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Quantum Information and Computing

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Modul No.03

Lecture No.12

Density Matrix - II

In the previous lecture we had introduced the idea of a density matrix the point that we try to make is that in most cases that we look at in a physical system the physical system is almost never an isolated system that is because it is always a part. Of a bigger system and it interacts with it is environment and so as a result the problem is that we have to make measurements generally on an ensemble and the other problem is that we could have a collection of different systems in the same ensemble and when you make a measurement it is not necessary that we are picking up the same state all the time in order to take care of these things we bring in the concept of a density matrix.

And as we will see later that the entire quantum mechanics can be restated in the language of density matrix which will be the more appropriate situation for talking about systems which are either parts of a bigger system or our members of an ensemble. So we had defined our density operator yesterday and so let us look at first we will spend some time on the density operator for the pure system where the system is described by a state vector so let us look at supposing.

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 $: g = | \Psi \rangle \langle \Psi |$ ${e_i}$ is a basis $\langle A \rangle = \langle \Psi | A | \Psi \rangle$
= $\sum_{i=1}^{n} c_i^2 c_i \langle e_i | A | e_i \rangle$
 $\langle e_i | \Psi \rangle$ $\langle A \rangle = \sum_{i,j} \langle \Psi | \hat{e}_i \rangle$

I have a system ψ system with a state vector ψ then the corresponding density matrix or density operator is simply given by ψ, ψ suppose I have in this situation supposing in the Hilbert space to which the ψ belongs supposing this is the basis.

Now emphases the basis let us look at what is the expectation value of an operator we know that this is simply given by ψ A ψ and if I now express the state ψ in as a linear combination of these basis states what we get is $\Sigma_i \Sigma_j c_i^* c_j$ and the matrix element of $e_i A e_j$ where this c_j for is the basic state scalars product with ψ and obviously your complex conjugate of that which is c_i^* will be ψ with e_i .

Now with this let us look at how much is the expectation value be so the expectation value of A we can rewrite this expression by plugging in these two things and what we get is $\Sigma_i \Sigma_j$ so we have got ψ e_i e_j ψ and of course the matrix element which is e_i A e_j now since these are scalars since these are scalars I can rewrite them by interchanging their orders and write it as $e_i\psi$, ψe_i .

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 $e\sum_{i} \langle e_i | \Psi \rangle \langle \Psi | e_i \rangle A_{ij}$
= $\sum_{i} \langle e_i | e_i | e_i \rangle \langle e_i | A | e_i \rangle$
= $\sum_{i} \langle e_i | e_i | e_i \rangle$
= π (eA) $40 = 0.52$ $(0.107)(4)$

So this is equal to so expectation value of A is given by Σ_{ij} so you notice this is $e_j\psi$, ψe_i and of course the matrix elements of A within the states i and j which I simply write it as this now this you notice is nothing but my density matrix ρ so therefore this expression is Σ_i and Σ_j e_j, e_j ρ e_i and this was e_i A e_i now what I notice here is that this cat e_i and bra e_i are together and nowhere else these summation over i appears so therefore the summation over i can be shifted there and you notice that if you take the Σ_i of this quantity that is nothing but the identity operator because of completeness.

So as a result this is given by Σ_j of $e_j \rho A e_j$ but some of the diagonal elements of diagonal matrix elements of an operator is nothing but the trace of that operator so this is trace of a ρ A so therefore if you know the density matrix we have proved it at least for the pure state case we will later on see that this is a relationship which is valid even for the general case that we will be talking about so this is what it is. Now taking the special case of A as an identity if you take A as an identity.

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Then you notice you get trace of ρ is equal to 1 now this will see is a property of density matrix which is always valid irrespective of whether the state is a pure state or a mixed it mixed yet we have not yet defined but we will do that look at the slides here.

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Which sort of gives you some of the properties that we have derived so far for the pure states the we had last time defined the density matrix for an ensemble or a mixed states as being given by Σ_i p_i, p_i is the probability with which the states ψ_i appears in an ensemble and so therefore the general definition of a density operator is Σ_i the probability i times $\psi_i \psi_j$.

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And for a pure States this obviously is simply ψ i and the expectation value of an operator we have just not shown it to be given like this. So with that let us go over now to the matrix representation of a density matrix, so obviously if I have a basis if I have a basis.

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3 e_i $= \langle e_m | \hat{e} | e_n \rangle$ Diagonal ele

Let us say $\{e_i\}$ or whatever now I define the mnth matrix elements as given by the matrix element of row in the states mn, so recall that row is my $|\psi\rangle \langle \psi|$ how so the diagonal matrix elements, are row let us say mm is em ψ then ψ em, so which is nothing but absolute value of $|\text{cm}| \psi|^2$. Now but however you recall that this was nothing but the definition of my probability in the bond interpretation of quantum mechanics.

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 ${e_i}$ $= \langle e_m | g | e_n \rangle$ Diagonal elements

So therefore this is nothing but am or cm as we wrote it cm absolute square, so this is the born probability of getting a state n when a measurement is made. Now that leaves us with off diagonal terms of the matrix elements of the density operator.

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So these off diagonal terms, if you look at a typical off diagonal terms suppose I say m is not equal to n, then let us write $C_m = |C_m| e^{i\phi m}$ we need C_m^* which is there so this is equal to $|C_m|$ e ^{i ϕ m}, So therefore my M&F matrix element is< em| ψ > < ψ en> so this is simply C_m C_n^{*} = |C_m| | $C_n|e^{i(\phi m - \phi n)}$ So you notice that the off diagonal matrix elements these depend on the relative phases between the states m and n.

And these result in the interference term, so the off diagonal matrix elements for m not equal to n these give rise to the interference term. So just give you some examples of a density matrix written in a for a single qubit system, so let us look at a state normalized state which is given by.

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 $|\Psi\rangle$ = suppose is write $1/\sqrt{2}$ $|0\rangle$ - i / $\sqrt{2}$ $|1\rangle$ this a normalized pure state, now according to our column vector representation this is simply given by $1/\sqrt{2}$ (1 and –i) So therefore the density matrix row is simply this product which is a matrix direct product which is equal to $1/\sqrt{2}$ and you can easily multiply the corresponding matrices namely $(1, -i)$ with the row vector $(1, +i)$ and that gives you $1/\sqrt{2}$ (1, i, -i, 1) notice one thing that the trace as expected is $1/2 + 1/2$ which is equal to 1.

The another point to notice is, the row is hermitian and this is again we will see is a property of a density matrix the Herman density of row.

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Let us look at these slides, so the point is this that if you are looking at the density matrix row I can of course write it like this as I have shown it to you earlier.

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And the diagonal elements of the density matrix gives you the boring probability of getting a state, the another point to notice this diagonal elements being $|C_n|^2$ there essentially non-negative quantity, so therefore the density operator is a positive operator this is another general property of the density operator.

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And the another point that we would like to make is that the density operator satisfies what is known as the Louisville equation, I am showing it simply in the slide it is a fairly straightforward algebra you should do it looking at the slide say since ψ is a state. So I have ih cross d ψ/dt is Hamiltonian acting on ψ taking the hermitian contribute of this I get – ih d/dt(ψ is brass i acted from the right with the Hamiltonian h.

And if you calculate what is ih cross off the density matrix row, this is simply done by a chain rule differentiation and you will find it is commutator of the Hamiltonian with row itself, one point to notice that it does not satisfy Heisenberg equation of motion even though ρ is an operator, and the main reason is this that ρ is an operator in the sense that it has the mathematical structure of an operator. But Heisenberg equation of motions which essentially said that ih x da /DTis commutated of a with the Hamiltonian is valid for the case where a is an operator representing a physical observable.

Now ρ though it has the mathematical structure of an operator it does not represent a physical of the pivot, and the equation that if satisfies is the liouville equation so the Schrodinger equation in my for the state is leads to the liouville equation for the density operator. So with this let us generalize to the case of a an ensemble, so in which case my ρ is sum over $\sum i p_i |\psi \psi|$

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Look at the slide, now clearly ρ is summation. And you can it takes a very trivial exercise to show that $Tr(\rho)=1$ which simply comes by taking the trace of both sides and using the fact that total probability sum over $\sum i p_i = 1$. Now one point is that for a pure state $\rho^2 = \rho$ that is fairly straightforward you have ψ , ψ , ψ get bracket is the structure and if you write ρ^2 then of course 1ψ and its bra and it's cat will come together giving me 1

So therefore $Tr(\rho^2)$ is same as Tr (ρ) and that is equal to 1 of course. Now since it is a positive operator its Eigen values are non-negative. Now this property, this property that $p=p^2$ is however not valid for the mixed state density matrix.

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And there is a matter of very simple way to look at it that the density matrix is actually sum over \sum ip_i| ψ ψ | so the point to notice a mixed state does not have a state vector, but it is described by a density matrix just to give you a general idea let us look at the following they suppose I have a an ensemble which has let us at 50% in state 0.

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And let us say another 50% in state $|0\rangle + |1\rangle / \sqrt{2}$ now I can individually calculate the density matrices for each one of them and then add them with the probabilities, so therefore my ρ would be the probability $1/2$ times the density matrix corresponding to this which is $|0\rangle > 0|$ plus the second states probability which is 1/2 this times $\langle 0|+ \langle 1|/\sqrt{2}$ multiplied with $|0|> + |1>/\sqrt{2}$ there you can open it up and write this, you notice there is a 1 over $\sqrt{2}$ up to 1 over $\sqrt{2}$ so there is a 1 over 4 there so i get 3 x 4 $|0\rangle$ <0|+1/4 $|1\rangle$ <1| there are cross terms here and this cross terms are 1/4 $|1 \rangle$ <0| +1/4 |0 > <1|. So if I now look at a matrix representation of this, this is clearly 3/4, 1/4 and 1/4 here and 1/4 here.

Look clearly that trace is still equal to 1 there are off diagonal matrix elements here, so therefore this is a partially mixed state why partial I will come to say it is a partially mixed state because the off diagonal matrix elements are there but they are not that big. For instance if you take an ensemble which has let us say 75% in state zero.

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 $757. 107$
25%. 117
9 = (344 0

And 25% in state 1, the corresponding density matrix would be a diagonal matrix 3/ 4, 1/4 00 notice we have reduced the amount of the strength of the optical elements, so and I have made it 0 so this is a completely mixed state. Now the case where the, it is still diagonal but the diagonal elements are all of equal strength that is called a maximally mixed situation. So this is what the density matrix for the mixed state is about.

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Having done that let us look at a representation of the density matrix, there is another point before I go over to that I would like to meet that suppose you have a situation where you find that $\rho1=p2$, the question is that does it imply the same state. Well, I have said that there is no concept of a state but does it imply the same mixture. The answer is no, $\rho1 = \rho2$ does not.

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es not two ensembles **SO/.**

Necessarily imply that the, the two an ensembles are the same this is an important point to note because for a pure system ψ 1= ψ 2 of course we have implied that the states are indistinguishable. And you can see it why, supposing I considered a case where 50% is in state 0 and fifty percent is in state 1. Now clearly this is a state in which I have got 1/2, 1/2 as the density matrix. Now on the other hand supposing I find I define a state in which ensemble in which 50% in state $0 + 1/\sqrt{2}$ and another 50% in 0-1 $\sqrt{2}$.

You can calculate the density matrix by the definition I have given and you will find I still get the same density matrix. Note again that we are saying that for an ensemble that concept of a state is not there. So an ensemble is given by a density matrix. And the postulates which we had corresponding to the state vectors the postulates of quantum mechanics can be replaced by the corresponding postulates for the density matrix. Now you can immediately see what those postulates should be, so you say that an ensemble is described by means of a density matrix which lies in a Hilbert space in which the state vectors corresponding to the component states are there.

The other thing is that the Schrodinger equation which every state satisfied is replaced by a the levels equation for the density matrix. And so therefore, this is some of the things that we need to talk about, just before we close this section let me give you an example from physics. Suppose I look at a coherent superposition of state + k and minus, so let me take a state size = $1/\sqrt{2}$ plus k + -k.

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 $\label{eq:psi} |\psi\rangle\colon \frac{1}{\ell k}\left[\begin{array}{c} | \psi k \rangle + | - k \rangle \end{array} \right]$ $P(n) = Tr [S |x\rangle\langle x|]$
= $\langle x | S | x \rangle$ $= 1 + \cos(2kx)$ Incoherent Superposition $S = \frac{1}{2}$ [IN> < N] + 1- W) $P(x) = 1$

That is equal momentum equal and opposite momentum added with the same. So you can calculate what is the density matrix corresponding to this, and find out what is the corresponding wave function, the wave function as you know is the projection of these states on to the position space that is the real space and you can calculate the probability of the density at point x, so which is given by remember that it should be corresponding to the density operator rho and of course the position operator XX for those of you who are not familiar with this part of physics can skip next couple of minutes.

But this is given by X by definition of the trace X and you can simply plug these numbers in size rho size calculate this and show that this quantity is equal to $1+$ cosine of 2 KX which obviously shows fringes that is because the intensity keeps on varying sense of that. Now if you took any

incoherent superposition that is instead of doing this, so we take for example a density matrix which is given by remember that when we have incoherent superposition I cannot define a state.

So this is $1/2$ kk $+$ -k,-k repeat the above calculation with this and you can find that PX will turn out to be equal to 1and there are no fringes here. So what we have done today is to define the density matrix corresponding to both pure state and an ensemble of pure states which are called next states and found stated that the when we look at systems which are collection of different types of systems different states an ensemble of different states.

What we need to do replacing the state vectors with this statements about the density matrix. We have related the expectation value of an operator to the trace of the operator multiplied with the density matrix. We have also pointed out the interpretation of the both the diagonal and offdiagonal components of the density matrix and we have seen that the density matrix is not unique in the sense to different ensembles could have the same density matrix. In the next lecture we will be looking at the relationship that the density matrix has for the single qubit systems with the Bloch sphere which we have discussed earlier.

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