Non Equilibrium Statistical Mechanics
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Lecture 15
Linear response (part 9)

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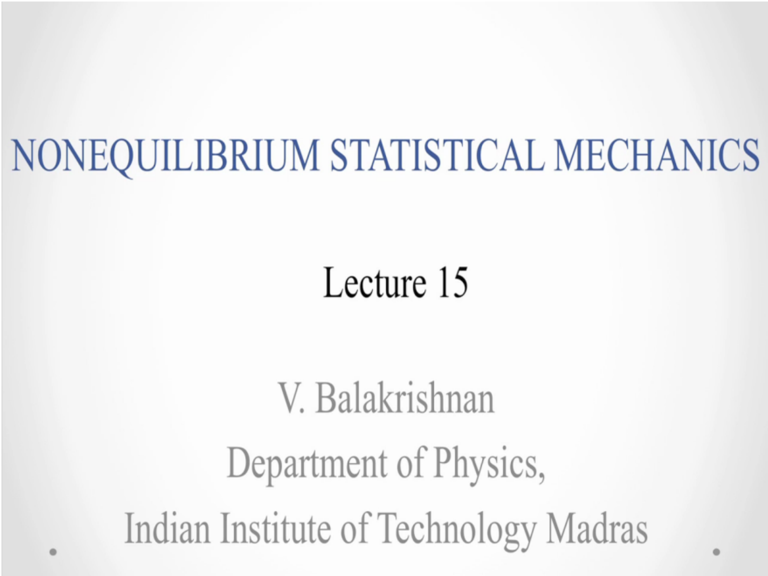

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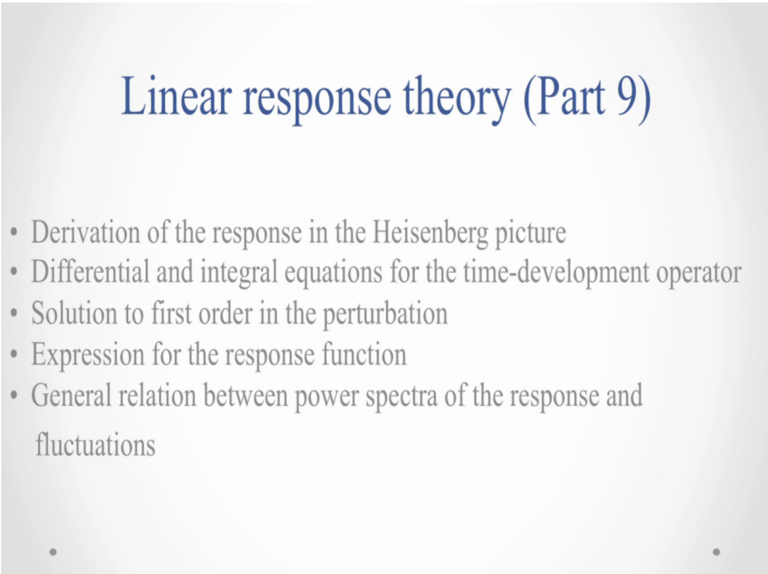

Right, so we have been looking at linear response theory from a specific point of view namely we decided to calculate corrections due to a small applied time-dependent perturbation to the Hamiltonian. We calculated corrections to physical quantities like the some arbitrary quantity B by computing things in terms of the change in the density matrix.

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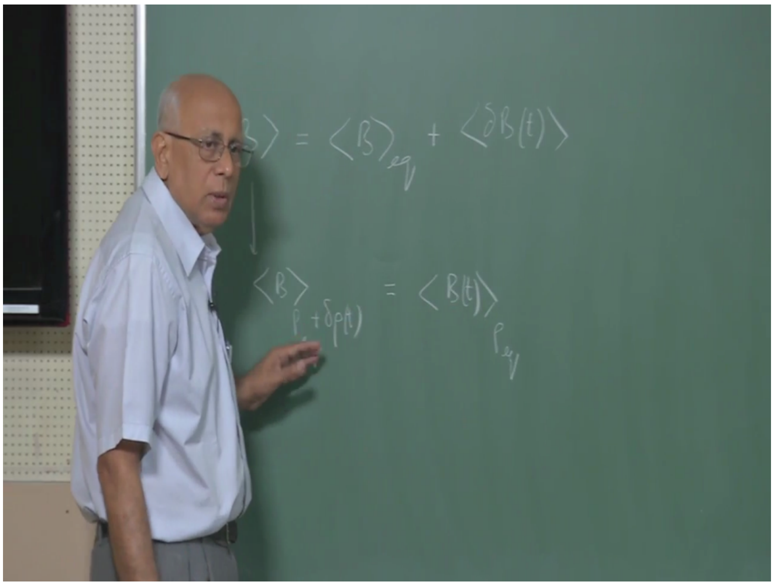

In other words if you recall what we did was to say that we start with some B and expectation value of this B was equal to B equilibrium plus a time-dependent part which we call Delta B and that would of course Bt and we computed averages and the statement was that this to first order in the applied force was computed by computing first the change in the density operator.

So in other words we use the fact that this was B with respect to rho equilibrium plus Delta rho of t and we know B rho equilibrium was the equilibrium value time independent and then we computed this using the (()) (1:38) to first order etc but you could equally, well, I have done this by working in a more active picture. In other words by working in terms of B of t itself in terms of rho equilibrium.

So this is, this means you would go to Heisenberg picture with the full time-dependent Hamiltonian, correct the first order in it and then compute averages with respect to rho equilibrium. We did not explicitly do this; we use this all this time. So what I would like to do is to make contact with what you would be more familiar with in the context of normal quantum mechanics and then we will put in the thermal fluctuations in average over things etc.

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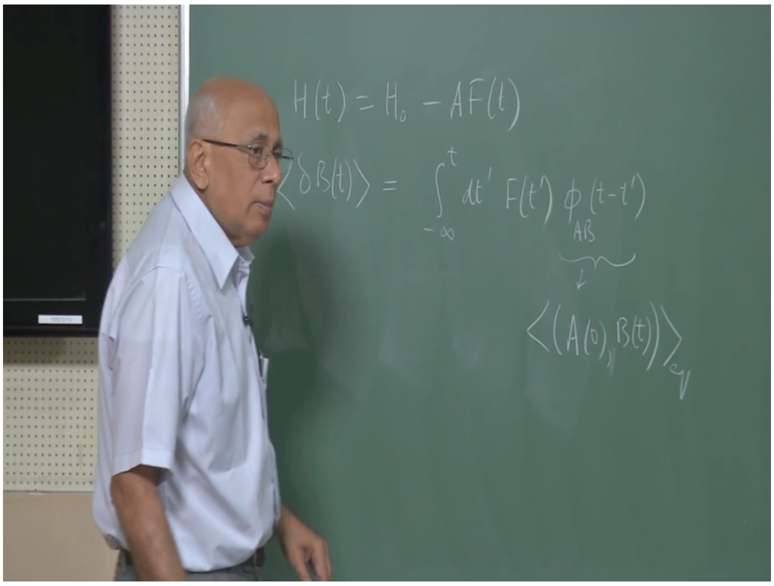

We know the answer already; we know the answer is given the Hamiltonian H of t equal to H not minus AF of t, we know that the change delta B of t on the average this is equal to an integral from whenever you switch on the force which we took to be minus infinity in the most general case up to t dt prime F of t prime multiplied by the operator part of it and the operator part of it was this response function phi AB of t minus t prime that was the result that we got.

And for these we (()) (3:07) the formulas among others for instance we discovered that this could be written as A of 0, B of t in the Heisenberg picture induced by the time independent part of the Hamiltonian trace with respect to the equilibrium density operator. So we had a formula like this and this we further simplified in the classical case in the quantum case and so on and so forth.

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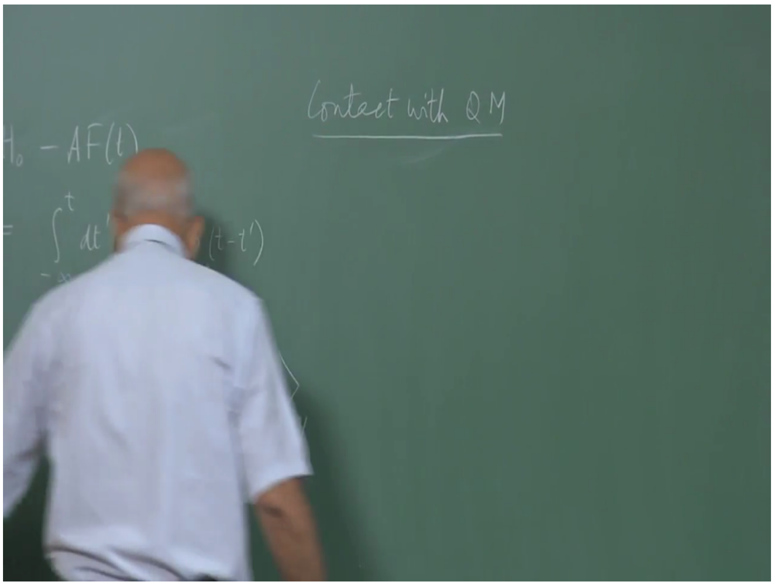

What I would like to do is to now establish contact with the usual way of doing 1 mechanics; we will do this in the Heisenberg picture just to clarify to you what we mean by going to the Heisenberg picture and so on. So it will become explicit in what I am going to do, so let me call this contact with quantum mechanics that the usual perturbation theory formula in quantum mechanics.

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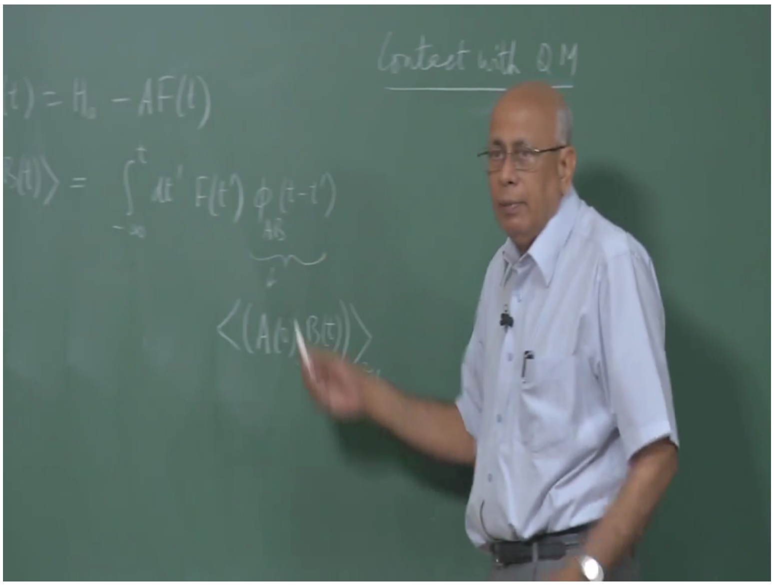

So I repeat we are just going to do something which will explicitly tell you how the commutator (()) (4:14) goes out here for this phi and we will re-derive this formula from a slightly different viewpoint, okay. This will make it go through more familiar ground and so that will you will operate itself.

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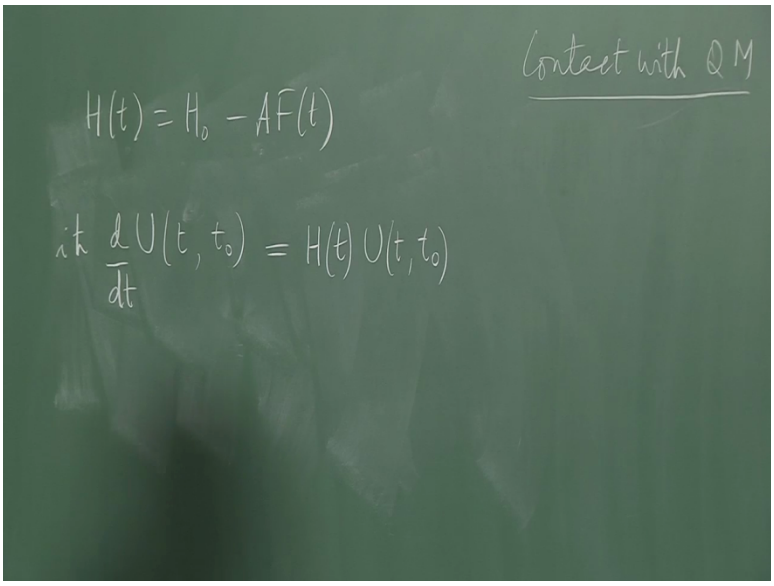

So again I start with this and when you do not put any subscript on any Hamiltonian it supposed to be in the shorting that picture, so this is a time independent. There is no explicit time dependence in this operator, it is physically observable and we will take this to be the physical case A is a hermitian operator, okay. So the Hamiltonian is a hermitian Hamiltonian.

If it is not I have the problem of writing this plus its conjugate (()) (4:58) to make the Hamiltonian hermitian but for simply city of notation we will take this to be hermitian operator here and the Hamiltonian to be hermitian, We will also take this to be real, so that the hermiticity of the Hamiltonian is ensured, right. Then we want to compute what the full system does?

And what would you normally do? You would say whatever state you start with, if you are starting with a state for example of the system then the shorting of equation would apply to the way that state evolves in time. So formally one can write down shorting of equation for the evolution of the state. Now it is convenient to introduce a time development operator U which is levelled by 2 time indices t and an initial time t not.

So I am going to take general initial time t not whatever be that etc. In general I take t not to be (()) (5:57) on the force and we will set it equal to minus infinity eventually but I want to make sure that we have general formalism in other cases where you switch it on at finite times and so on. So let us start with t t not, this takes you from the state of the system at t not to the state of the system at time t.

And it satisfies of course the equation d over dt equal to H in this case it is time-dependent U of t, t not, okay. So this is the equation satisfied by the time development operator U, okay. Because this is a hermitian Hamiltonian we know that this time development operator must be unitary operator, so that probability is conserved and so on, that is all we know about it to start with.

You also have a boundary condition on this operator which we will write down subsequently little later, okay. Now I repeat again there is the explicit time dependency here, so if you did not have this then the problem is utterly trivial completely trivial then the solution to this is with time-dependent Hamiltonian is just the exponential of this Hamiltonian multiplied by time, right?

But the question is, what is it with the time dependence present here? And we have to be careful because there is no guarantee that H at time t commutes with H at any other time, 2 operators at different (()) (7:36) need not commute, the same operator different instance of time did not commute at all because the Hamiltonian gets in between if you like. So what would one do? One would like to find a solution to this but first let see what happens in the absence of this fellow here.

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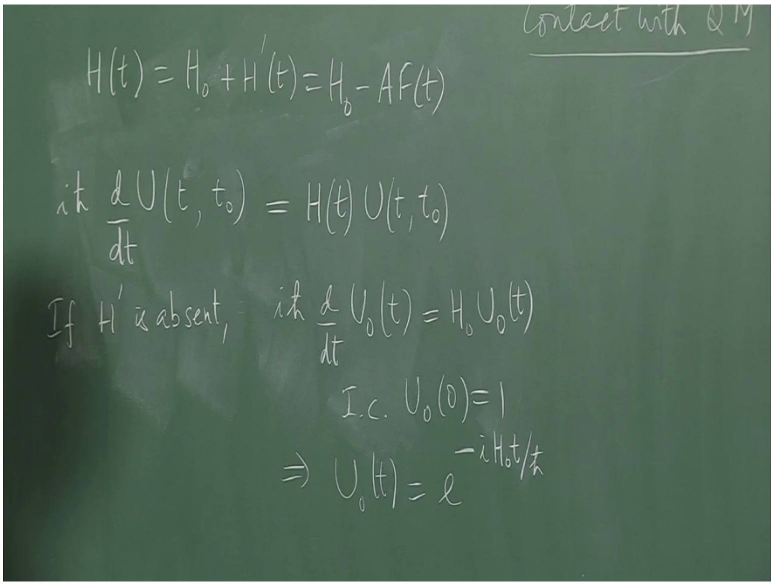

So if H prime, so this is what I call at H not plus H prime of t, if H prime is absent, then of course you have a time development operator d over dt and let us call that U not, the time development operator in the absence of h prime, okay the unperturbed problem and what would you do there? You would say this is t, let us take the initial time here there is no switching on force or anything like that.

So I will say that t equal to 0, the system is given to you and then I will look at it at any later time just to one Time argument over here, this is equal to H not U not of t, with the initial condition U not of 0 equal to1, okay. And then the solution implies U not of t equal to e to the there is H not divided by H cross, so it is e to the power minus i H not t over h cross t times U not of 0 which is 1, okay.

So that is a very trivial problem to do this, once you have this then I can go back and ask what is this look like the solution to this equation look like? But first let me define the Heisenberg picture for you.

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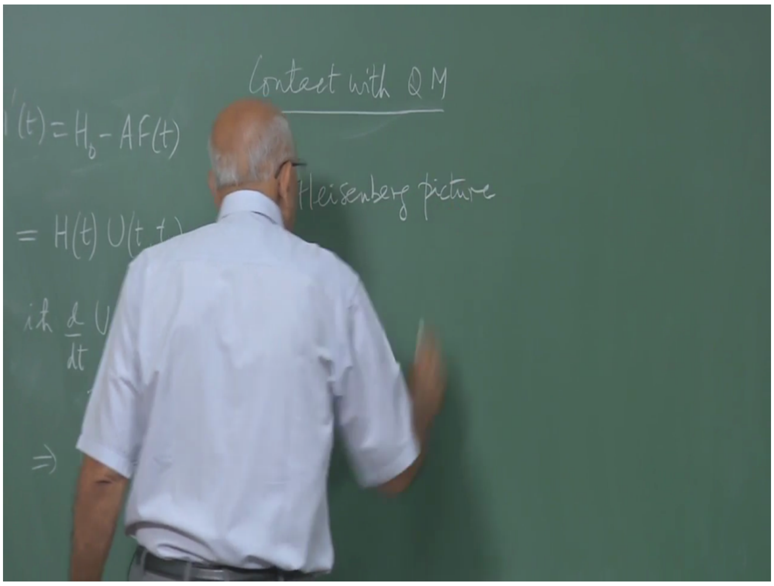

So the Heisenberg picture we are talking about is a transformation from the Schrodinger of picture to a time system which has time-dependence operators, the time dependence comes from H not alone as I have been saying.

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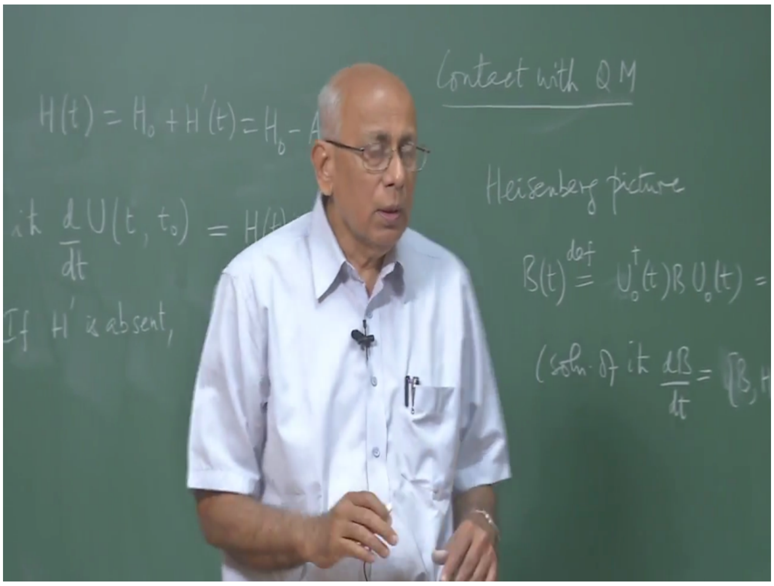

So any operator B now becomes time-dependent this is defined as e to the power as U not dagger of t B U not of t this is the definition or if you like I write a Heisenberg equation of (()) (10:33) this is solution of ih cross dB over dt is equal to B, H not that is a Heisenberg equation of motion, I solve this and I get this out here, okay. And this is equal to e to the power i H not t over h cross B e to the minus i H not t over h cross.

So if I write an operator without any Time argument at all by that I we mean the Schrodinger picture operator which coincides with the Heisenberg picture operator at t equal to 0, is that clear completely? So B of…

“Professor -Student conversation starts”

Student: We are doing the case where H prime is 0.

Professor: Yes, we are still doing the case where H prime is 0, okay. Because we are going to switch on H prime and I am still going to do this first and after that take care of H prime separately, okay. You will see as we go along what that end tells, okay.

“Professor-Student conversation ends”

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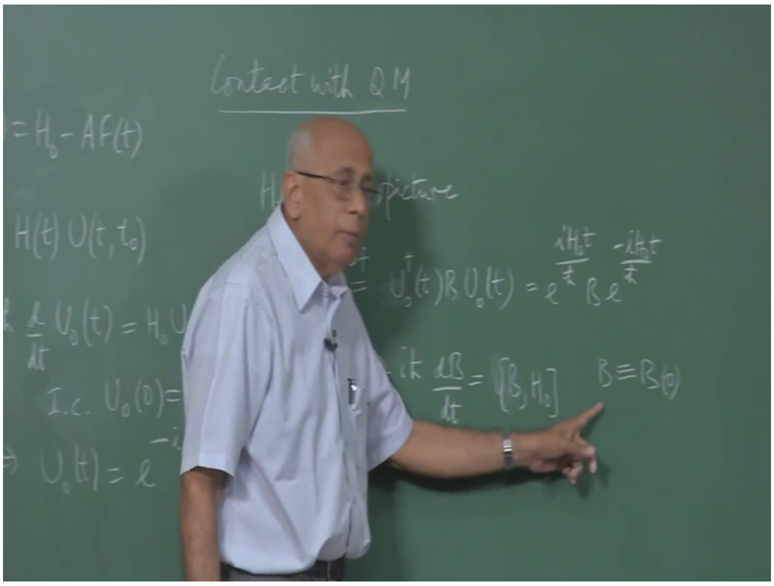

So we are still doing this and we are always going to continue to define a time dependence of an operator like B via this but of course once I switch this on.

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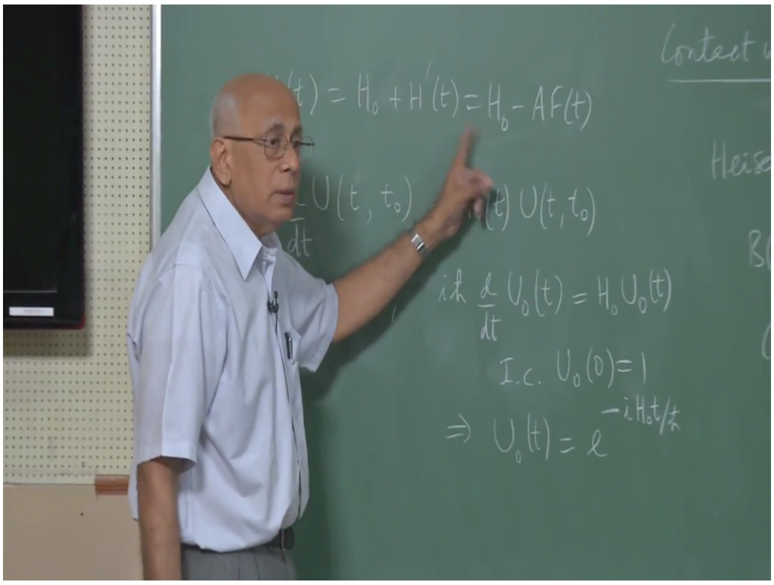

Once this is switched on, then there could be a time dependence in the operator coming from the fact that were in the time development operator is U and not U not I have to take that into account and I would like to do it to first order in F. So that is the problem really, no, of course you can also ask what is the general solution to this for an arbitrary H of t to all orders arbitrary H of t.

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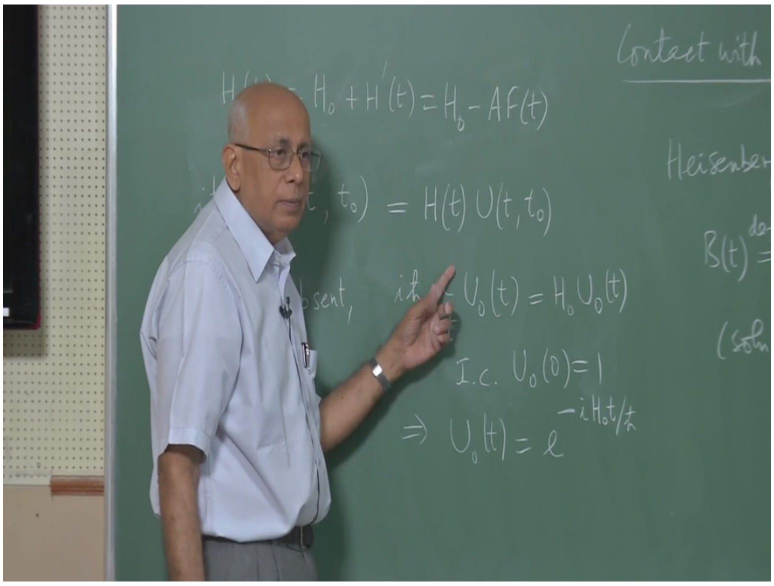

It is not an exponential because this fellow is explicitly time-dependent, you cannot trivially do that you need an integrating factor as you know.

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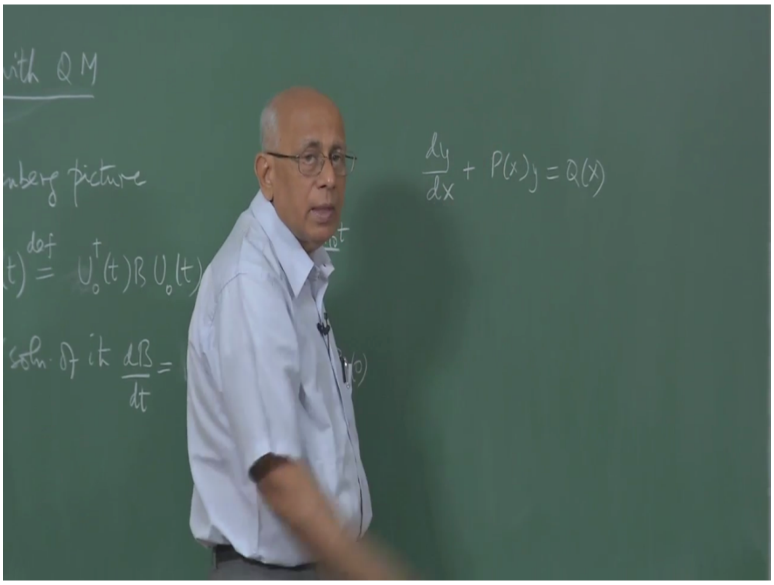

And even classically an even without operators along the line when you have a thing like dy over dx plus P of x y equal to Q of x if this were a constant this would be a trivial problem but if this were a function then of course you have an integrating factor to take into account, we have to do an definite integral of some kind, put correct boundary conditions and things like that.

Now it becomes much harder than the case of an operator because of this commutativity problem. You have a formal solution available it is called a disen time ordered exponential but we are not interested in that here, we are interested in things to first order in F, okay. So let us see what to do.

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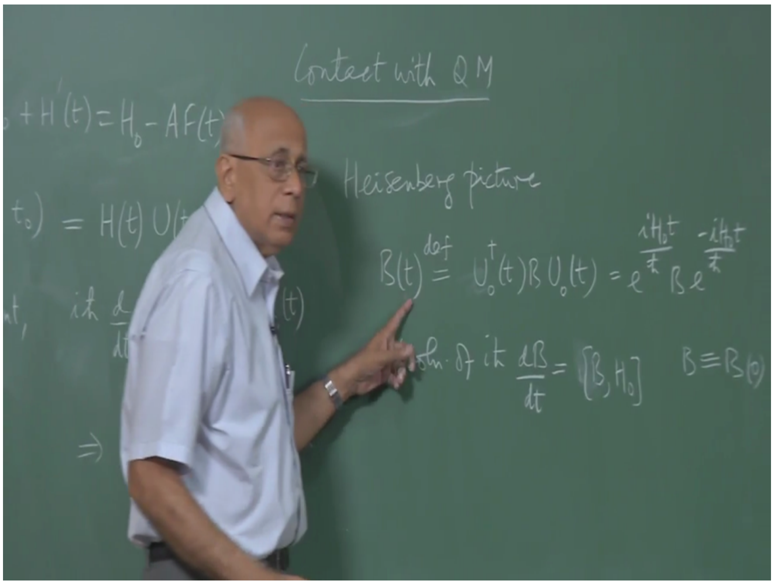

So is this clear, whenever I write this.

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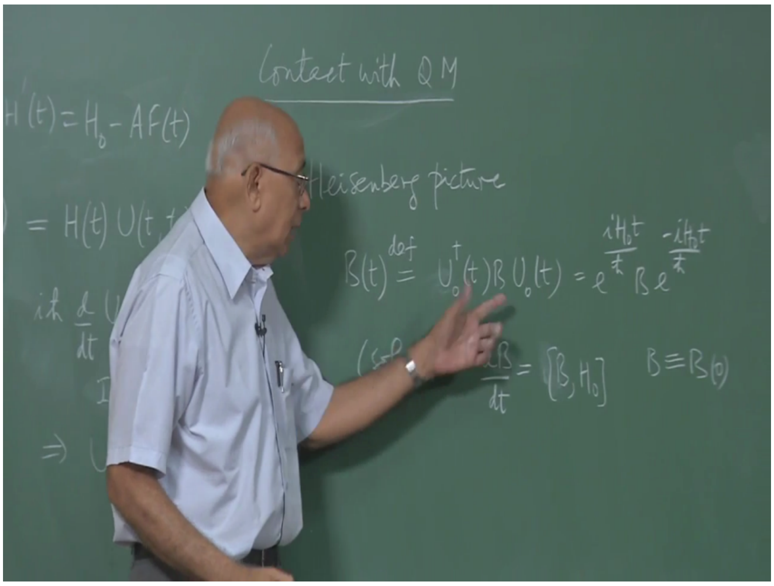

I mean this always and we will use that notation, okay. Of course when you switch this on B has time dependence because of this 2, this portion 2 I call that B total of t, the total time dependence if you like for lack of button notation.

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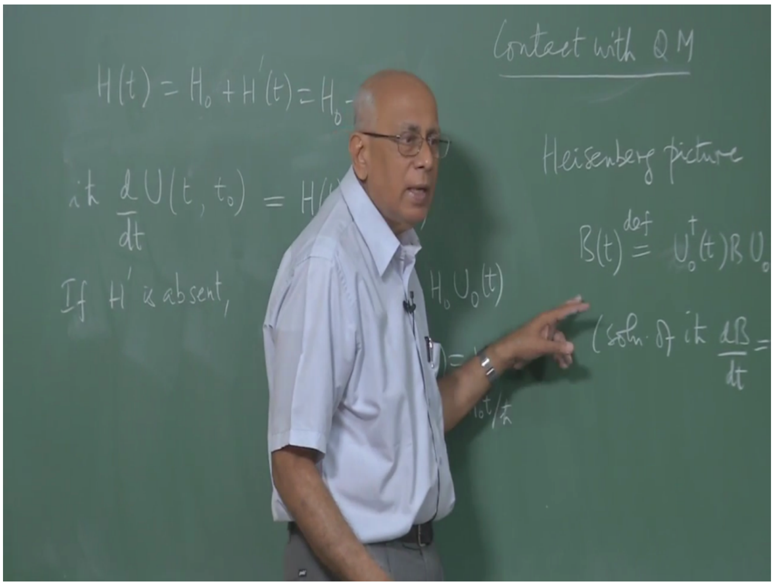

But I would like to retain B of t for this guy here, okay. And notice that they are not early derivations and linear response theory all the arguments of the function of the various operators refer to this kind of ring.

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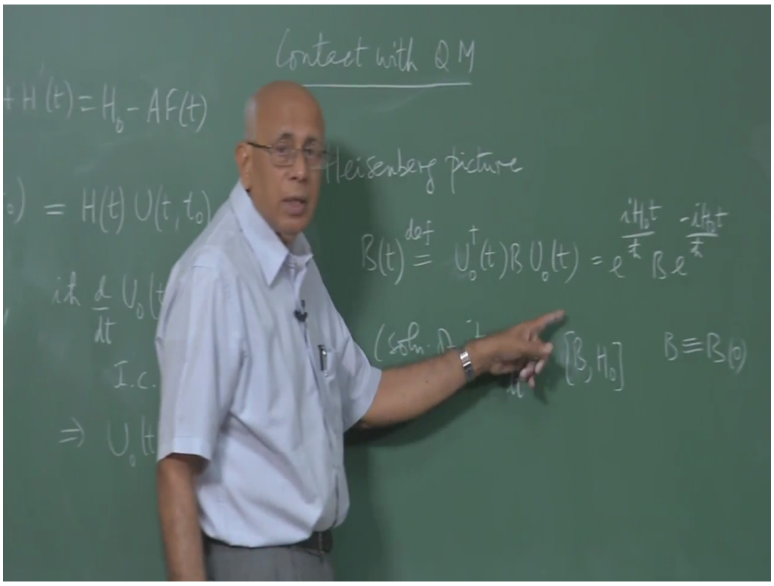

They all refer to this with an H not alone but I am now making this thing explicit here. You could ask what sort of picture is this where I take the time dependence of the operator to come from the unperturbed Hamiltonian but then I am including the interaction in some way, it is called the interaction picture, okay. But I am trying to do this without using that terminology but it will become obvious because I need only first-order, okay.

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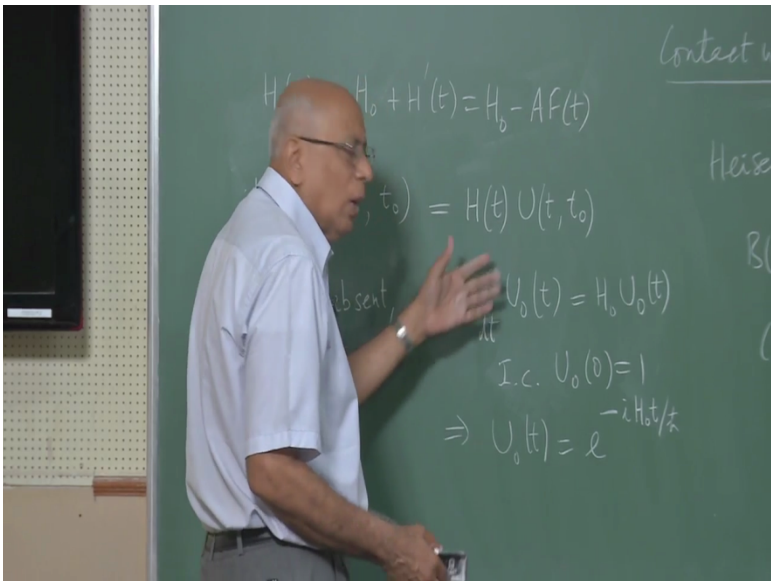

Now what should I do for this, I have to now do with this full problem.

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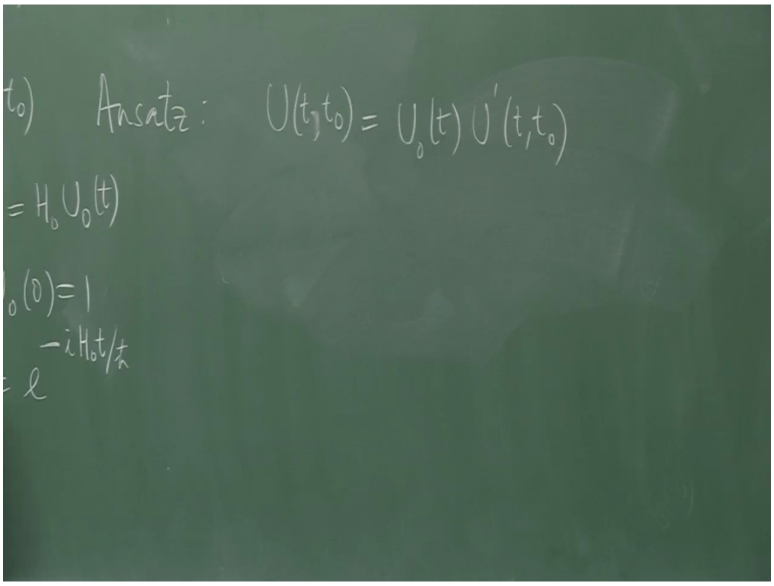

So let us use an Ansatz or trial solution and that would be, let us put U of t, t not to be equal to U not of t saying that this fellow will go on revolving due to H not all the times multiplied by U prime of t and t not that is a trial solution it may work it may not work we will see what happens, we know this, we know this function.

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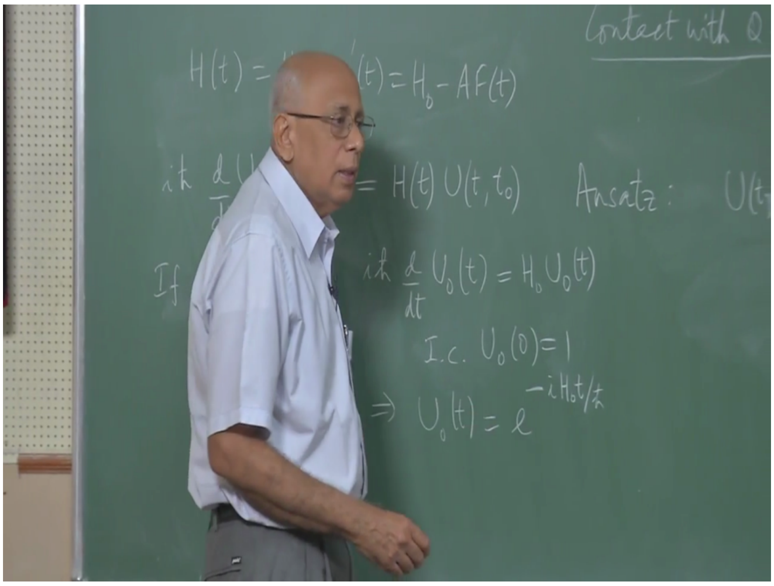

We know U not of t is this guy here explicitly. We need to put an equation for U prime, so what happens now?

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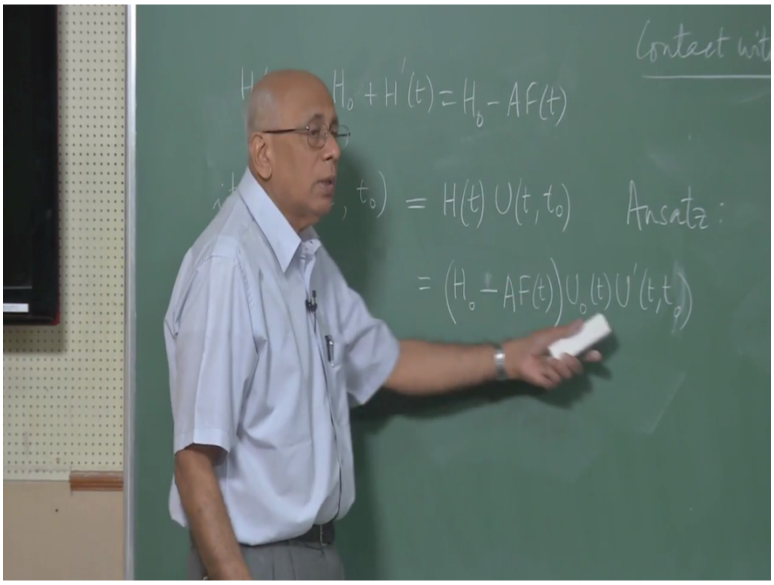

This is equal to H not minus AF of t in this fashion U not of t U prime of t, t not, okay. Just substituting for H and substituting this Ansatz for you.

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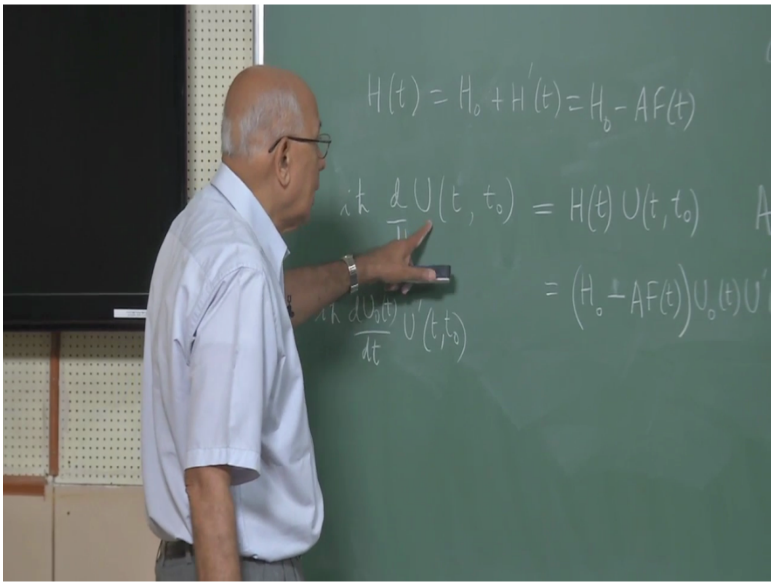

On the left and side I have ih cross d over dt, so you have dU not t over dt times U prime of t, t not that is the first term in the derivative here plus ih cross U not of t d over dt U prime of t, t not and that is equal to this fellow here, that is equal to H not U not of t, U prime of t, t not minus there is an F of t which comes out, A U not of t U prime of t, t not, just substituting but look at this term versus that.

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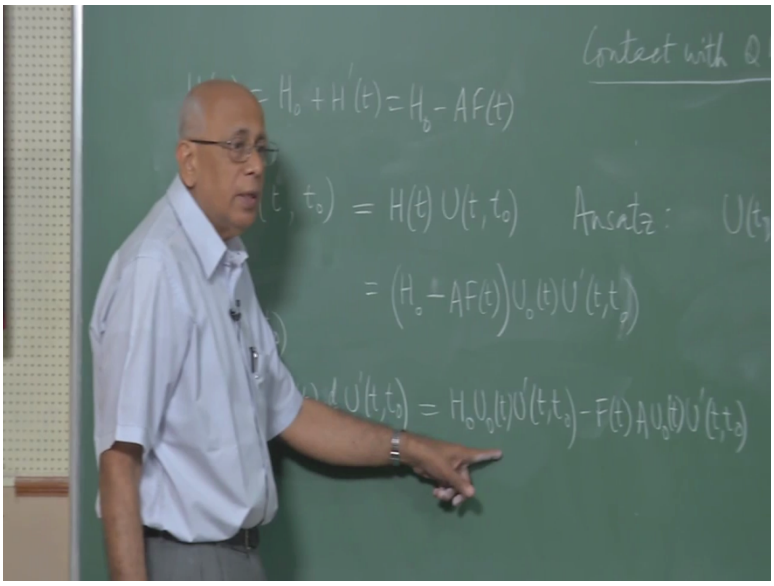

We already know ih dU not over dt is H not U not of t, we already know that. So this term says, this term cancels against that, even though they are operators, you operate on both sides of this equation, you operate with U prime of t, t not you get the same answer.

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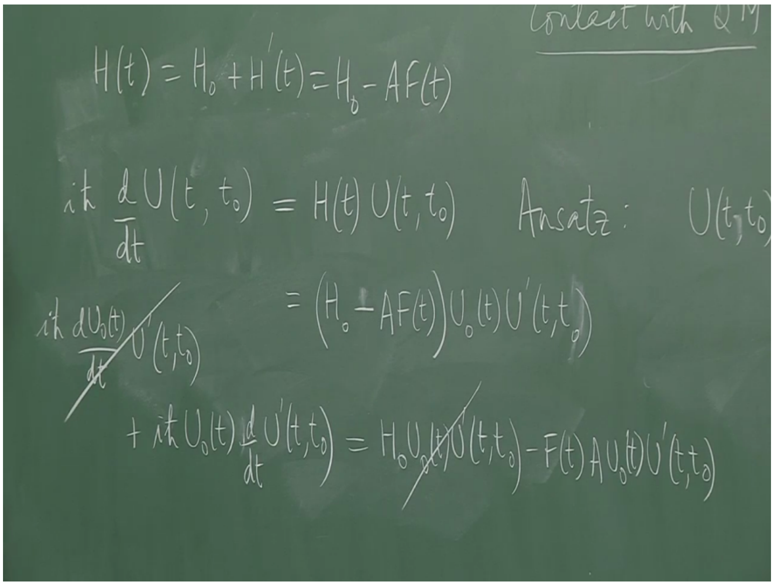

So this term cancels against this term, okay. And we have an equation for this alone but U not of t is a unitary operator its e to the minus iH not whatever it is.

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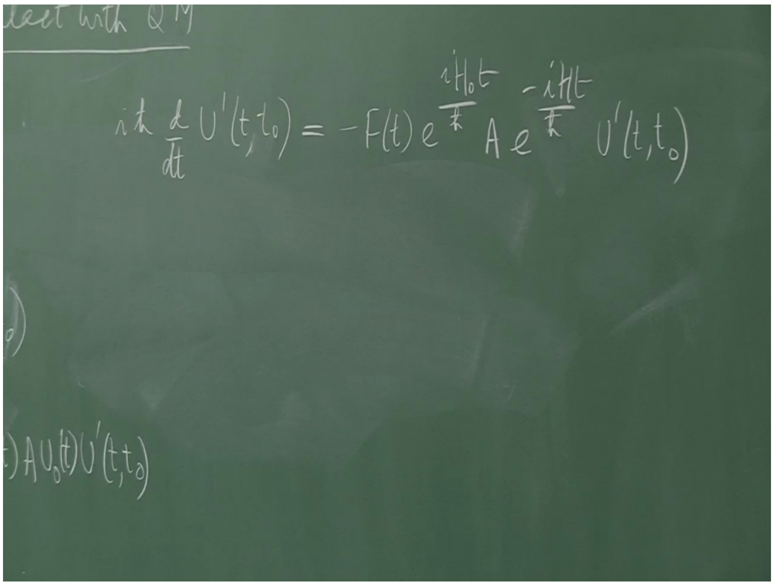

So this implies that ih cross d over dt U prime of t and t not this is equal to minus F of t and then e to the power let us move this U not to the other side that becomes U not dagger because U not is unitary, right? So this becomes e to the power iH not t over h cross A e to the minus iHt over h cross on this side, that is U not and then U prime of t.

“Professor -Student conversation starts”

Student: You forgot H not.

Student: Here.

Professor: Yes?

Student: Before iH not, A e for minus…

Professor: Oh! This is H not of t U prime of t, okay.

“Professor-Student conversation ends”

Which is of course this quantity here is what we have called A of t, for any operator that is the definition of the Heisenberg picture operator is induced by H not, okay. So this is equal to minus F of t A of t U prime of t, t not. Now what is the boundary condition on this fellow here?

Boundary condition U prime of t not t not equal to 1 because this is due to the switching on the perturbation and you switched on at time t not equal to at any t, t not, so at that instance of time it is the identity operator it starts with that and then it goes off to whatever it is.

“Professor -Student conversation starts”

Student: t not equal to 0?

Professor: No.

Student: that one is...

Professor: I am actually going to put t not equal to minus infinity, right now it is arbitrary, completely arbitrary I have defined my Heisenberg picture operator coincide with the Schrödinger picture operator at t equal to 0 is this convention.

Student: We do not want that (()) (20:28)

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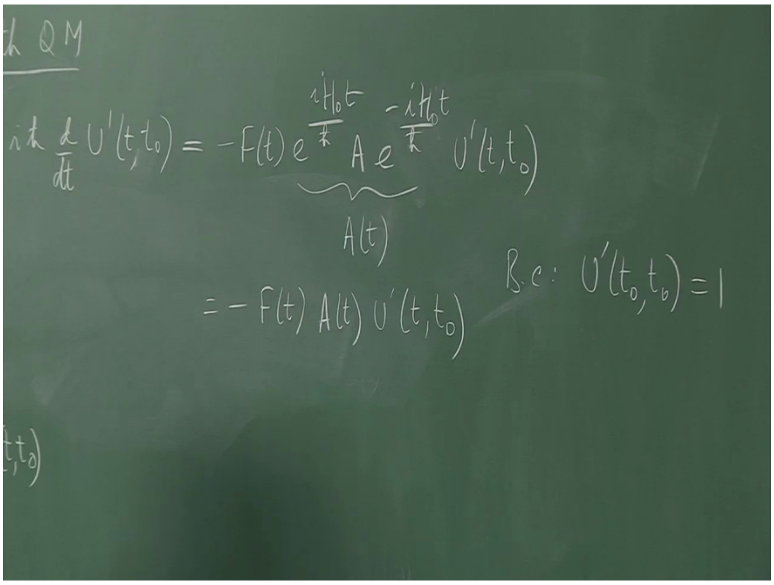

Professor: No because there is always this evolution due to H not going on, so I want to keep track of that and I simply want these 2 pictures coincide at some arbitrary t not t equal to 0 I call that the origin of time.

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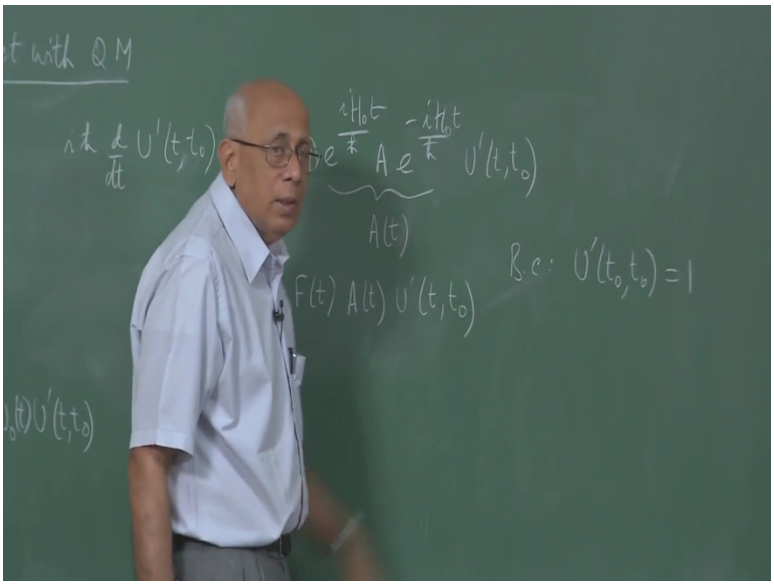

So this is the boundary condition I want to impose and that is a differential equation except this is an operator.

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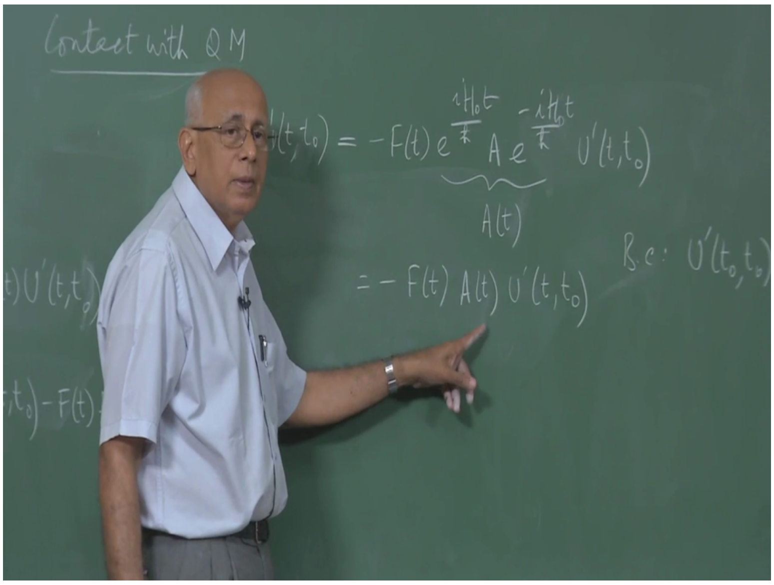

This fellow is an operator and we have to be careful, this is your number in some function it's a C number classical number. So we need to solve this equation using this condition and there is this ih cross setting here from this side. Now what is the way to solve this differential equation, it looks like I have exchanged one problem for another, this is again time-dependent and it is an operator and we do not know how it commutes with that, we have no idea at all at the moment.

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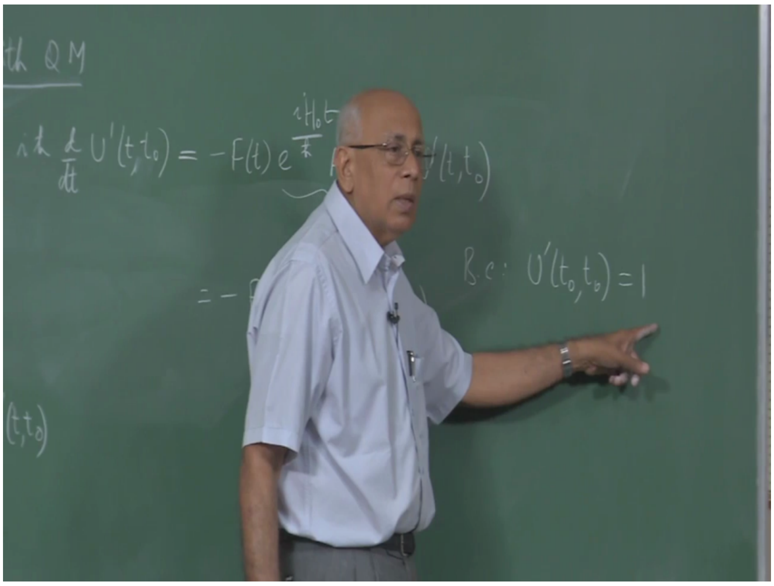

So we have not done anything significant except that now I am going to say let us convert this differential equation to an integral equation which will incorporate the boundary condition that U prime of t not t not equal to 1, okay.

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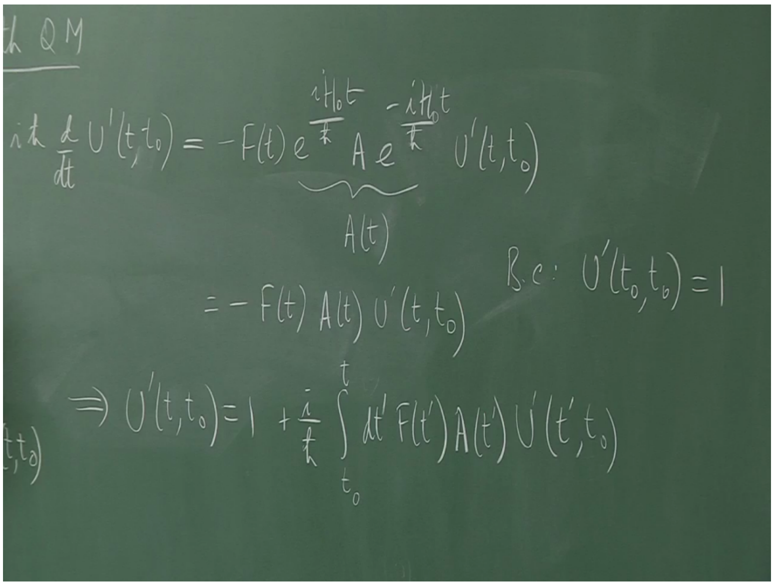

So this will imply, this thing implies that U prime of t t not equal to 1 and let us move the ih cross down here plus i over h cross integral from t not up to t because that integral whatever it is at t equal to t not will vanish and then you will get this equal to 1 at this side. So this is the correct in homogeneous term to take into account that boundary condition times Bt prime F of t prime A of t prime U prime of t prime t not.

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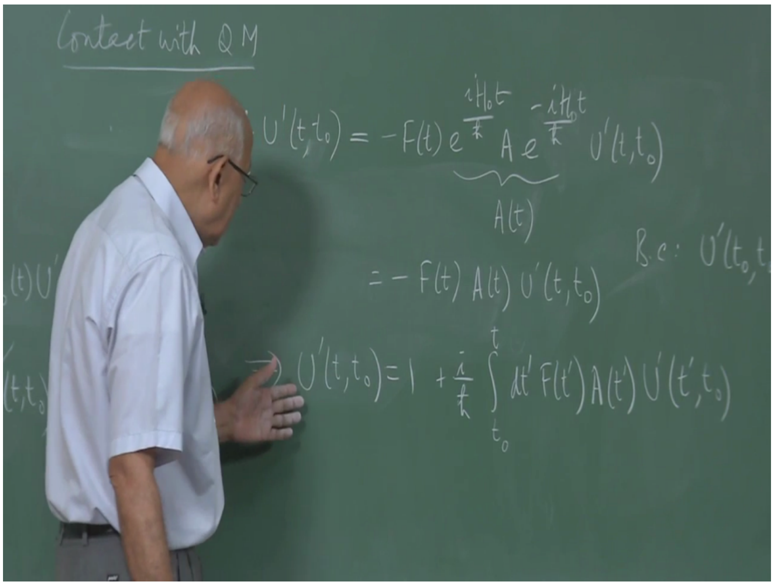

Why is that? Because if I, first of all if t not, t equal to t not this goes to 0 and U prime of t not t not equal to one which is our boundary condition.

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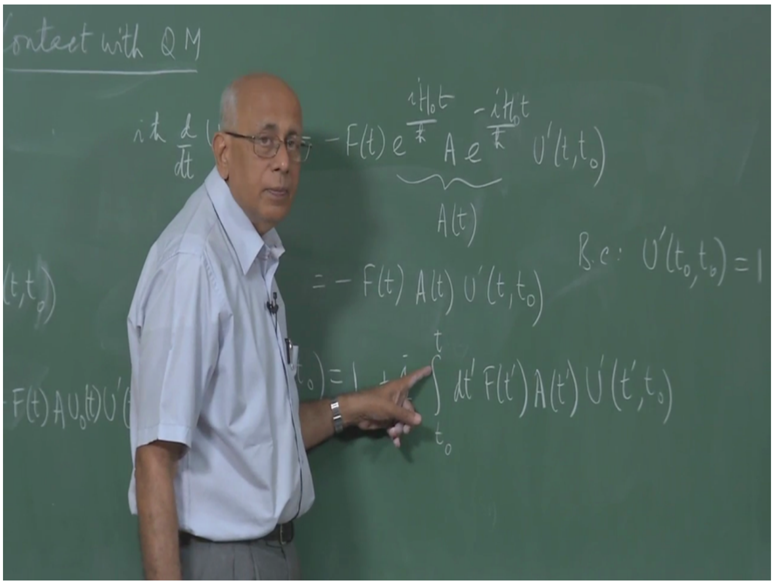

Second if I differentiate both sides, if I differentiate this fellow and multiply by ih cross I end up with precisely this because the only t dependence is sitting here and I use the formula for differentiation under the integral sign there is no t dependence here, so there is no partial derivative that is t dependence here and you are supposed to set the integration variable equal to this limit and differentiate the limit with respect to t which is 1 and if you do that, you get F of t A of t U prime of t. So the integral equation is exact, but approximation made here etc and it will tell you how this disen series is generated as you can see because now I solve this by iteration I say this is small, so I will do first-order, second order, third order etc and what is this to first order?

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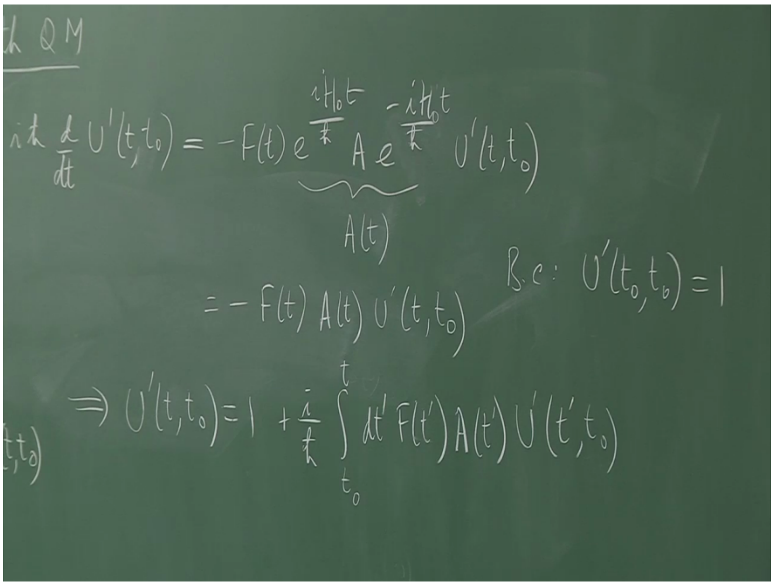

To zeroth order in F it is equal to 1, to first order in F, if it is an integral again with this quantity here with a second integration variable etc, right? So by iteration I can get the solution the exact solution but I am not interested in that, I am interested in it to first order.

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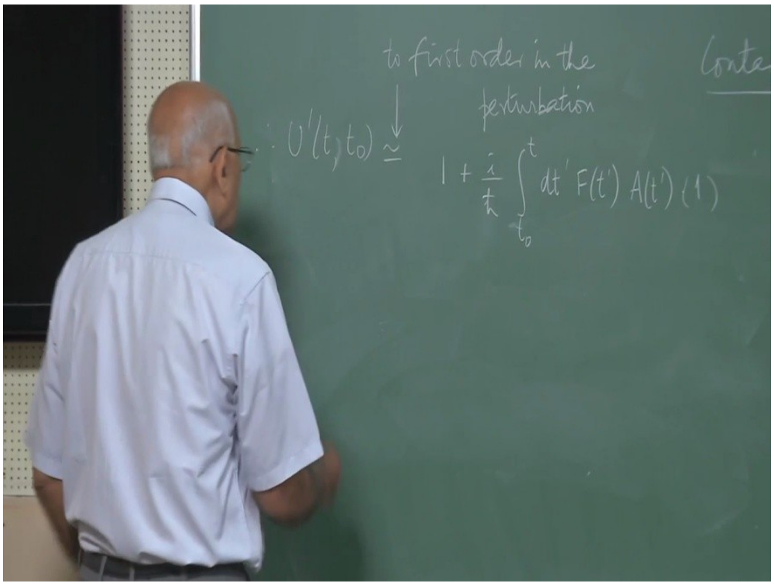

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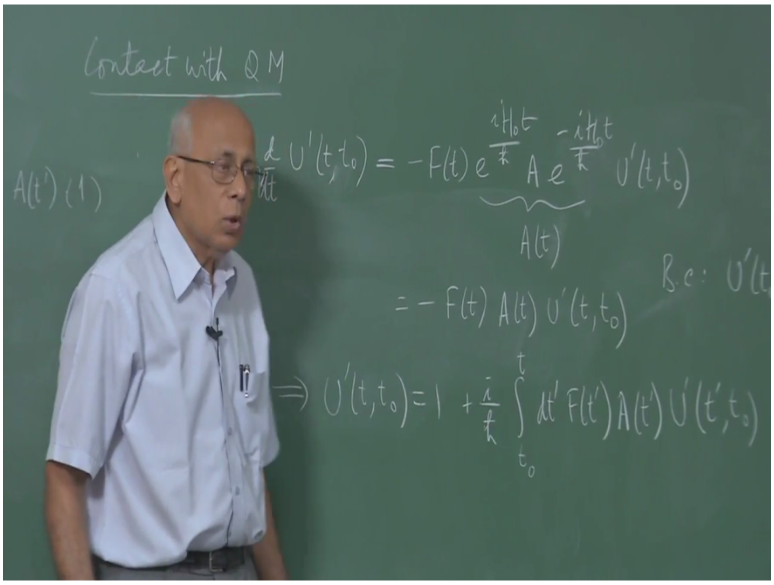

So therefore U prime of t, t not is equal to and this means to first order in the perturbation, this is equal to 1 plus i over h cross integral t not to t dt prime F of t prime A of t prime times 1 because that is the solution to zeroth order and there is already an F here, so if you retain this to zeroth order and F that is good enough plus higher-order is which I am not interested in.

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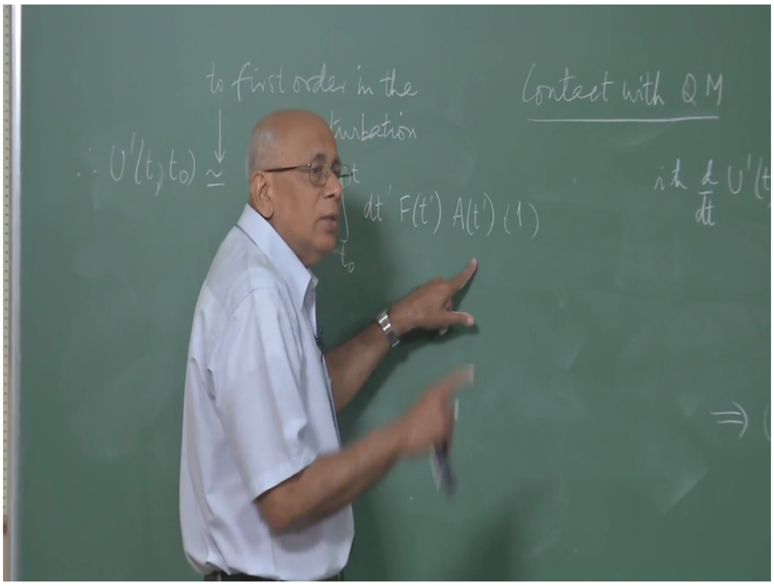

And what is A of t prime it is U not of t prime A, U not dagger of t prime A U not of t.

“Professor -Student conversation starts”

Student: e would be less than (()) (25:33)

Professor: We do not care at all. We do not care what it is and we do not care what t not is either, okay.

“Professor-Student conversation ends”

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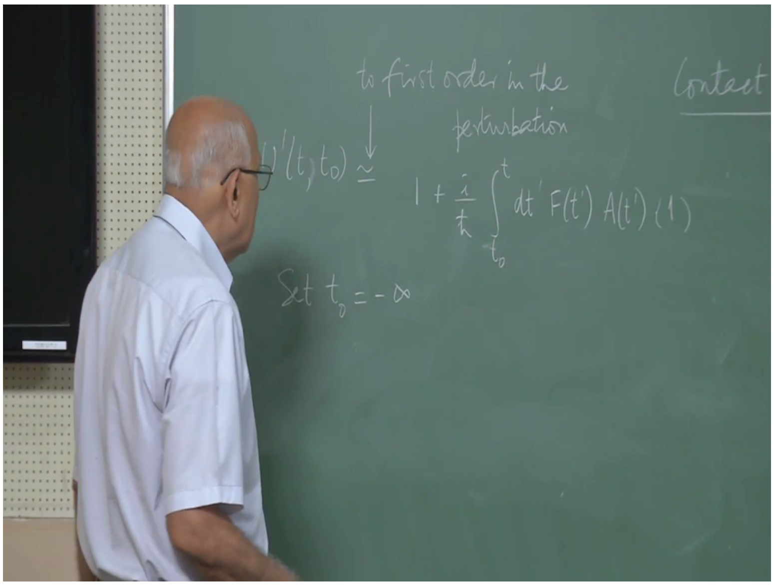

So now let us look at the case that we are interested in, so let us set t not equal to minus infinity, okay. That is the more general case I can of course put a Theta function, so that this ensures suppose this F is switched on at some finite time t not I can always put t prime minus t not here that is a unit step function here that will take care of it, so this is the most general case, we will do this, okay.

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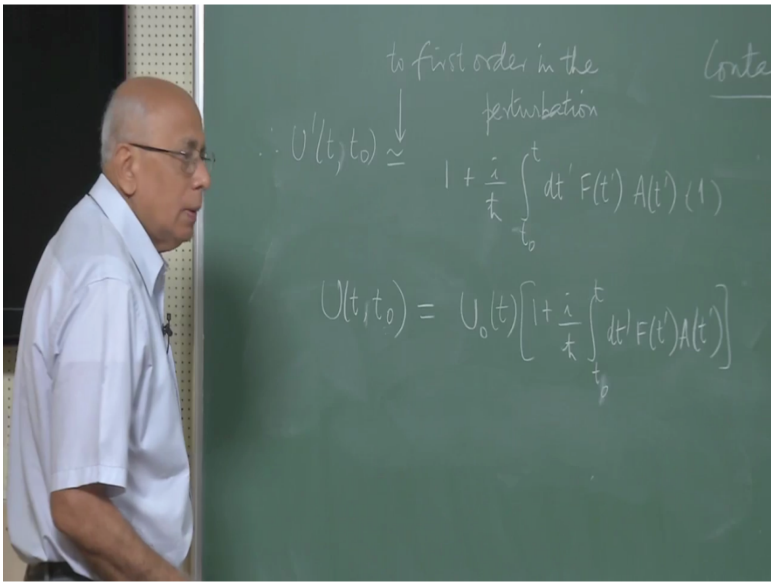

So what does U become even before I do that, what does U of t, t not, after all that is what we are interested in, what does this become? This quantity is U not of t is just sitting here multiplying this whole thing times 1 plus i over h cross integral t not to t dt prime F of t prime A of t.

Therefore U of t minus infinity is this, so we have our exact expression to first order the correct expression to first order and notice how the Heisenberg picture A has already got the Heisenberg picture evolution in it and the full-time development operator has a correction, this is the uncorrected one unperturbed part but then there is a perturbed part which is the product of this U of t with this integral all the way here.

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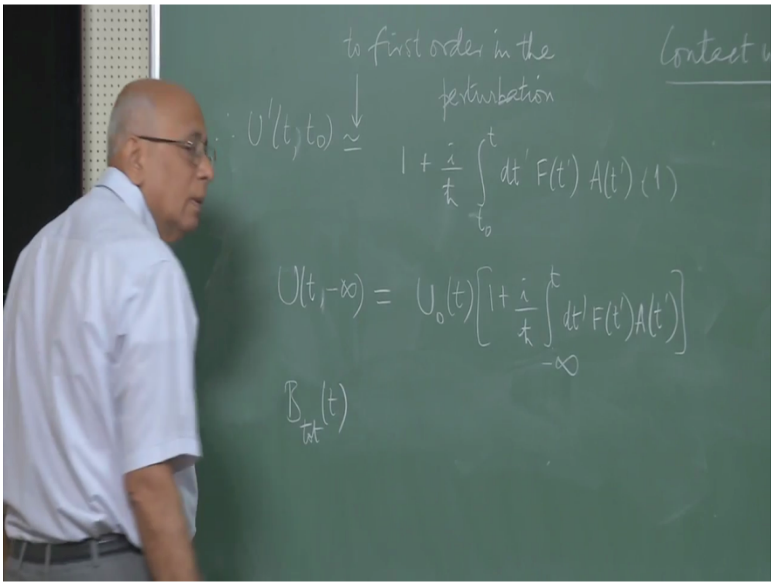

Now let us look at what time dependence of some physical quantity like Bs, so let us look at what is B? And I want the total of t. So let us put a total because I have already use the symbol B of t for this quantity.

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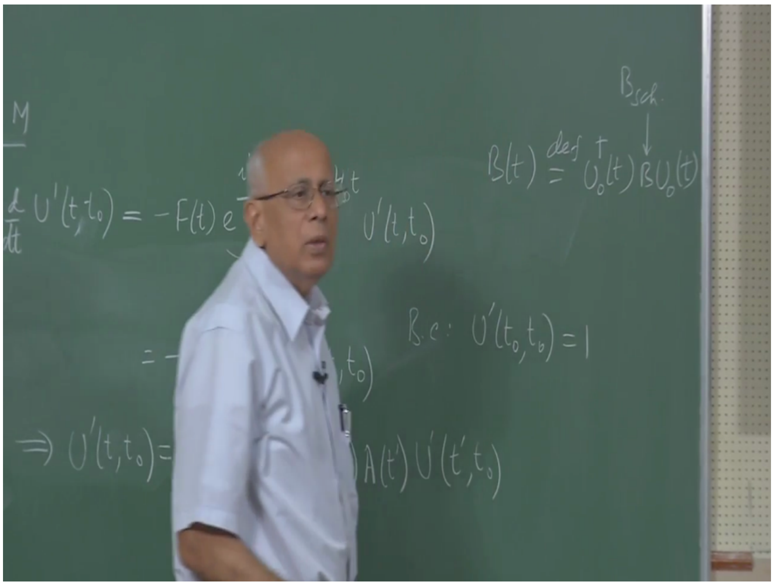

So I have already said B of t has been by defined by mean to be U not of t dagger B U not t and this is the B Schrodinger or B of 0, okay.

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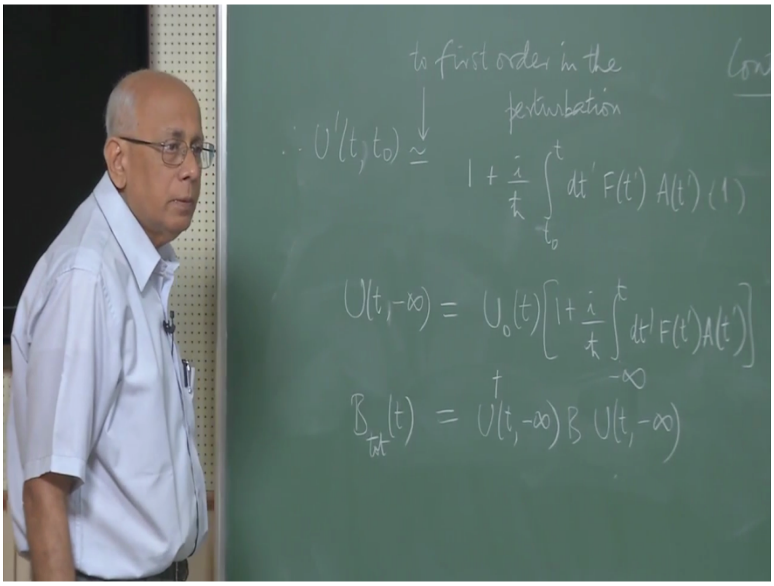

But now I want with this full thing here and what will this be, well if the state vector the states of the system are governed by the time development operator U then the operators are governed by U dagger operator U. So this of course is by definition U of t minus infinity B U of t minus infinity with a dagger here. Where I found this quantity to first order but had I found it to full glory to all orders I think this would have been the exact time developers in this point of any quantity here.

Pardon me, yes, we are going to check that, yes it will be as you can see because I have to take with him dagger of this, it will become this fellow will go on the right-hand side and then this will become minus and this is hermitian. So to first order it will be, to second-order you got to check order by order consistently but it is the full thing is, the full thing is as long as the Hamiltonian is hermitian, okay.

So the moral of the story is that if the Hamiltonian is time independent and hermitian then e to the power i Hamiltonian times t over h cross is a unitary operator but the statement is even if the Hamiltonian is time-dependent as long as its hermitian the time development operator is unitary, it is a complicated time ordered exponential but it is still unitary and you can show that order by order.

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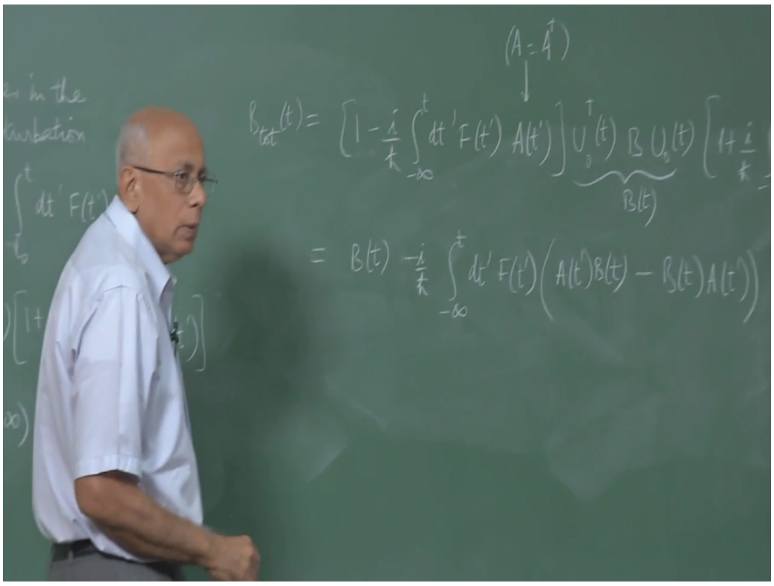

So now let us see what this fellow does, so this therefore implies that B total of t equal to U dagger, so if this fellow goes to the right-hand side and we have to write 1 minus i over h cross integral minus infinity to t dt prime F of t prime A of t prime because A equal to A dagger I have taken that to be the case, if it was not the case then you have to add a portion to the Hamiltonian which will make it hermitian.

So you will have to add minus AF of t minus A dagger F star of t, so that the sum becomes a hermitian quantity. Sometimes you would see in books plus HC show that it is a hermitian conjugate has been understood to be added but the fact is that I am now going to look at a simple where A is summation just for notational simplicity, so the minus and you have this multiplied by U not dagger.

So this is U not dagger of t and then that quantity B and then U which is U not of t on this side and then 1 plus i over H cross integral minus infinity to t dt prime F of t prime A of t prime, okay. But we have to give this only to first order for consistency, there is a second-order term here due to this F times that F but we have to throw that out because we do not have the answer correct to second-order.

We do not have the time development operator correct to second-order, so keeping that second-order term would be inconsistent which is equal to this times this will just give me B of t Schrodinger with the Heisenberg picture B of t governed by U not evolution and then we get this times that and then this times that, so let us put this times that first plus i over h cross integral minus infinity to t dt prime f of t prime times what?

Well, this is always B of t, so this portion is B of t I am multiplying 1 with B of t, so B of t and then A of t prime and in the opposite order it is A of t prime with B of t. So let us do following, let us write this as minus 1 over ih cross, is that correct? I have to be careful here I will not be careful, so let us let us not mess around with this signs, so let us take this term first.

So minus i over h cross integral minus infinity to t dt prime F of t prime, A of t prime, B of t that is this times that with a minus sign and taking it the other way there is an x i over plus i over h cross, so I will put a minus sign inside the bracket, okay.

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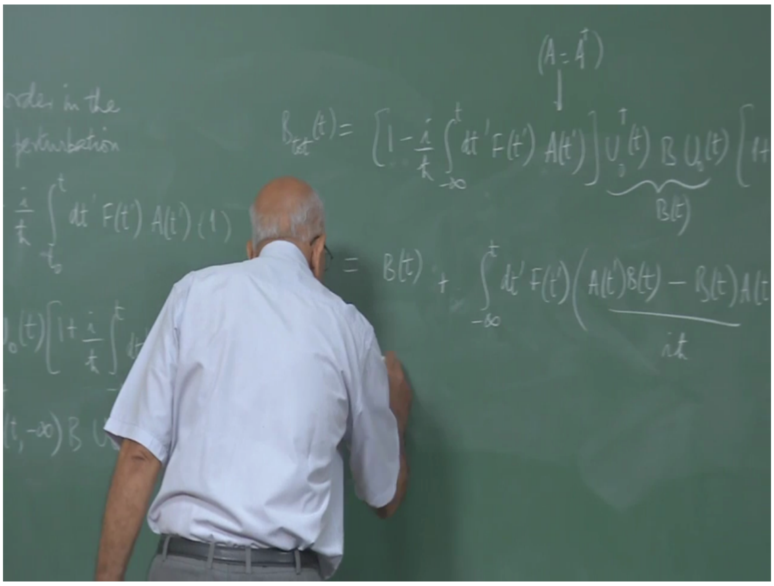

So let us just write this as plus over ih cross which is equal to B of t plus integral minus infinity to t dt prime F of t prime and then a commutator of A of p prime with B of t over ih cross but this is precisely what we call the response function?

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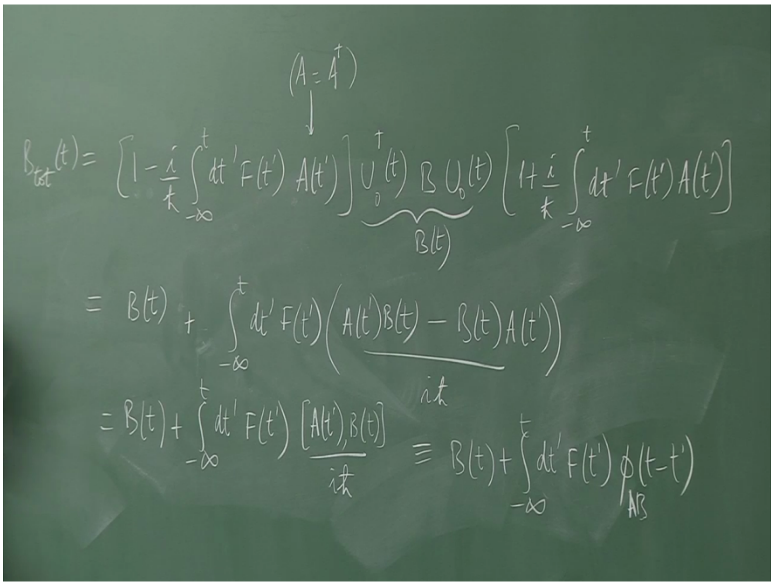

Well, it is actually t minus t prime that is not hard to show, that is not very hard to show, you put in those e to the ih's and etc not quite, not quite so let us not do that yet, that is not be in a hurry. So we have this expression here.

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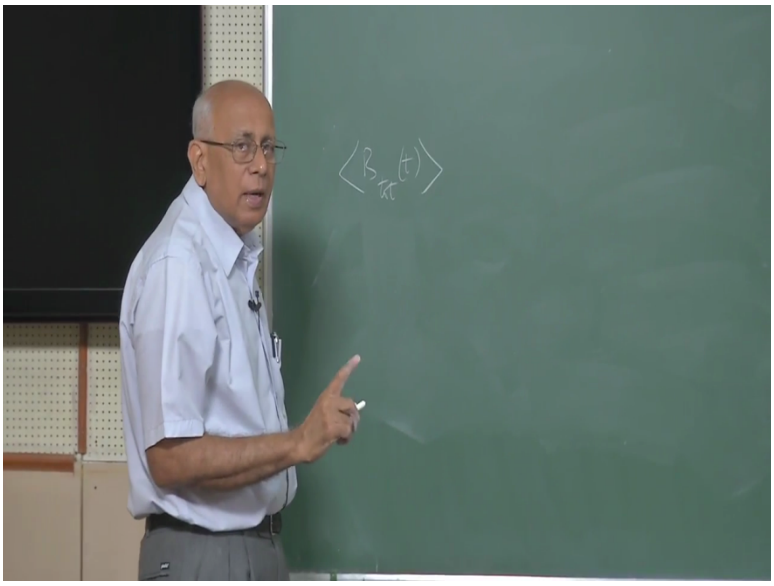

And now the last step is to say is B total of t average value, now we are going to take averages and with respect to what should be take the averages? With respect to here equilibrium because we have already put in all the time dependence in the operators. We have solve the equation of motion for the operators by writing the time development operator acting on the operators and finding out what that does explicitly and compute into first-order, okay.

So this average is now with respect to rho equilibrium that is equal to average value of B of t in equilibrium, rho equilibrium which I call equilibrium plus integral minus infinity to t dt prime F of t prime times the expectation value of A of t prime commutator B of t in equilibrium over ih cross. By the way this is time independent B equilibrium, this part of it is identically equal to B equilibrium.

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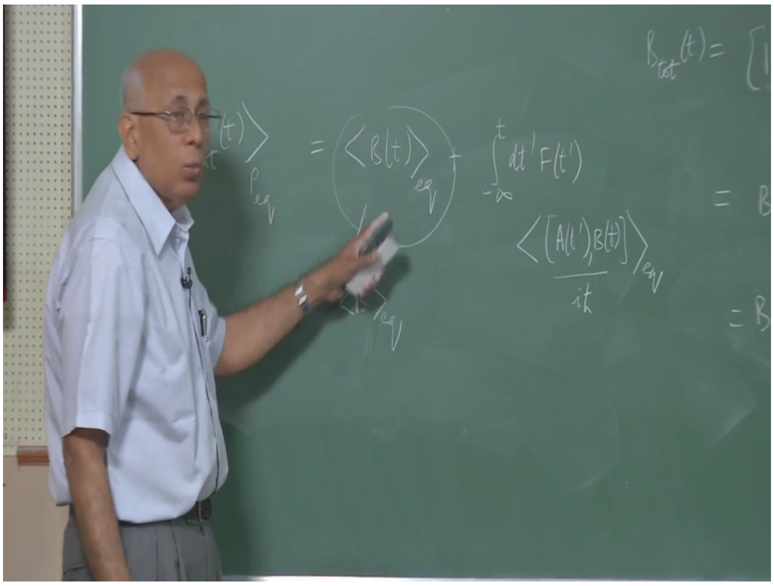

It is time independent, why is that? Why does that happen?

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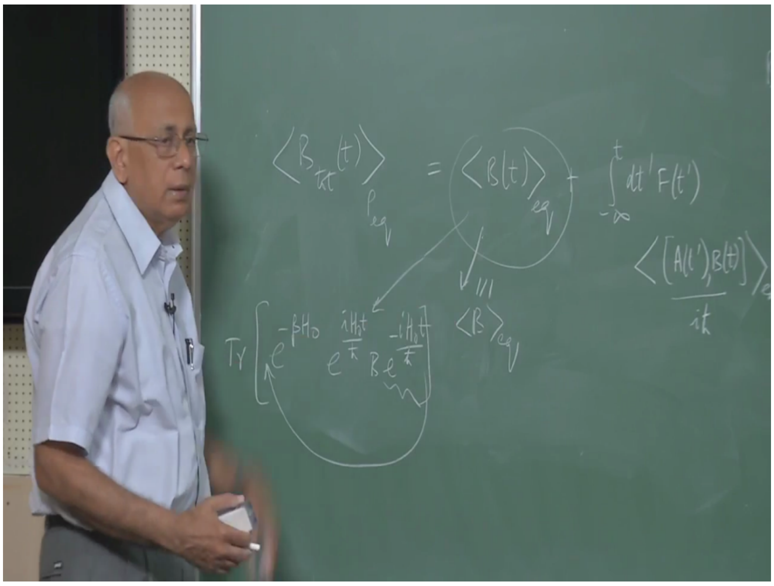

Because yes, because what you need here is e to the minus beta H not you got to take trace of e to the minus beta H not B of t but B of t e to the ih not t over h cross B e to the minus i H not t over h cross, by this cyclic invariance of the trace move this portion across to this side and of course it commutes with itself, if cancelled against this and you have traced e to the minus beta H not B which is equal to B.

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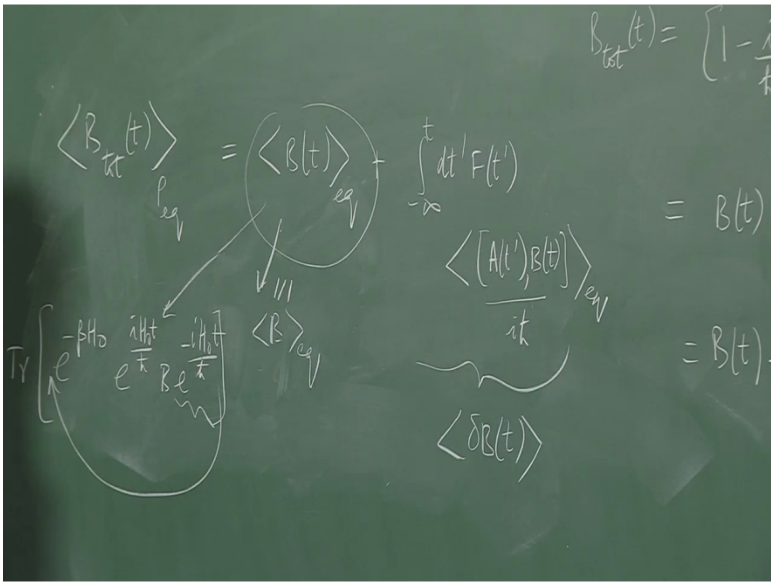

So this portion of it is harmless, this is just you can compute it at anytime it does not matter in the Schrodinger Heisenberg picture it does not matter, it is just the equilibrium average. So this part is what we defined as Delta B of t by definition this was the change and we are back to the formula we had for Delta B of t.

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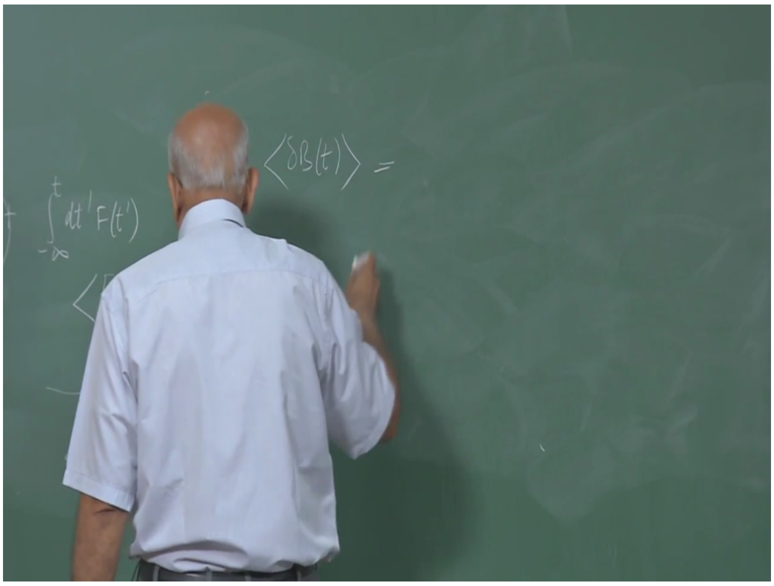

So delta B of t is going to be is ...“Professor -Student conversation starts”

Student: (()) (38:48)

Professor: Yes. Exactly, precisely, so this we can write now as integral minus infinity to t dt prime F of t prime phi AB of t minus t prime because the expectation value of A of b prime B of t commutator equilibrium is equal to and that we did, we explicitly did this, the road of this quantity and put in all the e to the minus beta H not sum took it across, that is how we that is one way of now explicitly derived.

“Professor-Student conversation ends”

So what have what have we done? We have done first-order perturbation theory in the Heisenberg picture. It also tells you how to generate the higher-orders, so in principle if you are interested you can go onto the next order and find out what is a correction etc. again go back to the integral equation for U prime and work out the solution to the second-order consistently, a lot of algebra…

“Professor -Student conversation starts”

Student: Linear (()) (40:11)

Professor: It will not be linear response theory anymore, definitely but it will be second-order perturbation theory, okay.

“Professor-Student conversation ends”

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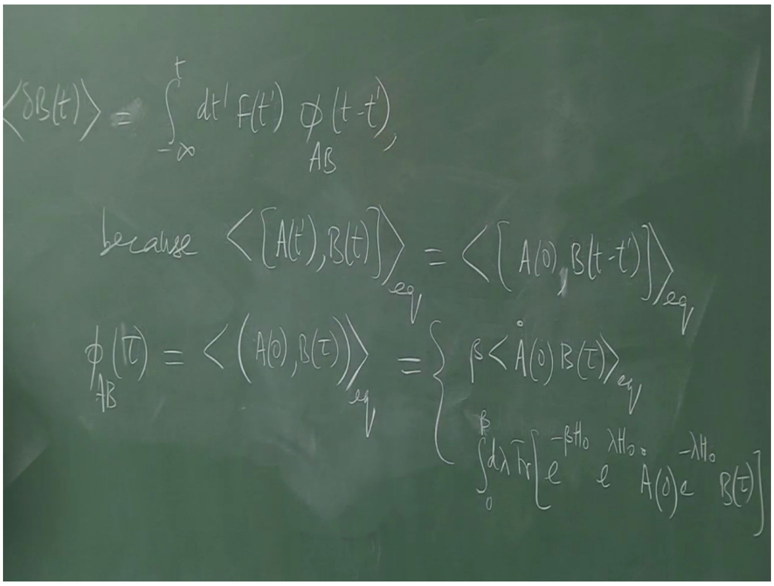

And then of course we also showed that phi AB of tau this quantity was equal to the bracket that we wrote here A of 0 B of tau this going to be in equilibrium, this was also equal to in the classical is just beta A dot of 0 B of tau equilibrium and the quantum case it was equal to integral 0 to beta B lambda trace of e to the minus beta H not times e to the lambda H not A dot of 0 e to the minus lambda H not B of tau greater towards.

Which we wrote as the same thing with this semicolon here by definition. So all the non-commutativity of quantum mechanics the complications arise from here from this expression, complicated expression relatively complicated expression because you have this sandwiching, this is sandwich between these 2 operators and then all the rest of the properties of this semicolon this comment, this response function namely the fact that it is stationary it is real for A and B hermitian its symmetric function if you interchange the A and B even though they do not commute with each other etc.

Those things follow because of the cyclic property of the trace, so (()) (42:16) I do this justice show explicitly that the same answer is obtained from perturbation theory, first-order perturbation theory by choosing the particular Ansatz for the time development operator, okay. And what is it that you are doing in choosing the Ansatz? You are simply saying that this operator is basically the unperturbed operator but for the perturbation you got an extra piece which satisfies a separated time dependent equation and that equation can be solved by converting it to an integral equation and iterating term by term. So that is one way of solving such operator equations with time-dependent inside the operator.

Now there is one more thing that we need to do and that is to connect this with this equation, after all there are (()) (43:03) force to the system, so there is some kind of energy that is either increasing or decreasing. Some energy is being dissipated and we would like to see how the system absorbs energy? If it is a quantum mechanical system it is obviously going to be able to absorb energy only if it takes you from one level to another.

Or brings you down from one level to another one of the 2, so we should be able to see that explicitly I am just going to outline the steps here and leave the rest of it as an exercise for you to work out.

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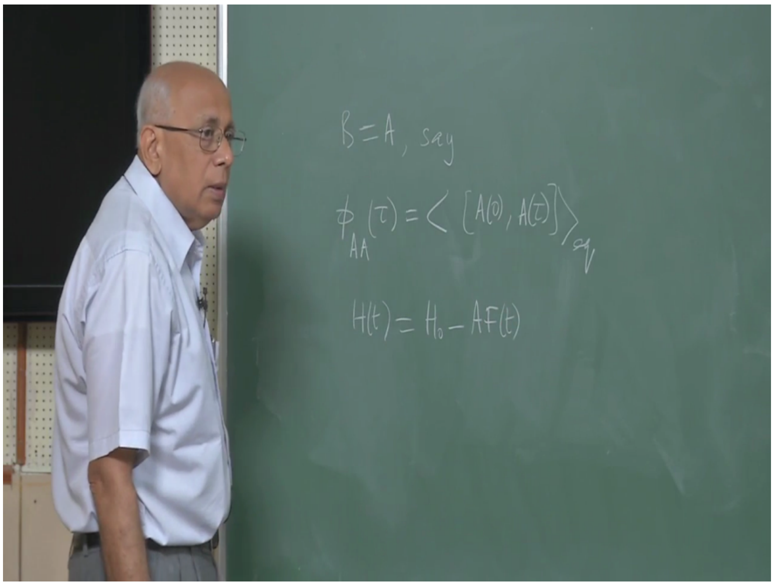

So let us do that case and for simplicity let us look at the case where B is equal to A itself. Then remember that Phi AA of tau equal to the equilibrium expectation value of the commutator of A of 0 A of tau and A is hermitian then what is it we want to compute? We have a Hamiltonian which is now time-dependent. So there is an H of t equal to H not minus AF of t.

We would like to find the rate of change of this the expectation value of this Hamiltonian of the internal energy of the system.

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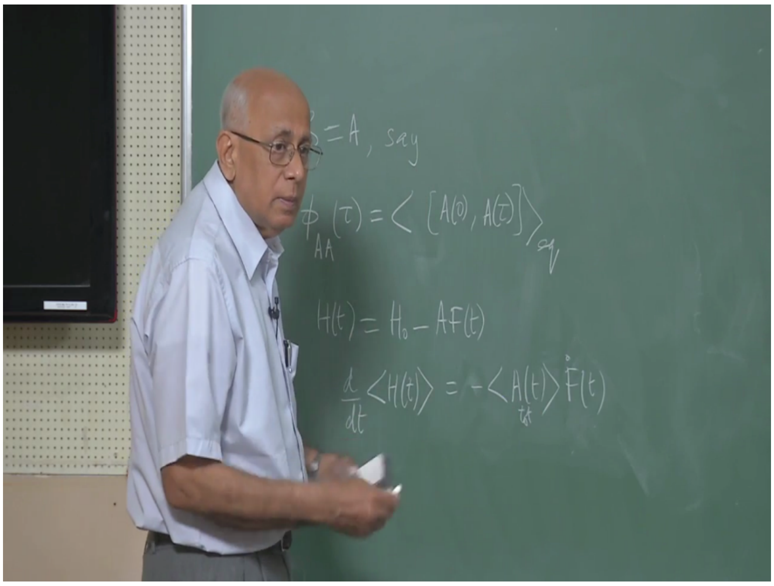

So we had like to find what is this? d over dt H of t and that comes from the time dependence here, so this quantity is minus A of t expectation F dot of t I should say A total and the explicit time dependence is sitting here and that is the quantity I want to compute.

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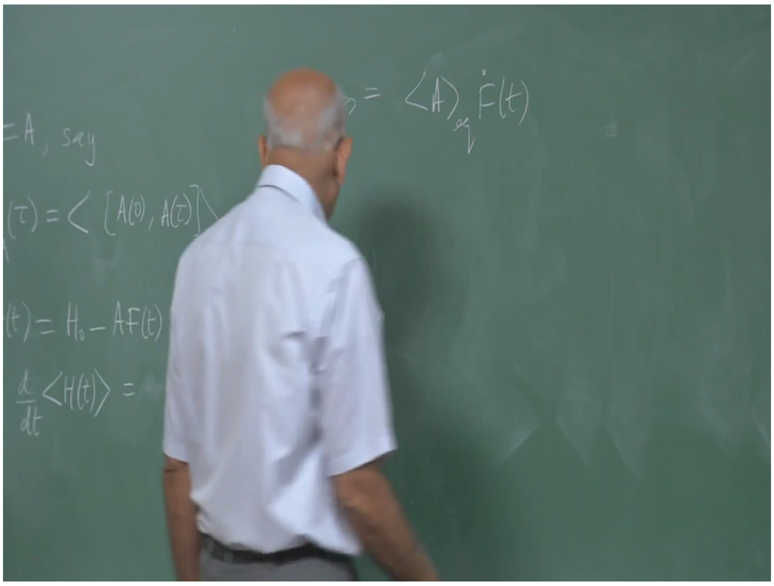

But this quantity, so this thing here is equal to, so let us compute minus of this one, this is equal to A equilibrium F dot of t is a term sitting here that is a harmless term you can see plus and this is the interesting part plus an integral from minus infinity to t dt prime F dot of P out here times phi AA of what? F dot of t minus t prime F dot t in the expression. We have an equation for this fellow here.

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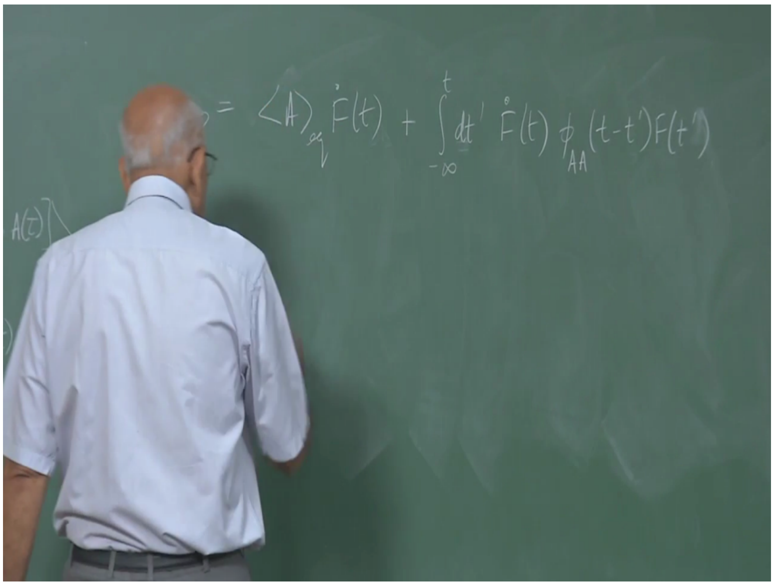

In fact we can go all the way back and write this expression in terms of the spectral function, they have an explicit expression for the spectral function in terms of e to the i omega tau and things like that and you can do this integral because the time integral finally this fellow here is a function of tau and that will become 0 to infinity in tau to the integral and it will essentially give you once you put in time dependencies here, if you put a Fourier mode it will give you the susceptibility at some temperature at some value of frequency.

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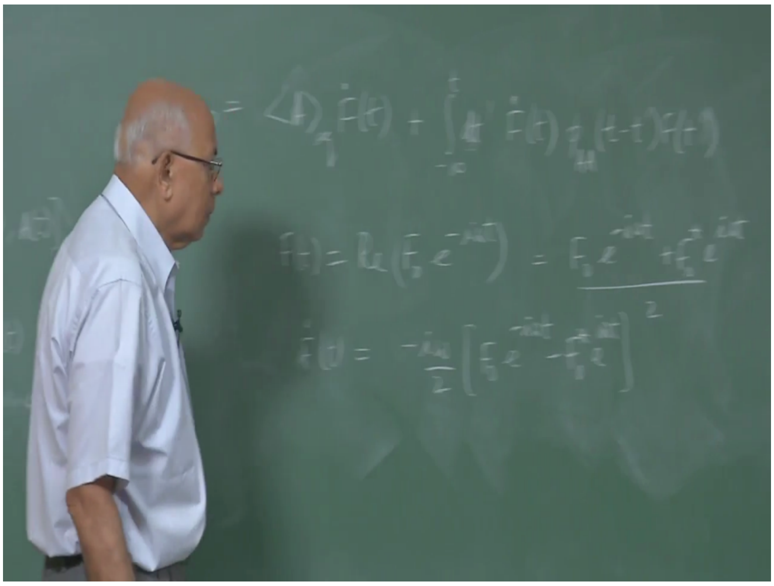

So now let us say, we now put in the physical case we say F of t equal to the real part of F not e to the minus i omega t. So I am trying to find out what happens if you hit the system with a force at some frequency omega which is equal to F not e to the minus i omega t plus F not star e t the i omega t over 2. So F dot of ps trivial this is equal to minus i omega over 2 times F not e to the minus i omega t minus F not star e to the i omega t.

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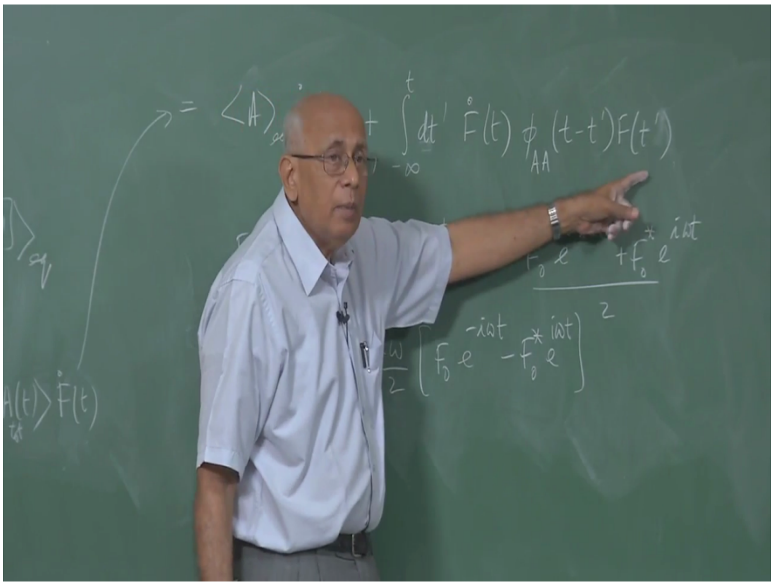

F not is some amplitude which is necessarily got to be complex because I want to the force to be real, so F not plus F not plug that in, put this expression in for F of t prime put this expression in for F dot of t t collect the exponentials together when you that you are going to get e to the i omega t minus t prime everywhere and sometimes t plus t prime 2 you that term as well, right?

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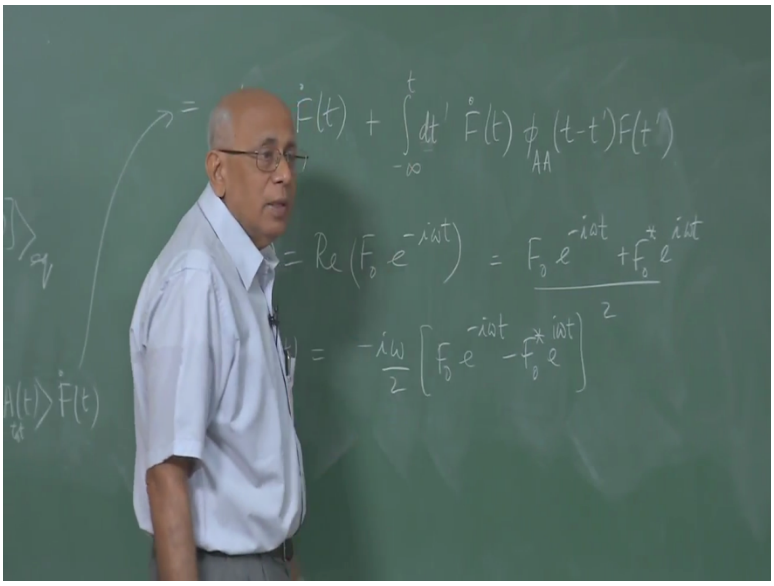

You are going to get both ends of terms in there, integral is minus infinity to t change variables to t minus t prime equal to tau and wherever you will recognize e to the i omega tau times phi AA of tau replace it with Kai of Omega, okay. And in terms with the wrong sign e to the 2 t plus t prime, what should you do? Subtract twice t, so make that t minus t prime inside and then there will be e to the 2i omega t outside, right?

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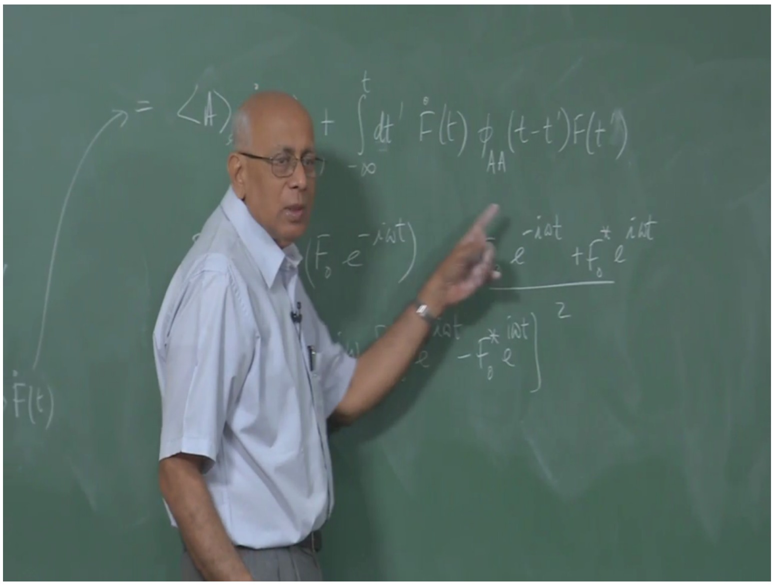

So that we have big mess that using, I do not want to write it down here because it requires a large number of terms due to this fellow here and what we want to find is the average rate of dissipation. So average then over time t comes 0 to pi over omega which is the time period, over a full cycle of this course that will give you the average rate of dissipation.

So are the steps clear? It will give you may be a constant, we do not know we will have e to the 2i omega t you have to integrate over a full period me give you 0 may not etc, so in general it will disappear as you can see.

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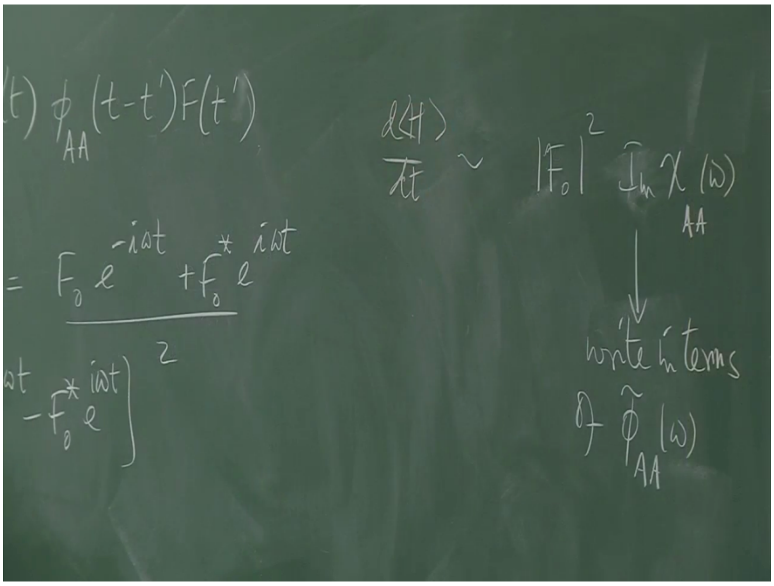

But at the end of the day you would expect this quantity to be proportional to mod F not square that is not too surprising, right? Times something which involves the susceptibility and I wanted to show that it is proportional to Kai imaginary times constant, so there is some omegas and stuff like that.

Now you can write this down in terms of the spectral function. So the spectral version is going to involve weight factors Anm Bmn those are going to now become Anm Bmn and then there would be summations and things like that, so those are called oscillator strengths and then there would be all the transition frequencies of the system. So that would be a term which corresponds to absorption and there would be a term which corresponds to emission.

The both are there in quantum mechanics, both, so there is always stimulated emission along with absorption and finally will discover that you got time dependent first order perturbation theory the Fermi Golden rule, so there are always things weighted by the Boltzmann factor. So compute this I am going to give this, write the answer down in the problem sheets and then you will see, check against what you have done.

So this kind of brings me to the end of formal linear response theory, the rest of it will be in the form of exercises which we will put in the notes but I would like you to go through this derivation step-by-step all over again and complete this, complete this piece of algebra I would do this except for the fact that they did not want you, that you carry over to next time and it is a lengthy, slightly lengthy piece of algebra but you see the strategy that is involved.

Once you do is for once frequency you know the answer for all frequencies because you so proposed for an arbitrary (()) (51:40), okay. That kind of completes what I wanted to say about linear response theory we still have to make contact with another way of doing this whole business which is to introduce a random force into the system and then compute various quantities once you have a stochastic model for the system including dissipation.

Now that is not easy to do in quantum mechanics because including friction in quantum mechanics is a nontrivial task you sidestep that task but the difficulty with that other more powerful, very powerful way of doing things is that you have to make some assumptions about the nature of the stochastic force that you have and then you have quantum mechanics you also have to worry about commutativity and so on, makes it more complicated.

The formalism of linear response theory on the other hand gives you a very general framework for solving such problems plus points and minus points this is more general than the other case but the other case is very specific and it will go further in terms once you make a detailed model of the stochastic force or whatever is driving that fluctuations then you can go little further here.

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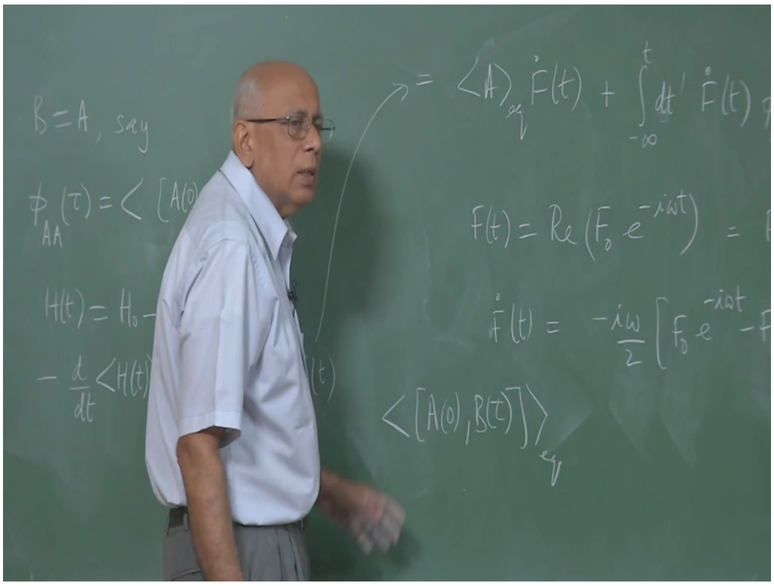

There is a fluctuation dissipation theorem here to and that is a relation between you already know in this case kind of intuitively you can see, we have a formula for this quantity, for A of 0 B of tau in equilibrium this was our response function and we have a formula for its Fourier transform which is essentially phi tilde of Omega, right? If you like that is like taking care of, this quantity here is taking care of the response of the system that is what the response is when you apply the force.

On the other hand the fluctuations themselves would be given by things like what happens under pure thermal fluctuations? Not the commutator but the anti-commutator would give you a measure of the fluctuations especially if you set A equal to B then you get mean square values that will give you fluctuations the variance of that quantity etc and you know that there is a relation which says that if you took the anti-commutator here.

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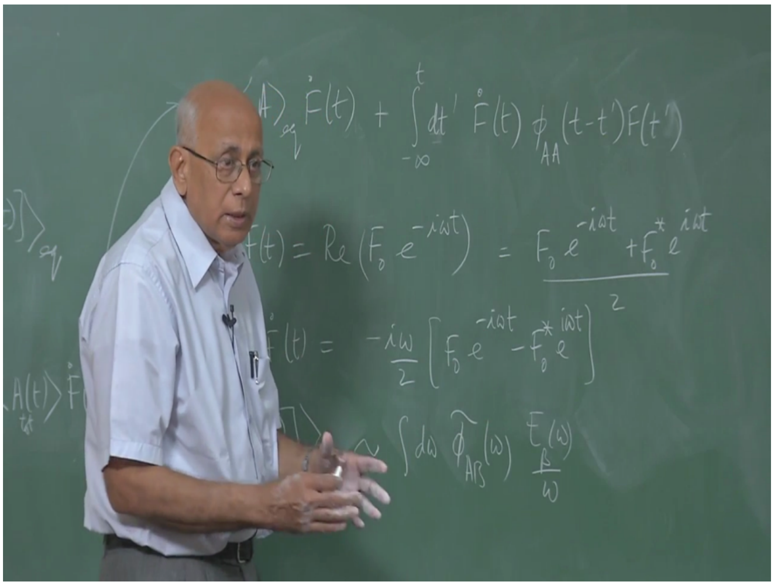

We could see that this went like an integral d omega phi AB tilde of omega times this quantity this e beta omega over omega whereas this fellow was just the spectral function the Fourier transform of the response function, right? Which measured the dissipation in the system if you like. So there is a connection which says that the power spectrum of this quantity which is its Fourier transform related to the power spectrum which measures the dissipation namely phi tilde by this formula.

One of them is phi tilde and the other is phi tilde times this quantity, so that is the generalized fluctuation dissipation theorem. We have not used when it is modelled for the random force or anything like that but it is a relation between fluctuations and dissipation.

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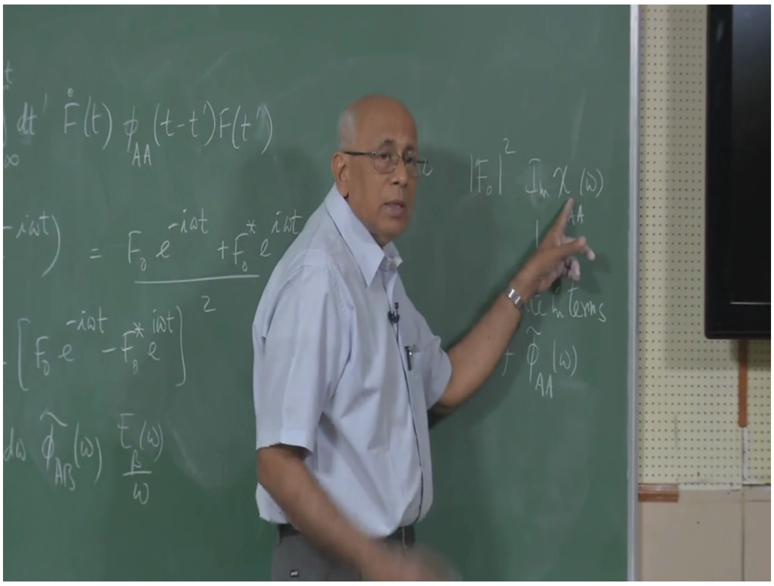

Because the dissipation is governed finally by this quantity which comes from the response function and the fluctuations are governed by the power spectrum of this one.

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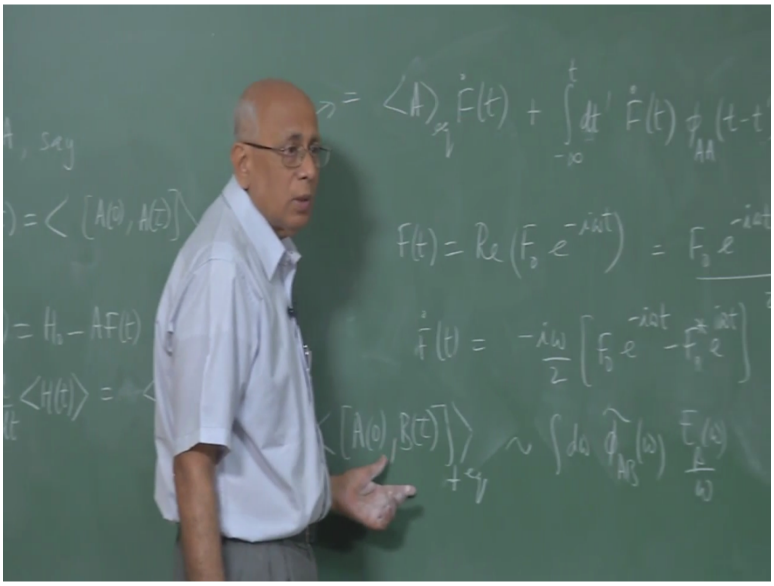

The Fourier transform of this quantity. So if you like that is the fluctuation dissipation theorem in this problem without any reference to the stochastic force or anything like that which is the way it appears in the Langevin model here, so this is intrinsic to it was not assumed any specific model of stochasticity and yet the thermal fluctuations are getting connected to the dissipation in the system.

So I will write that expression note explicitly in the hand out, so you can see and check what happens and you can also compute now things like the mean square displacement of a harmonic oscillator, quantum mechanical oscillator at finite temperature, at very high temperature this would be essentially kt and at very low temperatures it would be related to h cross Omega but in between temperatures it comes from using these some rules here for the spectral function, okay.

So some of these things I will give as exercises to check out, okay. So with that we stop here and the next thing we are going to do is to go back, backtrack a little bit and fill in the gap we had not filled in earlier which is to connect the Langevin model with the corresponding differential equation for the (()) (56:30) probability distributions and cells. So things like the Fokker Planck equation and so on and we take it from the next time.