FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

Dr. Sandeep K. Goyal
Department of Physical Sciences
IISER Mohali
Week-03
Lecture-08

Qubits: Density Operators - Part 01

So far what we discussed was what will happen if we perform a measurement on an ensemble of single photons. We need many, many single photons. They were in an unknown polarization state and we wanted to estimate the state of that polarization. So, we're using it in experiment, but we were assuming that all the photons are in the same state psi. What will happen if some of the photons are in state psi 1 and some other photons are in the state psi 2. So, the setup is such that we have stream of single photons coming, and with n1 of those photons out of total N, N1 of them are in state psi 1 and nN2 are in state psi 2.

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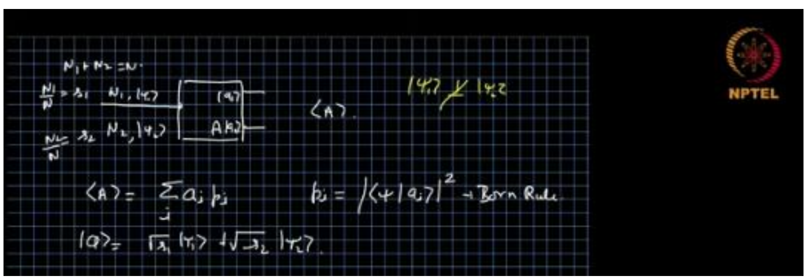

So, it is the N1 plus N2 equals N. This is the scenario we have here that out of total N, N1 photons are in state psi 1 and N2 photons are in state psi 2 or we can say that psi 1, photon can be found in the state psi 1 with probability s1, which is given by N1 over N, and probability s2 is for the photon to be found in the state psi 2. Now, if that is the case, then what can we say about the expectation value of an observable. And now our task is to find the expectation value of an observable. a1 and a2 are the eigenvectors of it.

So, ultimately, we want to find expectation value of A. Since we do not know what is s1, what is s2, whether the photons are in psi 1 or psi 2 or it is only one psi, it can be anything. So, without having any information about what is the situation of the incoming ensemble, incoming photon, we have to find the expectation value of A. And of course, the experimental setup should not care about the configuration in which we have prepared the photons, the set of photons. So, the expectation value of A, let us recall is given by sum over i, ai and pi, where pi is the probability of getting the outcome ai and it is calculated if the quantum system is in the state psi, then this is the probability of getting ai and this is called Born rule of probability. This is the axiom of quantum mechanics. Whatever we want to do, we have to use this. But the quantum mechanics never told us what will happen if we have more than one state. We cannot say that we can take the average state of it.

So, we call the state of the photon to be root of s1 psi 1, plus root of s2 psi 2. We cannot say that. Or even if we can say it, we have to prove it that this actually is the state. We are not assuming psi 1 and psi 2 are orthogonal. They need not be. They can be any arbitrary state as long as they are measured state it means they are normalized, okay and they belong to the Hilbert space of the interest. So, let us, the assumption we are making is a given photon is either in the state psi 1 or in the straight psi 2, so in the setup whenever one photon comes, then we get p1 probability which is psi 1 a1 mod square, the click will happen in a1 with probability p1 and click will happen with p2, with probability p2 in a2 in this. This is the born rule we are using, nothing else. And if the photon is in the state psi 2, then we get q1, which is psi 2 a1 mod square and q2, which is psi 2 a2 mod square. So, if psi1 comes, then the probabilities are p1 p2. If psi2 comes, then the probabilities are q1 q2. And since it's just a click, for every photon we will get just a click, either it will click here or here.

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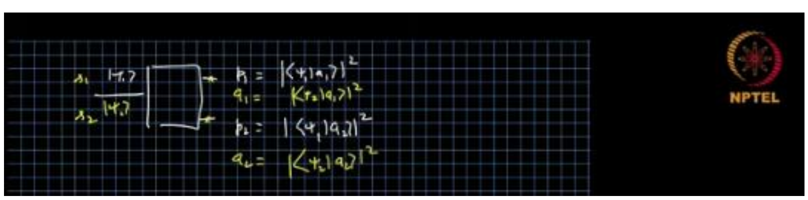

We do not know whether it was because of the probability p1 or q1 or it was because of the probability p2 or q2. From single click, we will never know. But with statistics also, probably we can find out, but we will see that. So, our photons are coming in states psi 1 and psi 2 and we get this probability. The probability of psi 1 coming is s1 and probability of psi 2 coming is s2.

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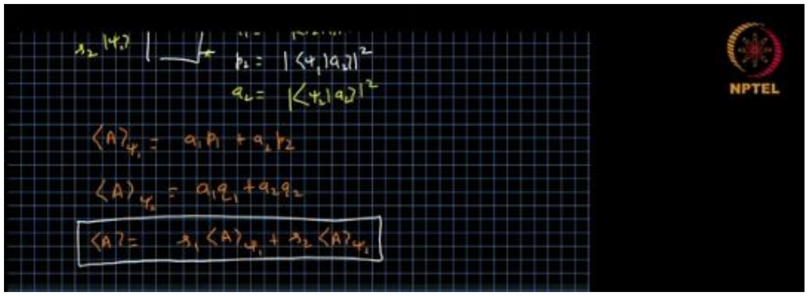

So, if the photon was in the state psi 1, then the expectation value, let us call it expectation psi 1, will be p1 a1 plus a2 p2. The expectation value when the photon was in psi 2 is a1q1 plus a2q2. And since we are repeating this experiment over many, many photons, very, very large number of photons, so the total expectation value will be s1 times the expectation value of A with psi 1 plus s2, the expectation value of A with psi 2. So, this is the expectation value we will get when we have an ensemble of photons in different states. Here we are taking simple case of psi 1, psi 2.

We can generalize to larger number also. So, in general, it will be A to be sum over i, si, A, psi i. The psi i's are the state in which the photons are prepared. They need not be orthogonal. They should be just valid states of photons, in anything, like we discussed the case of polarization. So, they can be polarization state of a single photon.

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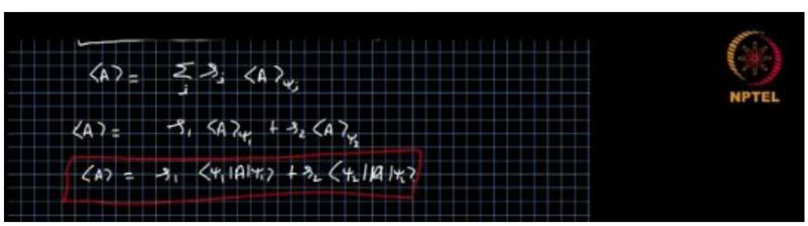

So, this is the most general expectation value of an observable for an arbitrary mixture of state. And you see, this is the first time we are seeing something beyond just psi. Now we have two psi's in the same ensemble. And we will reveal something very beautiful soon.

Now, let us write, we take a simple case of two, then we have a s1 A psi 1 plus s2 A psi 2.

And that we can write as a1 psi 1 A psi 1 plus s2 psi 2 A psi 2. What is the significance of this statement, this equation? The significance is, let us say there exists a state phi such that the expectation value of A can be written in this form. Let us say, it means we can choose phi to be s1, psi 1 plus root s2, psi 2. This does not mean, let us say it can be chosen this way, what will happen when we calculate phi A phi then we get s 1 psi 1 A psi 1 plus s 2 psi 2 A psi 2 plus root s 1 s 2 psi 1 A psi 2 plus psi2 A psi 1.

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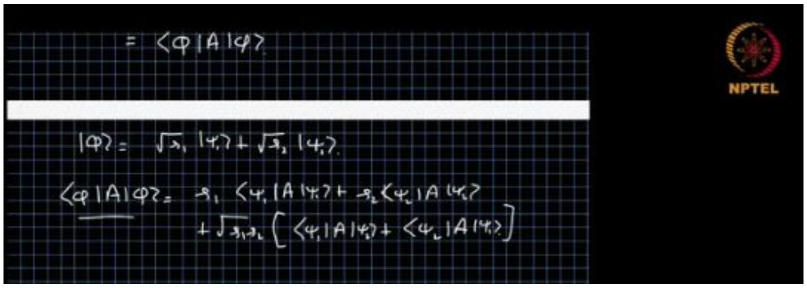

Now, if we compare this with expectation value of A, we see that these two terms are extra. They are not present in the original expression for expectation value of A. So, it means this choice of phi is not correct. Maybe we forgot, maybe instead of plus it should be minus sign or some other phase. So, we can choose phi, we can try with phi as a phase exponential of i gamma psi 2. And gamma is the relative phase between psi 1 and psi 2.

Again, if we calculate the expectation value of A with this new phi, we get s1 s2 plus root s1 s2. Even now, these terms are extra. These two terms are correct, but these two terms are not. They should not be present. But what does it mean?

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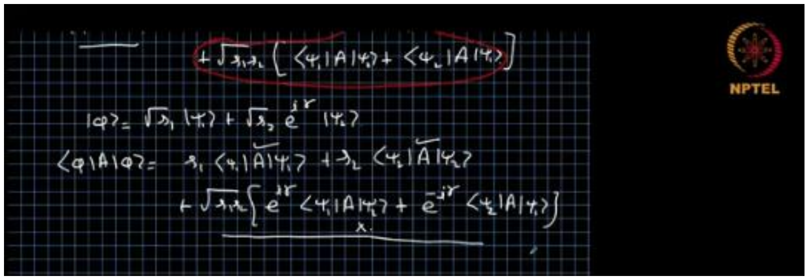

It means there does not exist any phi of this form which can yield the right expectation value for the scenario under consideration. Namely, we have a mixture of two pure states, psi 1 and psi 2, and we want to see what is the expectation value and we want to see what is the corresponding average state. But we can see one thing that if we average this expectation value over the whole range of gamma, then we get actually the right expectation value it means the two terms this and this disappear when we average over gamma. So, it means the state phi which is root s1 psi 1 plus exponential of i gamma, root s2 psi 2 for all gamma uniformly distributed, this is a valid state.

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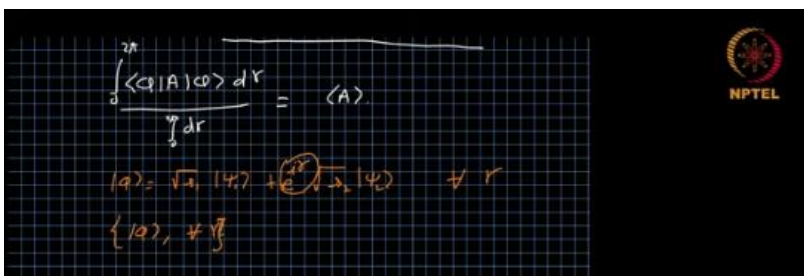

A valid representation for the scenario we have considered. So, it means what we are saying is that this gamma is completely random. We do not know what this is for any photon. That's why we have to take average. We have to average over all the gammas and that's how we can discard these two terms. So, we can say the phi for all gammas between 0 and 2 pi is the right representation for the ensemble of photons we have considered.

This is one way of saying it. We can also say that instead of working with pure states phi, we can develop another mathematical structure rho, as s1, psi1, psi1 plus s2, psi2, psi2. That is a statistical mixture of the two pure states. This is one state and the probability corresponding to it. This is another state and the probability corresponding to it.

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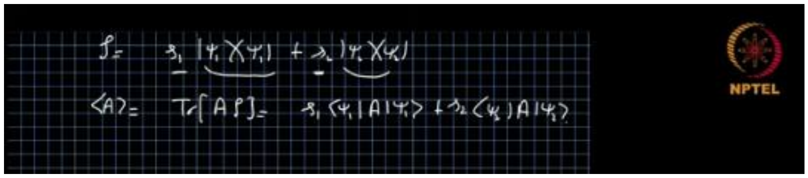

Now, the expectation value of A can be written as trace of A times rho, which will be s1 psi 1 A psi 1 plus s2 psi 2 A psi 2. This will give us the right expectation value for any arbitrary observable, okay. So, this operator is called the density operator and this is the more general way of representing a state of the quantum system. Here we are saying rho when we are writing it in this form sum over i, si, psi i, psi i. This is a mixture, a classical mixture of pure states or of quantum states psi i with probabilities si. This is called a mixed state. So, a very extreme example of a mixed state is a pure state, namely s1 is 1 and all the other si not equal to 1 is 0. So, in that case, our rho will be psi 1 psi 1 or any psi i, psi i, just that they know sum only one term.

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So, this is, here we are saying that all the quantum systems in the ensemble are in the same state. So, this is what we call pure state. So, if we don't have any summation here, then it's a pure state. If we have a summation, then it's a mixed state. So, in that way, this mathematical structure captures whatever have been discussed so far in terms of psi and beyond that.

Beyond that means these probabilities also it can handle and these are the classical probabilities. So, we have classical mixture and hence we have mixed state. So, what are the general properties of density operators. The more general density operator can be written as p i, psi i, psi i, where pi's are either 0 or closed numbers, sum over i p i is 1. So, set of pi's form a valid probability distribution.

Psi's are normalized states. Those are the only requirements we have for a density operator. So, that the pi should be positive and they should add up to 1 and psi i should be normalized. Psi i need not be orthogonal to each other, but they must be normalized. Now from here we can see that what is rho dagger.

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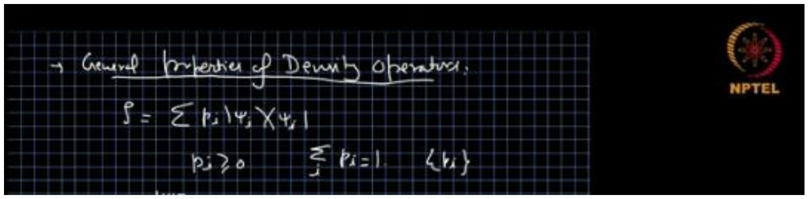

p i's are real, so p i remain p i, psi i psi i outer product will be, the dagger of it will be the same thing this is same as rho this implies that rho is Hermitian, so rho must be Hermitian now trace of rho will be sum over i p i trace of psi i psi i, you can check will be p i psi i psi i since psi is normalized we are left with sum over p i which is equal to one, this implies that trace of rho is one. So, rho should be Hermitian. rho should have trace 1. These are the two properties.

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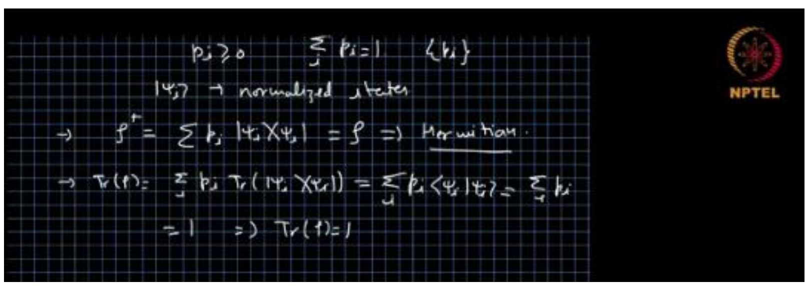

And third and foremost property is that rho, since it is Hermitian, so the eigenvalues of rho, let us call them lambda 1, lambda 2 and many, but for qubits only 2, lambda 1 and lambda 2. They should all be always be either positive or zero, so how we can say that since rho is Hermitian, we can always write a spectral decomposition for it, lambda i i, spectral decomposition. So, this is also a decomposition of rho in this form just that here accidentally psi i's are nothing but i's and they are orthonormal so if this this is the density matrix then lambda i must be positive and trace, the sum over lambda i's should be 1. It means lambda i's have to be positive semi-definite. Hence, and we know the property that Hermitian operator with positive semi-definite eigenvalues are positive semi-definite operators.

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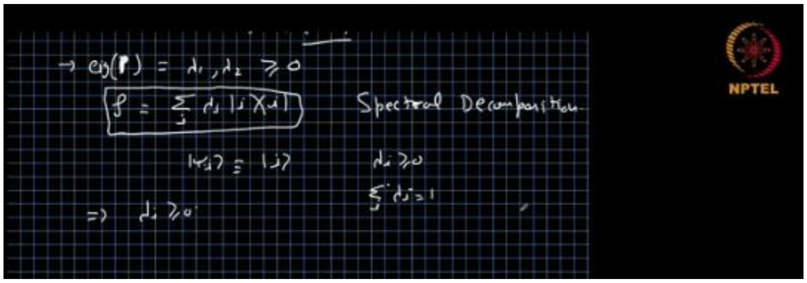

So, rho must be a positive semi-definite operator. The three properties we can summarize as rho is Hermitian, trace of rho is one and rho is positive. So, what we are seeing is if rho is written in this form, then it satisfies all these three properties not just that we are seeing the reverse also if against, if a matrix satisfy these three properties they are a valid state for a quantum system. So, any matrix which satisfies these three properties can be a bonafide state. How to prepare it and what to do with that is a secondary question, but that can be in principle a valid state for a quantum system.

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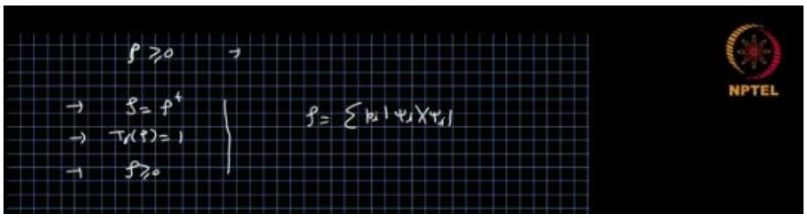

Now, rank of a matrix is the number of non-zero eigenvalues of the matrix. So, if rank of rho is 1, then it means it's a pure state. Pure state again let me reiterate pure state means it depends only on one psi, okay. So, this is equivalent to psi of course not mathematically but like the information in psi is same as the information in this rho. If the rank is not one then it's a mixed state. Now, since rho is Hermitian, we can write it in a very interesting way. First, let us say rho has an arbitrary form a, b, c, d and rho dagger becomes a star, a star, b star and d star.

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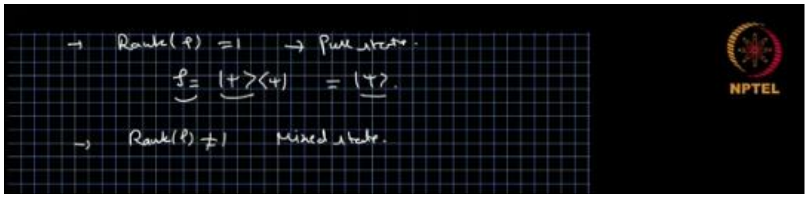

If rho equals rho dagger, this implies that A and D are real and B equals B star. It is a complex conjugate of each other. So, we can write rho as a, b, b star, d. Another thing is trace of rho is 1. This implies that a plus d equals 1. So, we can write rho as half times identity plus rx sigma x plus ry sigma y plus rz sigma z, how we can write this thing because first of all we notice that since the rho is a two by two Hermitian operator it can be decomposed as a sum of identity sigma x sigma y and sigma z because they form a basis for the Hermitian vector space. So, rx, ry, rz and the coefficient of identity should be, are yet to be found.

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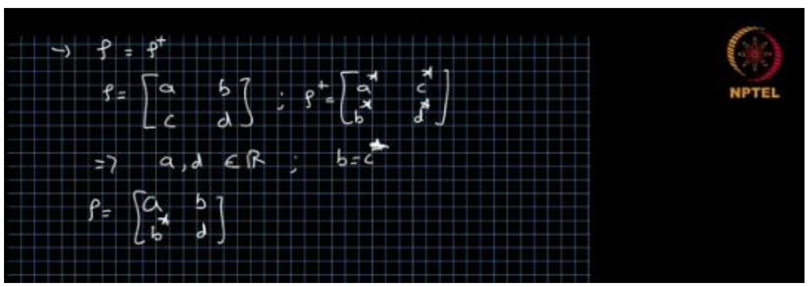

But since sigma x, sigma y and sigma z are traceless matrices, trace of sigma i is 0 for all i 1, 2, 3. So, the only matrix with non-square trace is the identity. So, the trace of identity is 2. So, the coefficient of this should be half. So, there is a half factor outside.

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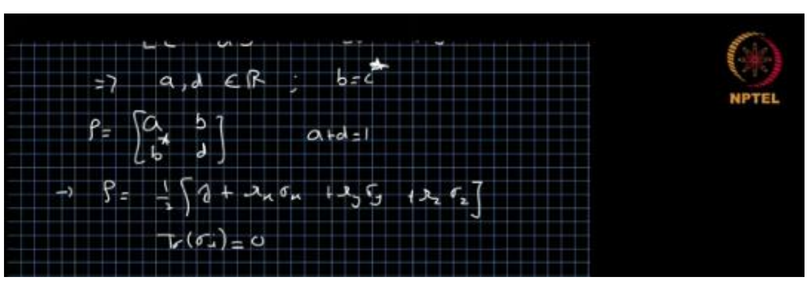

And other than that, there is no restriction over rx, ry and rz, just that they should be real. So, we can write rho in this form and it will satisfy the two conditions that its Hermitian and in that trace of rho is 1. Now, the next task is to find the eigenvalues of rho. And it turns out that it will be rx square plus ry square plus rz square square root over 2. So, there are two value values, one smaller, one larger.

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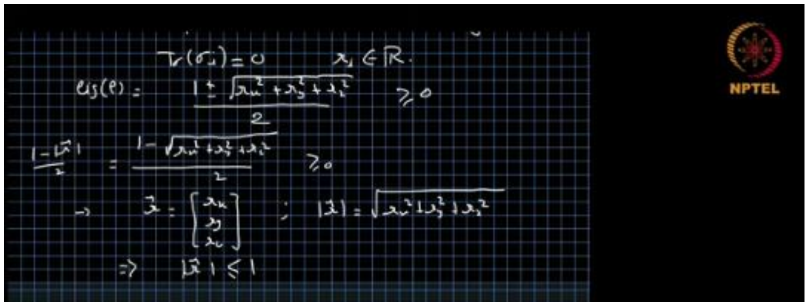

So, and they both should be positive. So, the smaller one is more likely to be negative than the bigger one. So, the smaller one is rx square plus ry square plus rz square over 2 should be a positive number. If we say r vector, if we define a r vector, which is a three-dimensional real vector, r x, r y, r z, then r vector mod will be square root of r x square plus r y square plus r z square. So, this becomes 1 minus r vector mod over 2 and from here we can say r vector mod should always be less than or equal to 1.

So, the positivity condition over the rho says that the r vector we have here in this decomposition, that should have magnitudes smaller than 1. So, this decomposition with the additional condition that r vector mod less than 1, less than or equal to 1, this is called block representation. Block representation or block decomposition of a qubit. Now, we see that r vector mod is less than or equal to 1. What will happen when r vector mod is equal to 1?

Then the eigenvalues of rho will become 1 plus minus 1 over 2 which is 1 and 0. Then the rank of the matrix is 1, hence pure state. So, till now we have seen mathematically how r looks like and how the density matrix can be represented and how density matrix rho is the more generalized form of representing the quantum state. But what is the physical significance of r, the rx, ry, rz? It turns out that the expectation value of sigma x is rx, sigma y is ry and sigma z is rz.

And this is a good exercise to establish this thing. Prove that expectation value of sigma x, sigma y, sigma z is rx, ry, rz, let me give you a hint that the expectation value of an observable is trace of A times pho. So, what we are seeing is the only quantities which we can measure in a lab namely sigma x, sigma y, sigma z or we should measure that has all the information, they are the direct coefficients of the density matrix rho in terms of rx, ry, rz. So, once we have rx, ry, rz and we plug it into the block decomposition, we get a 2 by 2 Hermitian matrix.

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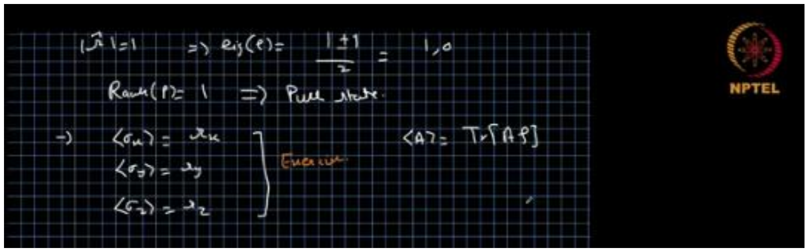

We find the eigenvalues of it and if the eigenvalue turns out to be 1 and 0, then we know that this rx, ry, rz correspond to the pure state, a pure state. And the eigenvector of rho corresponding to the eigenvalue 1 will be the pure state. So, in that way, this density operator representation of a state is more general and more useful way of writing the general states. So, if we are given an observable A with eigenvalues ai and eigenvectors ai and the state is given in the form of rho, then what is the probability of getting ai outcome? We know, we recall that for a pure state, the probability is given by the born rule, psi ai mod square.

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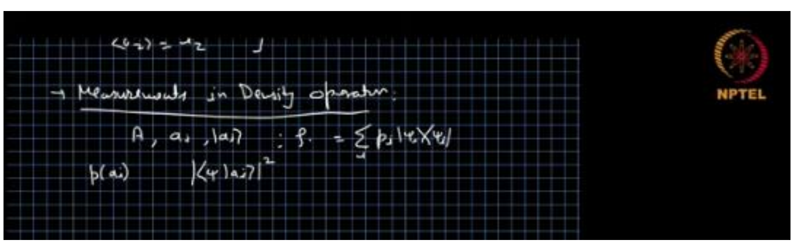

For a mixed state, where mixed state is given by sum over i, pi, psi i over psi i, it will be given by psi i, pi, sum over i, this factor. okay, so, we are assuming for each pure state we have probability psi i a let me say j not i we have different symbols psi j a i mod square and that state itself appear with probability pi, so the probability multiplies and we get the probability, the average probability of getting the output ai. This is the more generalized born rule of probability in terms of density matrix. But this is not very useful because we need to find the p i s and psi i s. So, we can expand it to make it simpler p j. We can say psi j a i and a i psi j which is ai sum over j pj psi j psi j ai and this is our rho. So, the probability of getting the outcome ai is actually the expectation value of rho in terms of ai This expression is interesting and I find it personally very interesting that here the role of the state and the quantity related to the observable have changed.

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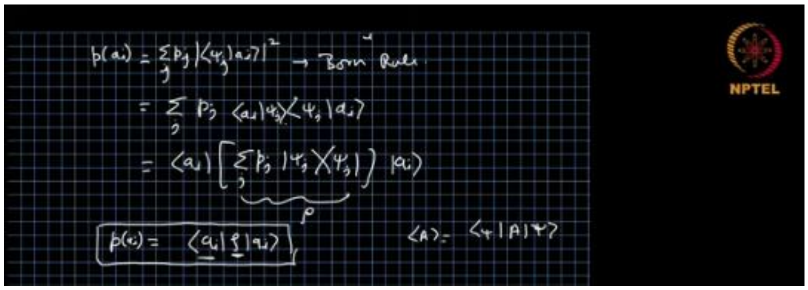

Till now we were saying that the expectation value of some observable is the expectation value of the observable of course the A sandwiched between the states psi, here we are saying rho is sandwiched between the eigen states eigenvectors a i okay, so we have flipped the role of observable and states although this statement has no material gain or any anything. But this is an interesting statement that here we have changed the role. Much later in this course, we will come to a duality in which we will show that a state of a quantum system can be thought of mathematically serve the operation on some other quantum system. Maybe these things are related and it should not come as a shock later on because we have seen something similar happening here. Okay but this was the new born rule of probability, the second part of the measurement postulate is the collapse, so what happens when we get the state a i, what happened to the state rho then rho goes to rho i which is given by a i outer product a i, rho a i outer product a i over p of a i now we see that this is just p of ai and we are left with ai ai over p we can cancel these and we are left with only ai ai.

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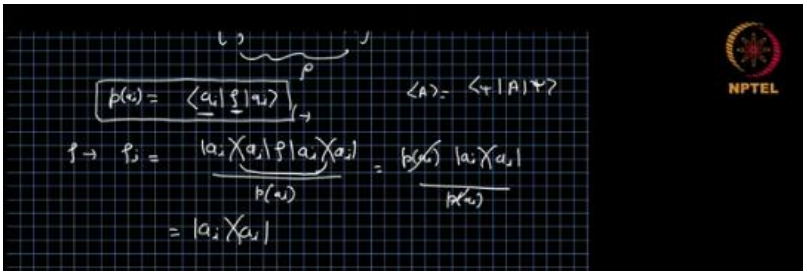

So, after the projection, the state rho collapses to pure state ai. And this is the original collapsible postulate in quantum mechanics. Then after measurement, the state collapses to the eigenstate of the observable.