

FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

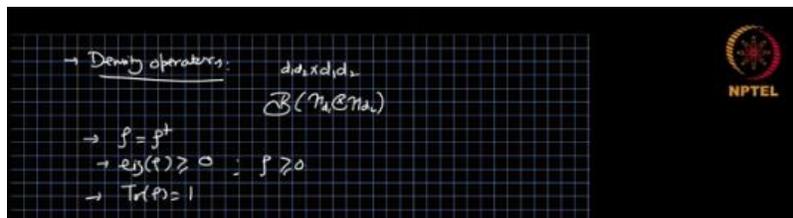
Dr. Sandeep K. Goyal
Department of Physical Sciences
IISER Mohali
Week-05
Lecture-14

Composite Systems: Density Operators

The density operators for composite systems are d_1 by d_1 , $d_1 d_2$ by $d_1 d_2$ matrices because they are the operators from the set of operators which are acting on the Hilbert space of d_1 dimension and Hilbert space of d_2 dimension jointly. The density operators don't act on anything but they are operators, so, they belong to the set of operators. As usual, as for any other density operator, the density operator of a composite system also satisfies the conditions that if ρ is the density operator, then it must be Hermitian, the eigenvalues of ρ should be positive semi-definite or in simple words ρ is a positive semi-definite matrix and the trace of ρ is one. So, it does not matter what kind of quantum system we are considering, it is a composite, it is pure, it is entangled, it is whatever it is. If there is a density operator, it has to satisfy these three conditions.

And any matrix which satisfy these three conditions is a bona fide density matrix of a quantum system. So, it has to satisfy these conditions. Let us take the example of qubits density operator ρ , of a two qubit system is a four by four matrix and since it is from the set of all the operators acting on H_{d_1} or H_2 tensor H_2 , so they form a vector space like all the 4×4 matrices, complex matrices form vector space. All the 4×4 Hermitian operator form a vector space, but all the states do not form a vector space because the trace condition, the trace has to be equal to 1. So, when we add two density matrices, the trace will not be equal to 1.

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It will become more than 1 or less than 1 or whatever we have. So, if we can still use some of the properties of the linear vector space of Hermitian operators, for example, the linear vector space of two by two Hermitian operators have the basis identity sigma x sigma y sigma z, which we have already discussed when we were discussing single qubit density matrices and single qubit operators or we al, like to call them sigma mu, where sigma 0 is identity, sigma 1 is sigma x, sigma y is sigma, sigma 2, is sigma y and sigma 3 is sigma z. So, mu runs from 0 to 3. So, we can extend this basis well, this was the basis for the set of operators acting on H2. Now we can have bases and two copies of those so it will be identity tensor identity, identity tensor sigma i, where i is x y and z, sigma i tensor identity again, sigma i can be sigma x sigma y sigma z and we have sigma i tensor sigma j, where i and j are x y and z. So, in that way we have 1 3 3 and 9 so total 16 operators short form we can write them sigma mu tensor sigma nu. So, this can very well serve as a basis for 4 by 4 Hermitian operators.

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\rightarrow 2-qubit system 4×4 matrix $\mathcal{B}(M_2 \otimes M_2)$
 $\mathcal{B}(M_2 \otimes M_2) \ni \{I, \sigma_x, \sigma_y, \sigma_z\} \otimes \{I, \sigma_x, \sigma_y, \sigma_z\}$
 $\{I, \sigma_x, \sigma_y, \sigma_z\}^{\otimes 2}$
 $= \{ I \otimes I, I \otimes \sigma_x, \sigma_x \otimes I, \sigma_x \otimes \sigma_x, \dots \}$
 $1 \quad 3 \quad 3 \quad 9 = 16$
 $\{ \sigma_{\mu} \otimes \sigma_{\nu} \}$

So, naturally, a density matrix can be decomposed in this form. One interesting thing is that the only trace non-zero matrix is this one, identity tensor identity, which has trace four. All other matrices are traceless, please verify it for yourself that all the other matrices are traceless, only, the trace non-zero matrix is the identity tensor identity. If we put the coefficient of identity tensor identity to be 1 over 4, then obviously the trace condition is satisfied for all the density matrices. Then we can have r dot sigma, that means rx sigma x plus ry sigma y plus rz sigma z tensor identity. So, we have taken these terms and we have combined all of them in one expression.

We can do the same for the other qubit. And we can write sigma ij and t ij, sigma i tensor sigma j. So, this is called the block representation of a two qubit system. Here this r vector is a three-dimensional real vector, s vector is a three-dimensional real vector and t

such that t_{ij} are the elements of this matrix is a three by three real matrix. From here we can see that the expectation value of σ_i tensor σ_j expectation value, which is $\text{Tr}(\rho \otimes \sigma_i \otimes \sigma_j)$, please verify it. Similarly, we can see identity tensor r or s dot σ or identity tensor σ_i expectation value

is s_i , σ_j tensor identity expectation value is r_j and identity tensor identity will have one expectation value one. So, we can again, in short form, we can write as $\frac{1}{4} \sum_{\mu, \nu} \sigma_\mu \otimes \sigma_\nu$, sum over μ and ν from zero to three. This is a simple form of like shorthand notation for the block representation. All the expectation values can be calculated here by the expressions given. And it is not very different from what we have been doing for single qubit. Just that here we are talking about two qubits.

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$$\rho = \frac{1}{4} \left[I \otimes I + (\vec{r} \cdot \vec{\sigma}) \otimes I + I \otimes (\vec{s} \cdot \vec{\sigma}) + \sum_{i,j} t_{ij} \sigma_i \otimes \sigma_j \right]$$

$$\vec{r} \in \mathbb{R}^3 \quad \vec{s} \in \mathbb{R}^3 \quad t = [t_{ij}] \quad 3 \times 3 \text{ Real}$$

$$\langle \sigma_i \otimes \sigma_j \rangle = \text{Tr}(\rho \otimes \sigma_i \otimes \sigma_j) = t_{ij} \rightarrow \text{Expectation}$$

$$\langle \sigma_i \otimes I \rangle = r_i$$

$$\langle I \otimes \sigma_j \rangle = s_j$$

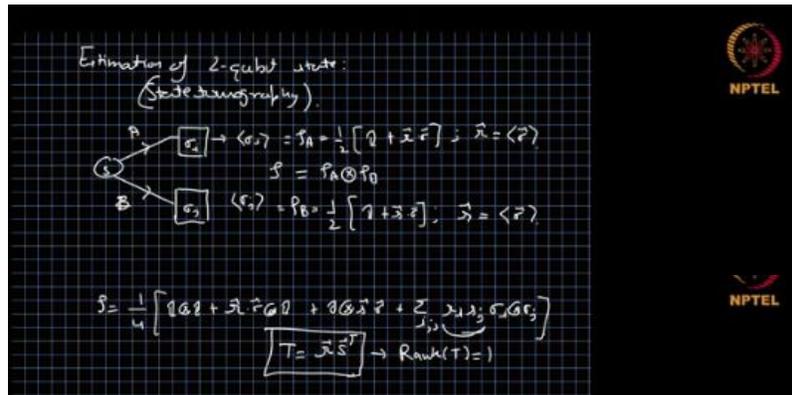
$$\rho = \frac{1}{4} \sum_{\mu, \nu} \sigma_\mu \otimes \sigma_\nu$$

Now, once we have represented the state, the question is how to estimate the state experimentally. To estimate the states experimentally, Estimation of two qubit state or state tomography. We can employ the techniques which we used for qubits. So let us say we have a source, which is producing one qubit and another qubit and sending them in different directions. This is qubit 1 and this is qubit 2 or A and B.

If we have qubit A and qubit B and it is sending it in the two different direction, we can perform measurements of σ_x , σ_y and σ_z on qubit A, and we can have the σ_x , σ_y , σ_z on qubit B. We get the output as expectation value of σ_i and expectation value of σ_j and from here the point is how do we calculate the density matrix. One way is on the subsystem A, we get the net matrix ρ_A , which is half identity plus r dot σ , where r vector is the expectation value of σ vector. Similarly, we have ρ_B here, which is half times identity dot s dot σ , where s vector is the expectation value of σ in the B subsystem. And we can see the ρ is ρ_A tensor ρ_B . And if we expand it, we get ρ to be $\frac{1}{4}$ tensor identity, r dot σ tensor identity plus identity tensor s dot σ plus sum over i and j , $r_i s_j$, σ_i tensor σ_j . So, if we perform local measurements on the two qubits and we get the

density matrices rho A and rho B, then this is the joint combined density matrix of the two qubits but this need not be the most general density matrix because the t_{ij} need not be of this form.

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t_{ij} can be any arbitrary three by three matrix or element from the three by three matrix and the matrix we can get from here, t because r , this from here we can write r vector and s vector transpose this is the rank one matrix. this is not the notion, so, our task is to estimate the most general density matrix. So, in order to do that, let us see sigma i times sigma j. Let us see that. We want to find the expectation value of that and that will be t_{ij} and this is, this need not be expectation value of sigma i times sigma j. This is what we have seen, if this were the case then the T matrix will be just r times s transpose, okay. T matrix will look like this t_{ij} element will look like $r_i r_j$. But this need not be the case. So, t_{ij} are more general, so we need to find the most general expectation value of sigma i times sigma j from a given experimental setting. So, in order to do that, let us take one example. Let us say we have sigma x tensor sigma z. Now, we can write the spectral decomposition of those sigma x is plus outer product plus minus minus outer product minus. This is the spectral decomposition of sigma x tensor spectral decomposition of sigma z is 0 0 minus 1. Now we expand this product, we get plus plus tensor 0 0 plus plus plus, this should minus tensor 1 1 minus minus minus tensor 0 0 plus minus minus tensor 1 1. This is what we get that the spectral decomposition of sigma x tensor sigma z can be written in this form.

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$$T = J S^T \rightarrow \text{Row}(T) =$$

$$\langle \sigma_x \otimes \sigma_z \rangle = \langle \psi | \sigma_x \otimes \sigma_z | \psi \rangle$$

$$\sigma_x \otimes \sigma_z = (|+\chi\rangle\langle +\chi| - |-\chi\rangle\langle -\chi|) \otimes (|0\rangle\langle 0| - |1\rangle\langle 1|)$$

We can simplify it. It will be here we have plus plus tensor 0 0. We can write it as plus 0 outer product plus 0. Okay, or this is plus tensor 0 outer product plus tensor 0. So, to save time and space we will write this way so we get the Sigma x tensor sigma z becomes plus zero outer product plus zero, minus plus one, outer product plus one minus minus zero outer product minus zero plus minus one outer product minus. The expectation value of sigma x tensor sigma z for a pure state psi is psi sigma x tensor sigma z psi.

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$$\sigma_x \otimes \sigma_z = (|+\chi\rangle\langle +\chi| - |-\chi\rangle\langle -\chi|) \otimes (|0\rangle\langle 0| - |1\rangle\langle 1|)$$

$$= |+\chi\rangle\langle +\chi| \otimes |0\rangle\langle 0| - |+\chi\rangle\langle +\chi| \otimes |1\rangle\langle 1|$$

$$- |-\chi\rangle\langle -\chi| \otimes |0\rangle\langle 0| + |-\chi\rangle\langle -\chi| \otimes |1\rangle\langle 1|$$

That will be psi plus 0 and plus 0 psi. So, it becomes mod squared minus psi plus 1 mod squared minus psi 0 minus 0 mod squared plus psi minus 1 mod squared. Now we see that this is the probability of getting plus in subsystem A and 0 in subsystem B. When we are performing measurement on sigma x in subsystem A and sigma z in subsystem B. This is the probability of getting plus in subsystem A and 1 in subsystem B. Similarly, this is the probability of getting minus in subsystem A and zero in subsystem B, and this one is the probability of getting minus in subsystem A and one in subsystem B and how do we get it?. We go back to our setup, let us repeat the setup, here we have a source descending two qubits qubit A and qubit B in two different directions. We put sigma x here and sigma z here. So, here, there will be two outcomes, one will be plus one may be minus and here it will be 0 and 1. we have detectors in front of them, so, when plus detector here clicks and zero detector here clicks.

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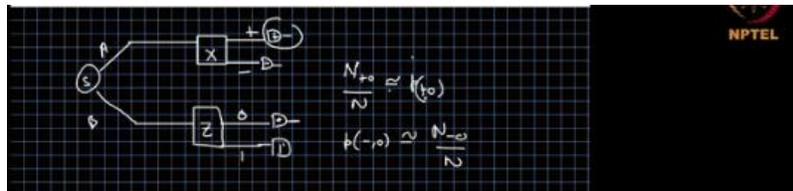
$$|+x\rangle|0\rangle|x_d = |+0\rangle \langle +0| \equiv (|\uparrow\rangle\langle\uparrow|)(\langle 0|\langle 0|)$$

$$\sigma_x \otimes \sigma_z = |+0\rangle\langle +0| - |+1\rangle\langle +1| - |-0\rangle\langle -0| + |-1\rangle\langle -1|$$

$$\langle +|\sigma_x \otimes \sigma_z|+\rangle = \underbrace{\langle \uparrow|\uparrow\rangle^2}_{p(+,0)} - \underbrace{\langle \uparrow|\downarrow\rangle^2}_{p(+,1)} - \underbrace{\langle \downarrow|\downarrow\rangle^2}_{p(-,0)} + \underbrace{\langle \downarrow|\uparrow\rangle^2}_{p(-,1)}$$

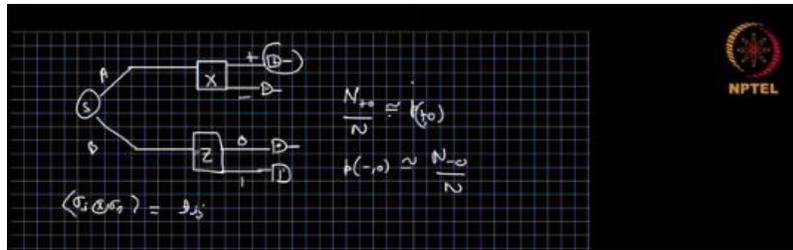
So, when plus and zero detectors click, we take all those incidences. When plus in the A and zero in the B clicks, and let us say it clicks for n number of times, n of, let me call it. n plus zero number of times and total number of pairs of the qubits were n, So, our probability of getting plus zero is very close to n plus zero over n. Similarly, p of minus zero is very close to number of clicks, simultaneous clicks in minus detector up there and zero detector in the B qubit, B subsystem, divided by the total number of input pairs. In that way, we can calculate all the relevant probabilities.

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And now we have to just take care of sign, p plus zero, comes with plus sign, p plus 1 comes with minus sign, p minus 0 comes with minus sign and p minus 1 comes with plus sign. This can be seen from the spectral decomposition of sigma x and sigma z. And with this, we can calculate the expectation value of sigma x and sigma z. This can be written as n plus 0 minus n plus 1 minus n minus 0 plus n minus 1 over the total number of pairs of qubits, n. So, the expectation value is the number of simultaneous clicks in these pairs of detectors divided by the total number of qubits. Similarly, we can calculate the expectation values of all the sigma i tensor sigma j and this will give us Tij. So, this is different from independently doing measurements on A and B. We have to see simultaneous clicks.

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$$\begin{aligned}
 \langle \sigma_x \otimes \sigma_x \rangle &= |t_0 \langle +|_0 \rangle - |t_1 \langle +|_1 \rangle| - |-0 \langle -|_0 \rangle + |-1 \langle -|_1 \rangle| \\
 \langle \psi | \sigma_x \otimes \sigma_x | \psi \rangle &= |\langle \psi | + \rangle|^2 - |\langle \psi | - \rangle|^2 = |\langle \psi | + \rangle|^2 + |\langle \psi | - \rangle|^2 \\
 &\approx \frac{N_{++} - N_{--}}{N} = \frac{N_{++} + N_{-+} - N_{-0} + N_{-1}}{N}
 \end{aligned}$$

Whenever we get a click, when we have a pair of qubits, we get a click in subsystem A. Corresponding to that, what was the click in subsystem B and what was being measured in subsystem B? We have to see this kind of correlated measurements and outcome of that. That will give us the real expectation value of sigma i tensor sigma j. But this is sigma i tensor sigma j. What about sigma i tensor identity? This is nothing but doing nothing literally doing nothing on the qubit B and performing measurement on qubit A of sigma in A. ,, whatever we give subsystem A does not care what is happening in subsystem B and calculate the probability of p plus and p minus and p plus minus p minus that will be the expectation value of sigma x for subsystem A.

Similarly, doing nothing on subsystem A and performing measurement of sigma j on subsystem B will give us expectation value of sigma j on B, that will give us the s j, that was r i. So, in that way we can calculate all the ri's all the sj's and all the tij's. So, this is how we estimate the state of a two qubit system. Now, one interesting thing came out of it is that if we want to find the state of only subsystem A we are not interested in the whole state of the A and B subsystems. Then we just need to perform measurement on sigma i tensor identity and calculate the expectation value. This will give us r i and from here we can calculate rho A to be half times identity plus r dot sigma. Similarly, rho B will be identity tensor sigma j, and this will be s j, this will be rho B equals half times identity plus s dot sigma.

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So, in that way, we can find the density matrices of subsystems, independent subsystems A and B. These two density matrices will not give you the, anyhow these two cannot give you the state of the total subsystem, because, you need joint measurement and the joint we mean by that, what we mean by that is what we described just now that the measurement should be correlated, they should be performed simultaneously. And if we are doing independent measurements and get rho A and rho B, it cannot give us the full information about the total state rho A, B. These states rho A and rho B are called the reduced density matrix. And we can see that we have rho a, b, the total state, which is 1 over 4, sum over mu nu, t mu nu sigma mu sigma nu, okay. Now, what will happen if we, sigma mu tensor sigma nu, if we take trace over subsystem B, that means we have 1 over 4 sum over mu nu, t mu nu sigma mu tensor trace of sigma nu. Now, trace of sigma nu, we know if nu is 0, it means if we have sigma 0, then the trace of that is 2. If mu is not 0 then the trace is 0.

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So, it will be 2 times delta nu 0. So, then we can take the sum over mu and wherever we have nu equals 0, that survives and everything else goes to 0. Factor 2 cancels. So, we get 1 over 2, sum over mu, T mu 0, sigma mu. Now, let us compare it with the block representation. T 0 0 is 1. T i 0 is r i.

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$\rho_A, \rho_B \rightarrow$ Reduced density matrices.
 $\rho_{AB} = \frac{1}{4} \sum_{\mu, \nu} T_{\mu\nu} \sigma_{\mu} \otimes \sigma_{\nu}$
 $\text{Tr}_B[\rho_{AB}] = \frac{1}{4} \sum_{\mu, \nu} T_{\mu\nu} \sigma_{\mu} \otimes \text{Tr}[\sigma_{\nu}] = \frac{1}{2} \sum_{\mu} T_{\mu 0} \sigma_{\mu}$
 $\text{Tr}[\sigma_{\nu}] = 2 \delta_{\nu 0}$
 $T_{00} = 1 \quad ; \quad T_{0i} = x_i$
 $\text{Tr}_B[\rho_{AB}] = \frac{1}{2} [1 + \vec{x} \cdot \vec{\sigma}] = \rho_A$
 $\rho_A = \text{Tr}_B[\rho_{AB}]$ Partial tracing of B.
 $\rho_B = \text{Tr}_A[\rho_{AB}]$

So, we have trace over B, rho AB to be 1 over 2 identity plus r vector dot sigma vector. And this is precisely rho A. So, we can say that the reduced density matrix of subsystem A can be achieved by partial tracing. Partial tracing of subsystem B. We trace out the subsystem B, we get the reduced density matrix of A. Similarly, rho B is trace over A, rho AB, the partial trace over A of the two subsystems. In the two subsystems, it will result in the density matrix of the subsystem B. Now, we have bipartite systems and we have discussed a little bit about the entanglement in the states of bipartite system.

If we are given the state rho A B, we can have this state of the form rho A tensor rho B. They are called, like we prepare them independently and we put them together and we get this kind of state rho A times the rho B. They are called product states. If we prepare, this is case 1, case 2, when rho AB is prepared like rho A in subsystem A and rho B in lab B. With this combination with probability pi and we then put them together, so, we prepare them locally and then we put them together by communicating locally uh communicating between the two labs Then, this preparation state is prepared by local operations and classically communicating between the two parties. So, local operations and classical communication and hence it does not require any quantum correlated correlation or any entanglement in it. So, this is called separable, this is a special case of separable states.

The case one when p one is one and all others are zero, then this is product state. So, we can call both of them as separable state, third case we have rho A B which cannot be written rho A i tensor rho B i. If a state cannot be written in the form of local operation and classical communication like sum over i, p i, rho a i, tensor rho b i, then it must be an entangled state. This is the definition of entanglement for mixed states. And of course, the pure state definition of entanglement is same as this one. This one is more general.

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$\rightarrow ① \rho_{AB} = \rho_A \otimes \rho_B \rightarrow \text{Product states, Separable.}$
 $② \rho_{AB} = \sum_k p_k \rho_{A,k} \otimes \rho_{B,k} \rightarrow \text{LOCC, Separable}$
 $③ \rho_{AB} \neq \sum_k p_k \rho_{A,k} \otimes \rho_{B,k} \rightarrow \text{Entangled state.}$

So, what we are trying to say here is there exists some state for which this kind of decomposition, this separable decomposition, sometimes it is called separable decomposition does not exist. And if by any method we cannot find or if we can prove that the separable decomposition of a state does not exist, then the state must be entangled. So, what does it mean? It means that if by some method we cannot find the separable decomposition, we cannot be sure that the given state is entangled or not. But if we can find even one separable decomposition, then we are convinced, we are sure that the given state is a separable state.

So, one decomposition, separable decomposition is enough to show that a given state is separable. Not coming up with a separable decomposition does not mean that it is a separable or entangled state. Now, if we look carefully, ρ_{AB} can be written as $\sum_i p_i \rho_{A,i} \otimes \rho_{B,i}$. And let us say ρ_{AB} can also further be written as $\sum_n \lambda_n |\psi_n\rangle \langle \psi_n|$. Combining these two, we get $\sum_i p_i \rho_{A,i} \otimes \rho_{B,i} = \sum_n \lambda_n |\psi_n\rangle \langle \psi_n|$. Or $\sum_m q_m |\phi_m\rangle \langle \phi_m|$.

So, in that way, this separable decomposition is one way of writing the preparation method of a bipartite system, state of a bipartite system. Let me remind you, when we say a preparation method, we mean a probability distribution and a set of pure states corresponding to them in such a way that we can retrieve the state ρ , mixed state from this combination. We are saying that the state ρ can be prepared by mixing set of state $|\psi_m\rangle$ with probabilities q_m . Now, we discussed earlier that for a pure state $|\psi\rangle$ or let me call it $|\phi\rangle$. I am writing the density matrix of the pure state.

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$③ \rho_{AB} \neq \sum_k p_k \rho_{A,k} \otimes \rho_{B,k} \rightarrow \text{Entangled state.}$
 $\rightarrow \rho_{AB} = \sum_k p_k \rho_{A,k} \otimes \rho_{B,k} = \sum_k p_k \left(\sum_m d_m |\psi_{km}\rangle \langle \psi_{km}| \right) \otimes \left(\sum_n e_n |\phi_{kn}\rangle \langle \phi_{kn}| \right)$
 $= \sum_{m,n} q_{mn} |\psi_{km}\rangle \langle \psi_{km}| \otimes |\phi_{kn}\rangle \langle \phi_{kn}| = \sum_{m,n} q_{mn} |\psi_{km}\rangle \langle \psi_{km}| \otimes |\phi_{kn}\rangle \langle \phi_{kn}|$
 $\{q_{mn}, |\psi_{km}\rangle, |\phi_{kn}\rangle\}$

We discussed earlier that for a pure state, the decomposition, the preparation method is unique. There cannot be more than one method. So given a pure state, this is the only way you can decompose it. There are no q ms, there are no p ms, there is nothing else. This is the only way you can write a pure state.

Now, if a pure state ϕ is entangled, let us say ϕ is, just take an example $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ then our $\phi \phi^\dagger$ outer product will be $\frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|)$. So, this is our state of two qubits and since this is a unique decomposition we cannot have any other decomposition and we can see that this decomposition cannot be written as $\rho_A \otimes \rho_B$, okay, so, it must be entangled. So, here is this state can be treated as an example of a state where the separable decomposition does not exist and hence it is an entangled state. So, here to prove that the separable decomposition does not exist, what we have used is that for a pure state there are no preparation methods or no non-unique preparation method, there is only one method that is preparing the system in that pure state. And separable decomposition is a way of writing the preparation method.

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$$\begin{aligned} \rightarrow \frac{|\Phi_{AB}\rangle\langle\Phi_{AB}|}{\langle\Phi_{AB}|\Phi_{AB}\rangle} &= \frac{1}{2} [|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|] \\ &\rightarrow \text{entangled} \\ &= \frac{1}{\sqrt{2}} [|00\rangle + |11\rangle] \neq |\psi\rangle\langle\psi| \\ &\neq \rho_A \otimes \rho_B \rightarrow \text{entangled} \end{aligned}$$

A unique way of having the preparation, the separable state decomposition for such cases will be the product form $\rho_A \otimes \rho_B$. ϕ_{AB} can only be written as $\rho_A \otimes \rho_B$ if at all. And as we know from our pure state experience that this cannot be written as some $\rho_A \otimes \rho_B$. Hence, the density matrix corresponding to the pure state cannot be written as $\rho_A \otimes \rho_B$. In this way, we have an example where the state does not possess a separable decomposition. Next, we will discuss something called purification.

For that, let us say we have a state ψ of two qubits, A and B. It is a pure state ψ of two qubits and let us say it is, let us decompose it as $\sum_{ij} \alpha_{ij} |i\rangle_A |j\rangle_B$. Now, the density matrix corresponding to this two qubit system will be $\psi \psi^\dagger$. I'm just not writing $\psi \psi^\dagger$ but you just assume there's $\psi \psi^\dagger$ always here and that will be $\sum_{ijkl} \alpha_{ij} \alpha_{kl}^* |ij\rangle\langle kl|$. Let me remind you that ij is just $i \otimes j$. Now, if we want to find the reduced density matrix ρ_A , then it will be $\text{trace over B } \rho_{AB}$. So, it

will be trace over B of sum over ij kl alpha ij alpha star kl, i outer product k tensor j outer product l. So, the trace will act only on the subsystem B. And when we take the trace of j and l, after taking trace, it will be delta of j l. So, it means we can take the summation over j or summation over l, and wherever we have l, we replace it with j. So, it becomes sum over i, j and k, alpha ij, alpha star kj, i outer product k. After taking the partial trace over B subsystem, this is the matrix we have.

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$$\rho_A = \text{Tr}_B[\rho_{AB}] = \text{Tr}_B \left[\sum_{i,j,k} \alpha_{ij} \alpha_{kj}^* (|i\rangle\langle i| \otimes |j\rangle\langle j|) \right]$$

$$= \sum_{i,j,k} \alpha_{ij} \alpha_{kj}^* |i\rangle\langle i|$$

→ Purification $|\psi\rangle_{AB} = \sum_{i,j} \alpha_{ij} |i\rangle_A |j\rangle_B$ $|i\rangle_B = |i\rangle \otimes |j\rangle$

$$\rho_{AB} = |\psi\rangle\langle\psi| = \sum_{i,j,k} \alpha_{ij} \alpha_{kj}^* |i\rangle\langle k| \otimes |j\rangle\langle j|$$

Now, we can see that we can write as i k sum over j, it is alpha i j alpha dagger j k i k. And this whole thing with the summation j can be written as alpha, or let us say matrix A times A dagger, the element i k, sum over i k. So, what we have assumed is alpha ij is an element of matrix A. This ij is element of matrix A. So, we have this alpha ij alpha dagger or it should be A dagger here A dagger j k, sum over j is same as A times A dagger i k element. So, our rho A is given by this expression. Since i k is a computational basis, 0, 0 and 1 at i-th place and everywhere else 0. Since it is a computational basis, rho A is same as A times A dagger when A is written in the computational basis.

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$$= \sum_{i,k} \sum_j [\alpha_{ij} (A^\dagger)_{jk}] |i\rangle\langle k| \quad [\alpha_{ij}] = A$$

$$\rho_A = \sum_{i,k} (A A^\dagger)_{ik} |i\rangle\langle k|$$

$$\rho_A = A A^\dagger$$

$$\rho_B = \sum_{j,k} \alpha_{ij} \alpha_{kj}^* |j\rangle\langle k|$$

Similarly, we can find rho B. Rho B will be again, we can see from here we take the trace over subsystem A and we get delta i k, the sum over i j k, j k l alpha i j alpha star i l. After taking the trace over A, we get this and here also again we can write as j l sum over i alpha i j alpha star i l j l. Now you can see what we have here is A dagger i i and A i j and sum over i, that becomes A dagger A i j, so j l and j l. So, A dagger A l j element is the coefficient of j l element of rho B, so it means we can say rho B is A dagger A transpose. So, in that way, if we have coefficient matrix A, then we can calculate rho A and rho B. Rho A will be A times A dagger and rho B will be A dagger A times A dagger A transpose, so, in that way we can find the reduced density matrix for A from for a pure state very easily. Why we have started this thing, because if we have, we have psi AB, which is sum over n, dn, en, fn, that is the Schmidt decomposition.

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$$\begin{aligned}
 |\psi\rangle &= \sum_{j,l} A_{jl} |j\rangle_A |l\rangle_B \\
 \rho_A &= \sum_{j,l} \left(\sum_{k,m} A_{kj} A_{ml}^\dagger \right) |j\rangle_A \langle l|_A \\
 &= \sum_{j,l} (A^\dagger A)_{jl} |j\rangle_A \langle l|_A \\
 \rho_B &= \sum_{j,l} (A^\dagger A)_{jl} |j\rangle_B \langle l|_B \\
 \rho_A &= (A^\dagger A)^T
 \end{aligned}$$

Then rho A will be dn squared, en, en, and rho B will be dn squared, fn, fn. Okay this is trivial to find out, so, and this is since en's are the orthonormal basis, this is a spectral decomposition. This is also a spectral decomposition, okay, and from the spectral decomposition we can find the eigenvalues dn square. That is, let us call lambda n equals dn square. Similarly, here it is same lambda n equals dn square and the eigenvectors en and fn. And from here, we can write the arithmetic composition of the 2-qubit system and that will be sum over square root of lambda n, en, fn.

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$$\begin{aligned}
 |\psi\rangle_{AB} &= \sum_n d_n |e_n\rangle_A |f_n\rangle_B \rightarrow \text{Schmidt Dec.} \\
 \rho_A &= \sum_n d_n^2 |e_n\rangle_A \langle e_n|_A & \rho_B &= \sum_n d_n^2 |f_n\rangle_B \langle f_n|_B \\
 & \quad \text{S.D.} & & \quad \text{S.D.} \\
 d_n &= d_n^2 |e_n\rangle & d_n &= d_n^2 |f_n\rangle \\
 \rho_A \rightarrow |\psi\rangle &= \sum_n \frac{1}{d_n} |e_n\rangle_A |f_n\rangle_B \quad \text{Purification} \\
 \rho_A &= \{|e_n\rangle, |e_m\rangle\} & \rho_B &= \{|f_n\rangle, |f_m\rangle\}
 \end{aligned}$$

So, in that way connection of rho A rho b mixed state to pure state psi is called purification. Let us say I am given rho and such that a_n are the eigenvalues and $|a_n\rangle$ are the eigenvectors of this density matrix. Then I can say that this is the density matrix system and there is an ancilla, there is another Hilbert sphere, another quantum system ancilla, which we do not know, which we do not care about. But it has a state with eigenvalue a_n and eigenvectors $|f_n\rangle$, some eigenvectors. This choice of eigenvector is completely arbitrary.

We can choose any orthonormal set $|f_n\rangle$. We are just interested in the eigenvalue a_n . Then we can say that the total state of system and ancilla is sum over n , square root of a_n , $|a_n\rangle$ which is given to us and $|f_n\rangle$ which we can choose arbitrarily as long as they are orthogonal. So, we can always say that the state, any state, mixed state of a given system can be thought of as reduced density matrix from a larger system which contains the system as well as ancilla are in the pure state and the state of that can be written as the state of the system and ancilla, the bigger quantum system can be written as pure state with coefficient, the Schmidt coefficient, root of, square root of a_n and the eigenvectors or Schmidt vectors $|a_n\rangle |f_n\rangle$. $|f_n\rangle$ is again arbitrary. We can choose it to be anything because ultimately it has to result in the density matrix, the physical density matrix rhos of the interest.

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$$|\psi\rangle = \sum_n \sqrt{a_n} |a_n\rangle |f_n\rangle \quad \text{Purification}$$

$$\rho_S = \sum_n a_n |a_n\rangle \langle a_n| \quad \rho_A = \sum_n a_n |f_n\rangle \langle f_n|$$

$$|\psi\rangle_{SA} = \sum_n \sqrt{a_n} |a_n\rangle |f_n\rangle \quad \text{Purification}$$

This process of connecting a mixed state to a pure state of a larger system, this is called purification. And this is used to simplify problems when we deal with open quantum systems, when we deal with more complicated quantum systems in mixed states.