

FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

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Qubits: Density Operators - Part 02

Next we will discuss something called the preparation methods in the density operators. Let us recall that the density operator ρ any entire density operator can be written as sum over i $p_i |\psi_i\rangle\langle\psi_i|$. This is the most general representation of a density operator. But if you recall how we arrived at this conclusion was that we have an ensemble of atoms, photons or whatever is our quantum system. And a few of them are in state ψ_1 , other are in state ψ_2 and ψ_3 and ψ_4 and so on. And their corresponding weight is probably given by p_1, p_2, p_3, p_4 .

Since all the quantum systems are indistinguishable from each other, we cannot say which quantum system is in state ψ_1 and which one is in state ψ_2 and so on. The measurement outcomes will give us an average answer. We will get an expectation value of an observable and it turned out that this density operator is one of the better ways of representing the state which will lead all the experimental results, namely the expectation values. And from here we saw that the expectation value of an observable is nothing but sum over i, p_i and expectation value of A in the individual state ψ_i , which can be written in a very short form as $\text{Tr}(A\rho)$ and trace over that.

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Preparation method: Density operator

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

$|\psi_1\rangle \rightarrow p_1$
 $|\psi_2\rangle \rightarrow p_2$
 $|\psi_3\rangle \rightarrow p_3$
 $|\psi_4\rangle \rightarrow p_4$

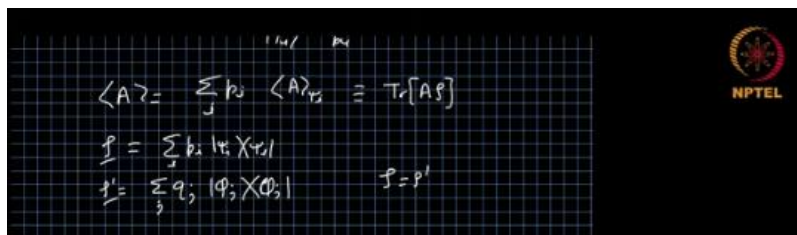
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Now we can see that in this way of representing a density matrix, it seems like some like there are quantum systems like for example photons, some of them are in state ψ_1 and

others are in the ψ_2 and ψ_3 with probability p_1, p_2, p_3 and for ψ_1 we have expectation value of A , for ψ_2 we have another expectation value and we take the weighted sum of that expectation values with the probabilities given by the preparation method. So, in that way this representation for a density operator can be thought of as a preparation procedure or method for a quantum ensemble, ensemble of a quantum system. So, this is a preparation method for a density matrix ρ or a quantum ensemble, state of a quantum ensemble given by ρ . Now, the question is, is this preparation method unique to achieve ρ ?

It means that if I have two, if I have two representations, one is $\sum_i p_i \psi_i$ and another $\rho' = \sum_j q_j \phi_j$, will they always be different states ρ and ρ' ? Is it possible to choose $p_i \psi_i = q_j \phi_j$ such that $\rho = \rho'$? So, can we prepare the state of a quantum system in more than one way is the question we are asking. So, that is what I like to call non-uniqueness, non-decomposition of density operators or non-unique ways of preparing state. To understand it or to get a feeling why we want to find out whether there is a unique method of preparing a state or a non-unique method, let us take one simple example, half times identity. It is a 2 by 2 identity, so this is a density matrix for a qubit.


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Here the r vector is zero like zero vector, all the r_x, r_y, r_z all are zero. It's a valid density matrix because it's the Hermitian, identity matrix is Hermitian, this is one and eigenvalues are half and half both are positive so ρ is positive operator so it satisfies all the three criteria for a matrix to be called a density matrix, in that way this is a valid density matrix. Now we can write half times identity as half times $|0\rangle\langle 0|$ plus $|1\rangle\langle 1|$ because $|0\rangle$ and $|1\rangle$ are the complete bases. So, $|0\rangle\langle 0|$ plus $|1\rangle\langle 1|$ is identity. Similarly, we can write it as half times plus plus, plus, minus minus since plus and minus are also complete places. So, we can write it as the summation of the mixture of plus and minus.

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→ Non-unique decomposition of Density operators
 → Non-unique method of preparing state ρ .

$$\begin{aligned}
 \rho &= \frac{1}{2} \rho & \vec{a} &= \vec{b} \\
 &= \frac{1}{2} [|0\rangle\langle 0| + |1\rangle\langle 1|] \\
 &= \frac{1}{2} [|+\rangle\langle +| + |-\rangle\langle -|]
 \end{aligned}$$


So, you see there are two decompositions for the same density matrix. So, probably we can represent one density matrix in more than one way. So, these are just the intuition and it is very simple example we have taken. We can have a very formal proof also. So, the proof of the statement of the non-unique decomposition of rho.



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Proof: $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ $p_i \geq 0$
 $\langle\psi_i|\psi_j\rangle = \delta_{ij}$ $\sum_i p_i = 1$
 $\langle\tilde{\psi}_i|\tilde{\psi}_j\rangle \neq \delta_{ij}$

$$\rho = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|$$


$$|\tilde{\psi}_i\rangle = \sqrt{p_i} |\psi_i\rangle$$

$\Rightarrow |\tilde{\psi}_i\rangle \rightarrow$ Neither Normalized Nor orthogonal

Let us say we have rho, which is given by $\sum_i p_i |\psi_i\rangle\langle\psi_i|$. So, p_i 's are the probabilities, and $|\psi_i\rangle, |\psi_j\rangle$ need not be zero, δ_{ij} , but $|\psi_i\rangle$'s are normalized. Normalization is important, orthogonality is not required. Now let us say rho is actually written as $\sum_i \tilde{p}_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|$, where we have defined \tilde{p}_i to be $\sqrt{p_i}$. So, $|\tilde{\psi}_i\rangle$ are neither normalized nor orthogonal. Okay, we have done it to make it look pretty that's all. Now let us define R_{jk} such that $\sum_i R_{ij} \tilde{p}_i = p_j$. Okay, so we are not putting any condition on R_{jk} whether they are orthogonal or normalized.

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$$\begin{aligned}
 |\tilde{\psi}_j\rangle &= \sum_k R_{kj} |\tilde{\psi}_k\rangle - \\
 \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| &= \sum_{j,k} R_{ij} R_{kj}^* |\tilde{\psi}_i\rangle\langle\tilde{\psi}_k| \\
 R_{kj}^* &= (R^\dagger)_{jk}
 \end{aligned}$$


They can also be neither normalized nor orthogonal. They are just some vectors we have defined as a superposition of ψ_i . Okay, now $\langle \psi_j | \psi_j \rangle$ can be written as $\sum_k R_{kj} R_{ki}^* \langle \psi_i | \psi_i \rangle$. We're just using this expression and plugging it in this sum over j , if we do we get $\sum_{j,k} R_{kj} R_{ki}^* \langle \psi_i | \psi_i \rangle$. Now, $R_{kj} R_{ki}^*$, if you refer back to our other lectures, we have $R_{kj} R_{ki}^*$, we can write it as $(R R^\dagger)_{jk}$. So, we have R dagger matrix and j element will be $R_{kj} R_{ki}^*$.

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$$R_{kj} = (R^\dagger)_{jk}$$

$$\sum_j |\psi_j\rangle \langle \psi_j| = \sum_{j,k} R_{kj} (R^\dagger)_{jk} |\psi_i\rangle \langle \psi_i|$$

$$(AB)_{ik} = \sum_j A_{ij} B_{jk}$$

We can substitute it here. We get sum over j , $\langle \psi_j | \psi_j \rangle$, sum over i and k and $R_{ij} R_{kj}^* \langle \psi_i | \psi_i \rangle$. Now if we have two matrices let us say A and B and we take the product of them and we want i kth element of them we get sum over j , $A_{ij} B_{jk}$, that will give us the i kth element of the product. we can use this thing we can say sum over j $\langle \psi_j | \psi_j \rangle$ equals sum over i k $R_{ij} R_{kj}^* \langle \psi_i | \psi_i \rangle$. So, this thing we can write as $(R R^\dagger)_{ik}$. That will be sum over j $R_{ij} R_{kj}^* \langle \psi_i | \psi_i \rangle$. Now, if $R R^\dagger$ is identity.

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$$\Rightarrow \sum_j |\psi_j\rangle \langle \psi_j| = \sum_{j,k} \left(\sum_i R_{ij} (R^\dagger)_{jk} \right) |\psi_i\rangle \langle \psi_i|$$

$$= \sum_{j,k} (R R^\dagger)_{jk} |\psi_i\rangle \langle \psi_i|$$

if $R R^\dagger = I$

Okay, then $(R R^\dagger)_{ik}$ will be δ_{ik} , this implies that sum over j $\langle \psi_j | \psi_j \rangle$ will be sum over i k $\delta_{ik} \langle \psi_i | \psi_i \rangle$, which will be sum over i $\langle \psi_i | \psi_i \rangle$. So, if $R R^\dagger$ is identity, we have sum over j , $\langle \psi_j | \psi_j \rangle$ is ρ , because this is ρ . What we have done here is we started with one preparation

method of rho where we had pi as the probability and psi as the states pure states and then we took we got a combination superposition of psi and we got phi and we found that that also is a valid decomposition of rho valid preparation method of rho as long as phi is related to psi by matrix Rij. And the condition over R is R times R dagger is identity. First of all, we should realize if R times R equals identity, this does not mean unitary.

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$$\begin{aligned} \text{if } RR^\dagger = I &\Rightarrow (RR^\dagger)_{jk} = \delta_{jk}. \\ \Rightarrow \sum_i |\tilde{\phi}_i\rangle\langle\tilde{\phi}_i| &= \sum_{i,j,k} \delta_{jk} |\tilde{\phi}_i\rangle\langle\tilde{\phi}_i| = \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j| \\ &= \rho. \\ \Rightarrow \text{if } RR^\dagger = I &\Rightarrow \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j| = \rho. \end{aligned}$$

In fact, this is identity only from one side, so it is called isometric matrices, not unitary. If it is R R dagger equals identity and R dagger R equals identity, then it is unitary. If only one condition is satisfied, then it is isometric. So, with this kind of condition, we can transform the state psi into phi and we still have the same density matrix. So, our new preparation method is sum over j, phi j tilde, phi j tilde.

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$$\begin{aligned} \Rightarrow \text{if } RR^\dagger = I &\Rightarrow \sum_j |\tilde{\phi}_j\rangle\langle\tilde{\phi}_j| = \rho. \\ |\tilde{\phi}_j\rangle &= \sum_i R_{ij} |\phi_i\rangle \\ \underline{RR^\dagger = I} &\neq \text{Unitary.} \\ &\hookrightarrow \text{Isometric Matrix.} \end{aligned}$$

And we did not assume they are normalized, but we can say they are normalized now by q j phi j, phi j, where now phi j are normalized and q j is nothing but the norm of phi j tilde. So, we have p i, psi i, one preparation method, and we have q j, phi j, another preparation method. Okay, and these two are related via transformation R, matrix R. And R is the isometric matrix. And how many isometric matrices are there?

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$$\rho = \sum_i |\phi_i\rangle\langle\phi_i| = \sum_j q_j |\psi_j\rangle\langle\psi_j|$$

$$q_j = \langle\phi_j|\phi_j\rangle$$

$$\{\psi_j, |\psi_j\rangle\} \mathcal{R} \{\phi_j, |\phi_j\rangle\}$$

Infinitely many. So, we have infinitely many ways of preparing a same quantum ensemble rho. So, what is the consequence of this statement that there are infinitely many ways of preparing a quantum ensemble? The consequence is the following. We prepare or an experimentalist prepares the quantum ensemble in a state, which is given by p i's and psi i's.

When we perform measurement and we calculate the expectation values and we reconstruct the state, we get a density matrix. So, we start with p i, psi i, and after measurement we reconstruct the state, we get rho. We don't get p i psi i, we get rho. And this rho can mean it is q j, phi j, it is r j, eta j, it can be many other methods.

So, we don't know which method was used to prepare the state. Once we prepare it and we forget about it, then we do not know what method was used to prepare and there is no way allowed in quantum mechanics which allows you to reconstruct the preparation method. Or we can say there is no way of retrieving the information about the basis used to create the state rho in a physical setting. If one can find any such method which can find out experimentally what base is, what psi is and what phi is are used to create the state rho, then that can be used for superluminal communication. It can violate many of the concepts of the principles in physics.

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$$\{\psi_j, |\psi_j\rangle\} \mathcal{R} \{\phi_j, |\phi_j\rangle\}$$

$$|\psi_j, |\psi_j\rangle\} \rightarrow \rho \rightarrow \{\phi_j, |\phi_j\rangle\}$$

And that will be one of the topic we will discuss in this course later on when we have learned about the generalized measurements and POVMs. So, these are very prominent profound consequences. So, which we will not discuss right now. So, let us say the state rho is that is given to us is p times 0 0 plus 1 minus p times plus. Let me remind you 0 is the eigenstate of sigma z and plus is the eigenstate of sigma x with plus 1 eigenvalue.

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Example: $\rho = b|0\rangle\langle 0| + (1-b)|1\rangle\langle 1|$
 3-pure states.
 $|y_1\rangle = |0\rangle \quad p_1 = b$
 $|y_2\rangle = |1\rangle \quad p_2 = 1-b$

$|q_1\rangle \quad |q_2\rangle = \sum_j R_{ij} |y_j\rangle$
 $|q_2\rangle \quad R = 2 \times 3 \text{ Matrix}$
 $|q_3\rangle \quad R^\dagger = 3 \times 2 \quad R R^\dagger = I_{2 \times 2}$

Now, this is one preparation method given to us. Now, our task is to find another preparation method with three pure states. So, it means we are given ρ_1 , which is 0, ρ_2 , which is plus with corresponding p_1 which is p and p_2 which is $1 - p$. Our task is to find ϕ_1, ϕ_2, ϕ_3 in such a way that ϕ_j is sum over $i, R_{ij} \rho_i$. From here, you can see that R has to be 2×3 matrix. So, R dagger will be a 3×2 matrix. So, R, R dagger is the identity which is 2×2 .

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$$\rho = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}; \quad \rho^\dagger = \begin{bmatrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{bmatrix}$$

$$\rho^\dagger = \begin{bmatrix} |y_1\rangle & |y_2\rangle \end{bmatrix}$$

$$R = \begin{bmatrix} \langle u_1 | \\ \langle u_2 | \end{bmatrix} \quad R R^\dagger = I = \begin{bmatrix} \langle u_1 | \\ \langle u_2 | \end{bmatrix} \begin{bmatrix} |y_1\rangle & |y_2\rangle \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \langle u_1 | y_1 \rangle & \langle u_1 | y_2 \rangle \\ \langle u_2 | y_1 \rangle & \langle u_2 | y_2 \rangle \end{bmatrix}$$

So, R will have the shape which is in this session, 2×3 matrix. And R dagger will have this shape. So, if we write, if we say R dagger is u_1 and u_2 , two vectors where u_1 and u_2 are the three-dimensional vectors, then R dagger or R becomes u_1 and u_2 and condition is $R R$ dagger equals identity which will be $u_1 u_2, u_1 u_2$ which will be $u_1 u_1, u_1 u_2, u_2 u_1$ and u_2, u_2 , which has to be equal to identity. It says that, this implies that u_1 and u_2

are normalized vectors and they are orthogonal to each other. So, we need to find two vectors, three-dimensional vectors, which are orthogonal and normalized.

So, there are many choices of vectors. For example, we can choose u_1 to be $1 \ 0 \ 0$ and u_2 to be $0 \ \frac{\cos \theta}{2} \ \frac{\sin \theta}{2}$, exponential of $i \phi$. We can choose this kind of vectors. So, there are many, many choices. Let us say one choice we are making u_1 to be $\frac{1}{\sqrt{2}} \ \frac{1}{\sqrt{2}} \ 1$ and u_2 to be $\frac{1}{\sqrt{3}} \ \omega \ \omega^2$, $\frac{1}{\sqrt{3}}$ it should be $\frac{1}{\sqrt{3}}$.

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Where ω is nothing but the cube root of identity. So, our matrix will look like $\frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{bmatrix}$. So, now ϕ_1 will be $R_{11} \psi_1$ plus $R_{21} \psi_2$, which will be ψ_1 plus ψ_2 over $\sqrt{3}$. ϕ_2 will be $R_{21} \psi_1$, $R_{22} \psi_1$ plus $R_{22} \psi_2$. That will be ψ_1 plus $\omega \psi_3$ over $\sqrt{3}$.

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And ϕ_3 is $R_{13} \psi_1$ plus $R_{23} \psi_1$, which will be ψ_1 squared here, plus $\omega \psi_2$ over $\sqrt{3}$. So, in that way we got the three five five one five two five three you can check they are not normalized so let me call them tilde they are not normalized wait a sec

we have made a small mistake this equation was for tildes and tildes were for the multiplications of probabilities also so tilde where psi i tilde root p i psi so we have to substitute that. And with this, we can, we have found a set of vectors, new vectors, phi i's, which there are three vectors now and with the corresponding probabilities, that will be the norm of phi i tildes. And we can check that the rho can be written as phi j tilde, phi j tilde. This shows that a given density matrix can be represented in more than one way.

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$$\rho = \sum_i |\tilde{\phi}_i\rangle\langle\tilde{\phi}_i| = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

→ Pure state: $\rho = |\psi\rangle\langle\psi|$

→ Spectral decomposition.

There is one exception to this rule and that is for the pure states. If rho is psi psi, then we cannot find any other representation for this state. It has to be just psi psi. We cannot find any other preparation method to prepare this state.

It will be just this psi-psi. But if there is any small amount of mixedness in the rho, any small amount of impurity, then this breaks down and we can find infinitely many ways of preparing the state, rho. So, till now we just saw that we can represent the density matrix in a mixture of two, mixture of three, we can have a mixture of infinitely many pure states also. That will be clear when we talk about the geometric representation of state, so we can represent the density matrix as a mixture of infinitely many states that's the upper bound, which is infinity. What is the lower bound?

How many pure states are required, minimum pure states are required to represent a density matrix rho. So, the minimum pure states required to decompose rho can be achieved from the spectral decomposition. Since rho is a Hermitian operator, so we can write rho as eigenvalues lambda i times the eigenvectors related to our eigenvectors. So, this is a spectral decomposition and in the set i is an orthonormal basis. Lambda i's are the eigenvalues which are positive and real.

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→ Spectral decomposition.

$$\rho = \sum_i d_i |\psi_i\rangle\langle\psi_i| \quad \{|\psi_i\rangle\} \text{ ONB}$$

Positive because it is a density operator. This decomposition will give us the minimum number of pure states required to decompose a density matrix ρ . We cannot go below this. So, this is the lower bound that is the that will be the equivalent that will be equal to the rank of ρ , for pure state rank is one, for mixed state rank is more than one, for density matrix for qubits the maximum rank is two. So, for qubits we need for full, for a mixed density matrix we need at least two pure states to represent the density matrix. And we can use as many pure states as we want to represent the density matrix. There is no problem.