**Question:** which matrices are both unitary **and** Hermitian?

**Answer:** reflections ( $\lambda_k \in \{+1, -1\}$ , for all  $k$ )

So, for unitary and Hermitian matrices we have normal matrices with respect to some orthonormal basis, there unitary which implies that lambda k square is equal to 1 for all the diagonal square of all of them are equal to 1 for k all k. Summation which means implies that is a the diagonal elements are all real for all k. And there are certain matrices which have both unitary and Hermitian for example, reflections where the diagonal elements are essentially plus 1 and minus 1 for all case; and so that is the way all things are.

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### Positive semidefinite matrices

**Positive semidefinite:** Hermitian and  $\lambda_k \geq 0$ , for all  $k$

**Theorem:**  $M$  is positive semidefinite iff  $M$  is Hermitian and, for all  $|\varphi\rangle$ ,  $\langle \varphi | M | \varphi \rangle \geq 0$

**(Positive definite:**  $\lambda_k > 0$ , for all  $k$ )

Now, there are these positive semi definite matrices also which we been often used in these kinds of studies in terms of gates and application for the quantum mechanical operations. So, positive semi definite means that they are Hermitian with the diagonal values of greater than 0 for all case. There exists a theorem where then normal matrices positive on matrix  $M$  is positive semi definite, if the normal matrix is Hermitian and for all values of ket  $\phi$  they will be positive. So, positive definite means that the eigenvalues will be greater than 0 for all  $k$ .

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**Projectors and density matrices**

**Projector:** Hermitian and  $M^2 = M$ , which implies that  $M$  is positive semidefinite and  $\lambda_k \in \{0, 1\}$ , for all  $k$

**Density matrix:** positive semidefinite and  $\text{Tr} M = 1$ , so  $\left[ \sum_{k=1}^d \lambda_k = 1 \right]$

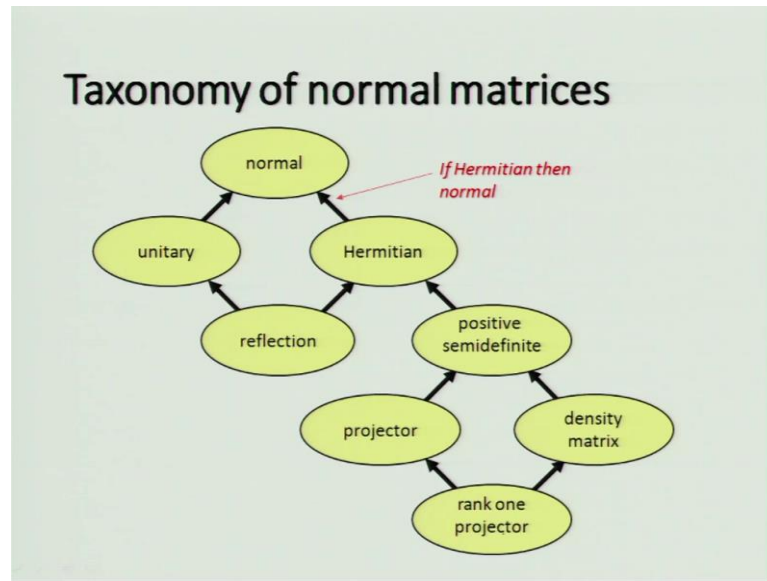
**Question:** which matrices are both projectors **and** density matrices?

**Answer:** rank-one projectors ( $\lambda_k = 1$  if  $k = k_0$  and  $\lambda_k = 0$  if  $k \neq k_0$ )

Now, one other very important thing which we have always used at the projectors and density matrices as we have been saying: the projectors are Hermitians and the square of them equivalent to the same, which implies that  $M$  is a positive semi definite and the eigenvalues are lies within 0 and 1 for all  $k$ . The density matrix itself is a positive semi definite and trace as it is trace of the matrix is 1, so as we know this.

And we both projectors and definite matrices for example, rank 1 projectors where the eigenvalues of 1 if  $k$  equal to 0 and it is equal to 0 if  $k$  is not equal to 0. So, these are basically the diagonal matrices.

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So, in some sense the concepts of the matrices nomenclature of matrices that we have been using; are of the kind where most of the matrices we use for quantum mechanical terms are normal and they are if Hermitian the normal then that is a Hermitian 1. Then there are these reflections which can be unitary and it can lead to normal matrices and there are these rank 1 projectors which can give rise to density matrices, projectors and the positives semi definite.

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## Review: Bloch sphere for qubits

Consider the set of all 2x2 density matrices  $\rho$

They have a nice representation in terms of the Pauli matrices:

$$\sigma_x = X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_z = Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \sigma_y = Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Note that these matrices—combined with  $I$ —form a basis for the vector space of all 2x2 matrices

We will express density matrices  $\rho$  in this basis

Note that the coefficient of  $I$  is  $\frac{1}{2}$ , since  $X, Y, Z$  have trace zero

The other very important part which we should refresh is the Bloch sphere for qubits which we have gone through several times, but it is also another place where the density matrix representation can make a big difference. So, if we consider a set of all 2 by 2 matrices of rho, then they have a nice representation in terms of Pauli matrices that we know it and those are the few Pauli matrices which are the gates that have been used all the time, sigma X or X gate which has all the diagonal says 0 and the diagonals as 1. The Z gate say call it which is basically the sigma Z, the diagonals as 0 1 and minus 1 with off diagonal 0 and sigma Y is the Y gate which has diagonals has zeros and off diagonals as complex conjugate of i.

These matrices combined with the identity forms a basis for the vector space of all 2 by 2 matrices and that is why these are very important. And we can express density matrices rho in this basis. Note that the coefficient I is half since X, Y, Z have trace 0. So, all the value of the trace from diagonals suppose to be 1 will have to come from I.

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**Bloch sphere for qubits: polar coordinates**

We will express 
$$\rho = \frac{I + c_x X + c_y Y + c_z Z}{2}$$

First consider the case of pure states  $|\psi\rangle\langle\psi|$ , where, without loss of generality,  $|\psi\rangle = \cos(\theta)|0\rangle + e^{2i\phi}\sin(\theta)|1\rangle$  ( $\theta, \phi \in \mathbf{R}$ )

$$\rho = \begin{bmatrix} \cos^2\theta & e^{-i2\phi}\cos\theta\sin\theta \\ e^{i2\phi}\cos\theta\sin\theta & \sin^2\theta \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + \cos(2\theta) & e^{-i2\phi}\sin(2\theta) \\ e^{i2\phi}\sin(2\theta) & 1 - \cos(2\theta) \end{bmatrix}$$

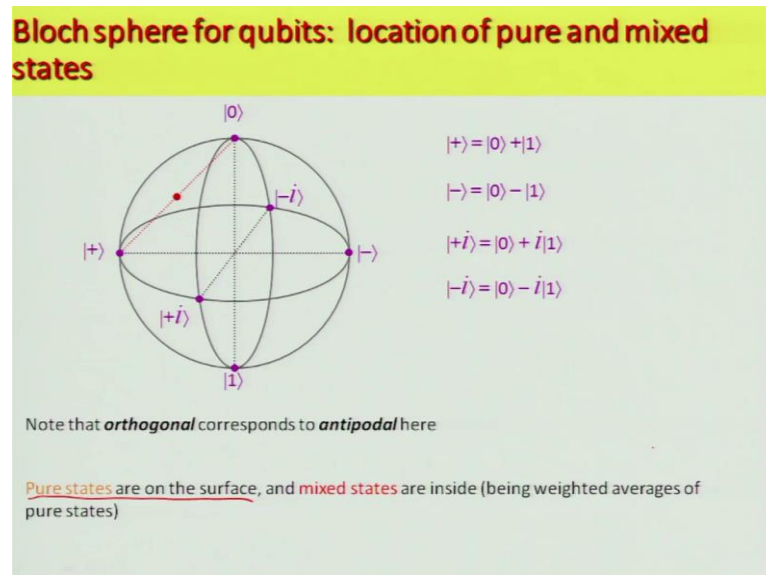
Therefore  $c_z = \cos(2\theta)$ ,  $c_x = \cos(2\phi)\sin(2\theta)$ ,  $c_y = \sin(2\phi)\sin(2\theta)$

These are **polar coordinates** of a unit vector  $(c_x, c_y, c_z) \in \mathbf{R}^3$

So, we can express the density matrix rho for a Bloch sphere for qubits along this form rho is equal to half with coefficient C x C y C z for X Y Z with I. Let us consider the case of pure state psi where without any loss of generality psi is equal to cosine theta 0 state times 2 power i phi sin theta I, so all these theta and phi are real elements. We consider that then we have a density matrix which looks like this form, which is possible

to equivalently write in this form. Therefore, we can get the coefficients  $C_x$  and  $C_y$  equivalently in between these 2 forms.

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These are the polar coordinates of the unit vector  $C_x C_y C_z$  which is in the real form. The Bloch sphere of a qubit's location of pure in mixed states can be looked at also in this sense. So, in the Bloch sphere we know that we have a 0 and 1 along the axis and we have these different notations where they you can have the super position of these states. The orthogonal corresponds to the antipodal here and the pure states are on the surface and the mixed states are inside being weighted average of the pure states.

So, this is how it can be looked at. So the mixed states are the ones which are inside this sphere as we show by the red line all the parts of it, whereas the pure states are always on the surface of this sphere. And most of the time when we essentially describe in initial terms how the Bloch sphere is and talk about the discussions about the vector motion and everything it is always with respect to the idea that the vector is pointing on or moving the state is always on the surface of this sphere which is what not true in case of the mixed state; as there being weighted average of the pure states

I think we have covered enough of these concepts where we have linked all the different aspects of the states that we have been; and the gates that we have been using in the terminology of the density matrices. And the next lecture we will be actually utilizing all these terminologies and the connections that we have established in this class to see how



measurements and the understanding that have been utilized in terms of the implementation are much more easily understood in terms of density matrices. See you in the next class.