Quantum Entanglement: Fundamentals, measures and application

Prof. Amarendra Kumar Sarma

Department of Physics

Indian Institute of Technology-Guwahati

Week-01

Lec 4: Mathematical Tools: Density Matrix-Part 2

Hello, welcome to part 2 of lecture 3. We will continue our discussion with density matrix formalism.

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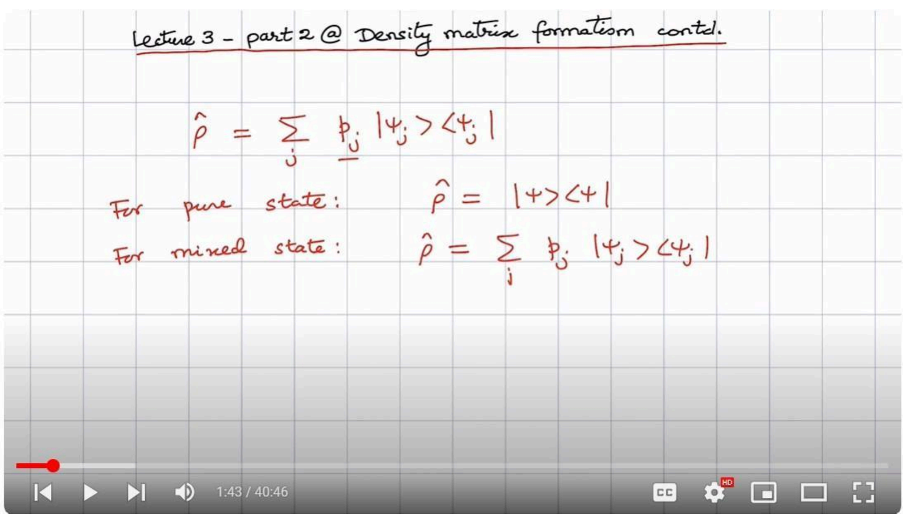

In the last lecture, we defined a density operator rho cap as follows. Rho cap is equal to sum over j Pj ket psi j bra psi j and it can be used to represent both pure and mixed states. For pure state the classical probability Pj is equal to 1 You just have only one state. So for pure state the density operator is simply ket psi bra psi the outer product and for mixed state this is exactly the definition that I have written but still let me write it once again. So, for mixed state we have rho cap is equal to Pj psi j psi j ok.

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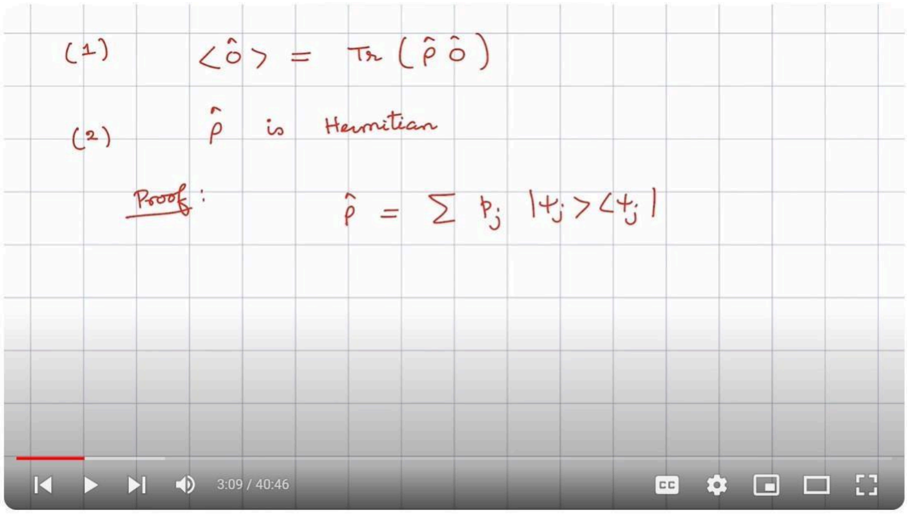

Now I shall discuss the important properties one by one which should be of course relevant to us. In fact one property already, I have discussed in the last class that is this that the expectation value of any observable I can write it in terms of density operator is this. That this should be basically the trace of the product of the density operator and the observable. Basically, the product of the matrices corresponding to the density operator and the observable and you just need to take the trace of the product of these two matrices. That is property number one. And second property is that this density operator must have to be Hermitian. In fact it is a Hermitian, rho is Hermitian and we can prove it and I will show you rho is Hermitian.

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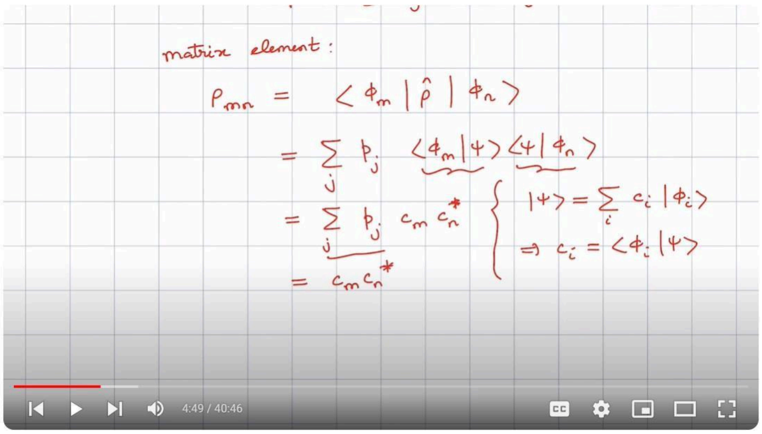

Let us prove. To be simple let us say, ok we will start with the definition rho cap is equal to Pj psi j psi j. Now if I consider the matrix element, suppose I consider the matrix element of the density operator or density matrix, let me say the matrix element rho mn in the orthonormal basis say phi, then this would be phi m rho phi n. So that is the density matrix element. Now if I put right, if I use this definition of the density operator here, so I have j Pj phi m psi psi phi n and already from our earlier class we have seen that this guy I can write it as this one I can write this is nothing but the coefficient Cm and this is the complex conjugate Cn*. If you have forgotten, just for your quick reference, this state arbitrary ket psi I can express it in the basis state phi as Ci ket phi i and from here I can write Ci is equal to the scalar product phi i psi, right? So using this now because of the fact that now sum is taken over all the classical probabilities, so that is going to be equal to one, so you will be left out with Cm Cn*.

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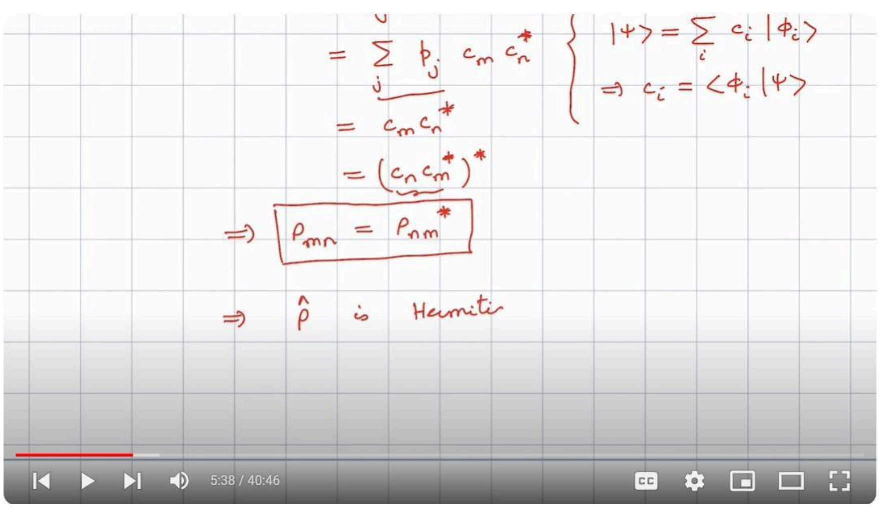

This one I can also write as Cn Cm*, then again the product of that and I again take the complex conjugate, this is nothing but rho n m*. So from here because it is now quite evident that if you take the density matrix and you take the transpose of the, basically if you rows becomes columns, columns becomes rows and then you take the complex conjugate then you are going to get the original matrix again, so that's why quite clearly it means that rho, the density operator rho is Hermitian.

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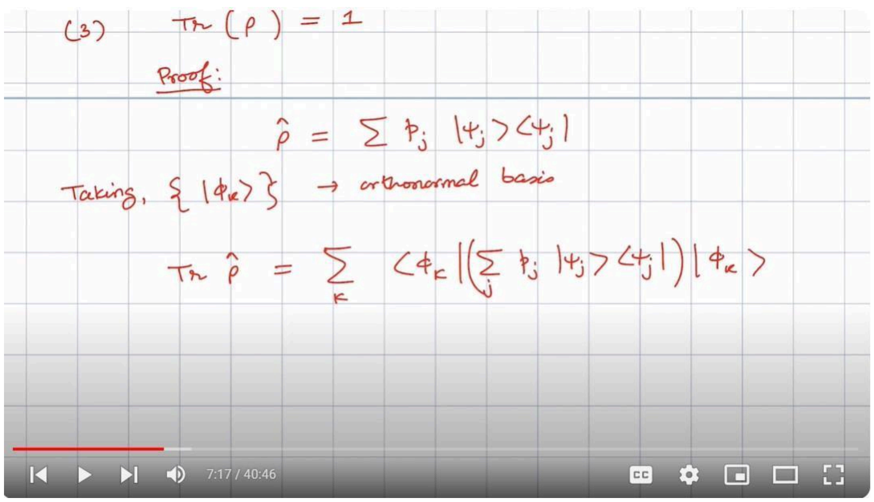

Okay, so now let me go to the other properties, now another important one is say the trace of rho trace of the density matrix is equal to one in fact from the physical significance of density operator that we have discussed in the last class as you remember that the diagonal elements of the density matrix represents the probabilities, so total probability has to be equal to one, so from there it is very clear, but let me now show it mathematically as well, that trace of rho density operator is equal to one, so again writing the basic definition we can start with that, so we have this alright, now taking the orthonormal basis state as say phi k, this is I am taking orthonormal basis orthonormal basis vectors okay, let me take the right trace of rho that would be equal to sum over k phi k and this is density operator let me put the whole definition here that would be j p j psi j psi j let me put actually it inside the bracket and I have here phi k, so because this is trace that's what I can write,

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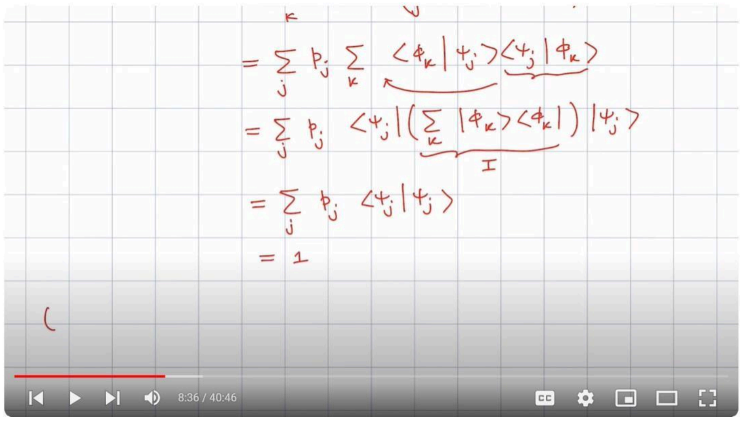

now I can just do little bit of manipulation here, I can write this summation here j let me take this side, the classical probability also let me take this way, take it out then I take the sum over k inside, so I have now phi k psi j psi j phi k alright, now as you can see I can again use the completeness condition for my advantage, so I write p j and I can, because this is just a number I can take it this side and if I do that I have here psi j and this summation over k I can take inside and I can write phi k phi k here and this would be psi j, now because of the completeness condition this is nothing but the identity, so therefore I will be left out with this is sum over j, so this is sum over j p j psi j psi j and as you can see this is this is obviously total is equal to 1,

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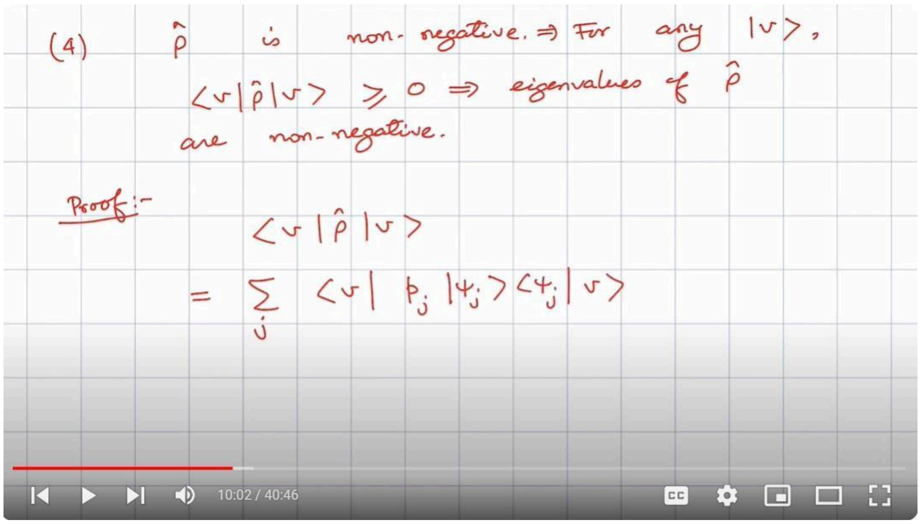

so one interesting property of density operator is that that density operator rho is non-negative what it mean? It means that for this actually imply that for any vector state vector say ket V we must have the expectation value of the density operator if we take that should always be greater than or equal to 0 it effectively means that the eigenvalues are non-negative or in other words, eigenvalues eigenvalues of the density operator rho are non-negative that means always positive it can never be negative it can be 0 but it cannot be negative. In fact the proof is very simple so let me show you that so let us find out the expectation value of the density operator for this vector V and that I can write as again invoking the definition of the density operator let me write it as this so you have p j psi j psi j V

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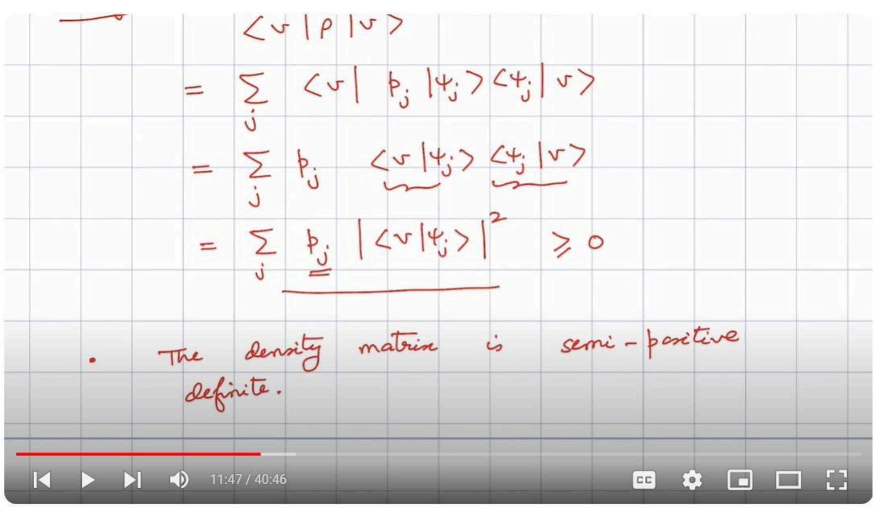

and just let me take the classical probability here p j then I have V psi j psi j V now as you can see this guy and this guy they are complex conjugate to each other so therefore immediately I can write summation p j mod of the scalar product of say V j V psi j okay so mod square now this is has to be greater than or equal to 0 since the right hand side this side you see is sum of numbers that are always positive or it may be 0 okay that's why this relation has to be always satisfied we have used the fact actually that the probability p j are real and non-negative and that is always the case now the fact that rho is non-negative is implies that as I said that eigenvalues of rho are non-negative so density matrix is that's why it is also said that density matrix is semi positive definite so this is another way to put the property the density matrix is semi positive definite semi positive definite so don't go by the you know it appears to be a technical word but it simply means that the eigenvalues of the density operator or the density matrix are always positive non-negative it cannot be negative.

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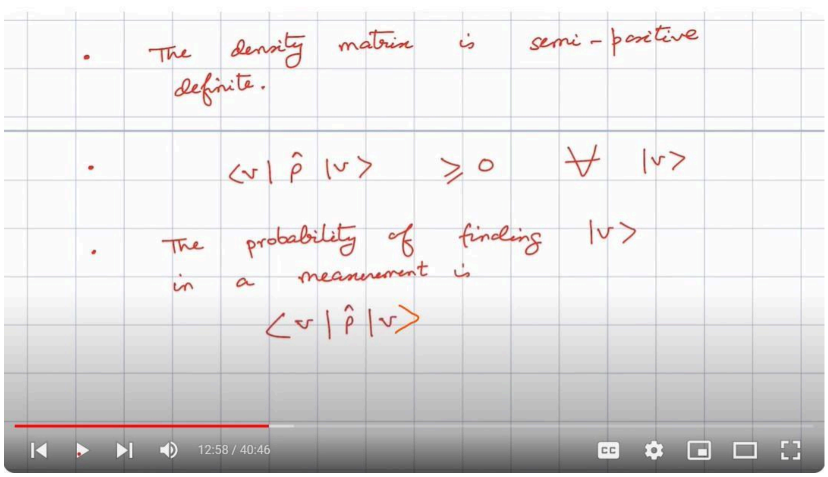

Alright now another thing is that one can always pick up any vector V and find out the expectation value of the operator rho and you are always going to with respect to this vector V state vector V if we find the expectation value then it is always going to be turn out to be greater than or equal to 0 for all vector state vector V in the Hilbert space in fact one important fact and interesting and very useful fact is that the probability the probability of finding let me just put it here finding the state V in a measurement in a measurement is simply you have to find the expectation value of it.

Now let us discuss how to distinguish pure and mixed test using density matrix formalism after that I will discuss some more interesting a couple of more interesting properties of the density matrix operator which are going to be very useful later on in our treatment of quantum entanglement .

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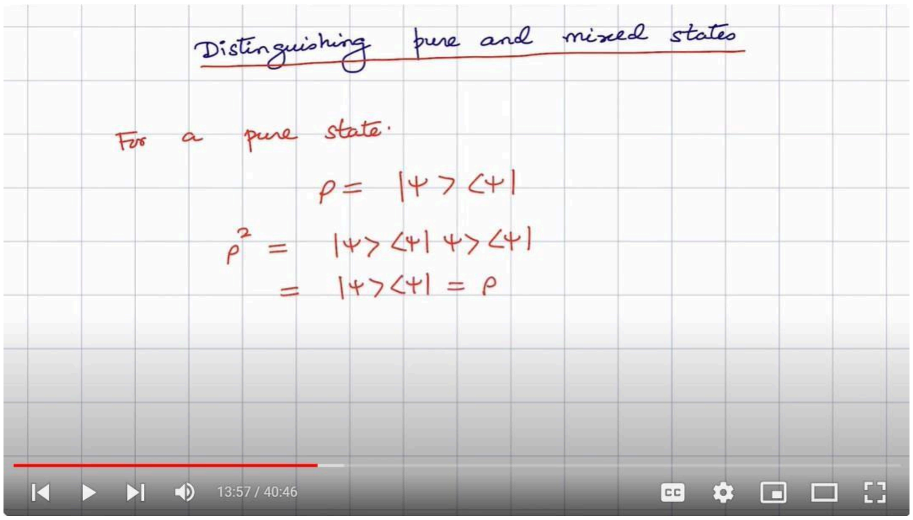

How to distinguish a pure and mixed state well it is easy for a pure state for a pure state the density operator rho is simply this as we all know if I find out what is rho square then you see that for the first rho I will have this and for the other one I will have this now because psi is normalize so you are going to simply get again this one and this is nothing but rho.

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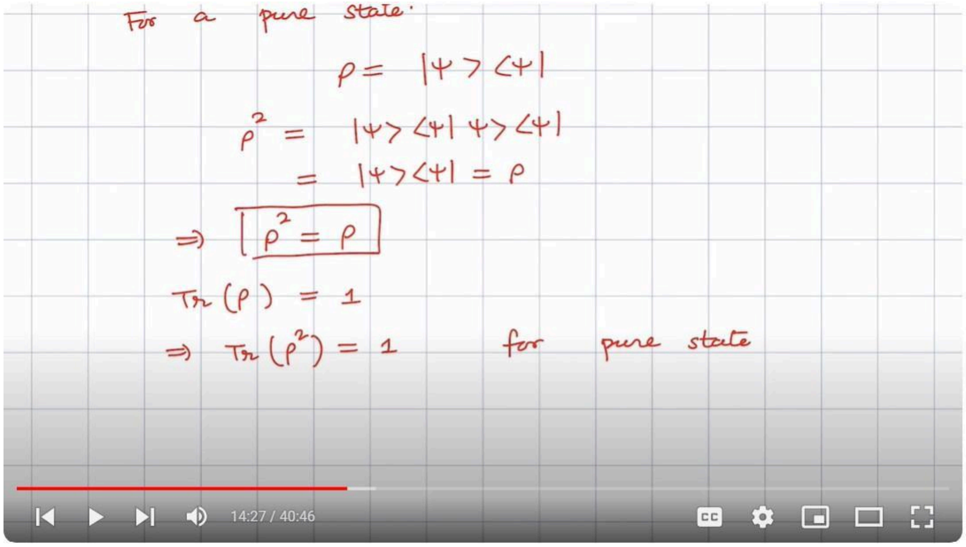

this implies that for pure state rho square is equal to rho on the other hand we also know that from the property of density operator that trace of rho is equal to 1 this implies that trace of rho square is equal to 1 for pure state this is because rho square is equal to rho I am using this property here ok.

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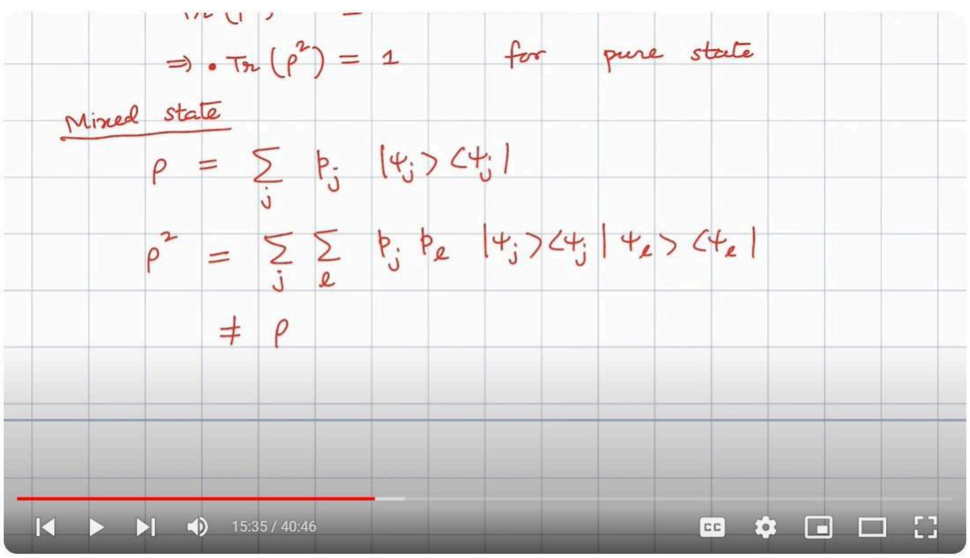

Now what about mixed state? for mixed state rho the density operator rho is I am not writing the operator sign any longer now so you can understand that I am talking about density operator so I have this sum over j pj psi j psi j and what about rho square? so this I am now talking about mixed state so what about rho square? so I have two rho's product of two rho's so let me just say for the first rho I have j for the second rho let me say invoke say l then I have here pj pl psi j psi j then psi l psi l alright now it is easy to see that this is definitely not equal to rho so rho square is not equal to rho for mixed state

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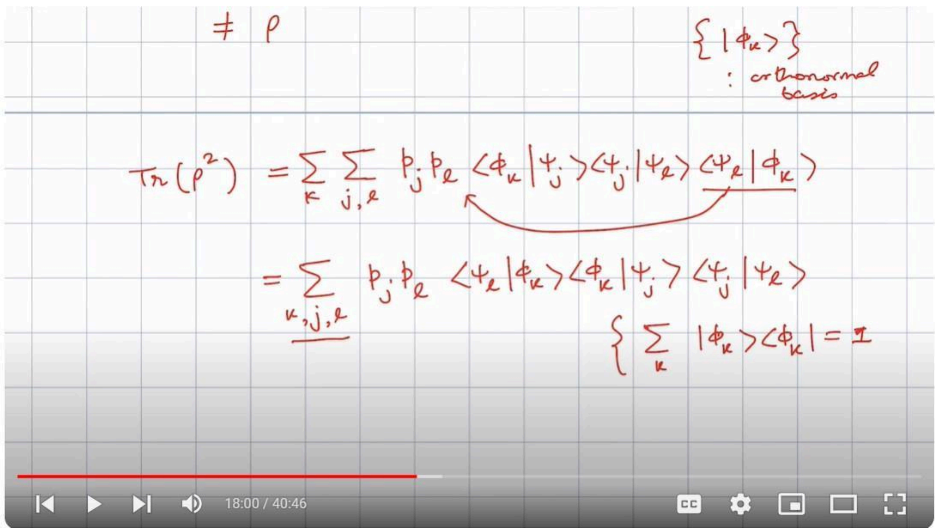

what about the trace of rho square? let us see check that trace of rho square if I take an orthonormal basis to be say if I take my orthonormal basis to be say phi k these I take my orthonormal basis orthonormal basis in that basis state trace of rho square would be sum over k rho square already I have written here so I am going to utilize it and so let me these two summations let me write as a one summation actually double summation is involved but for short hand notation I am using this to simplify the calculation so I have here pj pl and I am going to take just one minute let me take this up here to make the space okay pj pl then I have to take trace so I have here phi k psi j psi j just using this psi l psi l then phi k right I have to take the trace that way this is the way to take the trace and these are numbers so what I can do I can take it this side again I am going to utilize my old trick so everything now I can write as a single this thing but three summations are involved k j l and I have here pj pl and if I take this side then I have here psi l phi k phi k psi j psi j psi l right this is easy to understand now I can invoke because three summations are involved and I can invoke this orthonormal basically the completeness condition I can invoke that is I know that this relation is equal to one or identity.

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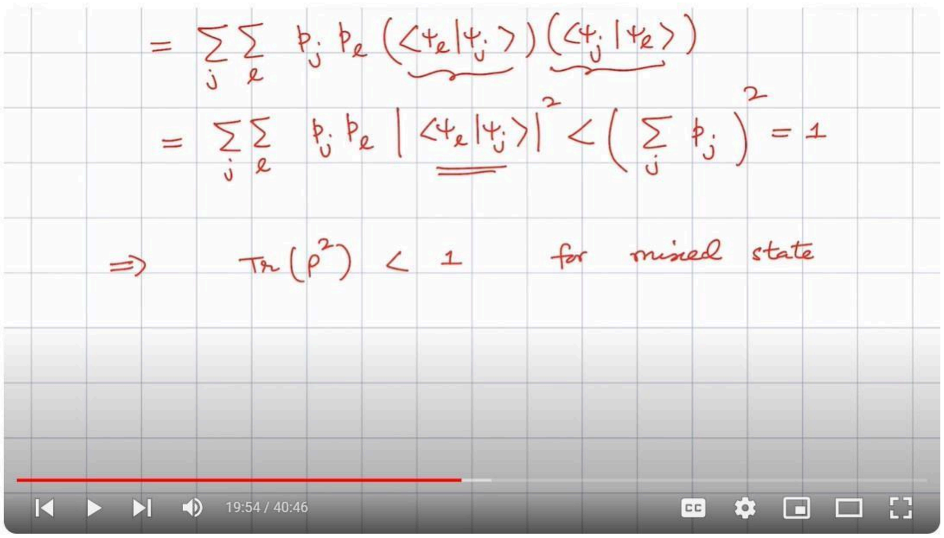

So utilizing this I will be just left out only two summations that is summation over j and summation over l I have here pj pl and I have here psi l psi j this is one term then other term would be psi j psi l now as you can see these are the complex conjugate of each other so this thing I can therefore write as j l pj pl and this would be mod of psi l psi j whole square right so because this is a positive quantity and this has to be as you can easily see that this has to be less than or equal to summation this is going to be equal to one if l is equal to j so maximum value would be one here so therefore it has to be less than or equal to this j pj mod whole square right I think is it when j is equal to l now this is sum over the probabilities classical probabilities that is equal to simply one so what you see ultimately you are getting we are working out trace of rho square for mixed state so this implies that trace of rho square for mixed state is less than one right less than one for mixed state for mixed state for pure state by the way this is of course I should better write one only for mixed state it is going to be because when for mixed state l is equal to j that is going to be equal to one trace of rho square be one so we just get a way using density matrix how to distinguish mixed state and pure state.

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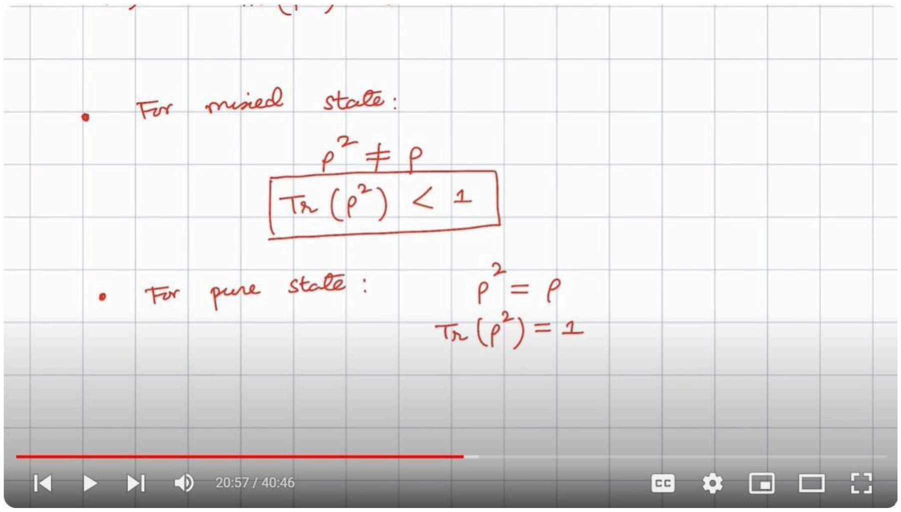

Let me conclude for mixed state for mixed state I must have rho square is not equal to rho and if I find out trace of rho square that is always going to be less than one by the way trace of rho is equal to one for both pure and mixed state because that is the property of the density operator and for pure state for pure state I have I must have rho square is equal to rho and trace of rho square should be equal to one that's the way we can distinguish whether a state is pure or mixed in fact this particular parameter trace of rho square is called the purity of the state right trace of rho square trace of rho square is termed as purity of the state purity of the state .

Before I go any further let me give you some examples to understand the properties and definitions that we have discussed so far in the context of density operator or density matrix.

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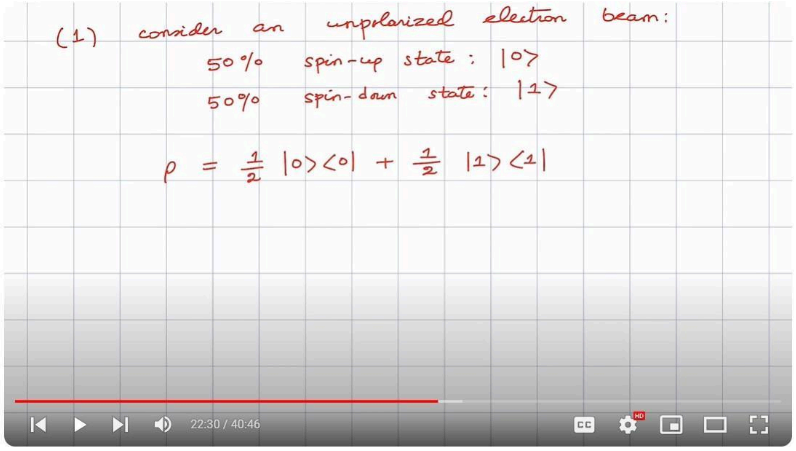

Consider an unpolarized electron beam consider an unpolarized electron beam consider an unpolarized electron beam where 50% of the electrons are in spin up state spin up state   that is we represent it up state by say ket 0 and 50% of the electrons are in spin down state   and spin down state is represented by say ket 1 so in this case the density operator of the electron beam   would be written like this 50% probability that is the classical probability   it is half so it is ket 0 bra 0 here for the second part we have half ket 1 bra 1 that's the density operator and it is clearly a mixed state and it should remind you about the box problem that I have discussed in the last lecture part 1 of this lecture.

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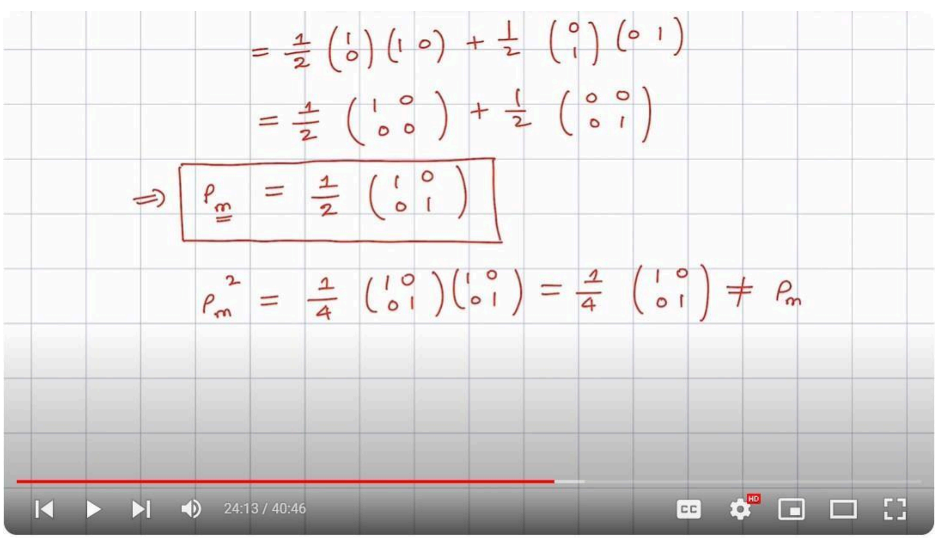

this I can further write in the matrix representation I can write it this ket 0 I can write as 1 0 and bra 0 would be 1 0 and here half ket 1 is 0 1 and this is the rho vector for the bra 1 and then I have 1 0 0 0 plus half 0 0 0 1 so finally the density operator I have is half 1 0 0 1 so what you should notice that this is a mixed state and I can prove it and also we can check whether the properties of the mixed state is obeyed or not what I mean by that is first of all if you calculate what is rho m square I am already putting this suffix here just to take that this is a mixed state I am talking about in fact if you find out what is rho m square you will find it will be 1 by 4 1 0 0 1 if you take the product you will get it will be 1 by 4 1 0 0 1 right and it is clearly this is not equal to rho m this is one of the thing that the mixed state has to obey.

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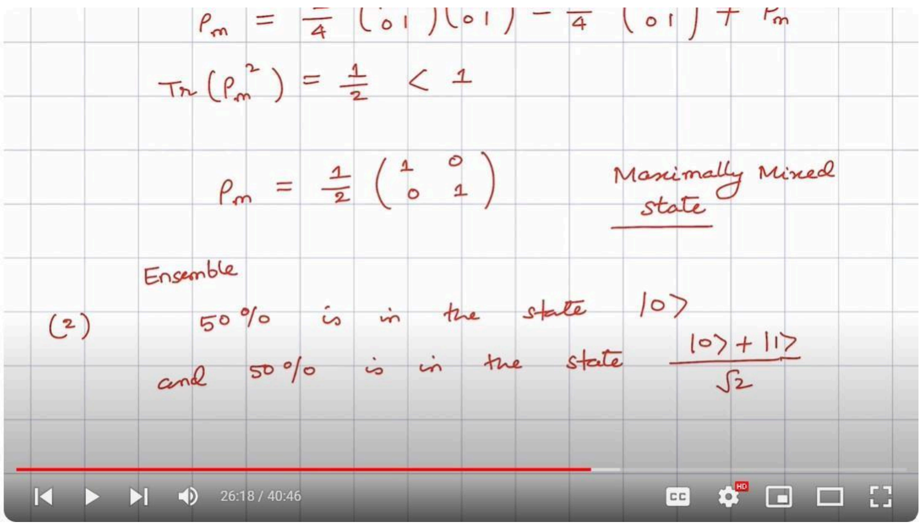

and also immediately you can see that trace of rho m square is equal to 1 by 4 plus 1 by 4 that is half and this is definitely less than 1 confirming that this state is mixed right rho m is a mixed state also you see that this particular state here there is no off diagonal elements that means no non zero off diagonal elements all the off diagonal elements here are 0 0 off diagonal elements and it has equal diagonal elements so this kind of states are called maximally mixed state ok so the definition of maximally mixed state is that where the off diagonal elements are 0 and all the diagonal elements are of equal value right so for example here we are having the off diagonal elements are half and half one half and one half ok let us consider another example consider and say ensemble where say there is again a 50% of the ensemble is 50% is in the state say ket 0 and 50% is in the state this time let us take a superposition state like this ket 0 plus ket 1 by root 2 so in this ensemble now we are talking about ensemble ok 50% whatever be the ensemble 50% is in the state ket 0 and 50% is in the state superposition state of ket 0 plus 1 divided by root 2

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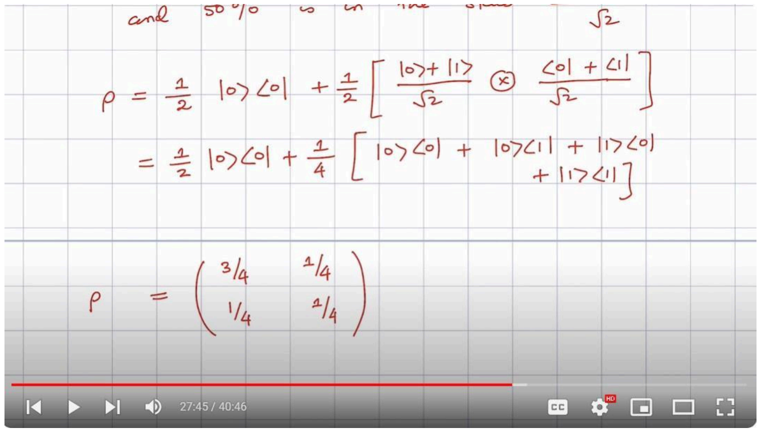

what about the corresponding density operator again it is a mixed state because this classical probability is here half ket 0 bra0 for the first part and for the second part I have half this is ket 0 plus 1 and in fact this is a direct product or tensor product so this is root 2 this bra 0 plus bra1 and if I open it up then I will get half ket 0 bra 0 plus 1 by 4 right and let me open it up the whole thing this would be ket 0 bra0 plus ket 0 bra1 plus ket 1 ket 0 plus ket 1 ket 1 and in matrix form you can easily write it and I leave it to you to show that you will get finally rho would be equal to 3 by 4 1 by 4, 1 by 4 1 by 4 now you see trace of rho should be equal to 1 and here indeed that is so this is a valid density matrix and also you see that the diagonal elements are positive here so it's a semi positive definite and this is because now you have a non zero off diagonal elements are there this kind of states are called partially mixed this kind of states are called partially mixed and in fact you can check all the other properties you can calculate what about the rho square and then you can find out the trace of rho square you will find that the properties corresponding to mixed states is going to be obeyed by this density matrix.

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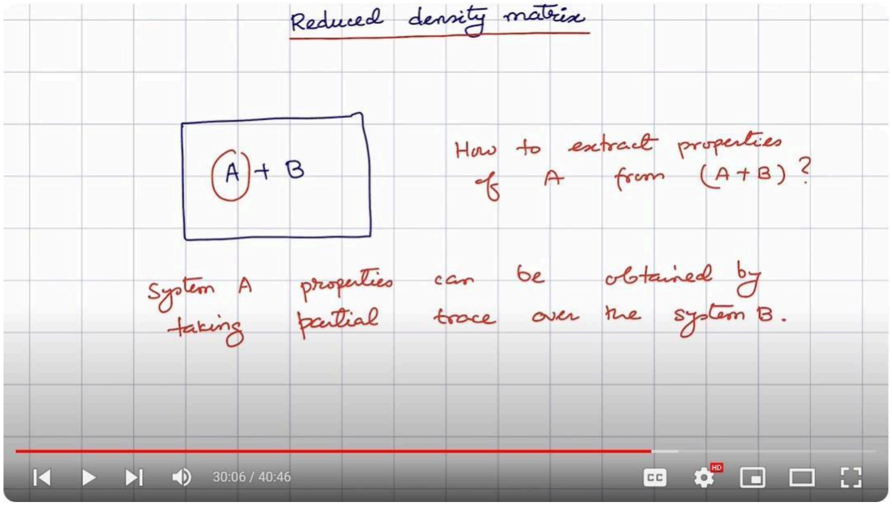

Now we are going to discuss about a very useful concept in density matrix formalism the so called reduced density matrix. Assume that we have a composite system A plus B but say we are not interested in the system B at all but we are interested in system A only, the question is then how to extract properties of system A from A plus B so the question is how to extract properties of A from A plus B from the composite system this is, this can be addressed by a prescription called reduced density matrix or reduced density operator, so in this by this prescription system A properties system A properties and it's an important point so let me write it, system A properties can be obtained by obtained by taking partial trace over the system B, partial trace over the system B,

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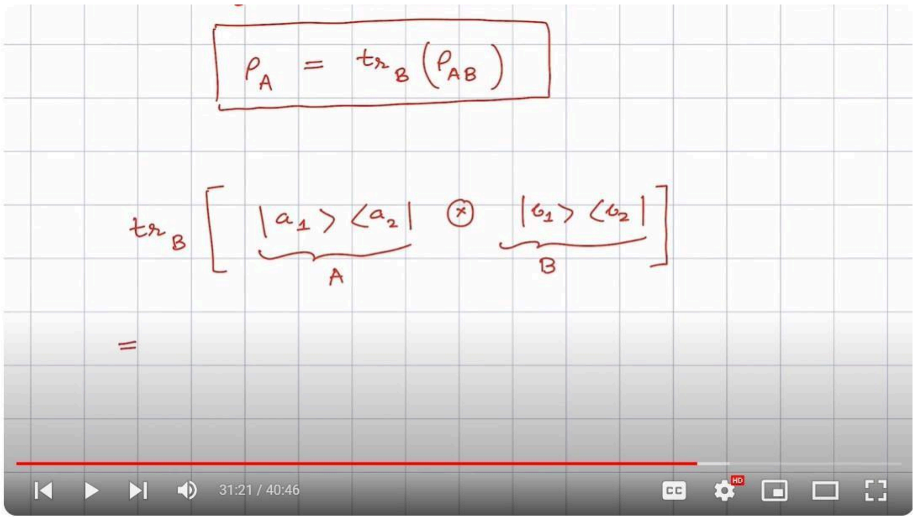

as I go along it will be more clear to you, thereby we can represent the state of the system A by a density operator rho A, so suppose the density operator of the composite system A plus B is rho AB then if I trace out B from that then I will be able to get the density operator for the system A, so this is what is called reduced density matrix, rho A is the reduced density matrix because you are getting it from the composite system density matrix rho AB, let me give a more clearer explanation of this partial trace issue to do that let us suppose that the composite system is represented by this way, I will explain what it is, so I am assuming that the system A and system B are separable, so this part refers to the system A and this part refers to the system say B, now if I take, this is how I represent the state of the composite system, now if I trace out B what I mean by tracing out B is I will take the trace over B only, so system A is not going to be affected by this trace operation, so I will take that out and I will take the trace over B so this is what I will have.

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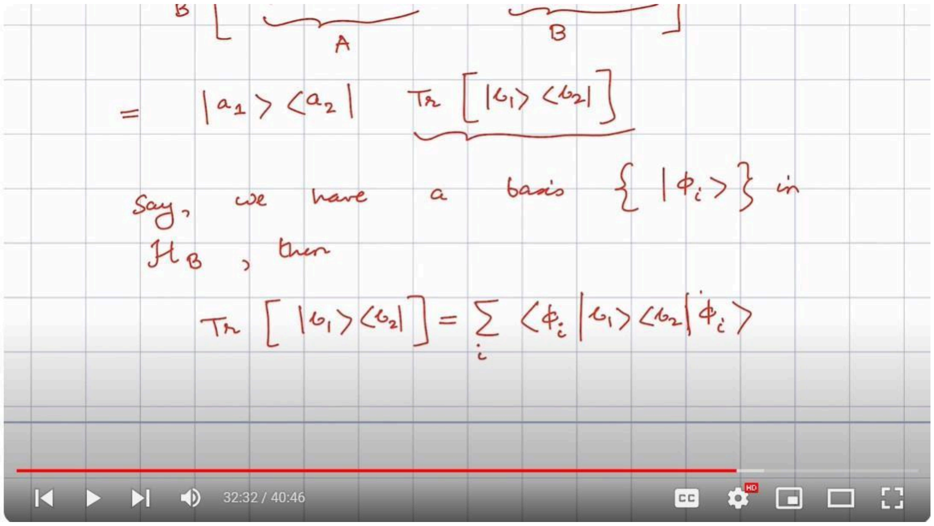

Now let us say let me now focus on this particular quantity here, trace operation, suppose we have a say, we have a basis so phi in the Hilbert space of B then the trace operation let me work out this in detail, the trace operation over B is going to give me you know how to take the trace operation by now, so I have here this phi i then B1 B2 here and this would be phi i right, that's what the trace operation means, basically you are summing up the diagonal elements of the matrix that is what we mean by taking trace.

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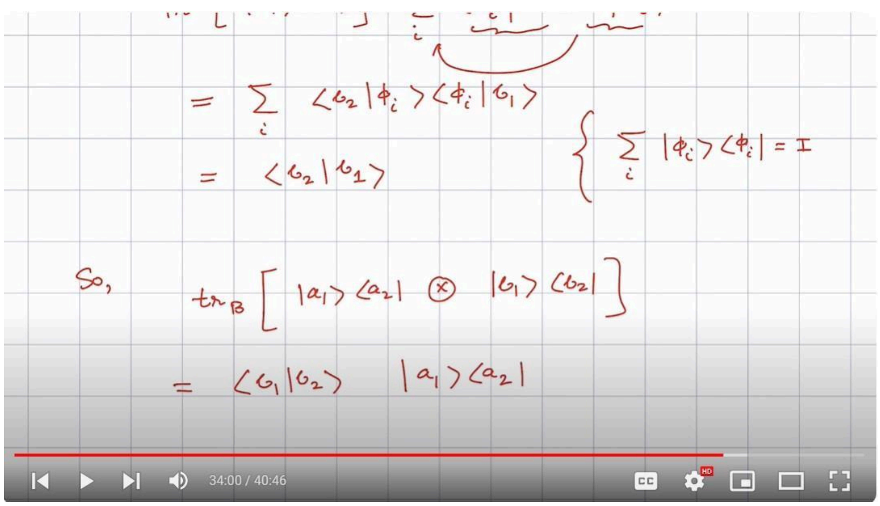

So this is what let me explain a little bit more, in fact I can simplify it further so this would be equal to, now because these are just numbers, so I can play my old tricks again I can take it this side and if I take that this side, so B2 phi i, here I have phi i B1, now impose the, or apply the so called completeness condition, that means we know that this guy is equal to identity, so therefore immediately you will get that this would be just a scalar product of B1 and B2 right, this would be the scalar product of B1 and B2 so tracing out B from the composite system is going to result in as we have worked out we will get the scalar product of B1 and B2 and outer product A1 A2, so partial trace essentially averages out the effect of system B and extract the properties of system A .

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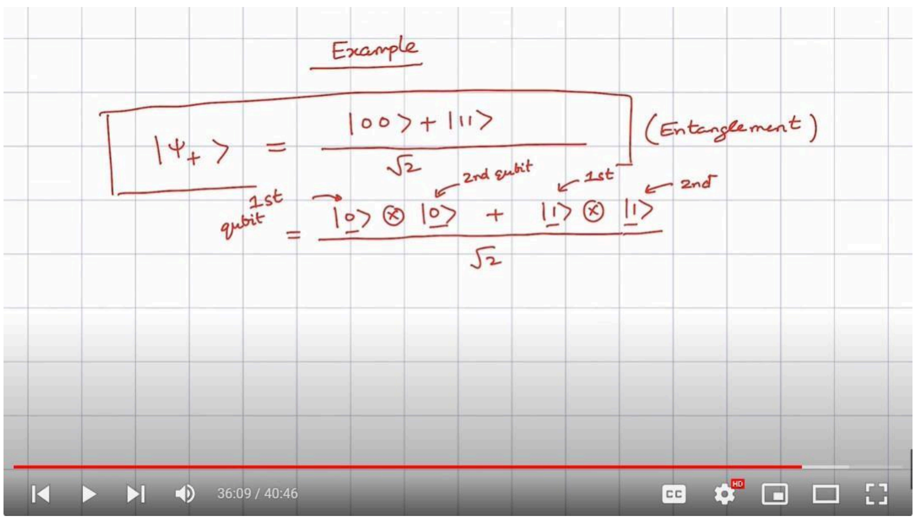

To illustrate it let me discuss an example and to do that, let us consider a state specified by this state vector and it's a two qubits system I am considering, so it is 0 0 plus 1 1 divided by root 2 so it basically short hand notation, if I write the full notation it would be direct product of 0 0 plus direct product of 1 1 divided by root 2 essentially the first part here represents the, refers to the first qubit and this one refers to the second qubit similarly here the same thing this is refers to first qubit and this refers to the second qubit, this state represents the fact that if the first qubit is in the state ket 0 then the second qubit is automatically in the state ket 0 or if the first qubit is in ket 1, the second qubit is automatically in the state ket 1, okay that means if we make a measurement and find that the first qubit is in the ket 0 which may refer to the ground state and the second qubit is also going to be found in the ground state and there is a 50 50 probability to have either to have either of this situation and this is an example of an entangled state, we are going to start discussing entanglement from the next module that is next lecture we will start module 2.

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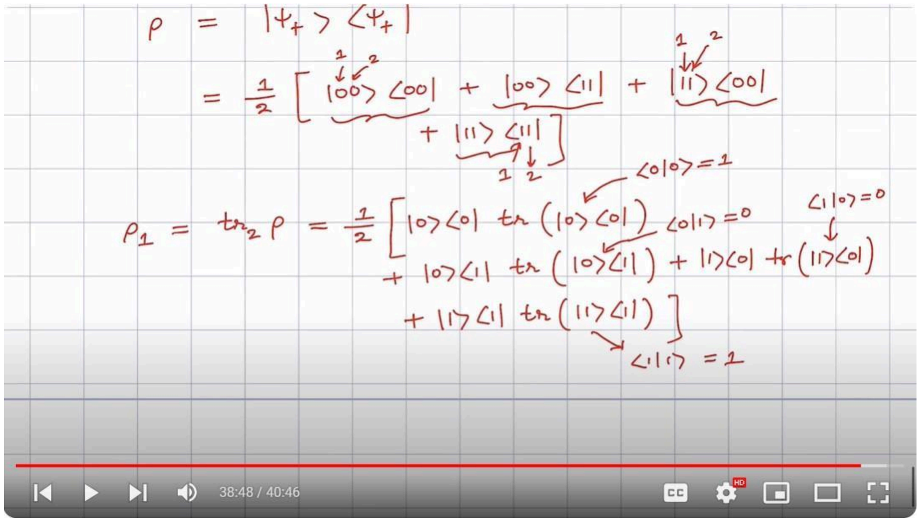

Now if I write the density operator for this entangled state it is easy to write, so density operator would be as per the usual definition, this is for the density operator and from here we can quickly get this would be 0 0 0 0 we have 0 0 1 1 plus 1 1 0 0 1 1 1 1, right? now again here the first 0 refers to the first qubit, second 0 refers to the second qubit and so on, so here say this is the first qubit, this is the second qubit, first qubit second qubit like this, okay? if I, we are interested only in the first qubit then we have to take the partial trace over the second qubit to get the density operator of the qubit 1, so this means that we have to trace out the second qubit from rho and if I if I do that then it is easy to we will just follow the prescription or the results that we have just worked out, the first qubit is going to remain unaffected so just let us concentrate on the first term how I do it so I have to take the trace over the second part so this is what I will have and let me now take this term, so here I will have the first qubit remains unaffected and trace operation would be over the second one similarly from the third I have 1 0 and trace over 1 0 and last term, last term will give me this now this trace operation we have already, we know the result this is the outer product and because of the trace you will get the scalar product of 0 0 which is obviously equal to 1 because of the normalization and this is going to give the scalar product of 0 1 and this is equal to 0 because of the orthogonality, similarly here this would be the scalar product 1 0, this is also going to be 0 and this guy, the scalar product would be 1 1 and this is going to give us simply 1.

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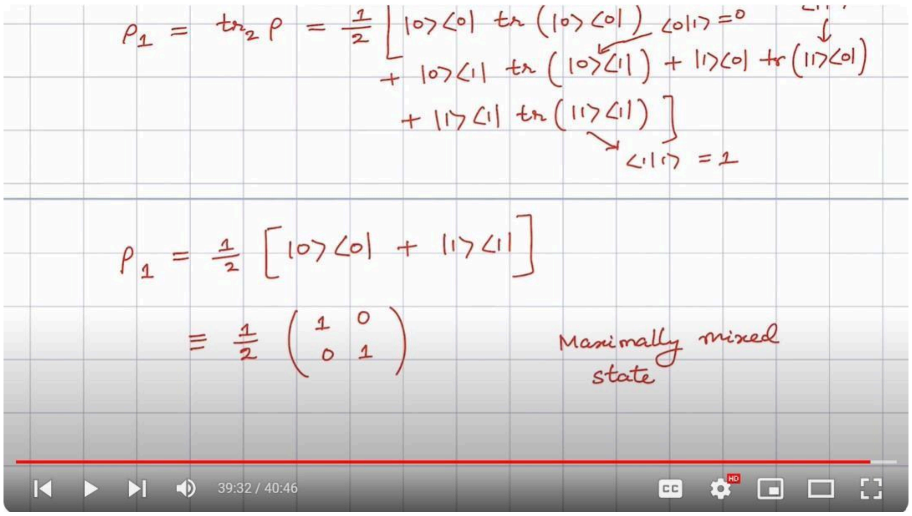

And because of this I will finally get rho 1 is equal to half 0 0 plus 1 1 and we have already seen this kind of a state and if I can write in the matrix form, this would be half 1 0 0 1, right, so it has half diagonal elements are 0 and diagonal elements are equal in magnitude and quite clearly this is a mixed state and this is a maximally mixed state maximally mixed state.

Let me stop for now, in this lecture we have learned, this was the part 2 of the lecture but overall in lecture 3 we have discussed the density matrix formalism which is going to be extremely useful, it is one of the most important tool for quantum entanglement, in the next lecture onwards we are going to start quantum entanglement, in fact from next lecture onwards the module 2 will start so that you understand the concepts that I have discussed in module 1, I have done some worked out examples in problem solving session, there I also discussed assignment zero problem solutions, so see you in the next lecture thank you.