Quantum Technology and Quantum Phenomena in Macroscopic Systems

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Lecture – 9

Density-Matrix Formalism.

Welcome to lecture 6 of this course. In the last class I introduced the concept of density matrix. In this class we are going to discuss the density matrix formulism in some more details. So, let us begin.

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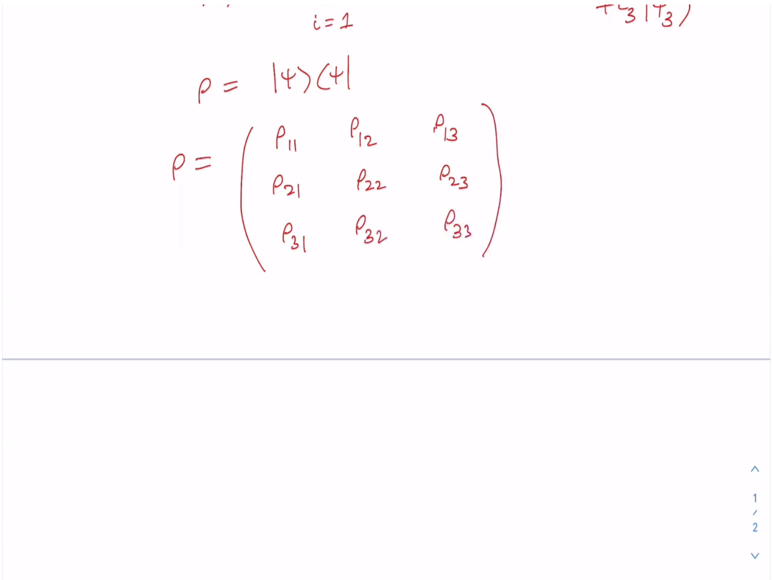

$i=1$

$$\rho = |\psi\rangle\langle\psi|$$

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{pmatrix}$$

In the last class we saw that the quantum state of a 2-level atom can be represented by the state vector psi is equal to say C g g plus C e e, right. So, g and e are the basis states of the 2-level atom. g refers to the ground state, e refers to the excited state, C g and C e are the complex coefficient and this is called a state vector representation or equivalently we also learned about another representation and that is called the density operator representation and in this case the density operator is defined as ket psi in bra psi.

So, this is an operator and here psi is a pure state. Actually, I will today discuss about mixed state as well. We will come to that little bit later. And in the basis ket g and ket e this density operator can be represented by this matrix rho, where these matrix elements are rho g g rho g e rho e g and rho e, and in fact, in terms of the coefficient rho g g is equal to C g C g star and rho g e is C g C e star rho e g is C e C g star and this one is C e C e star.

And also, we learned about the physical meaning of these density matrix elements. Now in general, irrespective of the nature of the atom if it is an isolated atom it may have many energy levels. So, the state of a pure atom, basically an atom which is not interacting with any environment in an isolated atom. So, it can be represented as a superposition of the state of the atom, or superposition of its eigenstates, right.

And this is the state vector representation and the corresponding density matrix representation or density operator representation would be this. For example, for say 3 level atom, the state vector psi would be it will go from i is equal to 1 to 3 C i phi i where phi i is at the eigenstate that means I can write it as C 1 phi 1 C 2 phi 2 and C 3 phi 3 where phi 1 phi 2 phi 3 are eigenstates and the corresponding density operator would be this.

And density matrix element would be represented by or the density matrix will be represented by 3 by 3 matrix with elements like this rho 11 rho 12 rho 13 rho 21 rho 22 rho 23 rho 31 rho 32 rho 33. So, this formalism can be extended to any number of energy levels.

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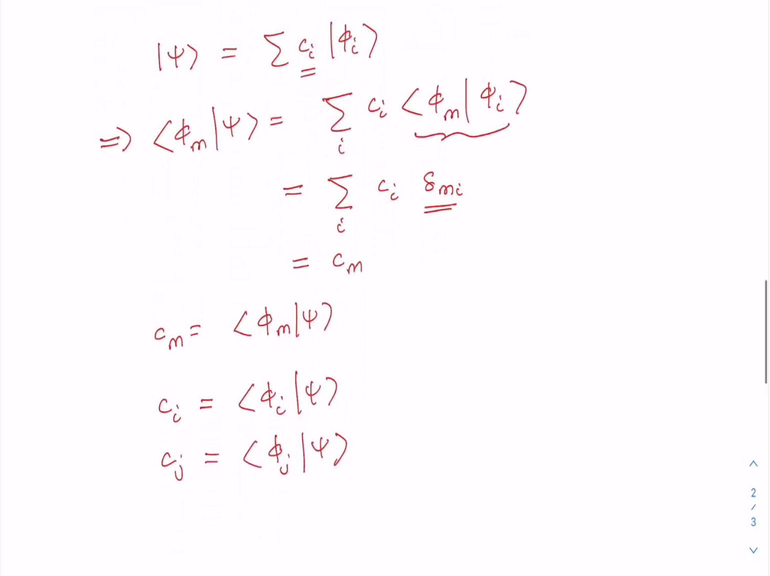

$$|\psi\rangle = \sum \underline{\underline{c_i}}\, |\phi_i\rangle$$

$$\Rightarrow \langle\phi_m|\psi\rangle = \sum_i c_i \underbrace{\langle\phi_m|\phi_i\rangle}$$

$$= \sum_i c_i\, \underline{\underline{\delta_{mi}}}$$

$$= c_m$$

$$c_m = \langle\phi_m|\psi\rangle$$

$$c_i = \langle\phi_i|\psi\rangle$$

$$c_j = \langle\phi_j|\psi\rangle$$

Now one great advantage of density operator is that we can find out the expectation value of any operator using this density matrix or density operator. So, suppose we have an operator A corresponding to an atomic system and then the expectation value of this operator would be given by just by taking the trace of the product of the density matrix rho and the matrix representation of the operator A. Then this is going to give us the expectation value of the observable A or operator A.

So, here actually many times I will not be going to write the hat. So, you just understand that we are discussing quantum mechanics so these are operators. Now let me actually prove it. This relation is very easy to prove. The expectation value of operator A is in the state vector formalism. It would be simply given by this where psi is equal to, I can write it as superposition of this eigenstates.

Now what I do I can just write it there are two, one is here bra psi and ket psi. So, let me use this but with different indices for bra part and the ket part. Then, I can write it by 2 summations say i and j here and here let me write C i star and other one would be C. So, therefore here I would have phi i A and this here would have phi j and then C j is coming out. I think it is easy to follow.

Now this coefficient also i can express in terms of these eigenstates because we have say psi is equal to say C i phi i. So, if I want to know C i, to know that let me multiply this by both sides by this bra phi m here and then the other side also I have to multiply it by phi m and you know that these are eigenstates. So, therefore these are C i. So, they are orthogonal. Orthonormality conditions I have to apply.

So, this would be C i delta m i. So, out of this summation, because of this Kronecker delta we will just get C m. So, this coefficient C m is simply given by phi m psi. So, therefore in this expression here C i C g C i would be simply phi i psi and C j would be phi g psi all right.

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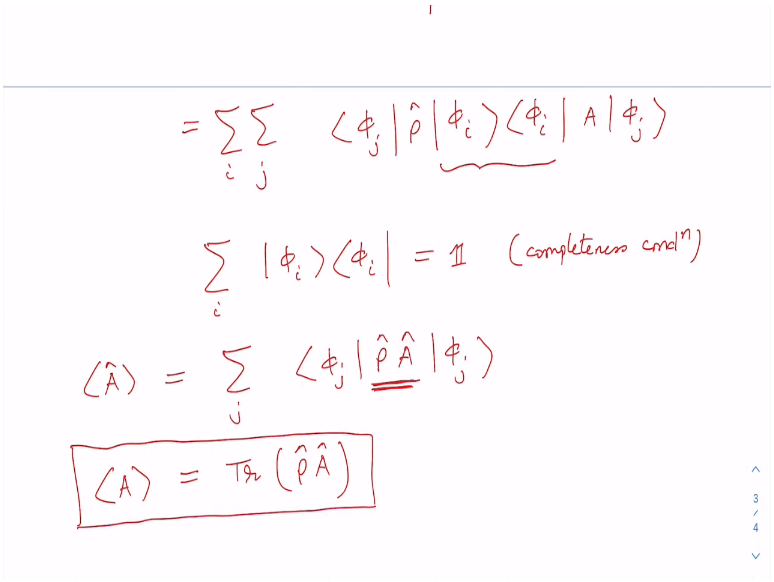

$$= \sum_i \sum_j \langle \phi_j | \hat{\rho} \underbrace{| \phi_i \rangle \langle \phi_i |}_{} A | \phi_j \rangle$$

$$\sum_i | \phi_i \rangle \langle \phi_i | = \mathbb{1} \quad (\text{completeness cond}^n)$$

$$\langle \hat{A} \rangle = \sum_j \langle \phi_j | \underline{\underline{\hat{\rho} \hat{A}}} | \phi_j \rangle$$

$$\boxed{\langle A \rangle = \text{Tr}(\hat{\rho} \hat{A})}$$

So, therefore if I put this, this implies that C i star is psi phi i. So, using this I can, let me just take it, I can just put these coefficients, okay. So, what I can do I can just write it as i j here C i star is psi phi i and C j is phi j psi. Remember these are just numbers and I have phi i A phi j. So, because these are numbers I can write them interchangeably. So, therefore if I just write it as phi j, if I take it this side this one phi is a psi and psi phi i okay then all right.

So, what I will have is phi i A phi j. We can see that this is nothing but the density operator rho. So, therefore we can write i j phi j rho phi i phi i A phi j. Now again if you see that this is actually I can invoke the so-called completeness condition because phi i are the basis states or eigenstates. So, therefore this is identity operator or identity matrix. So, using this identity matrix this completeness condition if I invoke then I can write the expectation value of the operator A as now I have j phi j rho A phi j.

And quite clearly as you can see this is nothing but the, these are some of the diagonal matrix elements of the operator product of the operators rho and A and therefore I can now write it as trace of the matrix rho and A. So, hence we prove that the expectation value of any operator can be written or can be found just by finding the trace of the matrix product rho and A. So, this is a very, very useful way to find out the expectation value of any operator.

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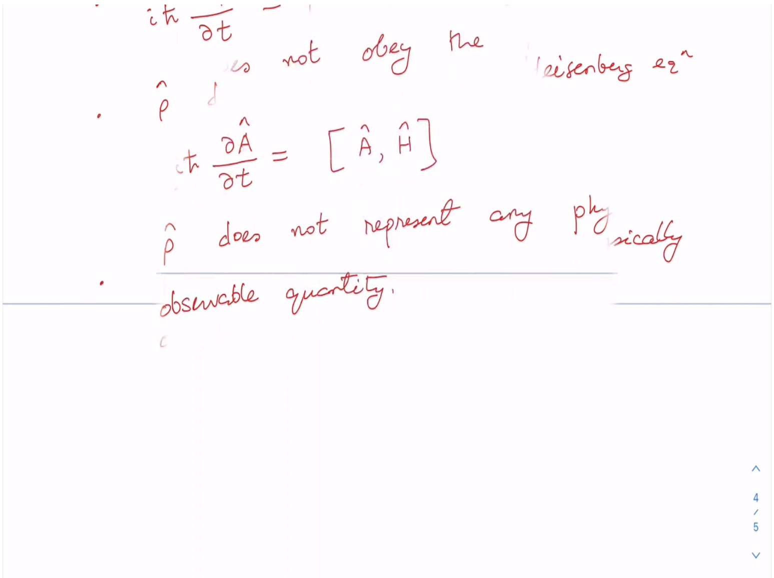

$i\hbar \frac{\quad}{\partial t}$

$\hat{\rho}$ d es not obey the eisenberg eq^n

$$i\hbar \frac{\partial \hat{A}}{\partial t} = [\hat{A}, \hat{H}]$$

$\hat{\rho}$ does not represent any physically observable quantity.

Now let me list out some properties of density operator or density matrix rho. Rho is an operator in the Hilbert space and rho is Hermitian. So, that means rho is equal to rho dagger that means if I take the complex conjugate of the density matrix and then take the transpose, I am going to get back the density matrix again, rho, and because rho is Hermitian, eigenvalues of rho are real and in addition to that they have to be non-negative and this comes due to the fact that the diagonal elements in the density matrix or density operator represents probabilities and probabilities cannot be negative and rho is normalized. Rho is normalized. This implies that if I take the trace of rho then we will get 1 and that is obvious because the diagonal element represents probability and total probability has to be equal to 1. One useful property to remember is that the probability to find the system in a measurement in the state say phi is given by just by calculating this quantity.

This is a very useful result in a way and property and it is worth remembering and we will utilize it later on. And finally, the evolution, the equation that density operator satisfies is the so-called Liouville equation and that is given by i h cross del rho del t is equal to H rho. This is called Liouville equation and if you see these equations carefully that this density or this is not Heisenberg equation by the way.

And rho in fact does not satisfy or obey the Heisenberg equation. Recall that if there is a physically observable quantity is there and it is represented by the operator say A in quantum mechanics then these operators satisfy this Heisenberg equation of motion if it is not explicitly dependent on time. But this rho does not represent any physically observable quantity that is why it does not satisfy the Heisenberg equation.

So, rho does not represent any physically observable quantity, all right.

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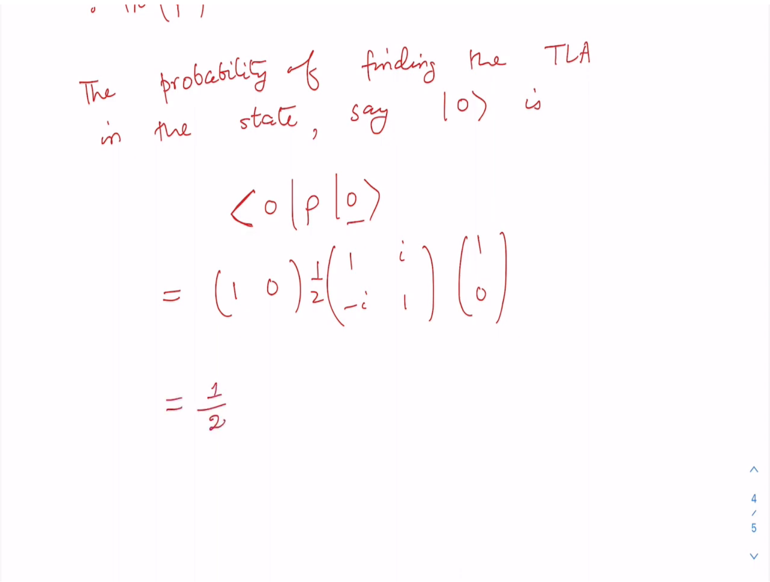

The probability of finding the TLA in the state, say $|0\rangle$ is

$$\langle 0|\rho|0\rangle$$

$$= \begin{pmatrix} 1 & 0 \end{pmatrix} \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \frac{1}{2}$$

To get an idea about the properties of rho, quickly. So, let us just consider this simple example say a 2-level atom is represented by this coherent superposition of state 0 and 1 and in terms of matrices, ket 0 is represented by the column vector 1 0 and ket 1 is represented by the column vector 0 1 and then this state vector of the 2-level atom can be represented by this column vector 1 minus i.

So, the corresponding density operator for this 2-level atom would be this ket psi bra psi and if you work it out then it would be 1 by root 2 1 minus i 1 by root 2 1 plus i and then rho would be represented by this matrix. So, this is the density matrix for the 2-level system that we are considering here. Now immediately you can see some of the properties are quite evident that rho is obviously equal to rho dagger. This rho is Hermitian and then trace of rho is equal to one.

And also, if I know the useful property that I mentioned earlier say the probability of finding the two-level atom in the state, just for illustration purpose, say in the state 0 is we actually already know the answer from the state vector the probability of finding the system in the state 0 is 1 by root mod square. So, that is obviously half but what about our formula? What it says that users have to calculate 0 rho 0 and which is I can now write it 0 as this bra as 1 0 this rho matrix rho is half 1 i minus i 1 and this 0 is ket is 1 0.

So, therefore if you actually work it out you are going to get a half. So, far we have confined our discussion to isolated or closed system and these systems are completely described by the so-called pure state but in reality, systems always interact with surrounding and it results in mixed states. So, let us now discuss density matrix formulism for mixed state.

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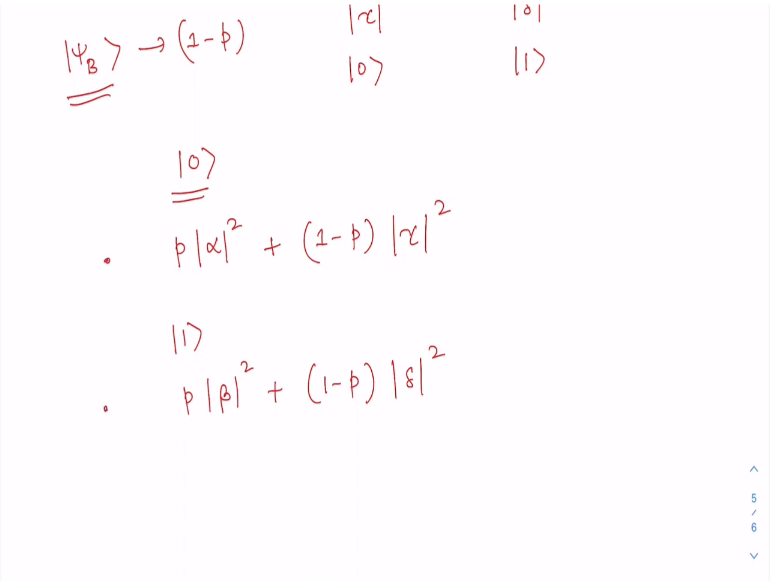

$|\psi_B\rangle \rightarrow (1-p)$ $|\gamma|$ $|\delta|$

$|0\rangle$ $|1\rangle$

$|0\rangle$

- $p|\alpha|^2 + (1-p)|\gamma|^2$

$|1\rangle$

- $p|\beta|^2 + (1-p)|\delta|^2$

Let us consider an ensemble of two 2-level atoms represented by state vector psi A and psi B. This is an ensemble of 2-level atoms. Two 2-level atoms we are considering say atom A and atom B or you can consider call them as subsystem A and subsystem B for the composite system A + B also then here A is represented by the state vector psi A which is a superposition of the ket basis state 0 and 1 ket 0 and ket 1 and psi B is also we can write it as a superposition of ket 0 and ket 1 with coefficients associated coefficients gamma and delta here.

Now from this ensemble the probability that one can pick up psi A is, say p and the probability that the state psi B is pick up is 1 minus p. These are statistical probability or classical probability. Now the question is that what one will get if a measurement is made in the basis states say ket 0 and ket 1? So, actually in this measurement 2 processes are happening, first of all one has to pick up either psi A or psi B from the ensemble and next make a quantum measurement, make measurement on the picked up state.

Now say psi is picked up from the ensemble with classical probability p. After it is picked up we make a measurement on the state psi A. Then because of the quantum measurement the measurement of the state psi A will either get collapsed to ket 0 or ket 1 with probabilities mod alpha square or mod beta square. So, with we will get either ket 0 or ket 1 and similarly in the other case if psi B is picked up and it would be picked up with classical probability say 1 minus p.

Then after we picked it up if we make a measurement either it will get collapsed to again ket 0 or ket 1 with corresponding probability mod gamma square and mod delta square. Now you see what would be the total probability that the composite system will be found in the ket state 0. Two things are happening. If we pick up say psi A, then the probability that it would be there in ket 0 would be p mod alpha square and if we pick up psi B then the probability would be 1 minus p mod gamma square.

On the other hand, the probability that we are going to get the ket state 1 would be p mod beta square and the other one 1 minus p delta square. So, these are the total probabilities. Either we are going to get the whole composite system either in the ket state 0 or in the ket state 1.

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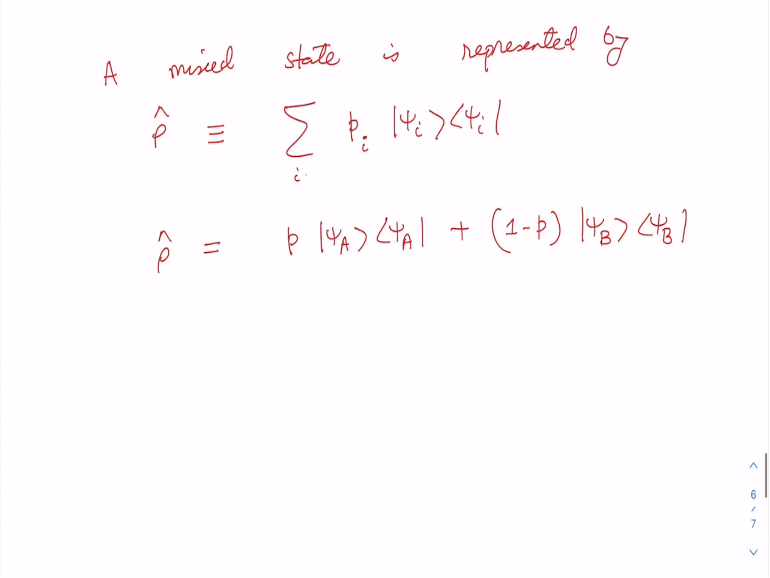

A mixed state is represented by

$$\hat{\rho} \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$\hat{\rho} = p |\psi_A\rangle\langle\psi_A| + (1-p) |\psi_B\rangle\langle\psi_B|$$

So, as you can now see that unlike in the case of pure quantum system, pure state cases, where the whole system is represented by the state vector psi that means if you have a box like this then every time you are going to pick up psi with hundred percent probability okay. So, that is why it is called pure state but now that is not the case here in the case of mixed state.

So, how to represent a mixed state? A mixed state is rather represented by density operator rho and this is where the biggest advantage of density operator formulism and this is for the mixed state case. It is defined as rho is equal to we have the corresponding classical probabilities and the state say psi i here. For example, in the above case where we have considered the density operator for this collection of 2-level atoms would be simply p psi A psi A and plus 1 minus p psi B psi B.

I am sure you know you have got the idea here and if we have, say n number of components in the ensemble. So, i is going to run from 1 to n.

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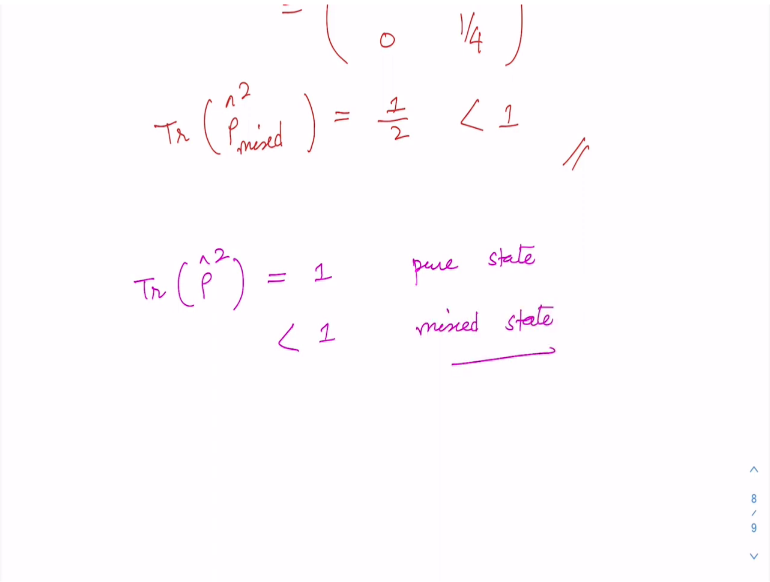

$$= \begin{pmatrix} 0 & 1/4 \end{pmatrix}$$

$$Tr\left(\hat{\rho}^2_{mixed}\right) = \frac{1}{2} < 1 \quad //$$

$$Tr\left(\hat{\rho}^2\right) = 1 \quad \text{pure state}$$

$$< 1 \quad \text{mixed state}$$

Now what about the expectation value in the mixed state? Expectation value of an operator, say o cap in the mixed state. So, that would be, let us work it out, given by this. So, the classical probability and the corresponding state you just have to sum it up. So, this is what you will have. Let us see whether we can get a compact form of this.

So, to do that let me invoke the completeness condition of basis state suppose I have the basis state phi k then I know that this completeness condition is satisfied. I can take advantage of this is equal to identity. So, therefore what I am going to do, I am just going to sandwich this here. This is running psi i and let me just do here k phi k phi k these are basic states, eigenstates.

So, this is what I have put here and then I have psi i. Now I can write it as follows: Because these are if you can see these are just numbers. This is a scalar product. So, I can take it like this. I can write i summation k p i. I can write it as phi k psi i. This one I am taking in here and then I have psi i o cap phi k all right. Now I can write it again as follows: k cap phi k. Let me write it as summation sign. Let me take inside here p i. I have here psi i psi i.

So, you have o cap and then phi k. I am just rearranging the terms there but you see that this guy is nothing but the density operator that as we have defined here. So, therefore I can write the whole thing as sum over k phi k rho o phi k. Now you can easily see that this is nothing but the summation of all the diagonal elements of this product of these matrices rho and o. Density operator in the operator observable. So, this is I can write it as simply trace of rho cap o cap.

So, this is the formula we have got even in the case of pure state and here also in the case of mixed state this is still valid. Now the question is how to distinguish a pure state from mixed state. If we suppose we are given a density of matrix or density operator then how can we distinguish a pure state and mixed state?

This is very easy because first of all both actually pure state and whether it is pure state or mixed state the trace of rho whether it is pure or mixed does not matter trace of rho is going to be equal to 1. Properties of the density operator or density matrix that I discussed previously is still valid and that means this density matrixes are normalized. Now to distinguish it what you have to do if you just take trace of rho square in the case of pure state it would be equal to 1 for pure state.

But trace of rho square for the mixed state if you take the density operator for the mixed state and multiply it twice and then take the trace then you are not going to get one. It would be less than one for the case of mixed state. Let me illustrate it by just giving an example. Let us say we have a 2-level atomic system or ensemble represented by the system. If I can write it as a coherent superposition of ket state 0 and 1.

Obviously, this refers to a pure state. I can define this state by state vector like this and then the corresponding density operator would be this ket psi and bra psi and if you work it out, immediately you will get it, it the density matrix of the pure state would be simply half half here half and half here. Now immediately you see the trace of rho is obviously one. What about rho square pure?

This would be simply the matrix multiplication of rho pure with itself. So, you have to take the matrix multiplication of rho pure with itself. So, this would be this one and if you do the multiplication you will see that you will get here 1 by 4 plus 1 by 4 1 by 4 plus 1 by 4 1 by 4 plus 1 by 4 1 by 4 plus 1 by 4. So, therefore we will just have one half one half one half and one half.

So, that means it is simply rho pure and quite clearly, we will have trace of rho square pure is equal to 1. Now what about the mixed state? So, let us say we have again a 2-level atom but the ensemble let me write here. Consider an ensemble of 2-level atom with equal mixtures of ket 0 and ket 1. So, that means there is a 50% probability or probability of half to get it in the state zero or which is represented by 1 0.

And there is a 50% classical probability of getting it in the state 1 which is represented as 0 1. So, what about the density operator representing this mixed state? That would be as per our definition of density operator for mixed statet. So, the classical probabilities are half in both cases. So, we have half 0 0 plus half. It would be 1 1 here. So, this I can represent in a matrix form and if you represent it in a matrix form.

So, in this case we have this mixed state. So, it would be half 0 0 half. Now you see again trace of this rho for the mixed state then it would be obviously equal to 1 but what about rho square if you take the product of this matrices. Matrix multiplication if you do what you are going to get is you are going to get here it would be 1 by 4 it would be 0 it will be 0 1 by 4 and quite clearly trace of rho square for this mixed state case you are simply going to get half which is less than one.

So, this validates what I said earlier that for the case of mixed state you just have to take the rho square. That means let me just conclude here just by saying this that to distinguish it you just have to find out trace of rho square if you are given a density operator. Just find out the product of the density operators. And then take the trace. Then if you get 1 then that is a pure state and if it is less than one that corresponds to a mixed state.

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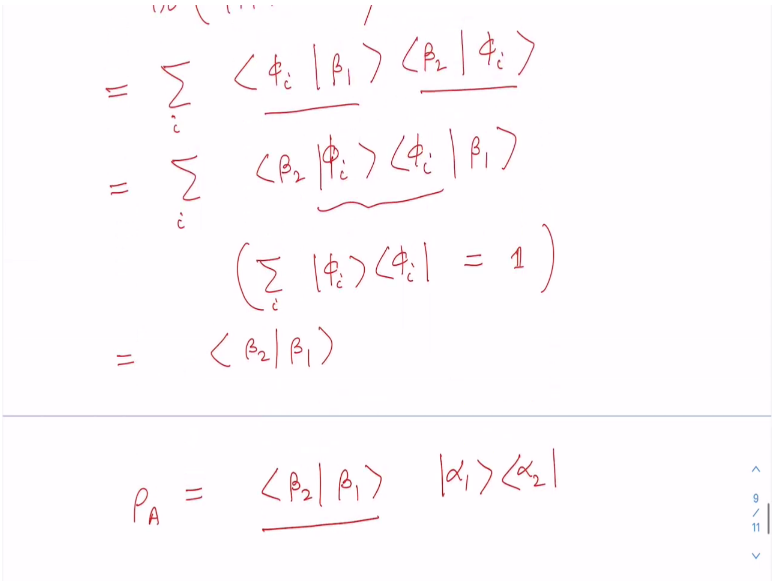

$$= \sum_i \underline{\langle \phi_i | \beta_1 \rangle} \, \underline{\langle \beta_2 | \phi_i \rangle}$$

$$= \sum_i \langle \beta_2 \underbrace{| \phi_i \rangle \langle \phi_i |} \beta_1 \rangle$$

$$\left(\sum_i | \phi_i \rangle \langle \phi_i | = \mathbb{1} \right)$$

$$= \langle \beta_2 | \beta_1 \rangle$$

$$\rho_A = \underline{\langle \beta_2 | \beta_1 \rangle} \, | \alpha_1 \rangle \langle \alpha_2 |$$

Let me now discuss an important concept called reduced density matrix. Reduced density matrix or reduced density operator. Say we have a composite system A plus B. Many a time what happens is that we may be interested in knowing only about the system A or only about the system B. For example, later on in this course we will have a situation where say we have a mechanical oscillator like this and this is interacting with a lot of photons or the mechanical oscillator is a bathed on a photon or surrounded by a lot of electromagnetic radiations.

Equivalently speaking, I can just depict the whole thing like this. Say I have this system A and it is surrounded by a lot of photons. So, this we may say to be as our surrounding and this as our system. So, now if we are interested only in the system, only the question is how to extract information about the system A from this composite system A plus B? or I mean to say that suppose I know the density operator for the composite system which is say rho A plus B, then how I can get information or how I can write the density operator rho A from rho A plus B? or similarly, if I just wanted to know about system B or I want to write the density operator for system B how I can do it if I know the density operator for the composite system? So, this is what is answered by the prescription called reduced density operator. So, how it is done?

So, properties of system B or A, say system B may be obtained by taking partial trace over the system A. I will explain it with some example of say system A. So, partial trace essentially averages out the effect of unwanted system and extract the properties of the of the system of interest. So, suppose I want to know about system B then I just have to take trace over A.

I have separated over A on the density operator rho A B and this is basically known as tracing out A or if I want to know similarly for system A then I just have to take trace over B. Let me explain it with an example. Let us say I have this composite system A B and it is represented by this density operator rho A B which is let me write it say a system A is say represented by say this ket alpha bra alpha 2 here and then this is a system A.

This is system A and system B is represented like this. This is my system B. Now when I say if I want to know about system A then I would just take trace over B, trace out B from A rho A B. So, I will just take trace. So, alpha 2 here cross beta 1 beta 2 taking trace over B means that I will just take the basis sets in the Hilbert space of the system B and then I will take the trace.

So, because I am just taking the trace over B only in this system, composite system A plus B. So, therefore this one that is belonging to system A would remain unaffected and I just have to take trace here on this beta 1 beta 2. So, hope this is clear. Now when I say taking trace over means I just have to deal with this guy here. Say, we have a basis state. We have basis states say phi i.

We have a set like this in the Hilbert space of the system B. Then trace over this system B, I can just write it like this. I will take it as phi i beta 1 beta 2 phi i and this of course I can write it just I can, these are numbers, so, I write beta 2 phi i phi i beta 1 then I can use the completeness condition as you know the completeness condition by now it is very well known to you.

So, I will simply get it as beta 2 beta1 and therefore I get my system density operator as beta 2 beta1. This is just a number and then I will be left out with this operator. That is how we can work out.

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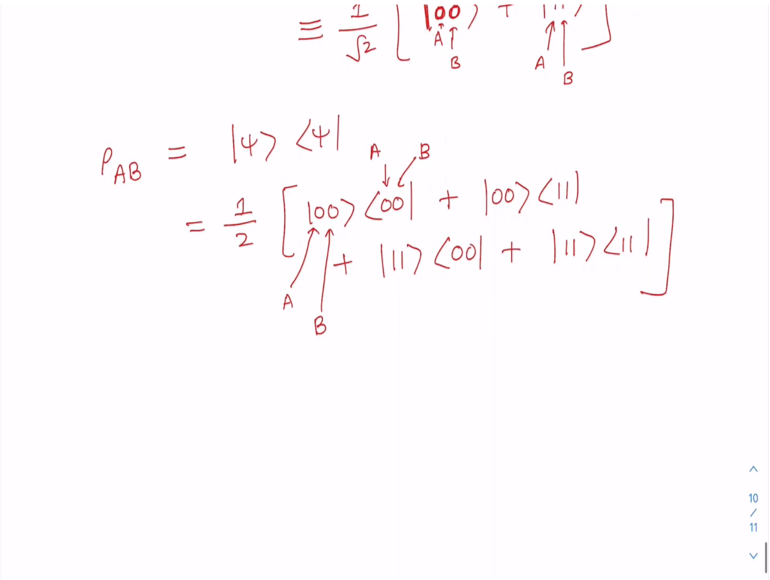

$$\equiv \frac{1}{\sqrt{2}}\left[\,|00\rangle + |11\rangle\,\right]$$

$$\rho_{AB} = |\psi\rangle\langle\psi|$$

$$= \frac{1}{2}\left[\,|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\,\right]$$

Similarly, system B if you work it out you will get it as alpha 2 alpha 1 and this would be beta 1 beta 2. I hope it is clear. So, let me give an example. Let us say consider two 2-level atoms, 2-level atoms A and B and say they are entangled and this entangled state for the composite system A B they are represented by this state. This entangled state is say in ket 0 and ket 0 1 basis. So, this is what I have this is the entangled state. That means if the system A is in the ket state 0, system B is also or the atom B is also in the ket state 0 and or if the atom A is in k state 1 then the system B is also automatically in ket state 1 okay. This is what it means. In shortened notation I can write it as 1 by root 2 0 0 plus 1 1. So, just understand that the first term, first element in this ket vector here represents it belongs to atom A and this belongs to atom A, this belongs to atom B.

And similarly, here this belongs to atom A and this belongs to atom B. So, these things just you have to remember. Then the density operator for this entangles system would be we can work it out very simply and that would be half if I expand I will get 0 0 0 0 plus 0 0 1 1 plus 1 1 0 0 plus 1 1 1 1. So, just remember that again let me emphasize that this is belonging to atom A, this one belongs to atom B, this belongs to atom A, this belongs to atom B and so on.

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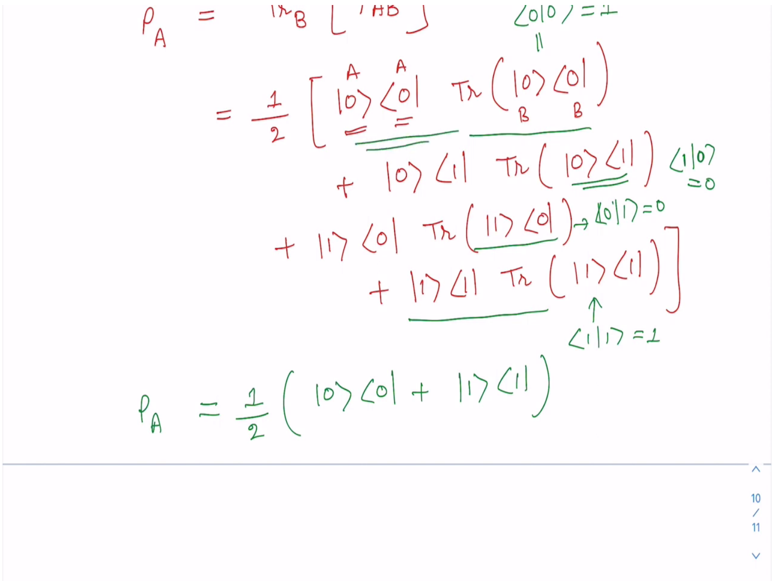

$$\rho_A = \mathrm{Tr}_B[\rho_{AB}] \qquad \langle 0|0\rangle = 1$$

$$= \frac{1}{2}\Big[\, \overset{A}{|0\rangle}\overset{A}{\langle 0|}\; \mathrm{Tr}\big(\underset{B}{|0\rangle}\underset{B}{\langle 0|}\big)$$

$$+ |0\rangle\langle 1|\; \mathrm{Tr}\big(|0\rangle\langle 1|\big) \qquad \langle 1|0\rangle = 0$$

$$+ |1\rangle\langle 0|\; \mathrm{Tr}\big(|1\rangle\langle 0|\big) \rightarrow \langle 0|1\rangle = 0$$

$$+ |1\rangle\langle 1|\; \mathrm{Tr}\big(|1\rangle\langle 1|\big)\Big] \qquad \langle 1|1\rangle = 1$$

$$\rho_A = \frac{1}{2}\big(|0\rangle\langle 0| + |1\rangle\langle 1|\big)$$

Now suppose if we are interested in the 2-level atom A only then if I want to extract the density operator for atom A then I just have to trace out atom B and that is now easy to do so let me show you how we will do that. You just have to take density operator rho A B is already I have written here, here I have written it. So, let me just write half and I will take trace over atom B.

So, a half here. This A would remain unaffected. So, A from here I take, A from here I take, this is what I take A A I have taken and then I will take trace on B and B part here. This I think you can easily see that this is your B and this is again from B and similarly I can just go on writing the other term 0 1. I have trace 0 1. You have to be careful and then you will have third term will give you 1 0 this belongs to system A.

So, I will take trace over this B 1 0 and then finally I have 1 1 and then I will take trace I have 1 1 all right. Now already I got this result that when we have taken trace here you see when I have taken trace like this. So, this would be simply this scalar product like this. So, this one is going to give me if I take trace this is going to give me 0 0 and I know that this is they are normalized.

So, this would give me 1. Here it will give me 1 0 and because this ket and this ket is orthogonal to each other. So, this is going to give me 0 and here also I will get it as 0 1 and this is going to give me 0 right and finally here I will get it as 1 1 and this is going to give me 1. So, therefore we are left out with this one that would be rho A would be equal to half 0 0 plus 1 1. So, these are the terms that will be left out and this is the density operator or density matrix for the system A.

Let me stop for today. In this class we have learned about the density matrix formulism. In the next class we are going to discuss about quantum harmonic oscillators which is actually one of the most important and critical component of quantum technology. In particular later we will learn that how electromagnetic fields could be modeled as an infinite collection of independent harmonic oscillators in the quantum regime, thank you.