Course Name: Quantum Entanglement: Fundamentals, measures and applications

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Week-01

Lec 3: Mathematical Tools: Density Matrix-Part 1

Hello, welcome to lecture 3 of module 1. In this lecture, we are going to learn some mathematical tools essential for the treatment of quantum entanglement. In fact, we are going to discuss the so-called density matrix formalism. In the last lecture, we learned, actually we know it from our elementary quantum mechanics, that all the information is, that a quantum system has, is contained in the so-called wave function or the state vector or state ket represented by the so-called ket psi. So ket psi represented like this contains all information about a quantum system.

When we can say with complete definiteness that a system is in the quantum state ket psi, that kind of state is called pure quantum state. There is no randomness in specifying the state of the system. Now this point would be more clearer to you when I am going to discuss about the so-called mixed states. But before I go to mixed state, let me say something more about pure quantum state.

A pure state psi can be represented or can be expanded as a superposition of basis state let's say C1 phi 1 ket phi 1 C2 ket phi 2 C3 ket phi 3 and so on. Here these phi's are, ket phi's are the so-called basis state C1 C2 C3 are complex numbers and I can write it, sort hand, notation as summation i Ci ket phi i. And you know the property that Ci has to obey this complex coefficient if you sum it, sum over all the complex coefficients mod squares would be equal to 1 because as you know C1 mod square gives the probability of finding this arbitrary state psi in the basis state phi 1. Then similarly C2 mod square is going to give the probability of finding the state in the basis state phi 2 and so on. Let me invoke the example of a qubit to understand some more useful concept.

In the last lecture we discussed a specific qubit system the so-called spin half quantum system. As we will see in this course many quantum entanglement concepts to understand we are going to use the example of a qubit system again and again in this course. Now let us consider a spin half system defined by this ket psi and we are going to take the basis state as say this up state up spin state and down spin state or also we can represent it say plus ket psi state and minus ket state as we have discussed it in the last class. So because we are considering this spin state spin system so this ket psi would be equal to say C1 up state ket up state and then C2 ket down state and if we take the up state this actually we have discussed all this notational thing we have discussed in the last class and the down state is 0 1 ok and then this ket psi can be represented in this basis by this column vector so C1 C2 would be its element and with the property C1 mod square plus C2 mod square is equal to 1. Now actually we can write say C1 is equal to because it's a complex coefficient I can write C1 as say cos theta by 2 and C2 I can write as sine theta by 2 e to the power i phi if I write in this notation immediately you can see that this particular condition is satisfied and it has its own utility when we write the arbitrary ket psi in the in this two state system which is in our case spin half system in this form so cos theta by 2 up state plus sine theta by 2 e to the power i phi down state ok so this is what we have now this actually gives us a very nice and intuitive picture of the state space of the spin half particle in fact any qubit can be represented in a nice you know diagram that I'm now going to discuss. By the way this particular state I can also write it in this form ket psi is equal to cos theta by 2 ket 0 which is referred to the up-state sine theta by 2 e to the power i phi that's the complex coefficient and this is ket 1. I think now onwards I'm going to use it for later part of my discussion here. I was talking about that particular diagrammatic representation it has a name it's called Bloch sphere. I will elaborate more on it on it but first let me draw a sphere like this let me consider it as you please consider it as a sphere it's a sphere of say unit radius that means radius one these are my axes, this is say x-axis this is y-axis you can recall the so-called spherical polar coordinate and suppose there is a let me use this different color now let us say this is a vector this vector is touching the surface of this a unit sphere and this angle is theta and if I take a projection here and this angle is the azimuthal angle say Phi now recall that we have we are now representing our two state quantum state this quantum system by this particular state now I you will see that this particular representation basically refers to the fact that every point on the sphere okay every point on the sphere is going to represent a quantum state depending on the angle theta and Phi okay just to give an example if I say if we say take theta is equal to 0 and Phi is equal to 0 then you see this ket psi would be equal to ket 0 right yeah it would be only become ket 0 because of from here you can see so this is going to represent the up state of the system that means the this spin half particle is its spin is directed along say in the z direction and it can it is basically referring to this particular point the northern hemisphere you can say this particular point is refers to the state ket 0 which represents in other words the up state of the spin or if I have say theta is equal to say pi and Phi is equal to 0 then this ket psi is going to represent the state again you if you look at it from this expression here theta is equal to pi so the first term is going to vanish so it will be and Phi I am taking to be 0 so this is going to represent the state ket 1 and which refers to basically the down spin right and this is going to represent this point here in the southern hemisphere so this is going to represent ket 1 in this way just by varying the angle theta and Phi the whole surface of the sphere can be covered and for a specific angle of theta and specific angle of Phi we are going to get a quantum state okay and this representation of the Bloch sphere is of immense importance in particular to quantum computation and it's very useful and let me give another example let us say if I what happens if I consider say theta is equal to say pi by 2 let me say theta is equal to pi by 2 and say Phi is equal to 0 in this case I will have this ket psi if again let me refer to this equation here now I am taking theta is equal to pi by 2 so therefore cos pi by 4 that is going to be 1 by root 2 right cos pi by 4 would be 1 by root 2 ket 0 plus sine theta by 2 that is sine pi by 4 that would be again 1 by root 2 e to the power i Phi is equal to 1 now because Phi is equal to 0 so you have this so you are getting a superposition state of ket 0 and ket 1 and this is a superposition state this one is going to be represented by this particular point this particular point here this is going to represent the superposition state 1 by root 2 ket 0 plus ket 1 ok this basically this particular vector is now going to point along this direction and it is touching the Bloch sphere the equator along the positive x-axis I hope you get the idea and you may be convinced also that this is a very powerful way to represent a two-state quantum system and this is known as this particular sphere as I said it is called the Bloch sphere it's basically the Bloch sphere representation of a qubit. Till now we are talking about a single component system for example when we talked about a two-state system for example the spin-half system that is a qubit a single qubit. Now let us consider two such qubits or two such quantum system one system is lying in the Hilbert space say H1 and another one is lying in the Hilbert space H2 such kind of composite systems are called bipartite systems now let me talk more about it and I will explain what we mean by bipartite system in detail because later on we are going to talk about bipartite entanglement. So let us say we have a system having two components, one component is lying in the Hilbert space say H1 another component is lying in the Hilbert space H2 say this is component number one and this is component number two. A system I think let me better write it a system composed of composed of two separate components separate components is called bipartite. Some of you may be hearing it for the first time but it's very simple as you can see a system composed of two separate components is called bipartite system then the system as a whole lives in a Hilbert space H is equal to tensor product of or direct product of H1 and H2 is called a tensor product. You need not have to bother much about it it's basically says that if we have a bipartite system so it again belongs to the Hilbert space and because one component belongs to H1 another one belongs to H2 so that's how overall it's basically lying in the Hilbert space right everything lies in the Hilbert space so you don't have to worry much I will actually give you some example then it would be more clearer what I mean by bipartite system now how to represent you know such kind of composite system what about the state vector remember as yet I am not talking about mixed state I am still talking about pure state so how to represent such kind of a composite system such kind of composite system if it is a pure so it can be represented by a state vector and the representation as will be like this and I will explain it it will look little bit complicated in the beginning but it will be clear to you if I give an example so say summation because there are two components one is over the summation i and then another is over the summation j say then there is complex coefficient I have say Cij for the one component let me write the basis state it's phi 1i and it is the tensor product direct product and that would be phi 2j okay here where actually these are this is ket phi 1i this is an orthonormal basis in the Hilbert space H1 on the other hand actually the same thing I am going to talk about the other state on the other hand this ket basis ket phi 2j is an orthonormal basis orthonormal basis in the Hilbert space H2 and also it may be clear to you that these coefficients must have to satisfy this particular condition you can consider it as a normalization condition and I think we have discussed it and this is a necessity okay and it should be clear now a state let me write here a state ket psi which belongs to the Hilbert space H which is basically the direct product or the tensor product of the Hilbert space H1 and H2 is written is written as a tensor product tensor product or direct product it's called tensor product or direct product of two vectors two vectors as I can write it as psi is equal to ket psi 1 with direct product ket psi 2 okay and if I can actually write it this kind of a state is called is called a separable state is called a separable state separable state or tensor product state tensor product state significance of this treatment or discussing whatever we are it will be clear to you some of you may find it difficult or it may be some most of a lot of you may be already aware but please just wait and just listen to these things carefully as I will give an example the things would be more clear to clearer to you so this is whenever we can write a composite system as a direct product of two state whenever we have a state like this and I can composite state like this say ket psi if I can write it as a direct product or tensor product of two ket state okay then this kind of states are called tensor product state or direct product state or of course in other words they are separable state as you can see I can write two separately it as a direct product of psi 1 and psi ket psi 1 and ket psi 2 and it has a very simple interpretation a separable state has a simple interpretation say the first system the first system is in the state ket psi 1 while the second system is in the ket psi 2 it is as simple as that okay. Again let us discuss the whole thing using a composite qubit system but before that let me comment on the notation in the case of the qubit composite system in the case of qubit composite system the state vector I can write as a ket psi is equal to summation i is equal to 0 to 1 you see because it's a two-state system I am talking about I have two qubits and every qubit I am just going to work on the basis state ket 0 and ket 1 that I am going to consider as my orthonormal basis state so for the first system i goes from 0 to 1 and the for the second system also because it is also again a qubit so it is also going from say 0 to 1 and I have this coefficient complex coefficient C i j for the first qubit I have this orthonormal basis phi 1 say i and it's a direct product or tensor product with the another qubit that is phi 2 j so this is the state vector representing this two qubit composite system I think it is easy to understand and again here this basis states phi 1 i say for the first qubit it has the basis states are ket 0 and ket 1 similarly for the state for this basis states phi 2 j the basis states are simply ket 0 and ket 1 ok. Now let me elaborate more about it what about the tensor product this tensor product can also be written in fact the tensor product of the two qubit system phi 1 i tensor product with phi 2 j that can also be written in a short notation rather than writing this big thing all the time I can just write it say phi 1 i phi 2 j ok this is a short hand notation so we can write the full state vector for the two qubit composite system as follows now I can write it as ket psi is equal to C 0 0 ket 0 ket 0 right I think it's now you can easily follow it just if you take a pen and paper and the you do it the way I'm doing it you'll be able to understand so C 0 1 ket 0 1 in fact should I ok let me just elaborate it this side also C 0 0 and this ket 0 0 is basically nothing but the direct product of ket 0 ket 0 ok you see here this also just look at that i goes from 0 to 1 j goes from 0 to 1 that's why I have C 0 0 then C 0 1 and I have other terms like C 1 0 ket 1 0 plus C 1 1 and ket 1 ket 1 or if I write it also the long notation also I can write this would be ket 0 this is what writing for this part direct product of ket 0 ket 1 and and so on ok let me just write it completely so it is ket 1 I am talking about this part here it would be direct product of ket 1 ket 0 and the last term would be C 1 1 direct product of ket 1 and ket 1 right also don't fail to see this that this coefficient has to satisfy this particular equation if you add up all the coefficients mod square of the modular square of the amplitudes so that would be has to be equal to 1 this condition has to be satisfied the formalism that we have discussed so far is applicable to the so called pure quantum state as you are already aware of for example a spin-half system it is being either in the up state or in the down state is a pure state even a complex superposition of the up state and down state is also a pure state however in most practical situation it is not possible to have complete knowledge of the system in other words the state in practice is not an eigenstate of the observable but mixture of various eigenstate each state having some classical probability such kind of states are called mixed states and we cannot specify a state vector for a mixed state and quite clearly the state vector formalism is not going to work if we want to describe a mixed state and we have to rely on a or we have to you know of course we have to invent a different kind of a formalism and it is already done particularly von newman contributed lot to develop this formalism and this formalism is called the density matrix or density operator formalism let us consider an ensemble an ensemble of two two-state system or two-level system okay two state systems say A and B say A and B all right these two states are represented by say two kets system A is represented by this ket psi in the basis say ket zero and ket one that is say alpha ket zero plus beta ket one because it's a two-state system and the probability that the system is here that you can define the the system by this ket psi with classical probability say p with i will explain what i mean by this just in a moment probability p probability p on the other hand the system B is represented by this state vector state ket say phi is equal to say gamma ket zero plus delta ket one with classical probability because either you are going to pick A or pick B for sure so its classical probability is going to be one minus p say this for simplicity purposes let us say and just for explanation of the concept that i am going to discuss now let us consider that these two systems are in a box and these systems A and B are there now the question is if we make a measurement in the box if we make a measurement in this box and ask these questions that what is the probability that you are going to get the system this ensemble system basically A and B in the ket state zero in the ket state zero ket zero or ket one what is the probability that you are going to find the system finally in this quantum state ket zero and ket one okay so basically this is a measurement problem and this is measurement processes involved and it involves a certain some steps the steps are as follows so first of all what you are going to do you are going to pick up either system A or system B so let us say that means you are either going to pick up say ket psi or ket alpha okay sorry ket phi from the box pick this is the measurement steps i'm now going to talk about from the box with probability say p probability of picking the state ket psi is p and ket phi is one minus p right this is completely a classical measurement and in the next step you are going to make a measurement on the picked up state so the next step would be make measurement make measurement on the picked up state picked up state that is ket psi or ket phi right so you may pick up ket psi with probability p and the probability of picking up ket phi the classical probability is one minus p now say you have picked up say you you picked up say you picked up the state psi ket psi and you know the ket psi is it is a superposition of the basis state alpha ket zero plus beta ket one now the question is what is the probability that the state collapse to the ket zero the probability the probability that the state psi after making the measurement ket psi collapse collapses to the state ket zero is obviously mod alpha square but then there is a classical probability is also involved because in the first place you have to pick up the state psi right ket psi you have to pick up and that's the probability is picking that up is p so the probability this is very important the probability that the state psi collapses to this basis state ket zero is p mod alpha square on the other hand if say you have picked up ket phi instead of ket psi if you and then make a measurement if say ket phi is picked up picked up and then the probability the probability that this phi ket phi collapses collapses to this basis state ket zero is how much that would be again it's very simple now because the probability of picking up the ket phi state is one minus p that is the classical probability then after you make the quantum measurement and getting the state ket zero is mod gamma square because recall that already we have written that ket phi is a superposition of ket zero and ket one and the coefficients involved where gamma ket zero and delta ket one right so this is the probability so overall then what is the total probability the total probability the total probability that the this ensemble state the ensemble of the system A and B the ensemble is in the basis state is in the basis state ket zero is p mod alpha square that means when you have picked up the ket psi and one minus p gamma mod gamma square if you have picked up the state phi and picking up the state ket phi is probably classical probability is one minus p so this is if you want to make the measurement this is basically the probability of getting the ensemble in the state ket psi similarly the probability probability of getting as a measurement getting the ensemble it is a easy guess now ensemble in the state in the basis state in the basis state ket one is so now again you look at it ket one the probability of picking up suppose you pick up ket psi then the probability is p and then if you make the probability of getting the state ket one would be mod beta square right on the other hand if you have picked up the ket phi state then the probability classical probability of selecting that is one minus p and then quantum measurement is going to give you mod delta square if you want to get the system or the state in the state ket psi so this is what is right it's simple this is what we talk about when we are dealing with a mixed state of this nature this particular treatment just i have discussed inspires us to define what is called the density operator the issue is say we have a random collection of quantum states is occurring with some probabilities the question is is there an efficient way to describe this affair rather than listing all the thousand quantum states and their corresponding probabilities the answer is yes let us define the quantity called density operator as follows density operator is follows density operator the symbol for density operator is rho because it's an operator we'll put a cap there and the definition is this sum over j pj ket psi j bra psi j it's an outer product as you can see it's an outer product so it's an operator and here this ket psi j is a state in the Hilbert space it's a state in the Hilbert space that means this state belongs to the Hilbert space H and it appears psi j appears with probability probability pj that's a classical probability as we have discussed in the last example and also it is assumed that this state psi j is normalized so the scalar product inner product this is equal to one okay now this formalism is quite powerful as we can calculate any expectation value of system operator by knowing the density operator so this definition you should must have to remember okay if we know the density operator then we'll be able to know the expectation value of any system operator let me invoke the case of pure state to illustrate this particular point let us say we have a pure state represented by the by ket psi as usual so let us say we have a pure state say ket psi and therefore the density operator for this pure state would be simply this outer product because the classical probability is definitely going to be 100 percent p is equal to one here in the definition of the density operator p is equal to only one state and it's a pure state so therefore in the box example that i have given earlier you are always going to pick up only ket psi okay because that is what is to be contained as a collection of the box is going to contain a collection of ket psi only and in the example that i have given the box example where we had the system A and B i discussed the system A is also in the state ket psi and system B is also in the state ket psi so therefore if we have to pick up we are always going to pick up only ket psi with 100 percent probability now anyway let us now calculate the expectation value of an observable let us say calculate the expectation value of an observable observable say O cap this is the operator representation of the observable O cap in the in the pure state in the pure state in the pure state ket psi okay so we know traditionally how operators you know expectation values are calculated but before i do that because this is an arbitrary state pure state i can always write it as an superposition of eigenstate this is anyway all of us are now quite expert i suppose have become expert so this is what i have and if i take the bra of this ket corresponding expression would be this so this would be c i star bra phi i so phi i is the basis state and traditionally if i say calculate the expectation value of the operator we know just we have to calculate this particular quantity okay now let me utilize this expansion here so first let me put the bra there that is summation i and from this ket i will have another summation say sum over say state j and for for the bra thing i will have say c i star for the ket I have c j and then I am going to have here it would be phi i o cap phi j right now because i have psi is equal to ket psi is equal to sum over c i phi i, I want to find out express this coefficient c i complex coefficient c i in terms of these states to do that let me multiply both sides of this equation by say let me take the inner product with the orthonormal basis say phi j then this is what i have because phi is a basis state phi forms the basis state so therefore i will have this inner product here phi j phi i and they are orthonormal so therefore i have this would be c i and delta j i okay if j is equal to i delta j would be equal to 1 if j is not equal to i they will be orthogonal to each other that would be equal to 0 and because of this the summation thing will become simply c j so therefore i have say c j I can express this coefficient I can express in terms of this arbitrary state psi and the orthonormal state say phi j like this all right and the corresponding c j star would be equal to bra psi and ket phi j this is what i think this is easy to understand now i can utilize it for calculating the expectation value let me once again write the expectation value of O would be operator would be the expression we have i j sum over i j c i star c j phi i operator O phi j okay and this i can then write it as summation i j c i star i can write it as this this expression i can write as you can see i can utilize it c i star would be bra psi phi i here and c j would be that would be phi j psi and then we have this expression here let me just write it phi i O phi j okay this let me simplify it further i have these are by the way just scalar product or inner product these are number so this number i can write this side and this number i can write this side okay this if i do then i will have phi j psi psi phi i and this guy is basically the matrix element i can write it as O i j and as you can see as per the definition for the pure state i think i have already done it or not okay let me yeah i have written that the for pure state psi the density operator would be this so therefore i can write it as i j phi j and this is the density operator this part is the density operator then i have here phi i O i j let me expand it once again write the full thing here that is phi i O phi j right now you see because of the fact that because the orthonormality condition phi i this outer product phi ket phi i bra phi i this is equal to 1 right or identity this is identity so therefore this is therefore this is equal to one this i can therefore write sum over j and i have phi j this is rho and then this is operator O and then this is phi j what you see that this is nothing but the sum of all the elements in the diagonal matrix of this product of these two matrices two operators so some of the diagonal elements in a matrix is called trace so therefore i can write it as a trace of the product of the two operators rho and O observable okay so what boils down as the expectation value of the observable O is simply the trace or trace of the product of the density operator and the observable operator basically the product of the it is the trace of the product of the matrix of matrix representation of the density operator and the matrix representation of the density operator okay then so it's now everything boils down very simply whenever we talk about finding out the expectation value of an operator using density matrix formalism is just to calculate the trace of the product of the density matrix corresponding to density operator and the matrix representing the observable so this we have actually discussed for pure state we have got it for pure state the question is is the same result applies for mixed state also now we'll see that as well we cannot specify a state ket or state vector for mixed state but certainly we can represent it by a density operator as follows rho cap is equal to sum over j p j that p j is the classical probability psi j direct product of this outer product of this this is the usual definition of density operator as you can see now let us calculate the expectation value of an observable O now for pure state if psi j is a pure state you know the expectation value of that operator would be simply this one but if it is a mixed state then it has every state size a appears with some probability p j then you just have to take the sum over all all of them and this is what the and how you calculate the expectation value of an operator in the for a mixed state right let us now expand it further and let me simplify it so this i can now write as summation j p j now here i'm going to apply a trick i can utilize the the so-called completeness condition let me explain it first let me write the expression psi j O cap here i put sandwich this orthonormal basis phi ket phi ket psi j i can always do this because of the fact that this orthonormal basis it satisfy the this completeness condition that means this basis ket phi k span the whole Hilbert space so this is identity therefore i can always put it there now from here i can i can let me take the summation now this side summation k summation over j p j you see this is just a number because it's a scalar product so i can write it this side so if i do that i have here i can write it phi k psi j and the other one just let me write it as psi j O phi k all right further i can uh write it this way summation over k let me take this guy out because some of our summation is taken over k and let me take this summation over j inside and i have here p j this is mathematically mathematical tricks and very easy to follow as you can see this is psi j i can write here okay and then i have this O cap phi k i hope you are able to follow it now this guy here in the bracket is nothing but the density operator as part of our definition so this expression therefore i can write that means the expectation value of this operator O in the mixed state i can now write it as sum over k phi k rho O cap phi k so what you see this is nothing but the trace of the product of the density operator and the observable operator and this i can simply write as trace of rho cap O cap okay and this result is identical with that of the one that we have discussed for the pure state so in general this is true that expectation value of an operator or an observable is simply the trace of the product of the density operator and the observable operator now finally let me throw some light into the physical meaning of various elements of the density matrix now consider okay i'm going to discuss about physical meaning of okay let me say matrix elements matrix elements of the density operator this is basically going to help you in understanding many of the concepts later on you can and i am going to consider the matrix element of the density operator say rho i j in the basis state say phi k so therefore i can write it as say phi i rho k phi j this is the matrix element rho i j for simplicity purposes let me consider a pure state for pure state i can write rho as this right this is the density operator for pure state phi j so for pure state rho is equal to this is the outer product right now again what we can write psi we can write it as a superposition of the basis states like this this i have already explained and from here just sometime back we got that ci i can write it as phi i psi and ci star i can write it as psi phi i utilizing this here in these two i can simply write the first one would be simply ci and the other one would be c j star okay now coming to the diagonal elements first diagonal element for diagonal element i is going to be equal to j right so that means rho ii would be equal to ci ci star that is nothing but ci mod square and you can recognize that this guy is nothing but probability this basically gives the probability of finding the probability of the probability of finding a state in the eigen state in the eigen state phi i all right and what about the off diagonal off diagonal elements refers to the fact that i is not equal to j so this would be rho i j is equal to ci c j star now because ci and cj are complex i can write ci as ci mod ci e to the power the phase would be say e to the power i theta i can write c j star would be mod cj e to the power minus i theta j that's the phase part i can always write any complex quantity as amplitude and an exponential of the phase right so this is going to give me ci mod ci mod cj e to the power i theta i minus theta j okay now what it basically means that it means that the off diagonal elements depend on the relative phase difference between the depend on the relative phases between the states phi k phi i and k phi j okay let me better write it the off diagonal as it is evident from this expression off diagonal elements depends on the relative relative phases phases between i hope you can write my read my handwriting okay it is between between the states ket phi i and phi j right and this is going to result in resulting in interference terms interference terms i think i will throw more light into it when we will do some example later on in this course let me stop for now in the part two of this lecture we'll continue our discussion on density matrix in particular its various properties and also we'll see how to distinguish between pure and mixed states so let us meet in the next lecture thank you so much now