Advanced Quantum Mechanics with Applications
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Lecture – 04
The Density Matrix Formalism, Expectation values of Operators

So, let us do some examples related to Density Matrix.

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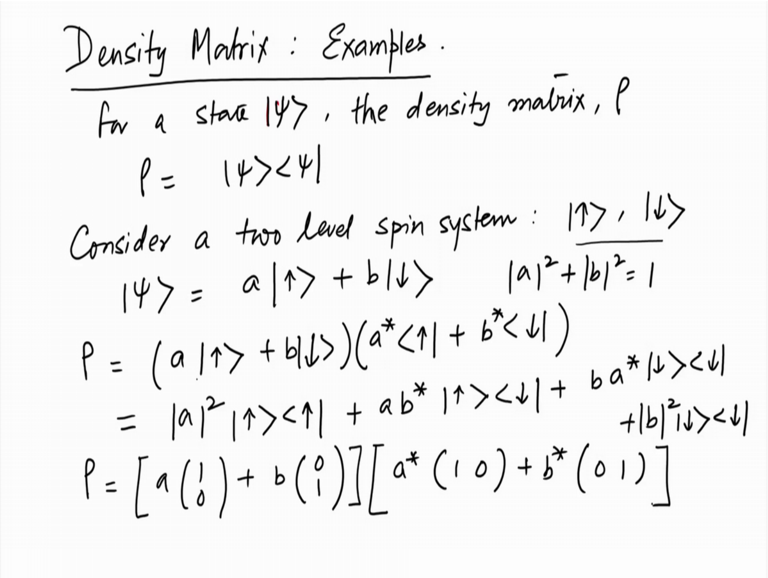

Density Matrix : Examples.

For a state $|\psi\rangle$, the density matrix, ρ

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

Consider a two level spin system : $|\uparrow\rangle, |\downarrow\rangle$

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle \qquad |a|^2+|b|^2=1$$

$$\rho = (a|\uparrow\rangle + b|\downarrow\rangle)(a^*\langle\uparrow| + b^*\langle\downarrow|)$$

$$= |a|^2|\uparrow\rangle\langle\uparrow| + ab^*|\uparrow\rangle\langle\downarrow| + ba^*|\downarrow\rangle\langle\downarrow| + |b|^2|\downarrow\rangle\langle\downarrow|$$

$$\rho = \left[a\begin{pmatrix}1\\0\end{pmatrix} + b\begin{pmatrix}0\\1\end{pmatrix}\right]\left[a^*\begin{pmatrix}1 & 0\end{pmatrix} + b^*\begin{pmatrix}0 & 1\end{pmatrix}\right]$$

So, that you understand that where these intimate density matrices are useful. So, as we have told that for a state psi the density matrix rho is defined as rho equal to this outer product of the states psi. This we have introduced earlier and just wanted to remind you that the density operator and density matrix these two words are used interchangeably; they mean the same thing for us.

So, now consider a two level system two level spin system. So, what we mean is that we have an upstate and a down state which are typically the spin states of spin half particle. And, let us write down a state which is a mixture of the up and the down states and of course, a square plus b square is equal to 1. Now, these a and b are complex coefficients or complex amplitudes. And now, we can define density operator or a density matrix as a up plus b down and multiplied by a a star now, with a conjugate up plus a b star and a conjugate down. And, this can simply be multiplied as a mod square and we have up outer product with an up and now we have a b star with an up and down and a b a star with a down and an up and plus a b mod square and a down ok.

So, now these are the elements or of the density matrix. So, as you see there are four elements and since the basis is very clearly defined by these a spin-up and spin-down as it is written here. So, we can write it down as a 2 by 2 matrix which is usually a practice to do in this case it is equal to a and an up is written as 1 0 and a b is written as a zee I mean a down is written as a with 0 1 and this will make things simpler.

So, we are writing an up spin with a 1 0 spinner two component spinner and the down spin is written with a two component spinner such as 0 and 1. And now, this has to be multiplied with a star. And now we have the conjugate of this spinner which is now written horizontally, whereas the original vector was written vertically. And a b star 0 1 and these two will have to be multiplied and when you multiply that. So, this can be now written as this rho is written as a 2 by 2 matrix.

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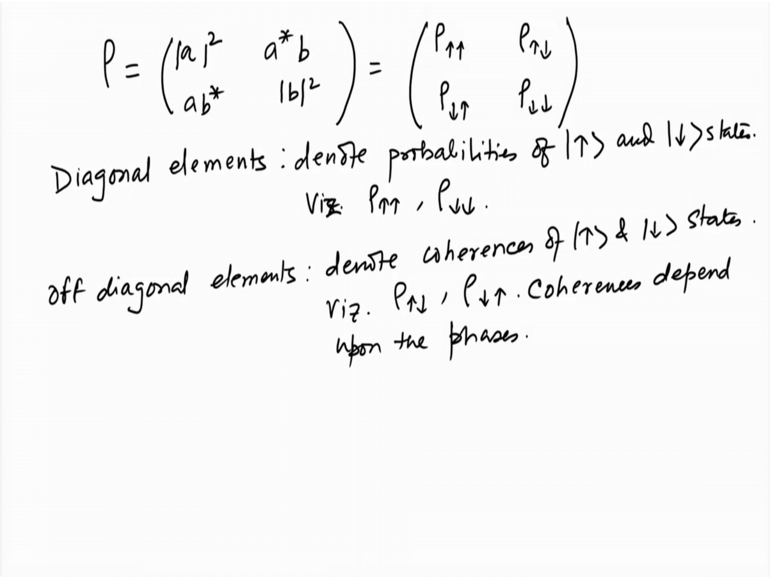

$$\rho = \begin{pmatrix} |a|^2 & a^*b \\ ab^* & |b|^2 \end{pmatrix} = \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix}$$

Diagonal elements : denote probabilities of $|\uparrow\rangle$ and $|\downarrow\rangle$ states. Viz. $\rho_{\uparrow\uparrow}$, $\rho_{\downarrow\downarrow}$.

off diagonal elements : denote coherences of $|\uparrow\rangle$ & $|\downarrow\rangle$ states. viz. $\rho_{\uparrow\downarrow}$, $\rho_{\downarrow\uparrow}$. Coherences depend upon the phases.

So, this density operator or the density matrix is now written as a 2 by 2 matrix with the amplitudes given by a mod square a star b and a b star and a b mod square. And, this could simply be written as up up and up down and a down up and a down down. So, these are the 2 or the 4 elements of a 2 by 2 matrix which here is the density matrix. So, we have a particular meaning attached to the diagonal and the off diagonal elements. So, the diagonal elements they denote the probabilities of the up and down states.

So, they are namely they are rho up up and rho down down and similarly the off diagonal elements they are written with so, they denote what are called as a coherences of up and down states. And they are of course, our rho up down and rho down up. Now, these coherences will be discussed in more details later on in the context of coherence and squeeze states etcetera. And so, these coherences depend upon the phase. And so, so these are the ways to write a density matrix in terms of a 2 by 2 matrix and let us just do another example here.

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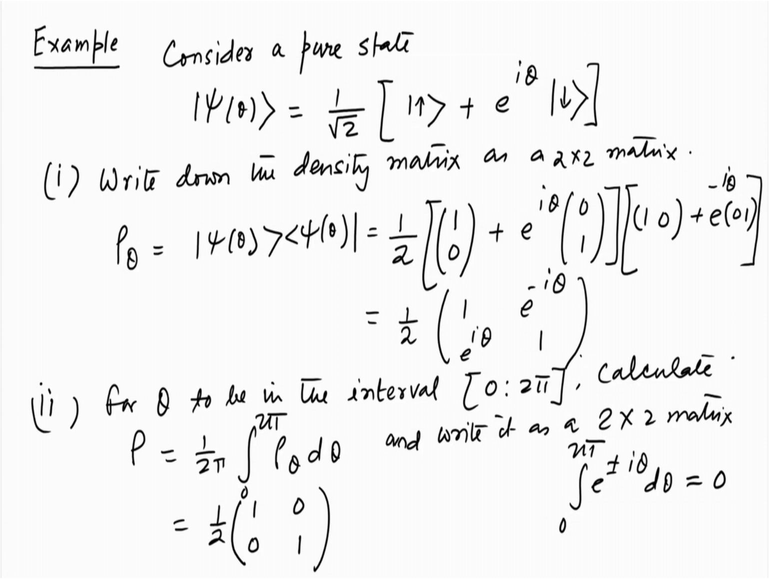

Example Consider a pure state

$$|\psi(\theta)\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle + e^{i\theta}|\downarrow\rangle\right]$$

(i) Write down the density matrix as a 2×2 matrix.

$$\rho_\theta = |\psi(\theta)\rangle\langle\psi(\theta)| = \frac{1}{2}\left[\begin{pmatrix}1\\0\end{pmatrix} + e^{i\theta}\begin{pmatrix}0\\1\end{pmatrix}\right]\left[(1\ 0) + e^{-i\theta}(0\ 1)\right]$$

$$= \frac{1}{2}\begin{pmatrix}1 & e^{-i\theta}\\ e^{i\theta} & 1\end{pmatrix}$$

(ii) for θ to be in the interval $[0:2\pi]$, calculate

$$\rho = \frac{1}{2\pi}\int_0^{2\pi}\rho_\theta\, d\theta$$ and write it as a 2×2 matrix

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

$$\int_0^{2\pi} e^{\pm i\theta}\, d\theta = 0$$

So, let us write down a question consider a pure state so, by the way what we are doing so, far concerns with the pure state. So, we have not seen as yet the notion of mixed states, but it is only that the mixed states will have to be now coming with a particular probability instead of state that we are writing. Consider a pure state here which looks like a psi of theta, where theta is an angle is defined as again it is a spin half system. But however, the spin down amplitude now comes does not come with half, but it comes with a factor that depends upon the angle.

So, the question is that first one write down the density matrix as a 2 by 2 matrix. And that is fairly easy because, you will write this as psi of theta and a psi of theta which will be simply equal to one half because, there are two factors of 1 by root 2 coming. And, if we write this as earlier as 1 0 as the spin up and its exponential i theta to be 0 1 now, this will be multiplied by a 1 0 and the plus exponential minus i theta and a 0 1. And, if you simplify this it will come out as half of 1 exponential minus i theta exponential i theta and 1. So, the important thing to notice is that this diagonal elements which are the probabilities they are half and half as it should be with the factor of half outside.

However, the probability or the coherence terms between the up and down spins now depend upon theta. So, a second question that can be asked is for theta to be in the interval 0 and 2 pi, we can calculate a rho which is an integral over the full range and a row theta d theta. Now, and write and write it as a 2 by 2 matrix that simply says that each of the elements will have to be integrated over 2 pi. Now, the diagonal elements of course, do not depend upon theta so, they will stay as what they are and a exponential minus i theta d theta over 0 to 2 pi gives me 0 and this is 0 as well exponential i theta.

So, exponential plus minus i theta d theta over 0 to 2 pi gives me 0 because i comes out and then there is an exponential i theta integral from 0 to 2 pi, at both the limits it is 1. So, that gives me 0 and we get back the density matrix that we have already said and now the coherence terms go to 0. So, as you integrate over all theta the coherence vanishes. So, basically the coherence is so, between 0 to pi will cancel with pi to 2 pi. So, that is the kind of understanding that we arrive at. So, let us just do a little bit of discussion on the mixed states.

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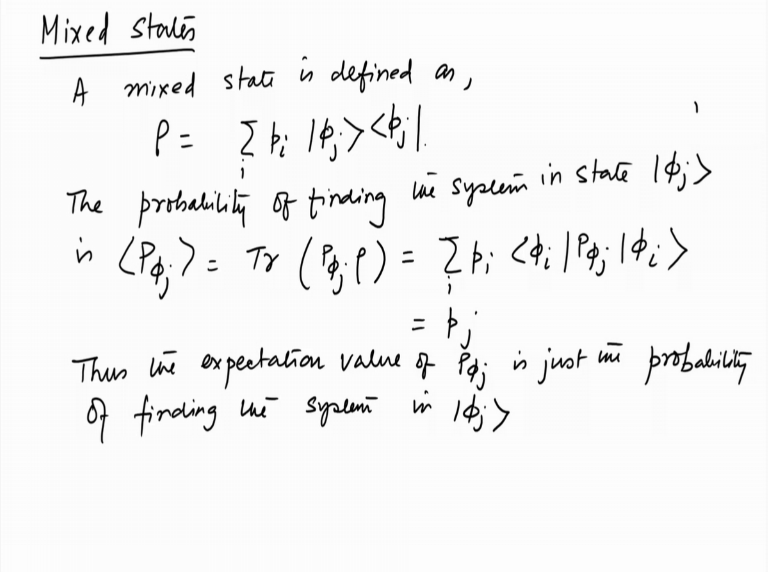

Mixed States

A mixed state is defined as,

$$\rho = \sum_i p_i |\phi_j\rangle\langle\phi_j|$$

The probability of finding the system in state $|\phi_j\rangle$ is $\langle P_{\phi_j}\rangle = Tr(P_{\phi_j}\rho) = \sum_i p_i \langle\phi_i|P_{\phi_j}|\phi_i\rangle$

$$= p_j$$

Thus the expectation value of P_{ϕ_j} is just the probability of finding the system in $|\phi_j\rangle$

So in fact, we are going to talk about a few disconnected small topics which are a important for later use and we will just introduce them and maybe use them more elaborately in subsequent discussions. So, a a mixed state is defined as so, it is the same thing excepting now there is a probability that comes with this. And so, this probability are p i is given by or rather this is defined as the probability of finding the state for rather finding the system in state phi j is a this P phi j which is nothing, but a trace of P phi j. So, this is by using the definition that the expectation value of any operator would be the operator multiplied by the density matrix and then the trace has to be taken over.

And this is nothing, but i and a p i and a phi i and P phi j and a phi i and this is nothing, but equal to p j. So, thus the expectation value of value of P phi j is just the probability of finding the system in a state phi j. We postpone any further discussion on mixed states and maybe we shall come back to it later. Now, we introduce another concept called as Reduced Density Matrix.

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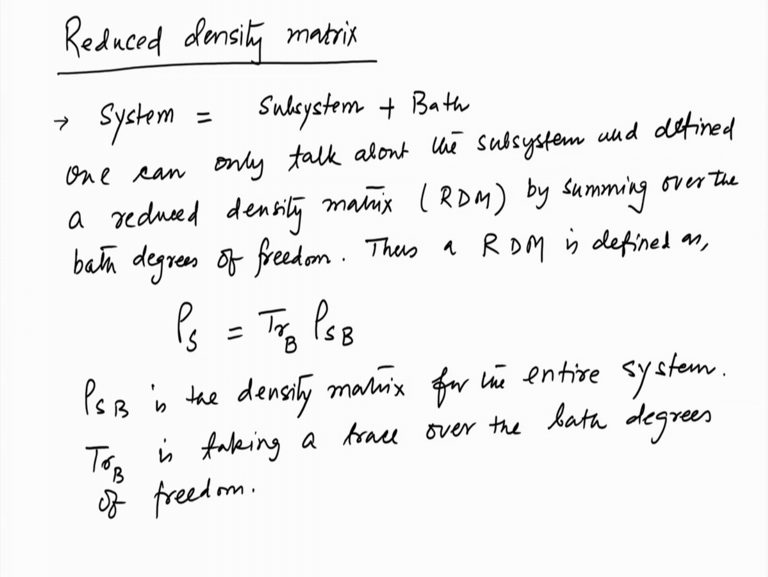

Reduced density matrix

→ System = Subsystem + Bath

One can only talk about the subsystem and defined a reduced density matrix (RDM) by summing over the bath degrees of freedom. Thus a RDM is defined as,

$$\rho_S = Tr_B \, \rho_{SB}$$

ρ_{SB} is the density matrix for the entire system. Tr_B is taking a trace over the bath degrees of freedom.

In statistical physics it is often used or rather introduced that a system is in a contact with a bath. And like for example, a heat bath suppose I keep a cup of tea on the table in this room or you keep a cup of tea in your room that you are sitting in and so, the tea is hot. However, if you keep the tea in that position or in that state for some time the tea will get cold however, the temperature of the room does not increase. So, this is the meaning of a bath or a temperature bath in this case is that it can extract as much of heat from a particular system which in this case your cup of tea, but it does not undergo any change in temperature. So, that is called as a bath.

And in canonical ensemble in statistical mechanics it is often used that a system is in contact with a temperature bath, such that the system is always at a given temperature t. And, even if you wait for long enough the system will still be at a temperature t because of the presence of the bath. So, sometimes the bath is not important for us to consider and one can actually sum over the bath degrees of freedom leaving only the system to be considered. In that case so, we can say that a system is equivalent to a subsystem which is actually the cup of tea in this case and a bath which is the room or the hall that you are sitting in at this moment.

So, one can only talk about the subsystem and define a reduce density matrix called as RDM, by summing over the bath degrees of freedom. So, thus RDM is defined as rho S that is the density matrix of the system only the system and we actually do a sum over the bath. So, B stands for bath S stands for system and S B is a the combined system and the bath the subsystem and the bath. And so, rho S B is the density matrix for the entire system and the entire system is defined in this in this first line here that we see here. So, that is the entire system and so, trace B is summing over or taking a trace over the bath degrees of freedom. Let us see some one example at least for a how one actually a sum over one particular degree of freedom.

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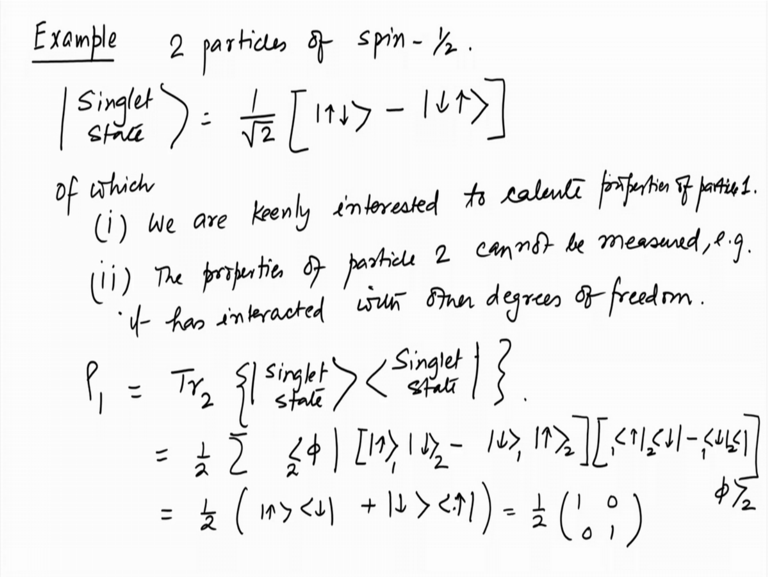

Example 2 particles of spin-½.

$$\left|\begin{matrix}\text{Singlet}\\ \text{state}\end{matrix}\right\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right]$$

of which

(i) We are keenly interested to calculate properties of particle 1.

(ii) The properties of particle 2 cannot be measured, e.g. ∵ it has interacted with other degrees of freedom.

$$\rho_1 = \mathrm{Tr}_2\left\{\left|\begin{matrix}\text{Singlet}\\ \text{state}\end{matrix}\right\rangle\left\langle\begin{matrix}\text{Singlet}\\ \text{state}\end{matrix}\right|\right\}.$$

$$= \frac{1}{2}\sum_{2} {}_2\langle\phi|\left[|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right]\left[{}_1\langle\uparrow|{}_2\langle\downarrow| - {}_1\langle\downarrow|{}_2\langle\uparrow|\right]|\phi\rangle_2$$

$$= \frac{1}{2}\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

Let us do that in a simple case that let us take again spin system now, is the spin system of 2 particles of spin half. So, this I am sure you have read in quantum mechanics or in atomic physics, that if there are or at least the spin angular momentum when you did is that when you have 2 particles of spin half there are the Hilbert space is actually a a four-dimensional. And, one can have 4 type of states of which 3 are called as the triplet states and that is why they are called triplet because, the 3 of them. And, there as a singlet state and now the singlet state is actually a antisymmetric with respect to a change in the spin indices, so whereas the triplet states are a symmetric.

So, let us talk about only a singlet state. So, this singlet state is written as with a normalization of 1 by root 2 and then there is a up down and minus down up. So, you see that so, these are the first on the left what we write is corresponding to the first particle and what we write to the right is that corresponding to the second particle. So, the first particle has spin half, second has spin down and the reverse in this case and they are there is a minus sign in between which makes it an antisymmetric because, if you change up to down there is a change in sign.

Now, say that particle 2 so, of which 1 we are keenly interested I am sorry to calculate or other know the properties of particle 1. And, second is that the properties of particle 2 particle 2 cannot be measured cannot be measured for a number of reasons. So, one of them could be that it has interacted with other degrees of freedom and has you know decayed in some sense ok. So, but of course, we are still interested in measuring the properties of 1. So, we will write down the density matrix of the particle number 1 by summing over or taking a trace over the singlet state. So, that can be written as half and there is a sum over and there is a phi 2 and this is a 1 1 and a 2 and a minus a down being a 1 and sorry this is written a little the kits are.

So, this is a 2 and this is a up 2 and now this is also that there is up and a 2 down and a minus down 1 and down 2 and then of course, it has to be a phi and then 2. So, this is what it is where phi is the state that we are summing over and this is equal to a half up and down and plus a down and up. And, this is equal to half into 1 0 0 0 1 which means that the probabilities of finding the states or the first particle in upstate is half and in the down state is half again.

And there is no we are not interested or rather we do not know how to calculate particle number 2 because, it has as I say it that it has interacted with other degrees of freedom ok. And, also we have introduced this but, just for the sake of completeness we are writing that the expectation values of any operator is a A t is equal to trace of A rho t.

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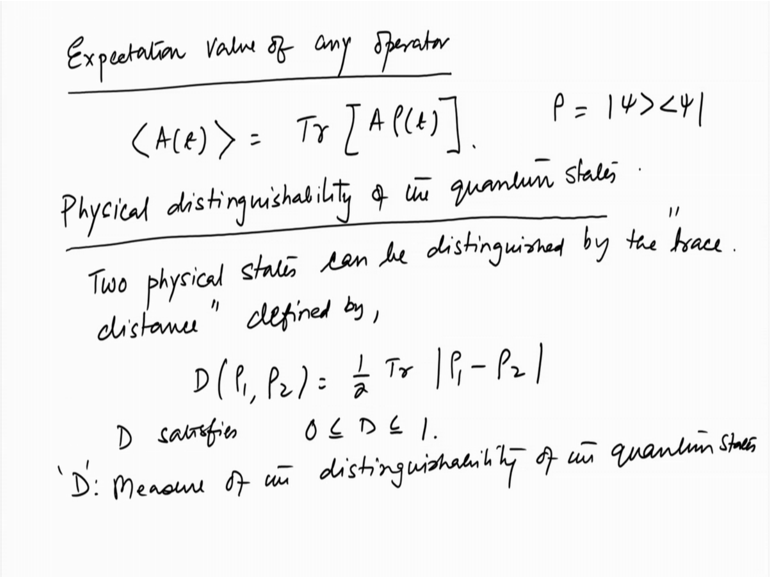

Expectation value of any operator

$$\langle A(t)\rangle = Tr\left[A\rho(t)\right]. \qquad \rho = |\psi\rangle\langle\psi|$$

Phycical distinguishability of the quantum states.

Two physical states can be distinguished by the "trace distance" defined by,

$$D(\rho_1, \rho_2) = \frac{1}{2} Tr\,|\rho_1 - \rho_2|$$

D satisfies $0 \le D \le 1$.

'D': Measure of the distinguishability of the quantum states

And so, it is enough to calculate the expectation value of any arbitrary operator just by knowing the density matrix for the system and the rho is of course, are defined as the psi and psi. So, let us take up another small topic for discussion which is called as the physical distinguishability of the quantum states. So, we want to asked the question that given two quantum states psi 1 and psi 2, how distinguishable they are or how what is the distance between them.

This word distance should not be actually sort of interpreted or misinterpreted as a physical distance. But, this is like how different they are is what we want to understand. And so, two physical states distinguished by the trace by the trace distance defined by rho 1 and rho 2, which is half the trace of rho 1 minus rho 2 and this distance satisfies a 0 less than D less than 1.

So, basically it is a measure of it is a measure of measure of the distinguishability of the quantum states as I already have said. So, it is clear that rho 1 and rho 2 are the density matrices for those quantum states that we talked about. So, one has to take a trace of this rho 1 minus rho 2 and multiplied by half. There is another way to talk about the distinguishability.

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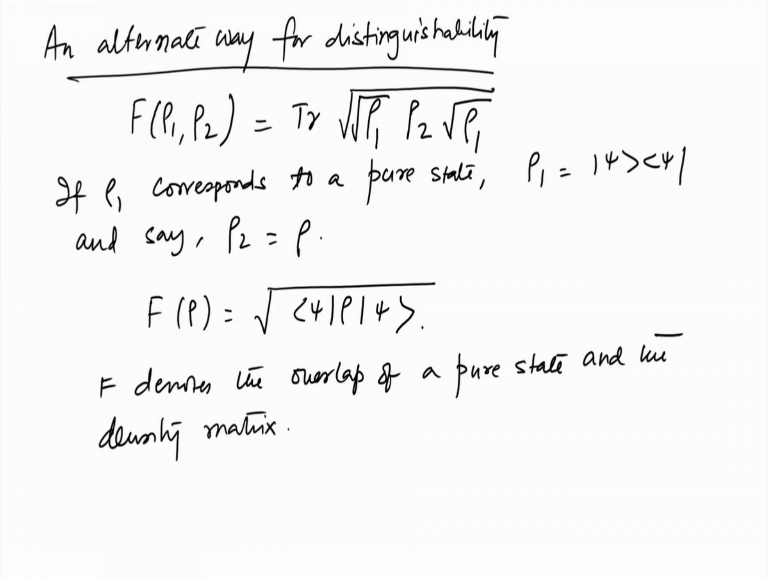

An alternate way for distinguishability

$$F(\rho_1,\rho_2) = \mathrm{Tr}\sqrt{\sqrt{\rho_1}\,\rho_2\sqrt{\rho_1}}$$

If ρ_1 corresponds to a pure state, $\rho_1 = |\psi\rangle\langle\psi|$
and say, $\rho_2 = \rho$.

$$F(\rho) = \sqrt{\langle\psi|\rho|\psi\rangle}.$$

F denotes the overlap of a pure state and the density matrix.

So, an alternate way and that is given by a quantity which is rho 1 rho 2 which is trace of rho 1 it is rho 1 square root rho 2 and a square root of rho 1. So, that is the definition of this distinguishability. And so, if rho 1 corresponds to a pure state rho 1 equal to psi psi and say a rho 2 equal to a rho, then the F rho is defined as square root of a psi and a rho and a psi. So, it is a, this F denotes the overlap of a pure state and the density matrix.