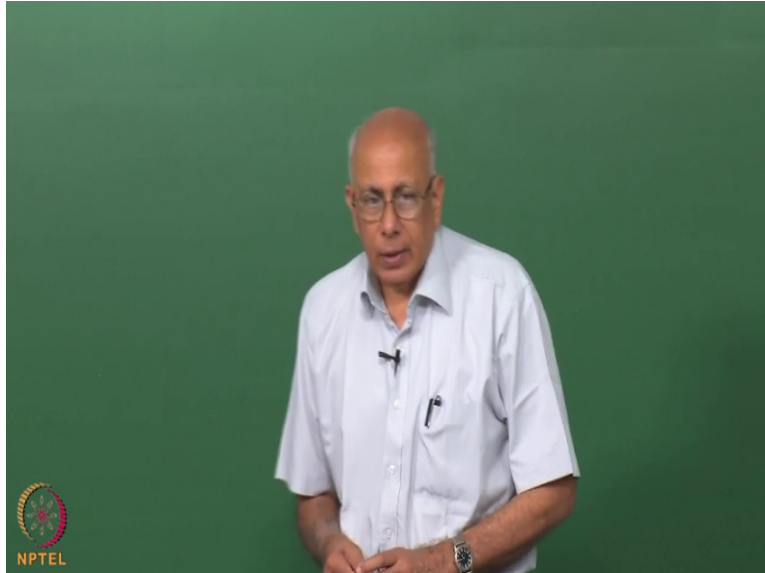


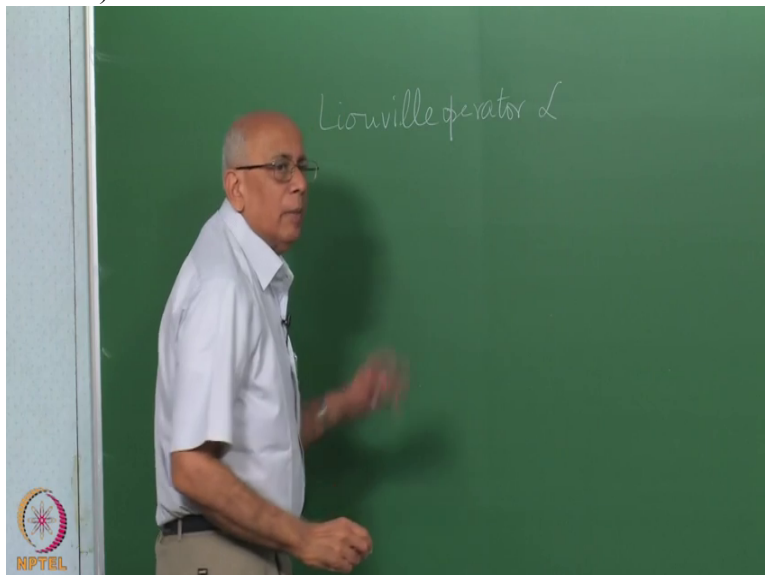
Nonequilibrium Statistical Mechanics
Professor V. Balakrishnan
Department of Physics
Indian Institute of Technology Madras
Lecture No 07
Linear response theory (Part 2)

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Right, so we had just started looking at the linear response theory and just to recapitulate what I said last time we had the Liouville operator L which determine

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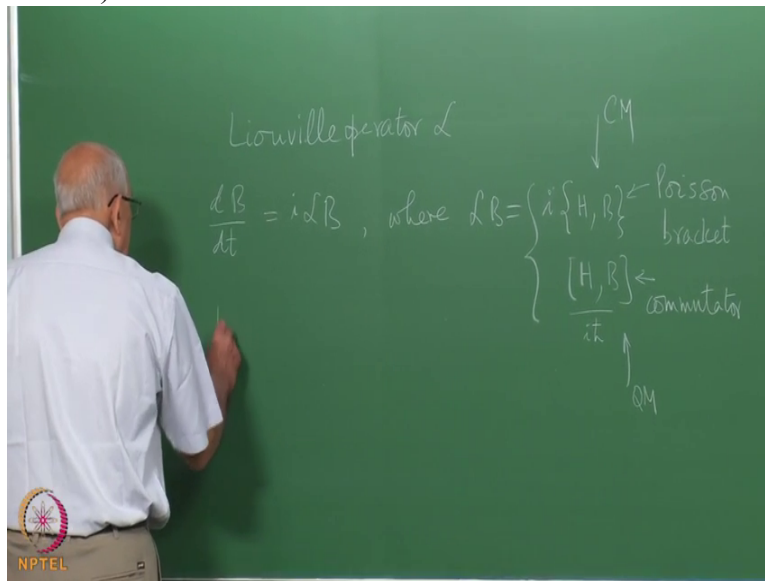


for any system, Hamiltonian system which determine time evolution. So the statement was that the time derivative of any observable, B for instance, $d B$ over $d t$ was equal to $i L$ acting on B and one has to solve this equation of motion if you like in abstract form 0:00:58.6 where

L on B was either equal to i times the Poisson bracket of, well, in quantum mechanics it was easier, it was H with B divided by i h cross in this fashion or in classical physics it was H with B Poisson bracket and this was the commutator where as this is the Poisson bracket.

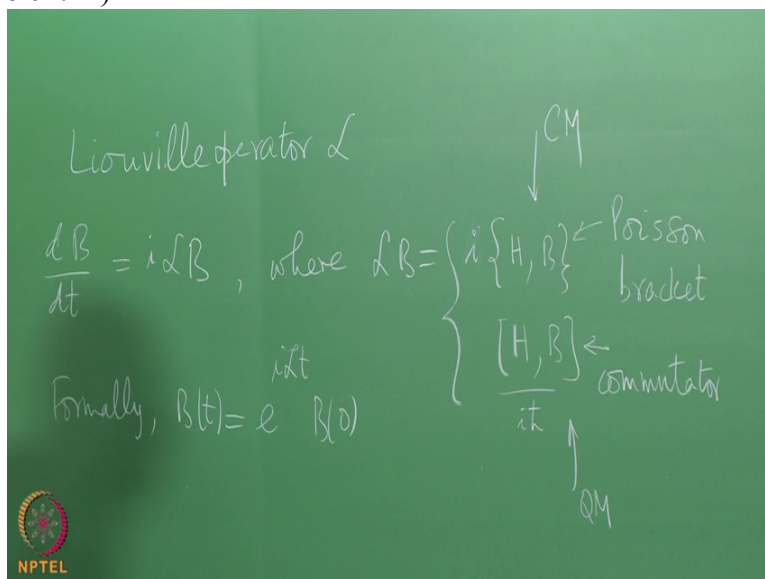
And whereas this was true in classical mechanics, this is true in quantum mechanics. That is the effect of this operation on any observable B but what you need to do for time dependence, explicit time dependence is formally

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B of t is equal to the exponential e to the i L t on B of zero. So one has to exponentiate this Liouville operator

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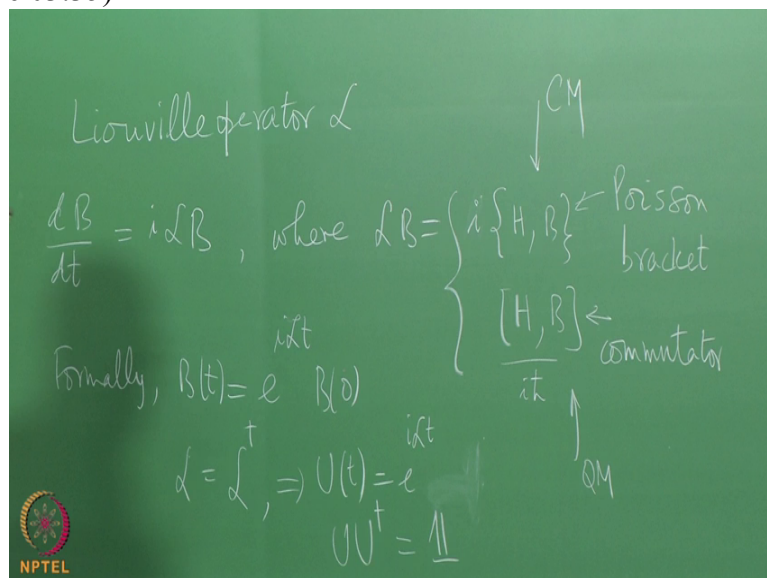


which is not always trivial to do.

In quantum mechanics, we know explicitly what this stands for, this fellow here, it is e^{-iHt} on either side of B of zero; in classical mechanics it means that you have to write down, and you write this down, you solve the Hamilton equations of motion and then you have B of q of t and p of t inside the argument, Ok. We will find it convenient to use this notation.

When we need to compute something we will go back and explicitly write out what these things are but till then the formal relation, this expression for the time development operator is very useful, Ok. We also saw this property that on a appropriate space, L was equal to L^\dagger implies that U of p which is e^{-iLp} is equal, is such that $U U^\dagger$ is equal to the identity operator, it is a unitary operator.

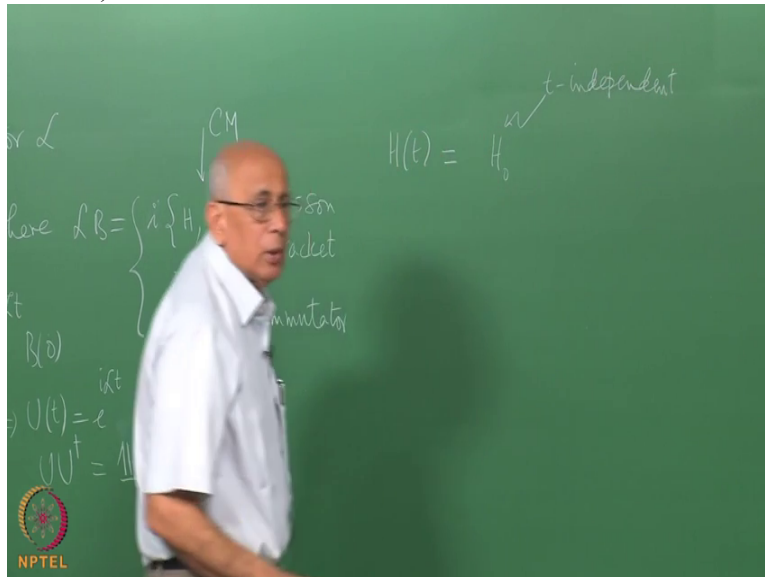
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And this came about, the interpretation of this fact is that probability is conserved or measure is preserved or whatever. Now having got this expression, what we would like to do is to extend this to a case where this L has become time dependent in an explicit way. So this is fine as long as the Hamiltonian we are talking about is autonomous, does not have a time dependence but the moment you have explicit time dependence in H then matters become more complicated.

So in particular if you notice we are interested in a situation where the Hamiltonian H of t is equal to H naught which is t independent, the unperturbed Hamiltonian

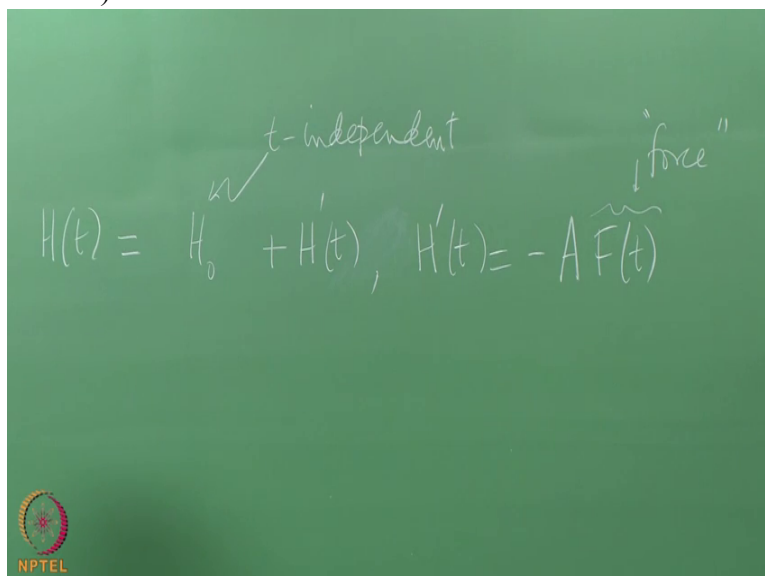
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and then a perturbation which is H' which is a function of t , where H' has the form minus some A times f of A . So it is some generalized force if you like and this is the operator pertaining to this system to which force couples, Ok.

So that is the form of the perturbation

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and we would like to solve the same problem, find physical averages of any arbitrary quantity in the presence of this time dependent perturbation.

So we start by saying, that at t equal to minus infinity the perturbation has not yet switched on, the system is in equilibrium. I could start from any finite time but if I set the stage where

the perturbation is switched on to the minus infinity then it is clear that every other case is the special case. I can switch it off till some time and then start it off and so on. We will see what transients we will do. So we will assume that, at t equal to minus infinity there is no perturbation.

The Hamiltonian is just H naught and the system of interest is in equilibrium in the canonical ensemble. So we will assume that, and the system of interest is in thermal equilibrium at temperature T ,

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$$H(t) = H_0 + H'(t), \quad H'(t) = -A \overbrace{F(t)}^{\text{"force"}}$$

$$\text{At } t = -\infty, \quad H = H_0 \text{ \& the system is in thermal equilibrium at temperature } T$$

Ok. Then the system's physical quantities are all, the average values are all specified by a thermal average with respect to the density operator of the canonical ensemble.

So, for instance the average value of B in equilibrium and I have used the subscript for equilibrium, this will be equal to, for any quantity B this will be equal to trace B times ρ equilibrium where we set trace ρ equilibrium to be equal to 1. We are always; we are going to normalize our density matrix so that the trace of this density matrix is 1, Ok.

So ρ equilibrium is equal to e to the minus beta H naught divided by trace e to the minus beta H naught. This part is a scalar, it is just a number. This is where the operator is, the trace of it is by definition 1. So this is what

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$$H(t) = H_0 + H'(t), \quad H'(t) = -A F(t)$$

At $t = -\infty$, $H = H_0$ & the system is in thermal equilibrium at temperature T

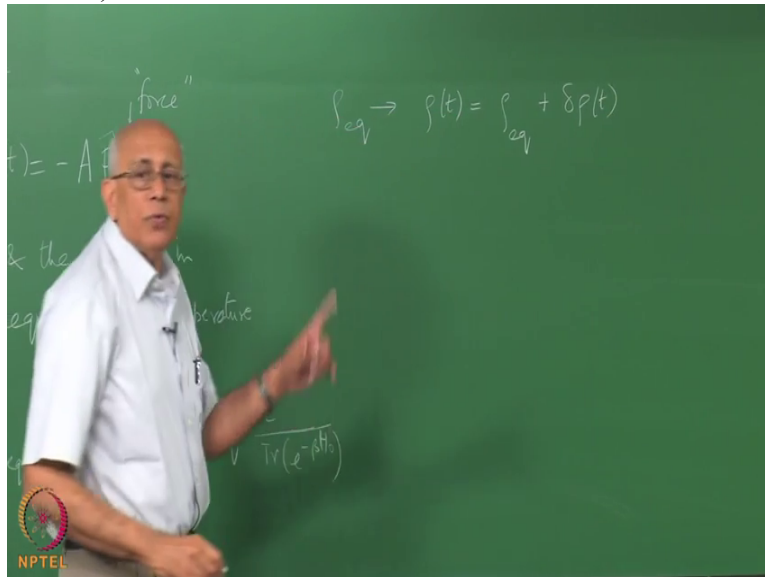
$$\langle B \rangle_{eq} = \frac{\text{Tr}(B \rho_{eq})}{\text{Tr}(\rho_{eq})}, \quad \text{Tr} \rho_{eq} = 1, \quad \rho_{eq} = \frac{e^{-\beta H_0}}{\text{Tr}(e^{-\beta H_0})}$$

we start with. System is in equilibrium at t equal to minus infinity. You switch on the perturbation and then you ask what is the value of, average value of any quantity of interest to you.

Let us take such generic quantity to be B . I want to distinguish it from this A because it does not have to be A itself. There could be a special case where B is equal to A . You are observing that quantity which appears in the Hamiltonian perturbation but in general it is some other quantity. We want to now know what the expectation value of this B is, out of equilibrium, away from equilibrium, in the absence of, in the presence of this perturbation here. We will assume that this perturbation is small in a very specific sense, in the sense that the second order terms in this perturbation will be neglected. So it is small compared to this and we want the correction to first order. So how does one go about it?

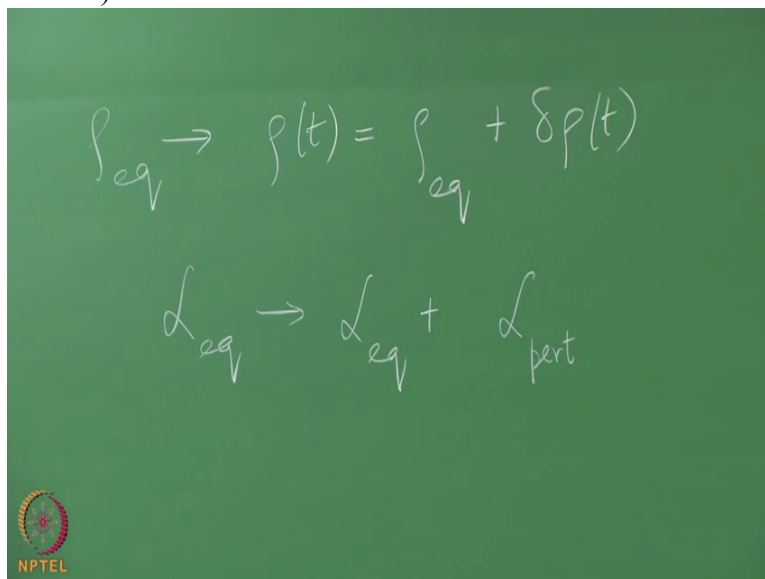
Well it is obvious that the density matrix itself will change. The new density matrix will not be the old density matrix at all with some new quantity of some kind, so ρ equilibrium will now go to ρ of p which is equal to ρ equilibrium plus a $\delta \rho$ of p

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correct to first order in the perturbation, right? Similarly the Liouville operator L , instead of the equilibrium Liouville operator the L will go to plus, let me use another term for it, let me call it delta L perturbation,

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the extra portion which comes because of this portion of the Hamiltonian, the H prime part
Ok.

Again L perturbation will be of first order. So now how would we compute the thing like this? Well you take this, now the quantum mechanical language makes these things explicit, you can see what will happen. These operators start with, at t equal to minus infinity they are at Schrodinger picture before you actually switch on the time dependent perturbation, Ok.

And once you switch it on they change with time and the change in time of any physical quantity can be done one of two ways. Either you have a time dependent density operator and you trace and you take expectation value with respect to that time dependent density operator or a time independent operator, the Schrodinger operator or you make the operator have time dependence to first order in the perturbation and compute averages with respect to the equilibrium density matrix. This would not matter, it does not matter which one you do, depends on what is convenient to you. But at a formal level, we could write the following.

We could write $\frac{d}{dt} \rho(t) = -i L \rho(t)$, so let me call this equal to L_{total} , $L_{\text{total}} \rho(t)$ that is the equation satisfied

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$$\rho_{\text{eq}} \rightarrow \rho(t) = \rho_{\text{eq}} + \delta \rho(t)$$

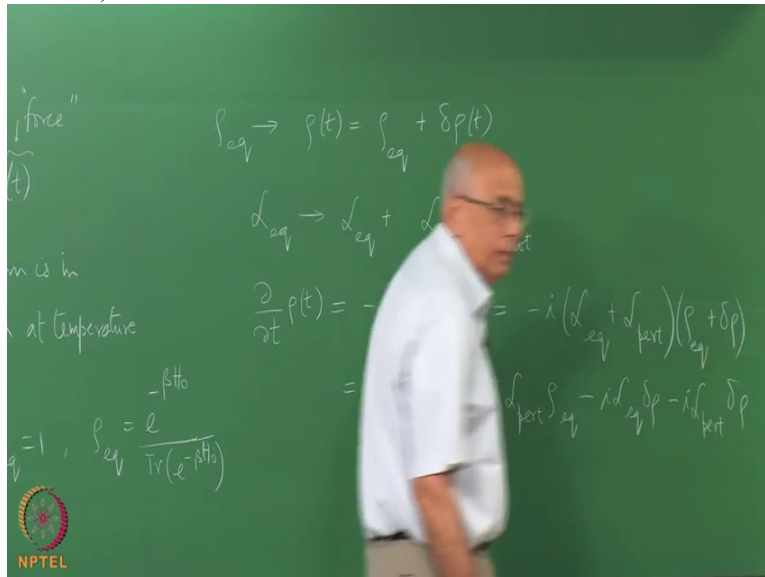
$$L_{\text{eq}} \rightarrow L_{\text{eq}} + L_{\text{pert}} = L_{\text{tot}}$$

$$\frac{\partial}{\partial t} \rho(t) = -i L_{\text{tot}} \rho$$

by the density operator. This here is called the von Neumann equation in quantum mechanics or the Liouville equation in classical mechanics. So this is equal to minus $i L_{\text{equilibrium}}$ plus $L_{\text{perturbation}}$ acting on $\rho_{\text{equilibrium}}$ plus $\delta \rho$ which is a function of t , formally.

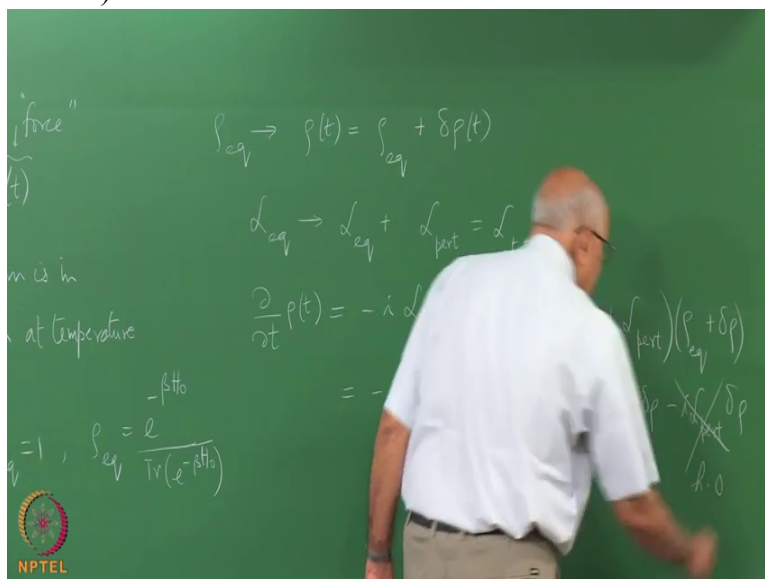
But this is equal to minus $i L_{\text{equilibrium}}$ acting on $\rho_{\text{equilibrium}}$, minus $i L_{\text{perturbation}}$ acting on $\rho_{\text{equilibrium}}$, minus $i L_{\text{equilibrium}}$ acting on $\delta \rho$ and then the last term minus $i L_{\text{perturbation}}$ acting on $\delta \rho$,

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Ok. There are 4 terms at a formal, in a formal sense. But this term is of higher order in the perturbation.

(Refer Slide Time 12:57)



Because this is perturbation and that is also perturbation. This is clearly of at least second order in the perturbation.

(Refer Slide Time 13:08)

$$\rho_{eq} \rightarrow \rho(t) = \rho_{eq} + \delta\rho(t)$$

$$d_{eq} \rightarrow d_{eq} + d_{pert} = d_{tot}$$

$$\frac{\partial}{\partial t} \rho(t) = -i d_{tot} \rho = -i (d_{eq} + d_{pert}) (\rho_{eq} + \delta\rho)$$

$$= -i d_{eq} \rho_{eq} - i d_{pert} \rho_{eq} - i d_{eq} \delta\rho - \cancel{i d_{pert} \delta\rho}$$

h.o.

So if I drop that term then this is an approximation correct to first order, Ok,

(Refer Slide Time 13:18)

$$\rho_{eq} \rightarrow \rho(t) = \rho_{eq} + \delta\rho(t)$$

$$d_{eq} \rightarrow d_{eq} + d_{pert} = d_{tot}$$

$$\frac{\partial}{\partial t} \rho(t) = -i d_{tot} \rho = -i (d_{eq} + d_{pert}) (\rho_{eq} + \delta\rho)$$

$$\approx -i d_{eq} \rho_{eq} - i d_{pert} \rho_{eq} - i d_{eq} \delta\rho - \cancel{i d_{pert} \delta\rho}$$

h.o.

right? What can I say about the first term?

(Professor – student conversation starts)

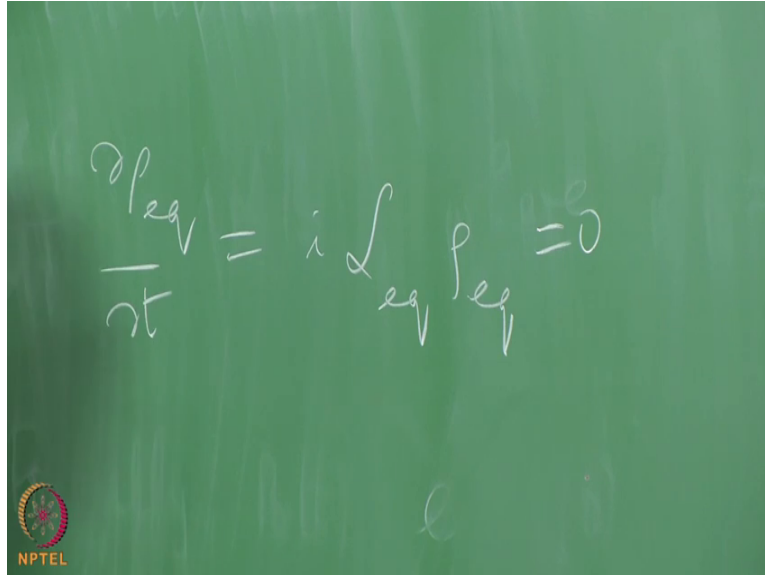
Student: 0:13:33.1

Professor: This involves here, a Poisson bracket or whatever of function of H H naught acting on H naught, ρ equilibrium is a function of H naught, right and H naught commutes with itself. So we know $\delta \rho$ equilibrium over $\delta \rho$ is zero because we know that, that must satisfy, this is a trivial statement but let me write it out, I mean formally $\delta \rho$

equilibrium over Δt equal to $i L$ equilibrium on ρ equilibrium and ρ equilibrium doesn't have any time dependence at all. This is zero, by definition.

(Professor – student conversation ends)

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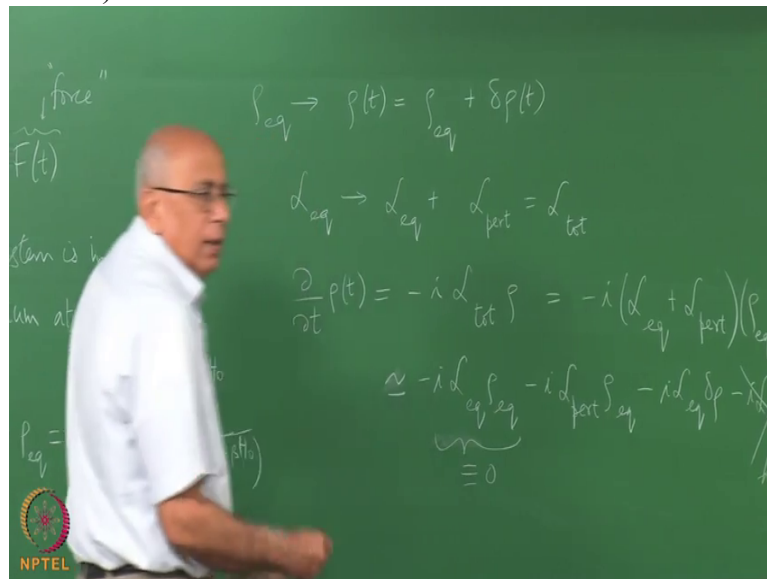

$$\frac{\partial \rho_{eq}}{\partial t} = i \int_{eq} \rho_{eq} = 0$$

This involves H naught, exponentiation etc. This involves H naught and they commute with each other. So this thing is zero, classical or quantum it doesn't matter, Ok. Incidentally going back to equilibrium statistical mechanics it is because this is zero that we can assert, and this involves H naught that we can assert that this must be a function of H naught, right?

I mean the equilibrium density matrix in the canonical, micro canonical whatever ensemble is a function of the unperturbed Hamiltonian always. What function it is cannot be given, got from this equation. This serves as the, equilibrium statistical mechanics density operator serves as a kind of boundary condition on this equation. At t equal to minus infinity it is some function of H naught and what function it is depends on the physics, depends on the ensemble and it is therefore put in not from this Liouville equation but from equilibrium statistical mechanics.

You need to derive that. So that's the standard derivation in equilibrium statistical mechanics. For us, we assume this is given. This quantity is given by the canonical ensemble, Ok. So this term is zero.

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It is identically zero, Ok. So that is a first order differential equation for this quantity in which this thing here acting on delta rho is something we know, we know what this L equilibrium does.

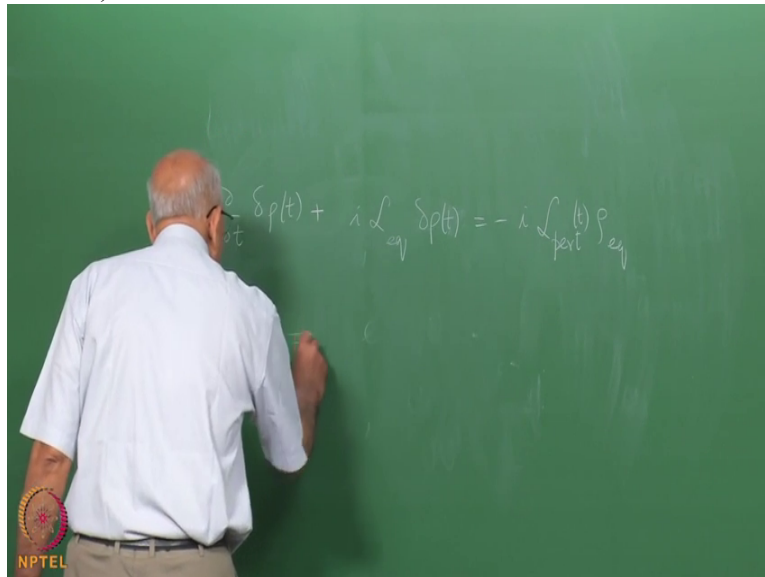
So I can write this down, that equation down as delta over delta rho, sorry, delta over delta t delta rho of t plus i L let me write this carefully, yes L equilibrium on delta rho is equal to minus i L perturbation on rho equilibrium. Is it right? Yes. Ok, right. So this function is known to me, this quantity is known to me and this term here, this delta term is unknown to me and it is the first order differential equation. Notice there is time dependence here. This is a function of t. There is time dependence here.

(Professor – student conversation starts)

Student: Are we supposed to take up the right kind of some source?

Professor: Yeah it acts like some kind of source. This term here is time dependence, delta rho has time dependence here and we can write the solution to this equation. So formally

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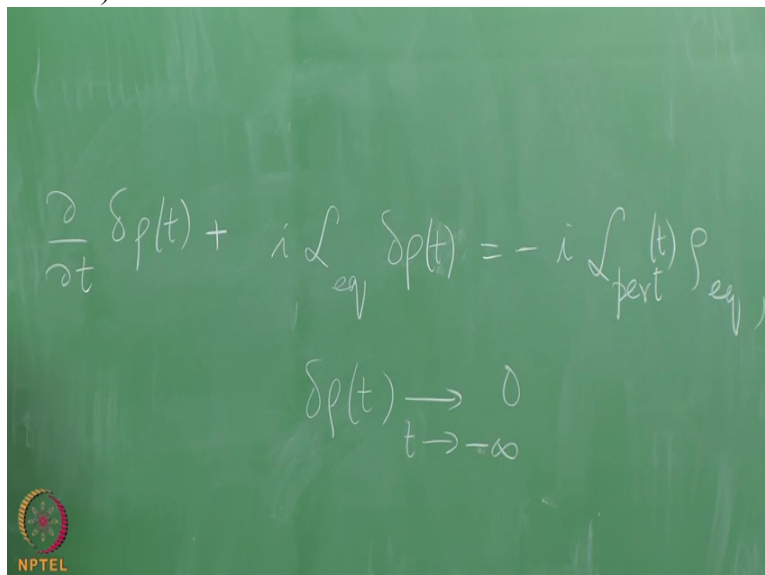


delta rho of t equal to, this is an inhomogeneous equation for delta rho, so the answer is a function, a particular integral plus a complementary function.

(Professor – student conversation ends)

But I am going to choose the complementary function such that delta rho is zero at t equal to minus infinity. That's the boundary condition. So delta rho is zero. Because at

(Refer Slide Time 18:27)



t equal to minus infinity the density operator was the equilibrium density operator. Therefore delta rho was identically zero. Together this now implies the solution, delta rho of t equal to only the comple/complementary only the particular integral, the complementary function has gone to zero by the boundary condition.

So it is an integral from minus infinity up to t dt prime times integrating factor, e to the p d x or whatever it is, the integrating factor here is e to the minus i L equilibrium of t minus t prime, times t minus t prime, sorry, so I better write it, not to avoid confusion, t minus t prime L equilibrium and that must act on this fellow. So it must act on minus i L perturbation and what time argument I must put in?

(Professor – student conversation starts)

Student: t prime 0:19:41.9

Professor: t prime, of t prime rho equilibrium, right?

(Refer Slide Time 19:54)

$$H(t) = At$$

$$\frac{d}{dt} \delta p(t) + i L_{eq} \delta p(t) = -i L_{pert}(t) \rho_{eq}$$

$$\delta p(t) \rightarrow 0 \quad t \rightarrow -\infty$$

$$\Rightarrow \delta p(t) = \int_{-\infty}^t dt' e^{-i(t-t')L_{eq}} (-i L_{pert}(t') \rho_{eq})$$

So notice exactly as we expected this portion involves the exponential of this Liouville operator. But the portion that involves the perturbation is linear, in this quantity as we expected; because we dropped this term. We dropped this term. Otherwise we would had to have exponentiate this term and since this is time dependent you cannot even write the solution that easily, you have to write a time ordered exponential or something.

So the formal expression is very complicated but to first order perturbation it is very simple. It is here. Now let us simplify that. So this gives you,

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$$\frac{\partial}{\partial t} \rho_p(t) + i \mathcal{L}_{eq} \rho_p(t) = -i \int_{pert} \rho_{eq}$$

$$\rho_p(t) \rightarrow 0 \quad t \rightarrow -\infty$$

$$\Rightarrow \rho_p(t) = \int_{-\infty}^t dt' e^{-i(t-t') \mathcal{L}_{eq}} (-i \int_{pert} \rho_{eq})$$

in the next stage, let us write down what this fellow is. Remember that \mathcal{L} , let me write this properly. Yes, remember that the Liouville operator acting on any function or operator was actually given by i times, remind me what it was here

Student: H with F 0:21:20.5

Professor: H with F or H with F divided by \hbar cross. That's what the Liouville operator did, Ok. The reason I am messing around is because this thing here is Hermitian.

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$$\mathcal{L} f = i \{H, f\}$$

$$\text{or}$$

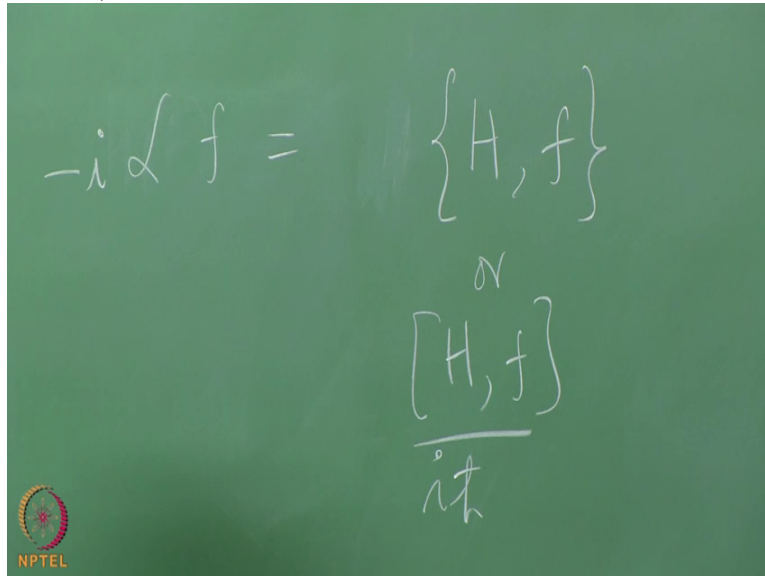
$$\frac{[H, f]}{\hbar}$$

So that is the reason I have to take out the i factor to make sure time development operator is unitary and it is nuisance keeping track of this i . So what does this become?

(Professor – student conversation ends)

Minus $i \mathcal{L} f$ becomes just this, do you agree? It becomes just this,

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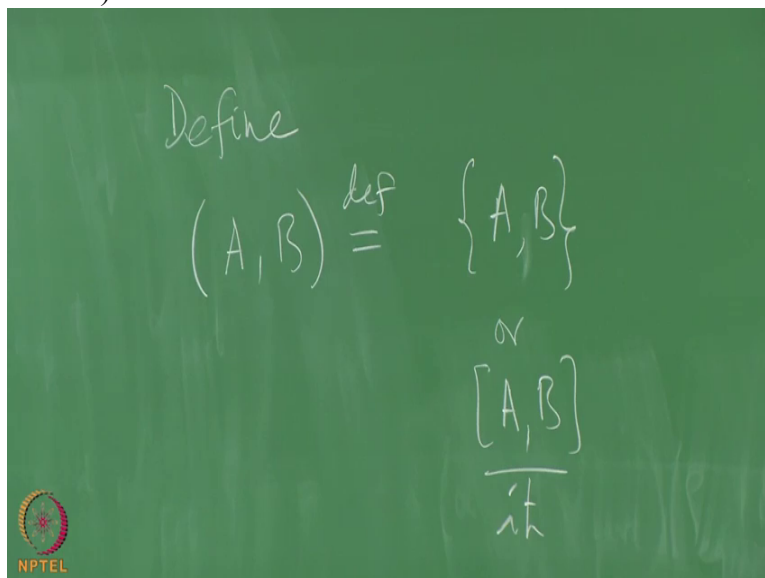

$$-i \mathcal{L} f = \{H, f\}$$

or

$$\frac{[H, f]}{i\hbar}$$

Ok. So let me define a bracket so that I stop carrying this symbol around all the time. So let's define, define the bracket of two quantities. Let us call it A and B to be by definition, equal to either the Poisson bracket or the commutator of A B over i h cross. Let me just use this round bracket as a symbol to

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Define

$$(A, B) \stackrel{def}{=} \{A, B\}$$

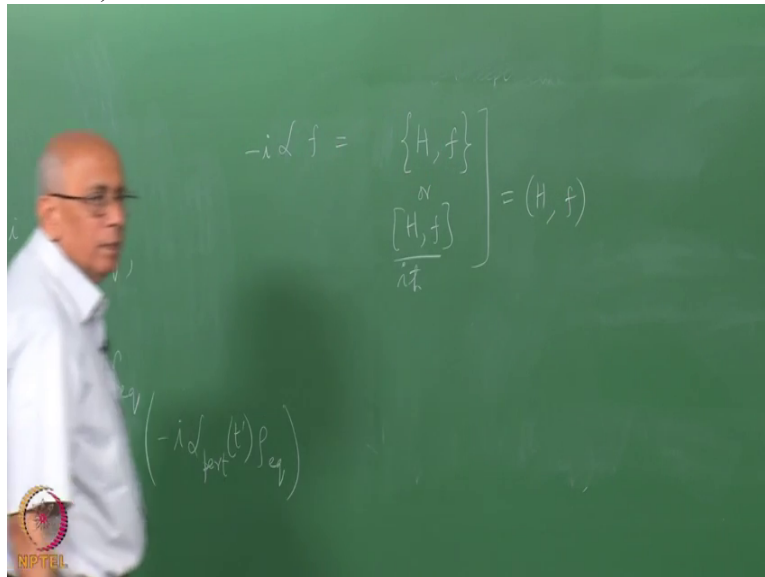
or

$$\frac{[A, B]}{i\hbar}$$

denote either the Poisson bracket or the quantum version of it which is the commutator divided by i h cross, Ok

So this L with minus i L f is H with f,

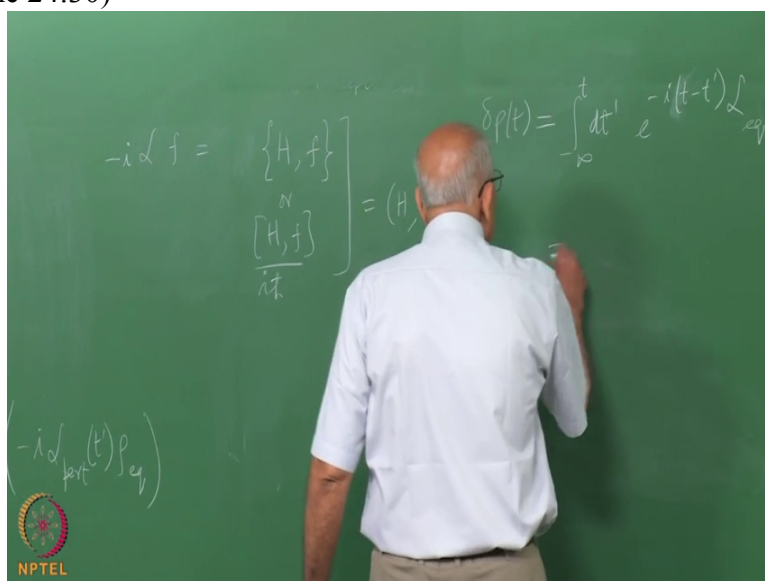
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right? So what happens here? Right, so let's write this out. So it says delta rho of t, just a bit of notation, I want to keep all the i factors right otherwise we run into trouble later on, so it is equal to this guy integral minus infinity to t d t prime e to the minus i t minus t prime L equilibrium times the bracket of minus i L perturbation times rho equilibrium and that is equal to H prime with whatever this is 0:24:01.0.

So this is the round bracket of H prime of t prime with rho equilibrium. Because that is my definition of this guy. For L perturbation, the Hamiltonian is H prime. So that's the 0:24:27.4. But we already know that

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this is equal to minus, integral minus infinity to t d t prime. Let us take out this guy, f of t prime because that is sitting here, the time dependence is in the scalar function, times e to the minus i L t minus t prime L equilibrium on A, the Schrodinger picture A rho equilibrium.

Now let us start, let me start inserting time arguments in this. This A that appeared in the Hamiltonian was in the Schrodinger picture, A at t equal to zero that is when

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$$\delta\rho(t) = \int_{-\infty}^t dt' e^{-i(t-t')L_{eq}} (H'(t'), \rho_{eq})$$

$$= - \int_{-\infty}^t dt' F(t') e^{-i(t-t')L_{eq}} (A(0), \rho_{eq})$$

I switched on the perturbation coupled to this dynamical variable here. So this is the formal expression, Ok but you could also write this as equal to minus integral minus infinity to t d t prime f of t prime.

Notice that all the operators are sitting here in the quantum case. In the classical case, the dynamical variables that evolved are sitting here. This quantity is the prescribed function. You have to tell me what is the time dependence of the force that you are applying, times e to the i t prime minus t L equilibrium acting on A of zero comma rho equilibrium.

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$$\begin{aligned} \delta p(t) &= \int_{-\infty}^t dt' e^{-i(t-t')} \mathcal{L}_{eq} (H'(t'), P_{eq}) \\ &= - \int_{-\infty}^t dt' F(t') e^{-i(t-t')} \mathcal{L}_{eq} (A(0), P_{eq}) \\ &= - \int_{-\infty}^t dt' F(t') e^{i(t-t')} \mathcal{L}_{eq} (A(0), P_{eq}) \end{aligned}$$

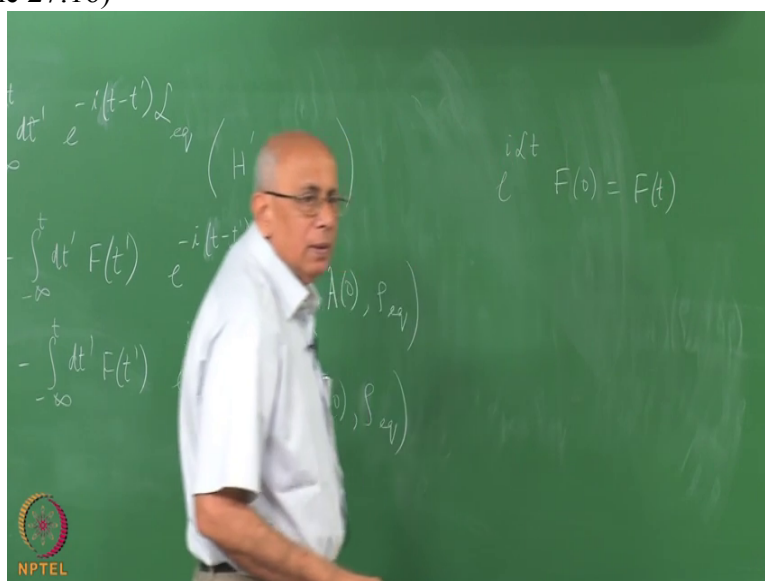
What should I do next? What should I do next? Pardon me?

(Professor – student conversation starts)

Student: 0:26:34.4

Professor: Well, do I have to expand it expon/exponentially? What is this acting on? What is this equilibrium going to act on? It is finally going to give some commutator, this fellow here is going to give some time dependence to quantities, will it change this at all? No. This is the argument that's going to change. This is the time argument. So what is e to the i L t on whatever is inside, on any F of zero equal to F of t,

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right? By definition. But now a subtlety, a little subtlety that arises; pardon me?

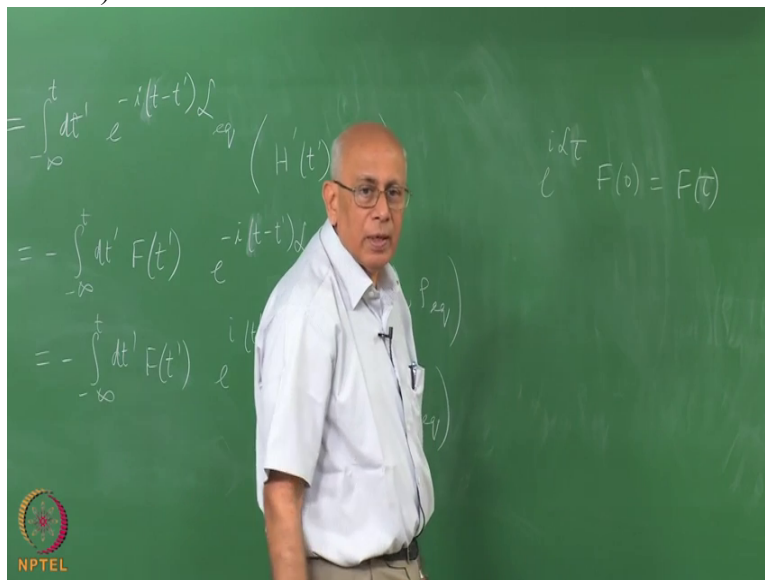
Student: 0:27:28.2

Professor: No, it is correct, it is correct. Because the

Student: 0:27:36.0

Professor: No, no, no. e to the i L remain neutral here. This is true for

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any operator right? Ok

Now what I have is L equilibrium. So this is the time dependence as per what Hamiltonian, H prime or H naught or the sum of the two?

Student: H naught

Professor: H naught, so really it is the Schrodinger picture operator which is going to the Heisenberg picture operator as governed by H naught. So the quantum way of writing it is easier. This thing here is equal to e to the power i H naught t over h cross F of zero tau e to the minus i H naught tau over h cross.

(Refer Slide Time 28:43)

$$F(0) = F(t)$$
$$= e^{iH_0 t} F(0) e^{-iH_0 t}$$

We know that the solution to the Heisenberg equation of motion for any operator in quantum mechanics governed by a time independent Hamiltonian H naught. So I have assumed that you already know that solution, Ok. Is everyone, does everyone feel comfortable with that or?

Student: interaction picture 0:29:04.7

Professor: Exactly, without saying so I am going to an interaction picture. I will explain in physical terms what this means. You see you switched on a perturbation. The Hamiltonian that you started with, H naught, you have added to it an H prime of t . If you did not have this, quantities will still evolve with time as governed by this Hamiltonian, by the unperturbed Hamiltonian. And we assumed that problem we can solve. Now we ask what happens if I switch on a time dependent perturbation to the Hamiltonian? Then it is convenient to do the following.

(Professor – student conversation ends)

When you are trying to find out the time dependence of physical quantities for the averages it is convenient to remove the known time dependence of those operators due to this part of the Hamiltonian. And then you ask what is the effect of the perturbation? It is like this.

Suppose you have a system which is static and then you set it rotating with some constant angular frequency. Then a convenient way of understanding the dynamics is to go to a co-rotating frame at which it appears to be at rest. And then if you perturb this system further there may be a little bit of jiggling etc etc and you can analyze that separately in the co-

rotating frame of reference. Once you have done that you can always go back to the original frame by undoing this rotation. Ok

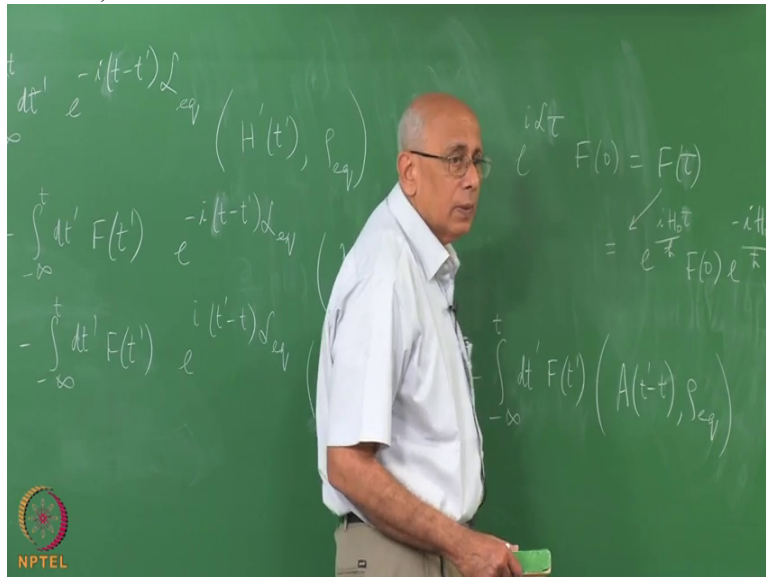
So this is what is the meaning of the interaction picture. When you have an interaction, when you have an interaction with an external force of this kind, then it is convenient to go to a frame of reference if you like, or a picture or a representation where the time dependence due to this routine evolution is already there, is known. It is like going to a rotating frame of reference, Ok and then you look at the perturbation alone.

So what I have been doing is to take these operators which are really in the so-called Schrodinger picture and then saying let us introduce a time dependence here defined in terms of L equilibrium here, Ok. So it stands for this. Whenever there is a time argument in any operator, it stands for this with H naught out here.

So with that understanding we can now write what this is. This will not be affected by this operator at all because you will have H naught and here you have $e^{-i H_{naught} t}$ and then $e^{-i H_{naught} \tau}$ and since H naught commutes with itself you can bring this across here and give it, gives you just $e^{-i H_{naught} t}$, right?

So the Hamiltonian itself will not change with time that is what it says when you go to the Heisenberg picture, right? So it doesn't act on this but it acts on this. Therefore you can write this as equal to minus and integral from minus infinity to t $d t'$ $F(t')$ bracket of $A(t' - t)$ equilibrium. You write in this form, where $A(t' - t)$, I mean precisely this;

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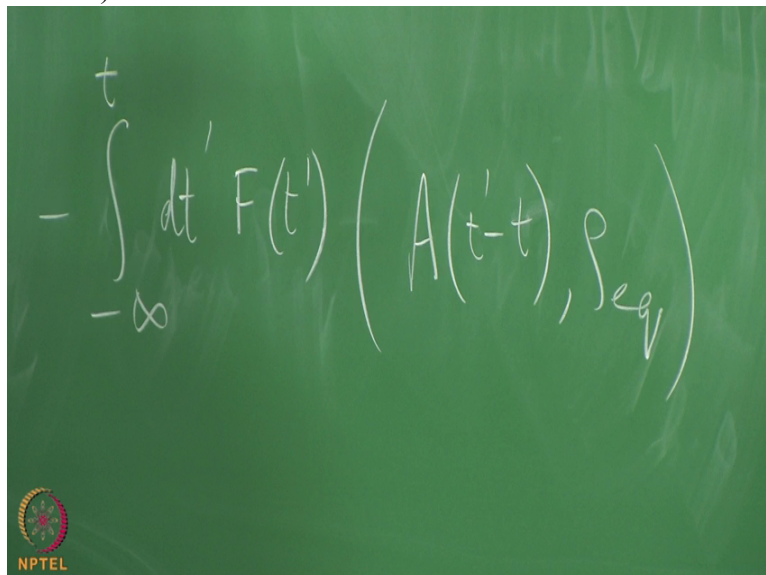
e to the i L tau, tau will be t prime minus t or whatever.

(Professor – student conversation starts)

Student: if the argument is not negative, right 0:33:16.9

Professor: t prime is always less than t. That's correct, that's correct, yeah. That's correct. We will see this explicitly, yeah. So this is t prime minus t, definitely. But it doesn't matter.

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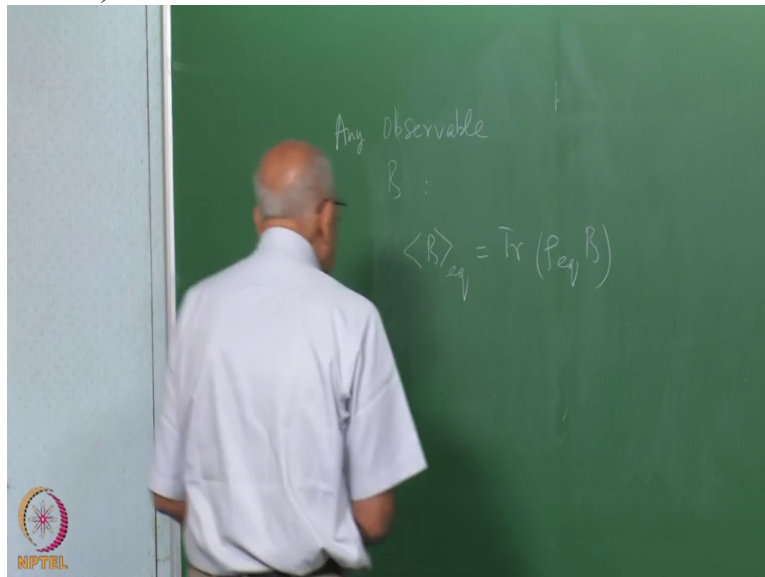
This argument, this formula is true whether tau is positive or negative, doesn't matter, Ok.

(Professor – student conversation ends)

Now let's go right back, that is delta rho of t. Now we want to know what is change in any physical observable. So if you give me an observable B, any observable B then B in equilibrium equal to trace rho equilibrium times t by definition because trace rho equilibrium is 1.

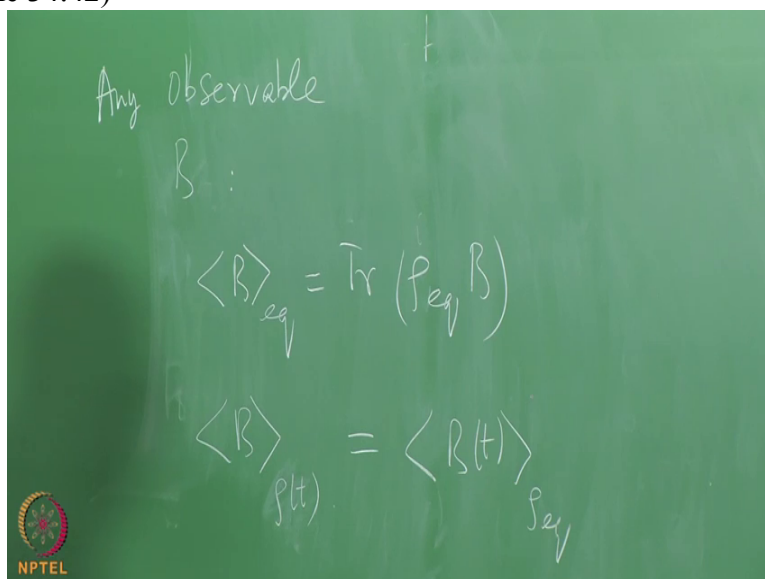
Now what is change in B in the presence of perturbation?

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So either I can compute B in terms of delta rho, sorry in terms of rho of t, this must be the same as B of t computed in rho equilibrium.

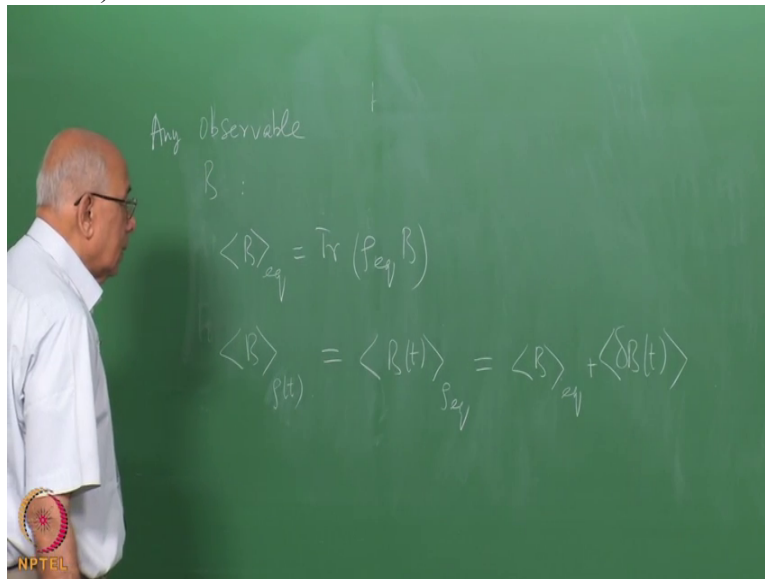
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Whether I put the burden of time dependence on the density operator or on the observable doesn't matter but I must do one of the two. I have just finished doing this because I have found what is delta rho.

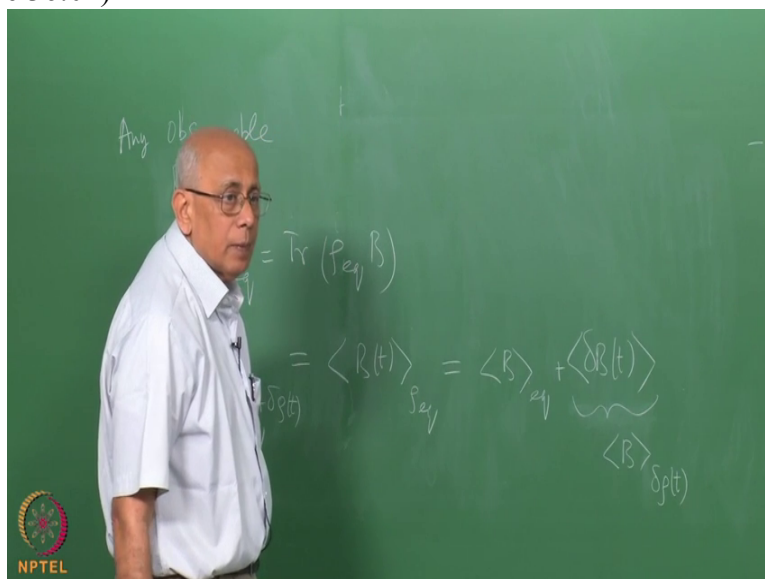
Because this quantity equal to B equilibrium plus delta B of t average value

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and it is this quantity that I have written, this thing here is what I have written by evaluating this in terms of, this is rho plus delta rho of t, Ok. B of t I have written, by definition equal to B plus delta B. But now the argument that I am making is that this quantity is the expectation value of B with respect to the change in the density matrix, the extra portion,

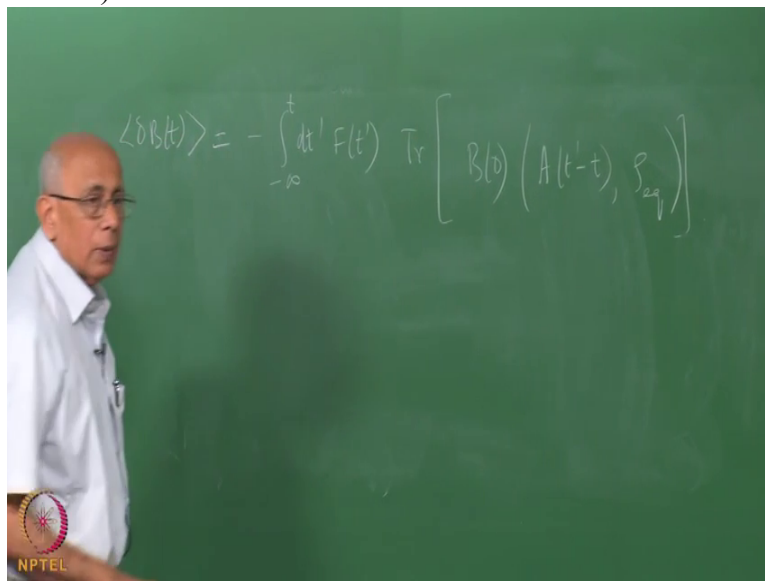
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by definition.

Because I don't know how to compute this, as so directly. So I chose to do this by changing, by finding the change in the density operator instead. So we are therefore home. All we have to do now is to say, Ok B average, therefore delta B of t equal to trace of B with respect to delta rho of t. This is all I have to do. But all these fellows come right through the trace so this is equal to minus, integral minus infinity to t dt prime F of t prime and then come the operator parts, so I have to take the trace of, of this quantity with respect to delta rho of t which is sitting here. So this is trace B of zero, is what that quantity is with respect to this guy here, A of t prime minus t rho equilibrium,

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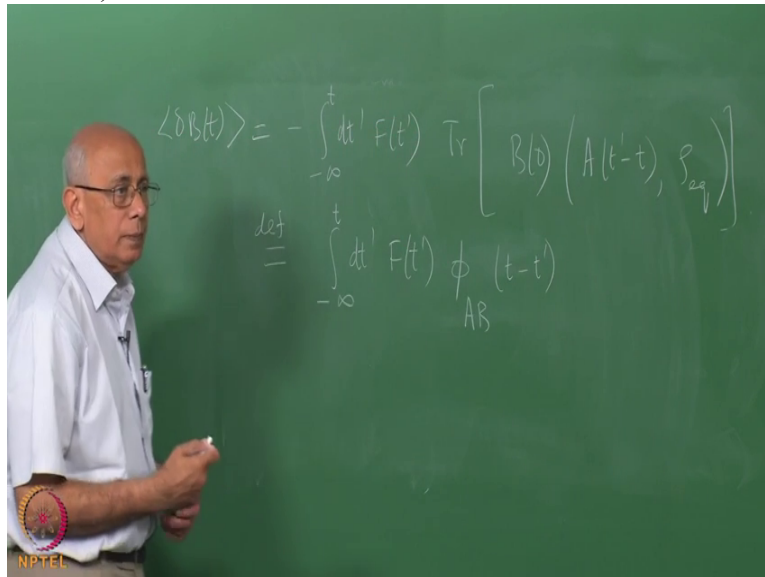
Ok?

If I write this by definition to be equal to the following physical quantity, minus infinity to t dt prime F of t prime times a portion which does not involve perturbation explicitly. This is found from the unperturbed Hamiltonian. This is found from the unperturbed Hamiltonian. This fellow is the original operator. That is weighted with this force.

So what we have is a situation where the change in the physical quantity at any time t, the first order change is an integral over all force histories from minus infinity to t gets cut off at t because of causality, the force at a time t prime greater than t cannot affect the response at the time earlier than t, right, at time t times a quantity which is completely independent of the perturbation itself, depends on A, depends on B and depends on the unperturbed Hamiltonian.

So let us call this phi A B of t minus t prime.

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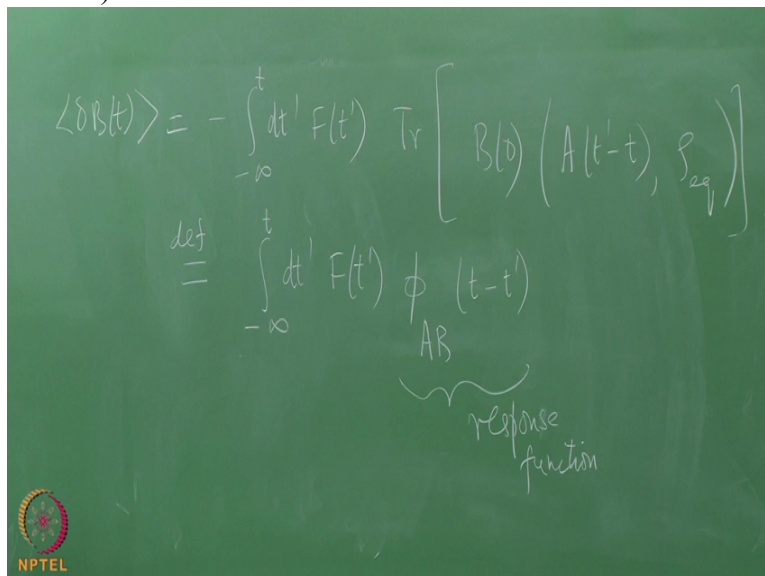
I have deliberately defined it as t minus t prime. Although what appears there is t prime minus t, doesn't matter, we will see in a minute, Ok. What would you call this function?

(Professor – student conversation starts)

Student: 0:39:40.5

Professor: Well it is some kind of response function of the way the variable B responds to the perturbation which involves the variable A. If A and B change to some other variables, you get a different response

(Refer Slide Time 40:06)



function. But the crucial thing, the important thing is that this fellow does not involve the perturbation at all. That's gone, that's here, first order and the perturbation and it is very physical now.

(Professor – student conversation ends)

It is a retarded response because if I can prove that this fellow is a function of t minus t prime then the response at time t depends on earlier force applied at any time t prime not dependent on t and t prime separately but how much time has elapsed between the cause and the effect. So it is retarded response to start with. It is linear response because it is first order in F . And it is causal because the effect gets cut off at time t , Ok. So we really have causal, linear, retarded response where this quantity is defined to be minus this guy here but now we have to write out what this is.

What is this response function? So let us write it,

(Refer Slide Time 41:24)

$$\langle \delta B(t) \rangle = - \int_{-\infty}^t dt' F(t') \text{Tr} \left[B(t) \left(A(t-t), \rho_{eq} \right) \right]$$

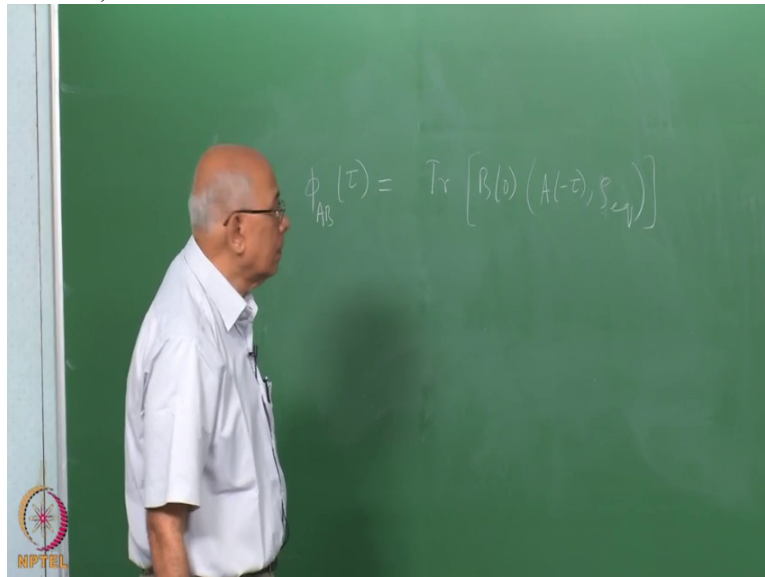
$$\stackrel{\text{def}}{=} \int_{-\infty}^t dt' F(t') \phi_{AB}(t-t)$$

response function

Causal, linear, retarded response

ϕ_{AB} of τ , let us put t minus t prime equal to τ , this here is trace B of zero A of minus τ rho equilibrium,

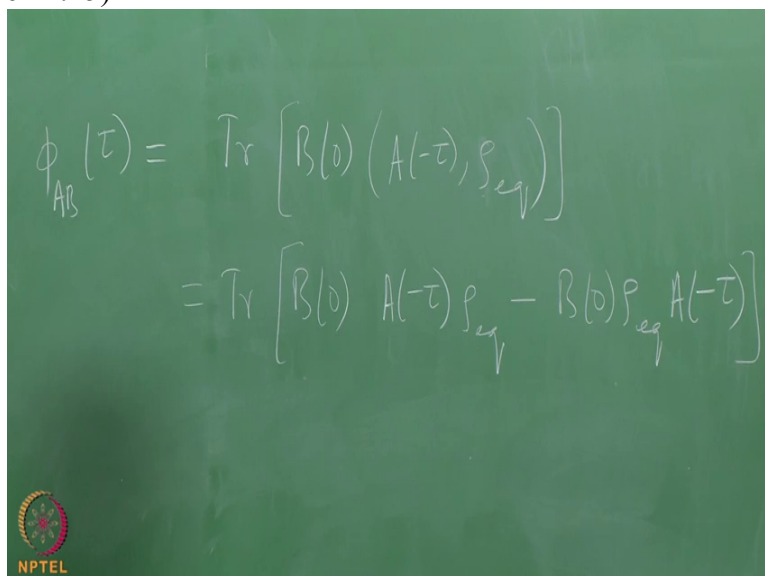
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Ok? You can rewrite it in many ways. So let us see first, or we should rewrite this in one particular way. This is equal to trace of zero. Let us do the quantum case because that is easier to write but it is exactly true in the classical case as well.

So this is A of minus tau rho equilibrium minus B of zero rho equilibrium A of minus tau. I have written out the commutator explicitly making sure that I don't take this B across because none of these fellows may commute with each other. So, especially in

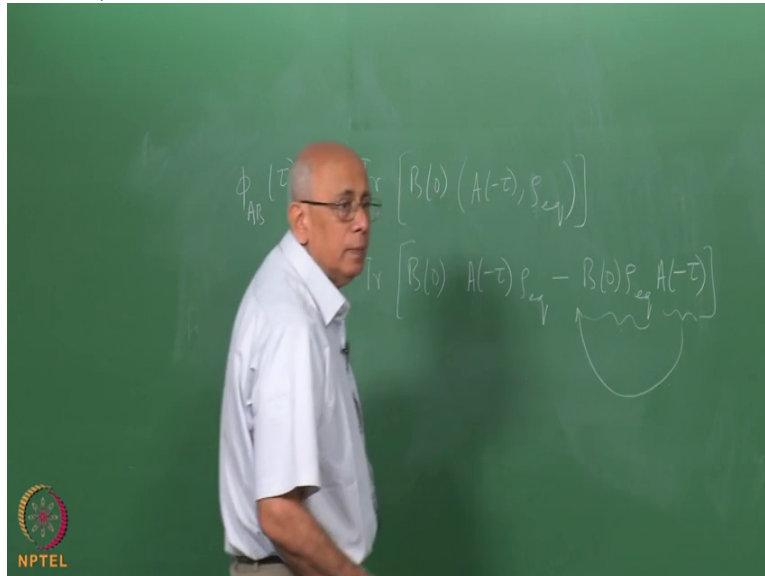
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quantum physics I have to be very careful about the order. Even in classical physics you know that the Poisson bracket of A with B is minus that of B with A. So I have got to be very careful with the order.

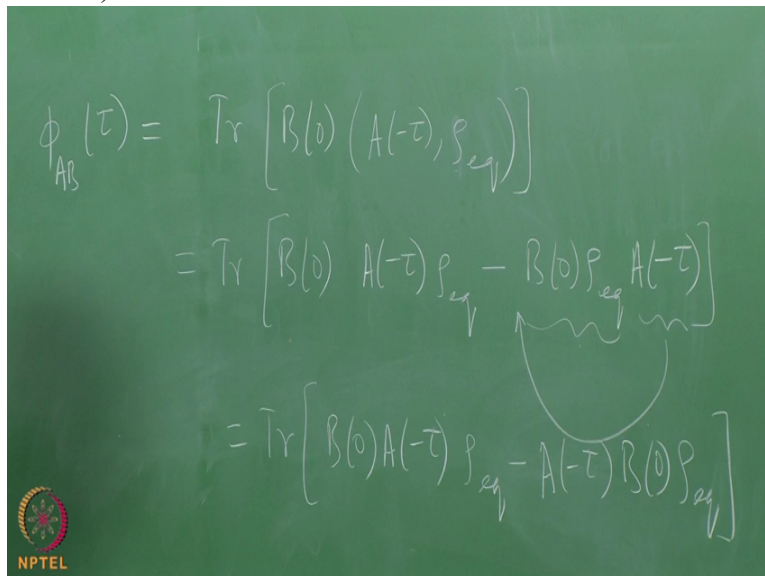
And now we use the cyclic property of the trace. So in this term I regard this as one unit and this as one unit and move this across here.

(Refer Slide Time 43:10)



So this is equal to trace B of zero A of minus tau rho equilibrium minus A of minus tau B of zero rho equilibrium.

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Trace A plus B is equal to trace A plus trace B of course. But I can take out the rho equilibrium common here and it is the commutator of B of zero with A of minus tau. So we have a very, very compact formula which says, uh, phi A B of tau is equal to the trace, the product of the commutator A of minus tau, uh there was a minus sign somewhere? There was minus

(Professor – student conversation starts)

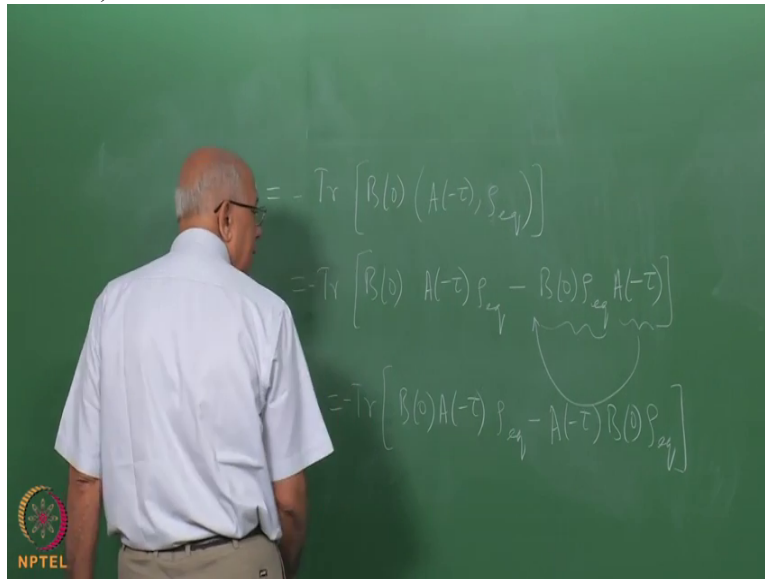
Student: Minus 0:44:18.2

Professor: There was minus here.

Student: Minus 0:44:19.1

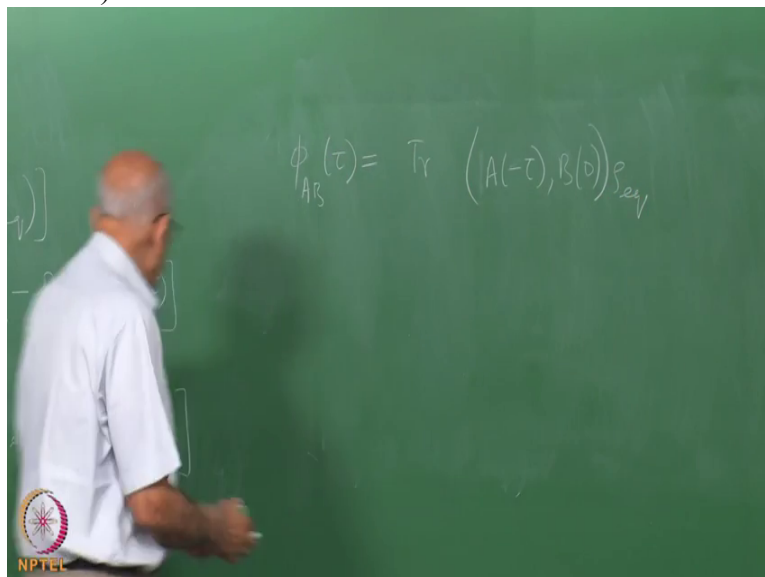
Professor: There is a minus here, right so this trace is, this is a minus, minus, minus

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everywhere, so this is equal to trace, the inner pro/product, Poisson bracket of A of minus tau with B of zero rho equilibrium with a plus sign because

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I inverted this. It became minus here and plus here. So it is the Poisson bracket or commutator of A of minus tau with B of zero. But what is this?

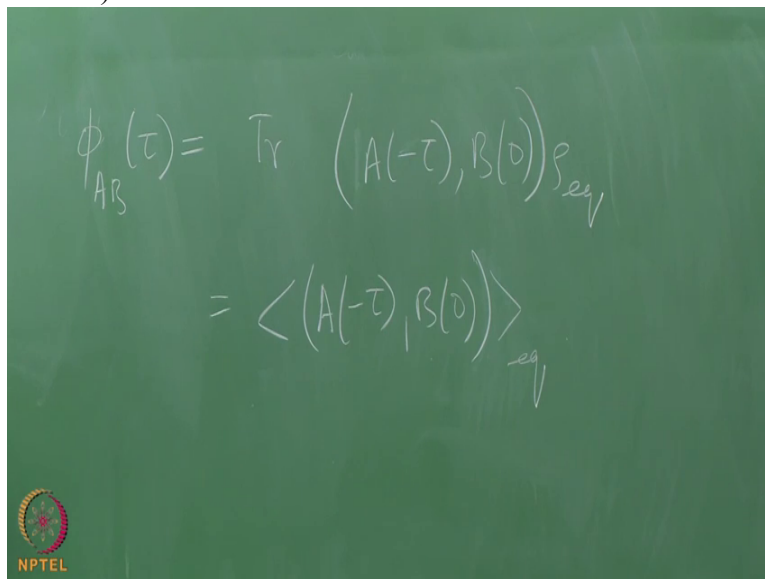
Student: 0:45:06.4

Professor: Trace of something times rho equilibrium

Student: It is the average 0:45:10.8

Professor: It is therefore the equilibrium average of this quantity, right? So this stands for, this is by definition equal to A of minus tau B of zero, the Poisson bracket or commutator bracket in equilibrium. So it is a remarkable statement.

(Refer Slide Time 45:37)


$$\phi_{AB}(\tau) = \text{Tr} (A(-\tau), B(0)) \rho_{eq}$$
$$= \langle (A(-\tau), B(0)) \rangle_{eq}$$

It says the response to an applied force is dependent; the response function which characterizes the response to an applied force is dependent only on the equilibrium average, thermal equilibrium average of this commutator bracket, Ok.

(Professor – student conversation ends)

The elapsed time is appearing here and now in some sense, you can see that while computing the average of the quantity B what is appearing here on this side is the average in equilibrium of the correlation of B with A in some sense, anti-symmetrised suitably to get you this Poisson bracket or commutator.

So this is the remarkable thing of causal linear retarded response that we will see the fluctuations govern this quantity. Because we are taking an average, average over what? Over thermal fluctuations in equilibrium. So the, it says the fluctuations are governing the behavior of the average. Fluctuations in equilibrium govern the behavior of the average away from equilibrium in the presence of the perturbation. So it is a profound statement.

It looks like a very simple derivation, but it is a, it is. It is first order perturbation theory plus statistical physics, that's all we have done but it is already a very, very deep statement here. But you can write this in other ways. You can also write this as equal to, you take this sequence, equal to trace A of minus tau B of zero, rho equilibrium is e to the minus whatever it is, so this is rho equilibrium minus B of zero A of minus tau rho equilibrium, trace of this fellow. Now write this fellow here

(Professor – student conversation starts)

Student: 0:47:52.5

Professor: Yes, it is true, classical and quantum

Student: Yeah what is the meaning of 0:48:01.1 Poisson bracket

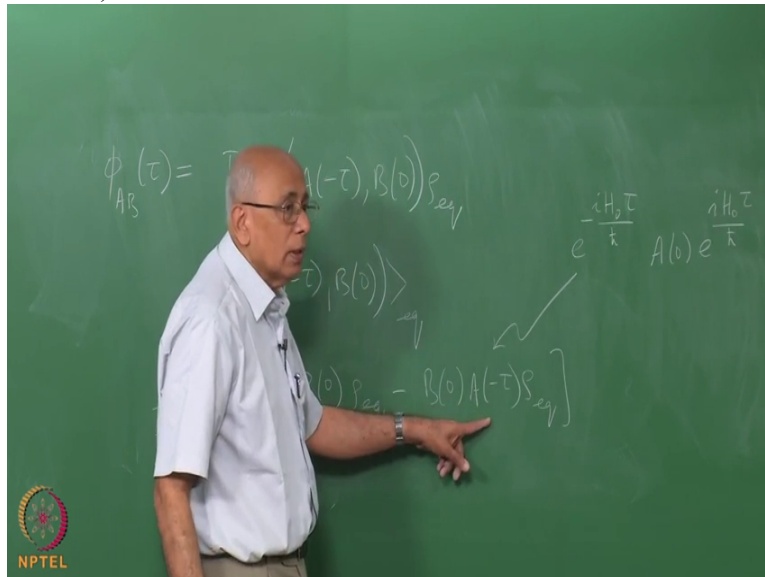
Professor: Yeah that's a Poisson bracket. I am doing only the quantum case here so that it is easier to understand. Otherwise I have to do classically; you have to do integration by parts etc. It is much messier notation. So all the while I am saying that we do the quantum case and then I let Planck's constant go to zero, things will go to Poisson's bracket etc.

It is the π/\hbar , just as we showed that L was a Hermitian operator in quantum mechanics it was trivial, in classical physics it was a little harder to show. The same thing is true here. I just want to show here what this will become. Now what you have to write, this fellow you write as e to the

Student: 0:48:44.3 divide by $i \hbar$ bar.

Professor: Yes, you have to divide by $i \hbar$ bar, yes definitely. Yeah so this is e to the power $i H$ naught tau over \hbar cross with a minus sign A of zero e to the minus $i H$ naught tau over \hbar cross with the plus sign on the right hand side, this fellow here.

(Refer Slide Time 49:14)



You put that in here and use the fact that this is a function only of H naught. Then you can move this factor out to the right hand side because it commutes and then by cyclic invariance you bring to the left hand side here where it will hit this B so you will have e to the $i H$ naught τ by \hbar cross B of zero e to the minus $i H$ naught t τ over \hbar cross times A of zero. So it will transfer the time argument to this quantity and ditto here.

Student: 0:49:51.4 Can't we use 0:49:51.8 invariance

Professor: I don't know that yet.

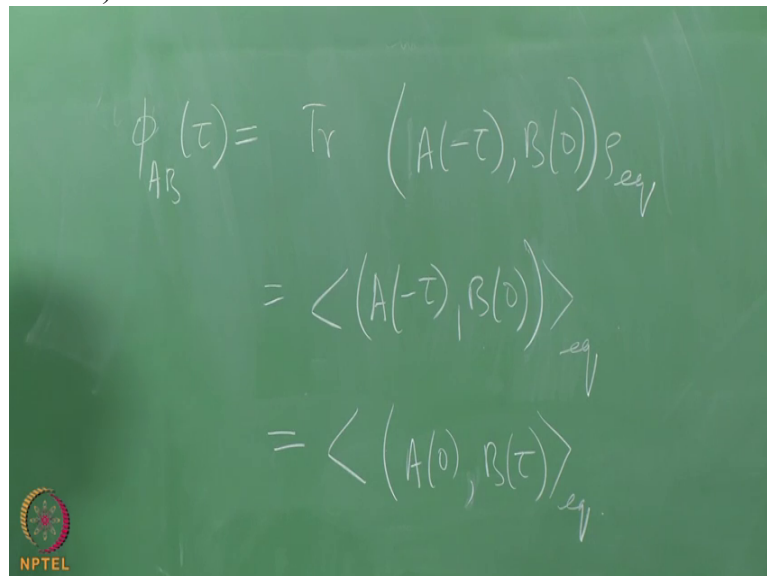
Student: 0:49:54.0 Because you already said that H naught is time independent.

Professor: H naught is time independent. But I don't know what these quantities will do. Yeah you are right. Finally it arises from the fact that H naught is time independent and therefore these correlations will all become stationary. They will become independent of the time argument but this is an explicit demonstration of that.

(Professor – student conversation ends)

So this quantity here, and I will stop with this, this is also equal to expectation value of A of zero B of τ in equilibrium,

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$$\begin{aligned}\phi_{AB}(\tau) &= \text{Tr} \left((A(-\tau), B(0)) \rho_{eq} \right) \\ &= \langle (A(-\tau), B(0)) \rangle_{eq} \\ &= \langle (A(0), B(\tau)) \rangle_{eq}\end{aligned}$$

The image shows a green chalkboard with three lines of handwritten white text. The first line is $\phi_{AB}(\tau) = \text{Tr} \left((A(-\tau), B(0)) \rho_{eq} \right)$. The second line is $= \langle (A(-\tau), B(0)) \rangle_{eq}$. The third line is $= \langle (A(0), B(\tau)) \rangle_{eq}$. In the bottom left corner of the chalkboard, there is a small circular logo with the text 'NPTEL' below it.

Ok which is a little more physical to understand because this says, whatever tau appears here is due to the unperturbed Hamiltonian and its correlation with the original Schrodinger operator A is what is giving you, in thermal equilibrium, is what is giving you the response function, Ok. So we will start at this point next time, Ok.