# Implementation Aspects of Quantum Computing Prof. Debabrata Goswami Department of Chemistry Indian Institute of Technology, Kanpur

# Lecture – 34 Concept of Density Matrix for Quantum Computing

We are coming towards the end of this series of lectures for this course. We have already covered ten weeks of learning about quantum computing and its implementations and in the last week, we were going over some of the basics to make sure that we understand the concept of implementation again based on some of the basics. And as we have been interacting more and more with the students, we have also come to know that there are certain aspects which would help if we relook at them a little bit more. One of the key elements of that happens to be density matrices and density operators.

So, we start this week's lecture with this concept of density matrices and density operators. We have introduced this earlier and mentioned certain aspects a bit in relation mainly with respect to NMR and here we will be doing a little bit more understanding a bi so that the missing elements or the implementation parts that we used density matrices implicitly can become clearer.

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So, when we talk about density matrix; a quote comes to mind that again is related to Richard Feynman where he made this statement that when we solve a quantum mechanical problem, what we really do is divide the universe into two parts; the system in which we are interested and the rest of the universe. So, this was quoted from his statistical mechanics lectures back in 1972; essentially stating that whenever we are going to talk about density matrices, we are going to discuss about the statistics and the collective aspect of the part.

When we include the part of the universe outside the system, the motivation of using the density matrices becomes clear. So, that is the basic idea that whenever we are going to include the part of the universe outside the system alone, then the motivation of using density matrices becomes very clear. And actually this is very pertinent to quantum computing as we will discuss here. So, essentially let us look at what these mean.

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So most cases density matrices and density operators are used reversibly and often are used in one and the same way for both the cases. So, in general the statement that was made in the last slide is sort of more clearer in this term of Venn diagram, where we have an ensemble of the states that we are talking about with some probability for each of the states and that essentially forms the quantum system and that interaction of the quantum subsystem, as a result of probabilities and their interactions is the fundamental point of view that we are taking.

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So, let us see what we will be mostly doing in this lecture and why we are doing it. Most of this lecture will be spent on mastering density matrices and the density matrix and so we would need to master a rather complex formalism in some sense and that is the reason why I thought I will go back on this now, where it has become an important point to understand.

Might seem a little strange since the density matrix is never essential for calculations, it is a mathematical tool introduced for convenience and in our particular case the convenience meant that we were more inclined to use it for implementation aspects. And mostly we have to bother with it as already we know because we have gone through the implementation processes. But let me actually point it out again, that the density matrices although it seems to be very deep abstraction, but once you have mastered the formalism it becomes far easier to understand many other things including the concepts of quantum entanglement and quantum communication; which we have already gone through before.

So, that is the reason why we are relooking it and that is the reason why I had initially introduced it but never really gone deeper into it. But before closing our entire series of concepts on quantum computing, I thought we need to really look at it once more.

Let  $|\varphi_i\rangle$  be a complete set of vectors in the vector space describing the system, and let  $|\theta_i\rangle$  be a complete set for the rest of the universe. The most general way to write the wavefunction for the total system is  $|\psi\rangle = \sum_{ij} C_{ij} |\varphi_i\rangle |\theta_j\rangle$ Now let A be an operator that acts only on the system, is A does not act on  $|\theta_i\rangle$ A  $|\phi_i\rangle|\theta_j\rangle = \sum_{ii'j} A_{ii'} |\phi_i\rangle |\theta_j\rangle \langle\theta_j| \langle\phi_{i'}|$ Now we have,  $\langle \psi | A | \psi \rangle = \sum_{ij'} C_{ij'}^* C_{i'j} \langle \varphi_i | A | \varphi_{i'}\rangle$   $= \sum_{ii'} \langle \varphi_i | A | \varphi_{i'}\rangle |\phi_{i'i}\rangle$ Density Matrix

So, mathematically if we consider says phi i and theta i to be the complete set of vectors in vector space describing the system. So, mathematically let phi i be a complete set of vectors in the vector space describing the system and theta i be a complete for the rest of the universe. The most general way to write the wave function for the total system is generally written in this form, where both phi i and phi theta j are composing the total system.

Now, let A be an operator which acts only on the system that is A does not act on theta i, then what will happen is the operator A acting on the system would give rise to a result which would be given by this form of equation. So, when we apply this then we will have the observable; would be having the form as given in this equation where in we will find that this particular part can be represented in terms of the density matrix as we call it and that is the definition in how we start discussing about it.

So, once again we have the vector space describing the system by phi i and the complete set of the rest of the universe as theta i, then the most general way to write the wave function of the total system is a composite of the 2 psi then we use an operator which acts only on the system, which is how most of the operators that we choose, work and then what we find is that we will be having a situation where if we find its expectation value for the wave function, it will end up producing result; where we will be having the resultant coming from the part where the system is being interacted by the operator resulting in a part corresponding to this kind which is the density matrix that we are looking at.

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So, we basically have defined the operator rho to be such that; it is going to be having a form of this kind with the understanding that rho is going to be Hermitian. So, once we look at this one again where we have defined this part, then we get doing a little bit of math as we show here that the trace of the operator on the density matrix will give rise to the expectation value of the operator that we were looking at.

So, due to the Hermitian nature of rho it can be diagnosed with a complete orthonormal set of eigenvectors with real Eigen values wi, so that the final density matrix would look like this rho.

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So, we have  $\langle \psi | A | \psi \rangle = \text{Tr } A \rho$  and  $\rho = \sum_{i} w_{i} | i \rangle \langle i |$ If we let A be 1, we obtain  $\sum_{i} w_{i} = Tr \rho = \langle A \rangle = \langle \psi | \psi \rangle = 1$ If we let A be  $| i^{i} \rangle \langle i^{i} |$  we have  $w_{i} = Tr A \rho = \langle A \rangle = \langle \psi | A | \psi \rangle = \sum_{j} (\langle \psi | i^{i} \rangle | \theta_{j} \rangle)(\langle \theta_{j} | \langle i^{i} | \psi \rangle))$   $= \sum_{j} | (\langle i^{i} | \langle \theta_{j} | \rangle) | \psi \rangle |^{2}$ Therefore, we have  $w_{i} \ge 0$  and  $\sum_{i} w_{i} = 1$ Orthonormal set of eigenvectors and real eigenvalues.

So, we have essentially stated that the expectation value would be the trace of operator A with rho and rho which is our density matrix will be of this form and if we let our operator to be just identity then what we will get is the sum of all the eigen functions would be equal to just the expectation value, in this case it would be 1 because it is the we have taken the operator to be 1 unity.

And if we let A to be of this form then we will have the eigen functions to follow as a result of this trace application a form which would be of this kind which means that our eigen functions are going to be either equal or greater than 0 and the sum total of each of the eigen values would be equal to 1. So, it is an orthonormal set of eigenvectors and real Eigenvalues are the solutions which are with respect to the density matrix that we have defined rho.

So, that is the first criteria that we have to understand that the density matrix would always give us orthonormal set of eigenvectors and real eigenvalues. So, that is what we are getting. Any system is described by a density matrix  $\rho$ , where  $\rho$  is of the form  $\sum_{i} w_{i} | i \rangle \langle i | and$ (a) The set  $| i \rangle$  is a complete orthonormal set of vectors. (b)  $w_{i} \geq 0$ (c)  $\sum_{i} w_{i} = 1$ (d) Given an operator A, the expectation of A is given by  $\langle A \rangle = Tr \rho A$ Notice that,  $\langle A \rangle = Tr \rho = \sum_{i'} \langle i' | \rho A | i' \rangle = \sum_{i'i} w_{i} \langle i' | i \rangle \langle i | A | i' \rangle = \sum_{i} w_{i} \langle i | A | i \rangle$ Thus,  $w_{i}$  is the probability that the system is in state  $| i \rangle$ . If all but one  $w_{i}$  are zero, we say that the system is in a *pure state*; otherwise it is in a *mixed state*.

Any system that is described by density matrix rho, where rho is of the form that we have just now defined summation all over i for the eigen function w i with for the bracket notation that we have used, the set ket i is a complete orthonormal set of vectors. So, these are the rules that we finally, get out as the result of this mathematical understanding.

And given an operator, the expectation value of A is given by trace of rho of A and we also notice that this can be rewritten in this format which gives rise to the fact that w i is a probability that the system is in state i if all, but one w i are 0 then we say that the system is in a pure state, otherwise it is in a mixed state.

So, this definition allows us to find out that the probability of the system and its weightage factor and if it is only one state as we have just discussed that w i is the probability if it if all, but one is 0, then that particular state is the only one which represents the state and therefore, it is a pure state otherwise it is in a mixed state; that is the basic idea.



So, in that sense density matrices of pure states are then represented as in terms of the vectors that we are doing the ket vectors psi and all such states are called pure states. An alternative way of representing quantum state in terms of density matrix therefore, are the way that we have just introduced and it is also as I mentioned reversibly used with the term density operators. So, the density matrix of a pure state is the matrix written in this form which as its summation can be written in terms of the weightage factor for the states which are composing the psi state. This is a particular way of representing density matrix, which we will get into more in detail.

Now, as an example the density matrix of say alpha 0 plus beta 1 can be written simply in this terms and which will then be the coefficient squares along the diagonals and their products along the off diagonals. So, the summation part of the statement that we have shown at the very beginning can also be summarized in the matrix notation as we shown here.

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(1) Consider a pure state: 
$$|\psi\rangle = \frac{1}{\sqrt{2}} (\uparrow\rangle + |\downarrow\rangle)$$
  
 $\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ 
Notice that  $\rho^2 = \rho$   
and  $\frac{1}{Tr\rho = 1}$   
(2) Consider a mixed state: 50%  $|\uparrow\rangle$  and 50%  $|\downarrow\rangle$   
 $\rho = \frac{1}{2} (|\uparrow\rangle\langle\uparrow|) + \frac{1}{2} (|\downarrow\rangle\langle\downarrow|)$ 
Notice that  $\rho^2 \neq \rho$   
and  $\frac{1}{2} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ 
Notice that  $\rho^2 \neq \rho$   
 $p = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ 

For a pure state for example, we have conditions where we can have wave function which is a composition of 1 over root 2 normalization factor; upward spin and downward spin. If we take this wave function then the density matrix can be written in this form and we find that the square of the density matrix is equal to itself and its trace is equal to 1; trace is by the way the sum of the diagonals.

If we consider a mixed state of 50 percent upward spin and 50 percent downward spin, then we have a case which looks like this and in this case the matrices will turn out to be in this fashion such that the final result of the density matrix will come out as this and in this case the rho's square is not equal to rho although, the trace rho is equal to 1 as before.

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Again if you take a 50-50 mixture of ket psi as we had shown before of spin going one direction versus the other direction and another wave function get phi as 1 over root 2 spin going up versus spin going down and the negative sign between them. Then if we look at the density matrix, we once again find it comes out to be a density matrix as given in the last case which is a mixed case and we find that rho square is going to be not equal to rho again and the trace is again going to be equal.

So, now the diagonal elements are always equal to 1 essentially that is a reflection of the fact that this diagonal elements are essentially giving the populations of the state, so the total population irrespective of how we look at it which is the trace is always going to be 1 and the off diagonal elements are the ones which will indicate something else and as we come to this is known as the coherence; how much they are correlated to each other, the correlation between these states because they are essentially corresponding to the coefficients of the two different states and their complex conjugate product and therefore, when they have some correlations then that will represent the coherence of the states.

It is important to note that in both the cases, we describe a system which we know nothing about is total of total ignorance because what we have done is we have put mixed states in case of the second and the third case whereas, in the first case where it was a pure state, where rho square in the first case; this was a case where we only had one state to look at is. So, opposition state, but it is essentially one state of spin going up or down, but this is a state which is a pure state.

However in the cases where we looked at later on, they were all mixed states and therefore, we know nothing about those states. It is a state of total ignorance and that is why it is important to get into the concepts of density matrices because for pure states it perhaps would not matter much as to what we talk about their properties and things like that, but for mixed states; the difficulty is that we cannot really come up with a way as to how to understand them. So, density matrices are ways where we can get to know about mixed states first of all identify them because whenever we find that the rho is equal to rho square, which we saw in density matrix; we know that it is a pure state whereas, whenever it is rho not equal to rho square, then we know that it is a mixed state and so that gives us some indication as to how to look at these states.

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Now, in the case of a matrix which we have been using a lot; I just wanted to say just keep the clarification as I mentioned before it is the sum of the diagonal elements which for example, in this case has been identified as the diagonal elements and it has some interesting properties which is that its associative, it has; so A times B and B times A; all these laws for multiplication, addition these things work and also the unitary laws work with this. So, unitary operator acting on the state inside the trace would make it remain

the same and the trace of a matrix essentially can also be represented as the expectation value of the wave function as long as this is an orthonormal basis phi i for instance.

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So, in terms of notation of density matrices and traces this is how we go about doing it. We generally represent as we have been saying the ket wave function as a super position of two other states with their coefficients and we can have them written as we have shown here that these coefficients are nothing, but which can be written in these terms because they are orthonormal sets. So, the probability of getting 0 when measuring this can be found out by using this kind of a mathematical form and what we find is that in this form also when we arrive at; we get that the density matrix is the form that we are get arriving at where we are getting that the density matrix is what we are using when we use the trace.

So, whenever we are going to make a measurement of a particular state that is where the density matrix appears. We have; this is a definition which we had already used that the probability of a particular measure is always the square of the coefficient and that is what we are utilizing and we can always find that in order to get the value of that, we can always use the density matrix and that is one of the ways of saying that the density matrix would automatically help us in finding the probability of the or the contribution of a particular state to the composite state.

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Density matrix: Eigenstates of density matrix form complete basis for subsystem block Eigenvalues give the weight of a state Keep the m eigenstates corresponding to m highest eigenvalues Eigenstate of the whole system thus given by:  $|\psi_0 \gg \sum_{\alpha} \sqrt{w_{\alpha}} |\phi_{\alpha} > \chi_{\alpha} >$  Schmidt decomposition The optimal approximation Entanglement states (mutual quantum information):  $S(\rho) = -Tr(\rho \log \rho) = -\sum_{\alpha} w_{\alpha} \log w_{\alpha}$ DM can be defined for pure, coherent superposition or statistical averaged states

So, the Eigenstates of density matrices form complete basis for subsystem block that we have already seen. The Eigenvalues give the weight of the state that is what we had discussed earlier and we can keep the m Eigenstates corresponding to the m highest Eigenvalues; m is just the running number here, running digit. Eigenstates of the whole system can thus be given by for instance the wave function which is equivalent to the root, since the weightage factors or the weightage of the state are essentially the probability; the amplitude of it would then be square root of this weightage, times the individual states that they are made of and this is the famous Schmidt decomposition that has been sometimes eluded to when we were doing our steps or processes in quantum computing or quantum information processing.

This is an optimal approximation; however, because we are making a statement that we understand that they can be made to be decomposed in this kind of a state. In case of entangled states, the mutual quantum information is carried in terms of the entropy of the state which is often written in terms of the way how entropy is often defined and since trace allows the logarithm to go through this kind of a process. So, we can this is the property of the trace that we looked at earlier. So, we can instead write the trace as in this form minus rho log; rho and this will be equivalent to the weightage factor terms the log of that.

So, density matrix can be defined for pure coherence to a position of statistical average states and so it is a very powerful approach. Whereas, in case of looking at the state alone; it might often be difficult to find out what to do with them. So, the idea that these kinds of definitions work for all the cases whether it is pure, whether it is having a coherence super position or whether they are a statistical average of many states, it gives us the advantage of using the density matrix formalism.

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Now, when we have the concept of pure states, it is much easier to understand because as we said that they basically represent one particular state; however, when we have mixture of pure states, the state is described by a state vector and is called a pure state. If we have a qubit which is known to be in pure state psi 1 let us say with probability p 1 and in psi 2 with probability p 2; what will happen. So, that is the question to ask when we have a state which is described by a state vector, but can be in the mixture of pure states.

So more generally we considered the probabilistic picture of pure states called mixed states, which is then given in terms of the overall wave function psi, which is now going to have the probability of each wave function in terms of the particular composition. So, for example; psi 1 with probability p 1 psi 2 with probability p 2 and so on and so forth.

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So, we have these contributions which make up the final mixed state which is the psi state. So, that density matrix of this mixed state would be having a probability distribution on pure states and it is called a mixed state. The density matrix associated with such mixed state would then be given as sum total of the probability times the inner product of the two wave functions the ket and the bra.

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So, the density matrix for say this particular mixed state 0 with probability half and 1 with probability half can be written in this form. So, the density matrix of the mixed state

would then the probability of measuring the 0 would be given by the conditional probability such that, it is probability of measuring 0 given the pure state psi i. So, then we can go ahead and find that this will be basically as we did this exercise before; the probability of measuring the state 0 given the pure state psi i; would be the trace of the state 0 that the inner product of the two and the density matrix.

So, the density matrix is again coming into this picture whenever we want to measure the probability of the state whenever we have bunch of other states available and we can always come back to this picture, where the wave function is a composition of the probability of the inner product of the composite wave functions to give rise to the solution. So, density matrices contain all the information about an arbitrary quantum state.

Now, this is one of the most important parts of studying density matrices because as I mentioned earlier, we have limited information on the states as soon as they are going to become mixed states. So for pure states, it is possible to get enough information about the state and we can do operations to get the results out of it. However, for mixed state the only way to get information about it is as we have been showing is through the density matrices.

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So, now let us look at what it me implies; it implies that we can now work with operationally indistinguishable states which are these are expressions in terms of density

matrices alone, independent of any specific probabilistic mixtures states with identical density matrices are operationally indistinguishable. Now this is the corollary of the fact that the density matrices essentially carry all the information because in other words of saying that those states, where the density matrices are going to be the same; we will have very little to do with their particular understanding because if we are going to rely on the concept of density matrices to understand them; so all the states where they have identical density matrices then they are operationally indistinguishable for us to start off with their studies.

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When we apply unitary operator to a density matrix of a pure state, the resulting state is essentially the result of the unitary matrix with the density matrix. So, when we apply this we basically get the unitary on operation on the density matrix.

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When we apply unitary operator to a density matrix of a mixed state say for example, a state which has this kind of a behavior, the resulting state is going to have the density matrices which will have the property which are going to be given by dependency on the density matrix alone.

So, if you notice the difference in the earlier case when we applied the unitary operation to the density matrix of a pure state. The pure state is essentially the only state that existed in the wave function, so the unitary operator essentially resulted in only providing the information about the pure state directly. The entire wave function could be operated on by the unitary operator; however, in this case when it is a mixed case. So, with the application of unitary operation, we always get the result which is expected that the density matrix is being applied; the unitary operator works on the density operator in this form. (Refer Slide Time: 28:03)



Now when we do this; this is always true and let us look at how this works the operational density matrices for mixed state essentially results in unitary operator working on the density matrices and which is still true, as a result of that the effect of measurement on a density matrix would end up measuring the state rho with respect to the basis say phi 1; all the way to phi d still we will yield the kth outcome with probability phi of k rho phi of k ket.

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Because the effect of measuring measurement on a density matrix measures the state rho with respect to the basis yielding the kth outcome with probability this; this is because the operation of the density matrix essentially means that we are applying this particular wave function as a result of that which means that I have basically ended up producing this particular state and the state is collapsing to this particular kth state and therefore, it is always measuring the probability of the kth state collapsing into that final state and would give the kth outcome with the probability and this is the reason why this is a universal measurement which works with the density matrices whenever we use a quantum operations using of density matrices.

And this is something which would work universally whether it is a pure state or a mixed state and that is the basic idea; this is collapses to this particular state. So, with this I would like to end today's lecture because we were planning to just give you the introduction to the density matrices, its necessity to be one of the important parameters that we have been using and time whenever we talk about collapse, whether we are doing a pure state or mixed state and in terms of communications and in many times of the computing, it has been very important that the overall property or the overall result which we have looked at are the important properties that we looked at and in many cases it was possible to have a solution only, because we were able to use density matrices.

And so that is why I wanted to give you some important ideas about the density matrices before we go further. We will meet you more on these issues in the next lecture.