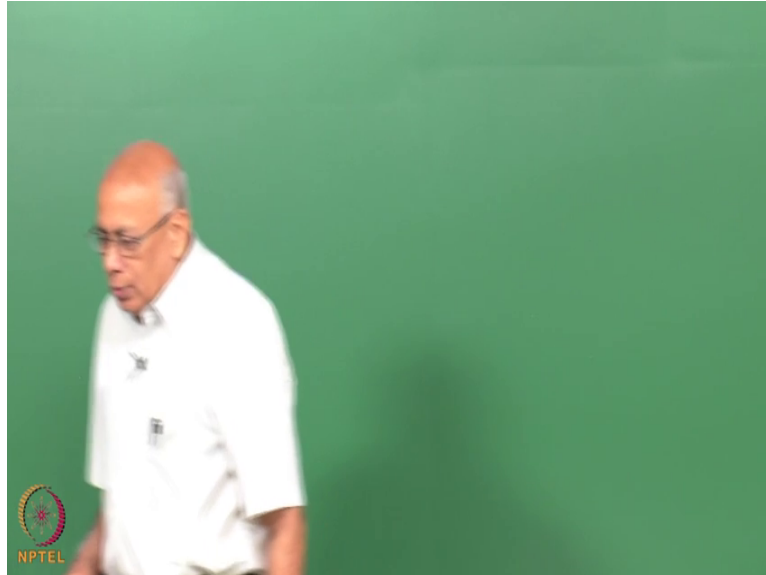


Nonequilibrium Statistical Mechanics
Professor V. Balakrishnan
Department of Physics
Indian Institute of Technology Madras
Lecture No 10
Linear response theory (Part 5)

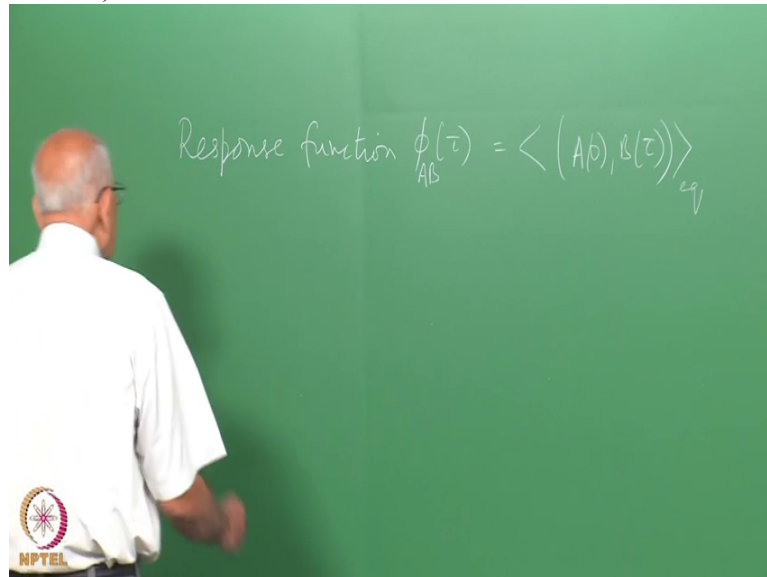
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So to recall what point we had stopped at last time we discovered that the correlation, the response function $\phi_{AB}(\tau)$ which was formally equal to the equilibrium expectation value of A of zero B of τ in equilibrium, we wrote this in a number of ways in terms of trace with $\rho_{\text{equilibrium}}$, with A of zero bracket with B of τ and so on. We have several representations for it.

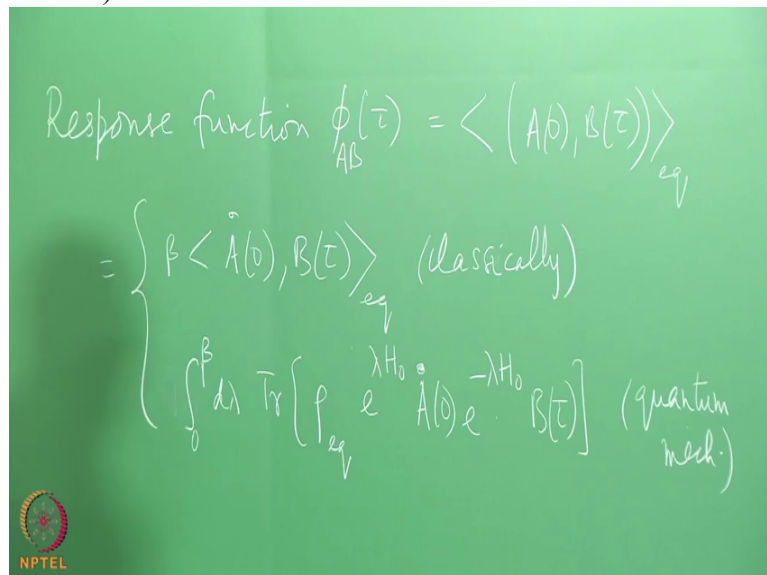
But we discovered

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that this became equal to, in classical mechanics, it reduced to just the correlation between A dot at zero and B at time tau. In equilibrium, this was classically. Quantum mechanically we had a somewhat more complicated formula and quantum mechanically it was equal to trace, well, it was equal to an integral from zero to beta d lambda and then trace of rho equilibrium times e to the lambda H naught A of zero, A dot of zero, e to the minus lambda H naught and then a B of tau like this, and this was in quantum. This was the quantum mechanical case.

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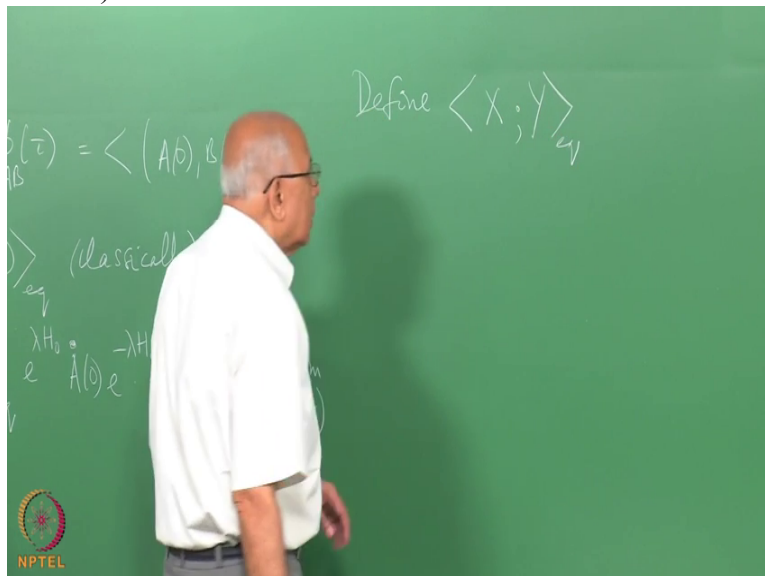
So it is like some kind of 0:02:16.6 transform with the e to the lambda H naught here, minus lambda H naught and then integrate it over lambda from zero to beta in this fashion and then you take the trace of this fellow here, Ok. It is very convenient, the whole combination

appears over and over again, so it is very convenient to give it a small notation, introduce some notation.

But notice that in the classical case where things commute with each other, this will cancel against that. You just have A dot of zero, this gives you an integral beta and that gives you this factor and you are back to this out here. So classically this formula reduces to the classical formula but this is the more general formula.

So it is convenient to introduce what is called the canonical correlation. So let us define $\langle X; Y \rangle$ in equilibrium

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with arbitrary time arguments, whatever be the time arguments of these dynamical variables, if X and Y are observables, operators in the quantum case define this to be equal to 1 over beta times an integral zero to beta d lambda and then trace rho equilibrium X, sorry e to the lambda H naught X e to the minus lambda H naught Y.

So define with a semi-colon here, I don't want to put a comma because that stands for things like Poisson brackets and so on, or a commutator but define this $\langle X; Y \rangle$ for arbitrary time arguments of the observables X and Y just defined in this fashion here. Then this thing here

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Define $\langle X; Y \rangle_{eq}$

$$= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr}[\rho_{eq} e^{\lambda H_0} X e^{-\lambda H_0} Y]$$

(quantum mech.)
NPTEL

in the quantum case becomes equal to this thing here, becomes equal to beta times, as you can see it becomes A dot of zero semi-colon B of tau,

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function $\phi_{AB}(\tau) = \langle A(0), B(\tau) \rangle_{eq}$

$\langle A(0), B(\tau) \rangle_{eq}$ (classically)

$\frac{1}{\beta} \int_0^\beta d\lambda \text{Tr}[\rho_{eq} e^{\lambda H_0} \dot{A}(0) e^{-\lambda H_0} B(\tau)]$ (quantum mech.) = $\beta \langle \dot{A}(0); B(\tau) \rangle_{eq}$

Define $\langle X; Y \rangle_{eq}$

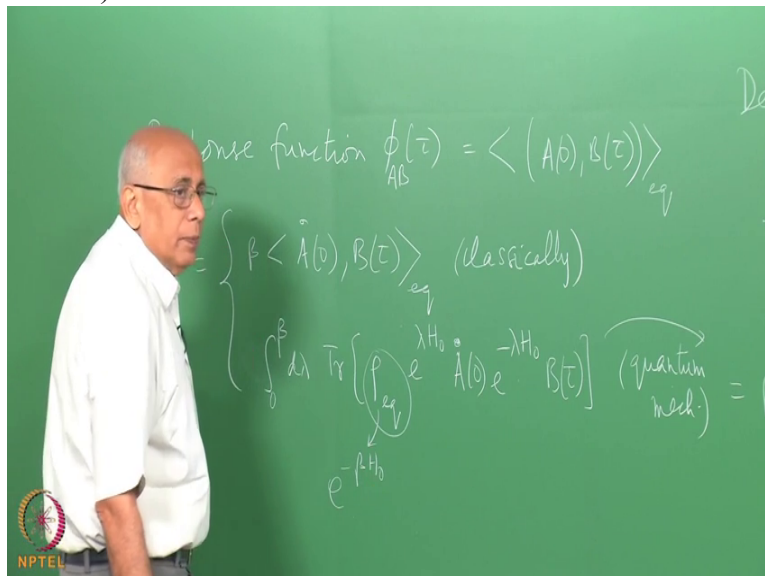
$$= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr}[\rho_{eq} e^{\lambda H_0} X e^{-\lambda H_0} Y]$$

(quantum mech.)
NPTEL

by definition.

So this whole rigmarole with rho equilibrium which is e to the, this quantity remember, is e to the minus beta H naught

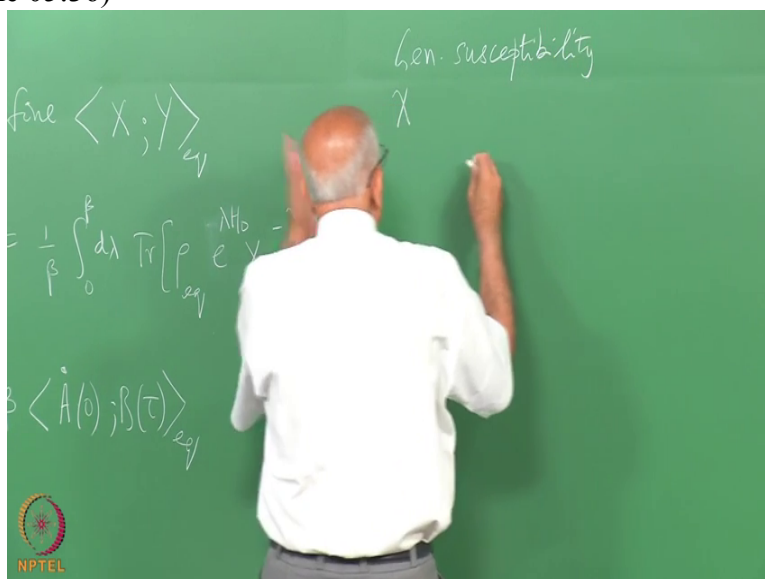
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normalized such that the trace of this quantity is 1. So this makes sure that both the classical and quantum cases look alike. In the classical case the semi-colon is just deleted. It is just gone. It reduces to just the product. In the quantum case you have to order these operators in this careful fashion here.

Now the advantage of doing this is that this response function has a very compact form now. So it immediately tells you that this is a very important formula that the generalized susceptibility corresponding to

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these observables A and B of ω has the compact form $\int_0^\infty d\tau e^{-i\omega\tau} \phi_{AB}(\tau)$ but that is $\beta \langle \dot{A}(0); B(\tau) \rangle_{eq}$ in equilibrium.

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Gen. susceptibility

$$\chi_{AB}(\omega) = \beta \int_0^{\infty} d\tau e^{i\omega\tau} \langle \dot{A}(0); B(\tau) \rangle_{eq}$$

NPTEL

So that is a very compact formula and then the job reduces to computing this number. In a sense it summarizes all of linear response theory. The derivation of this formula here, where this semi-colon bracket has this very specific meaning. Now what is the advantage of doing this?


Well this thing here has lot of interesting properties. To start with, it is stationary, immediately follows that it is stationary. Because let us see what happens to it. This thing here, I want to show that X of any arbitrary t naught Y of t nau/naught, plus t equilibrium, we want to show if it is stationary, it means you can subtract the same time argument from both time arguments here, same constant and you get the same answer.

So this will be equal to X of zero, Y of, you know, t alone. That is stationarity. So this is equal to, Ok.

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Gen. susceptibility

$$\chi_{AB}(\omega) = \beta \int_0^{\infty} d\tau e^{i\omega\tau} \langle \dot{A}(0); B(\tau) \rangle_{eq}$$

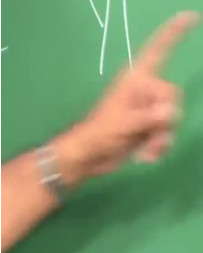
$$\langle X(t_0); Y(t_0+t) \rangle_{eq} = \langle X(0); Y(t) \rangle_{eq} \text{ (stationarity)}$$



I urge you to try and show this is so. What would you do? You would go back to the definition, you go back to this thing here, put in the time arguments in these places and then we know what X of t naught does, for instance this quantity here is equal to e to the i H naught t naught over \hbar cross X of zero, sorry t naught over \hbar cross e to the minus i H naught t naught over \hbar cross.

That is the meaning of X of t naught in the Heisenberg picture,

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$\chi_{AB}(\omega)$

$$\langle X(t_0); Y(t_0+t) \rangle_{eq} = \langle X$$


$$e^{iH_0 t_0/\hbar} X(0) e^{-iH_0 t_0/\hbar}$$


driven by an evolution governed by the unperturbed Hamiltonian, Ok. So for this quantity substitute this in the bracket, in the definition of this semi-colon, for this quantity X of t

naught, put in this quantity here. Because we finally want to show that something involves X of zero alone.

Then for the y part, put in the same thing but with t naught plus t in the exponents. So you get a long, big expression here and then remember that H naught commutes with itself. So e to the $A H$ naught commutes with the e to the $B H$ naught where A and B are scalar numbers. So you can move those two brackets around, those two factors around. And then use the cyclic invariance of the trace.

Whether operators commute or not, $\text{trace } A B$ is $\text{trace } B A$ always. So you should take certain packages, certain parts of this and blocks of these operators and you can transfer it to the left, 0:09:17.9. When you do that, you should get this back again, Ok. So all the H naughts will go away except the one that involves this time argument Y , and you should get this expression here, Ok.

You could also further write this as X of minus t Y of zero. You can subtract anything, same argument; same constant can be subtracted from the two time arguments in this two point correlation, Ok. So the first important quantity of this is stationarity; that helps the great deal, Ok.

The second property is symmetry and this follows in the following way. So let me show this, so the first property is stationarity and the second property is X independent of what time argument you have, regardless of what time argument you have, X of anything Y of anything else, so let us call it X of t_1 Y of t_2 , independent of what t_1 and t_2 are, by the way this is a function of t_1 minus t_2 alone, this quantity is equal to Y of t_2 X of t_1 .

So there is the symmetry property which is a huge


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Gen. susceptibility

$$\chi_{AB}(\omega) = \frac{1}{\beta} \int_0^{\infty} dt e^{i\omega t} \langle \dot{A}(0); B(t) \rangle_{eq}$$

$\lambda H_0 \gamma$ (i) $\langle X(t_2); Y(t_0+t) \rangle_{eq} = \langle X(0); Y(t) \rangle_{eq}$ (stationarity)

(ii) $\langle X(t_1); Y(t_2) \rangle_{eq} = \langle Y(t_2); X(t_1) \rangle_{eq}$ (symmetry)

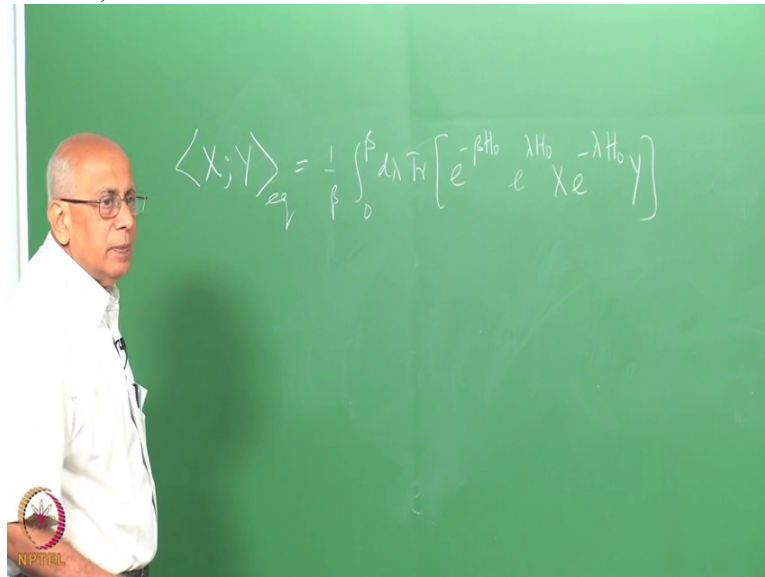


help because it says you can actually commute these fellows around, when you have suscepti/susceptibility, when you have this response function here, for this formula for phi A B, you can, it does not matter which order you put this in here, Ok. Now how do you go about showing that? Well, we really have to go back here and show that this is equal to Y X independent of time arguments etc.

So let us start at this point and this is just a mathematical trick, so it is not very, let us write it out here. X semi-colon Y in equilibrium is equal to 1 over beta, that is the 0:11:43.0 zero to beta d lambda trace e to the minus beta H naught e to the lambda H naught X e to the minus lambda H naught Y, that is this quantity X semi-colon Y, I want to show it is Y semi-colon X, so clearly I am going to exploit the cyclic property of the trace bringing something here and putting it on this side.

So how do you go about it?

(Refer Slide Time 12:17)



I need these lambdas to act on this Y but remember that these two factors do not; these two don't commute, because they do not commute with X necessarily. Of course these two commute, these two do not commute and so on. So H naught X and Y in general are operators which do not commute with each other. How would you then produce, how do you get this across this fellow here? The trick, pardon me?

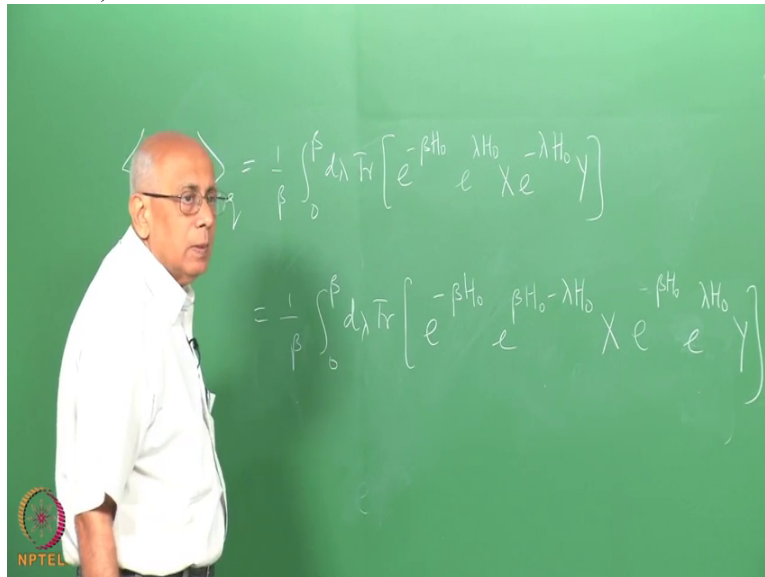
(Professor – student conversation starts)

Student: 0:12:52.0

Professor: Change of integration variable, exactly so set, let us set beta minus lambda to be the variable of integration. Then this is a minus d lambda prime if you put lambda prime is equal to beta minus lambda, the integration runs from zero to beta here, so the minus sign cancels and so this thing is the same as 1 over beta integral zero to d lambda trace e to the minus beta H naught e to the, instead of lambda I should write beta minus lambda, Ok.

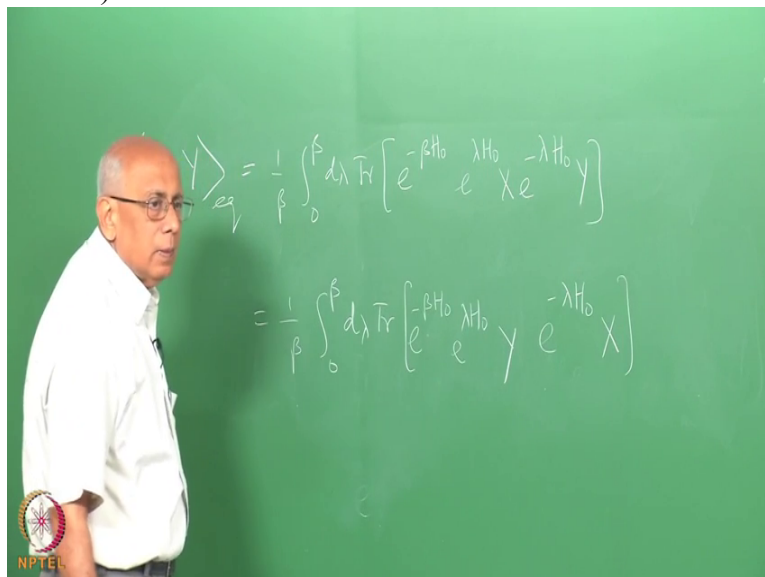
(Professor – student conversation ends)

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Just changing variables of integration. I remove the prime after I change the variables. So these factors go away and you have e to the lambda H naught here and now move this across to this side. So you have e to the minus beta H naught Y e to the lambda H naught, sorry, so I move this whole block as it is, e to the lambda H naught Y and that's gone.

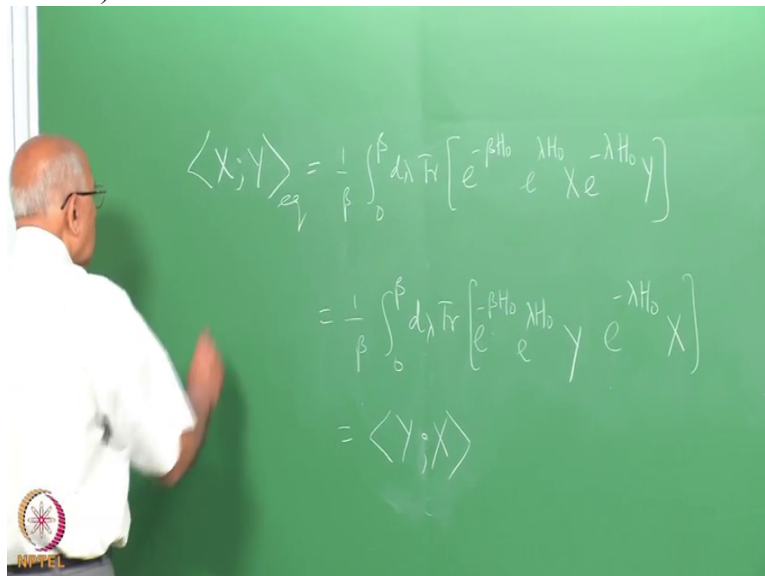
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This is Y semi-colon X.

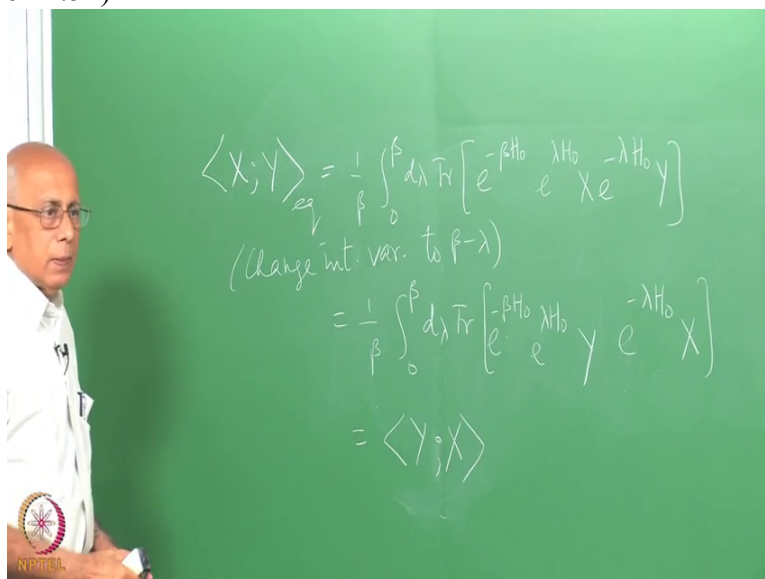
So there is a

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$$\begin{aligned}\langle X; Y \rangle_{eq} &= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[e^{-\beta H_0} e^{\lambda H_0} X e^{-\lambda H_0} Y \right] \\ &= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[e^{-\beta H_0} e^{\lambda H_0} Y e^{-\lambda H_0} X \right] \\ &= \langle Y; X \rangle\end{aligned}$$

change of variable here, change integration variable to beta minus lambda.

(Refer Slide Time 14:51)


$$\begin{aligned}\langle X; Y \rangle_{eq} &= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[e^{-\beta H_0} e^{\lambda H_0} X e^{-\lambda H_0} Y \right] \\ &\quad \text{(change int. var. to } \beta - \lambda \text{)} \\ &= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[e^{-\beta H_0} e^{\lambda H_0} Y e^{-\lambda H_0} X \right] \\ &= \langle Y; X \rangle\end{aligned}$$

That gives you the symmetric property. So you can see the great advantage of defining the semi-colon bracket because it is almost behaving classically. You can put these two fellows in either order, you don't care. It is stationary, it is symmetric.

Once you have that notation in place, then actually you can play around with it as if these are classical objects provided you have that semi-colon in between 0:15:22.0. And it has got another very important property, the third one which is the following.

I expect, I expect that this, if A and B are observables, they are represented by Hermitian operators if they are physical observables, real physical observables. I then expect that if I apply a real force the response should be real, real quantity. So I want certain reality properties of this whole thing. I would like to show that the response function must satisfy certain symmetry properties in order that the response to real force be real, Ok.

So let us do that in slow steps. Let us first take what happens if you take the complex conjugate of this semi-colon bracket. So let us find $\langle X \rangle_{eq}$ semi-colon $\langle Y \rangle_{eq}$ star complex conjugate. This is equal to 1 over beta, zero over beta d lambda e to the, trace H naught this fashion, sorry. Trace of this fellow

(Professor – student conversation starts)

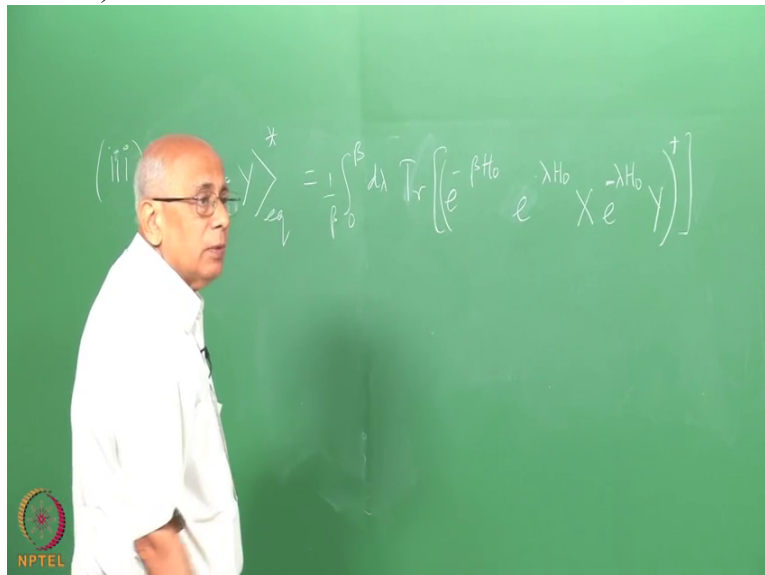
Student: lambda is not the 0:17:08.2

Professor: Pardon me?

Student: Lambda is not X e power minus 0:17:13.0

Professor: Oh yeah, this is plus and this is minus, thank you, right. And I need the Hermitian conjugate of this.

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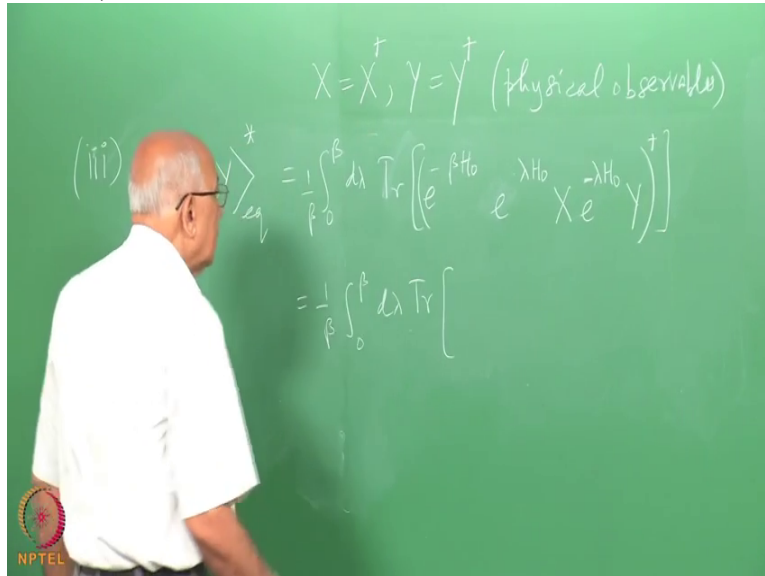


So that is equal to 1 over beta integral zero to beta d lambda trace, then of course when I take the Hermitian conjugate of a product of operators, they appear in the reverse order. So now we are looking at what happens if A and B are, X and B are, X and Y are Hermitian.

(Professor – student conversation ends)

So X equal to X dagger, Y equal to Y dagger. These are physical observables. So once I have this,

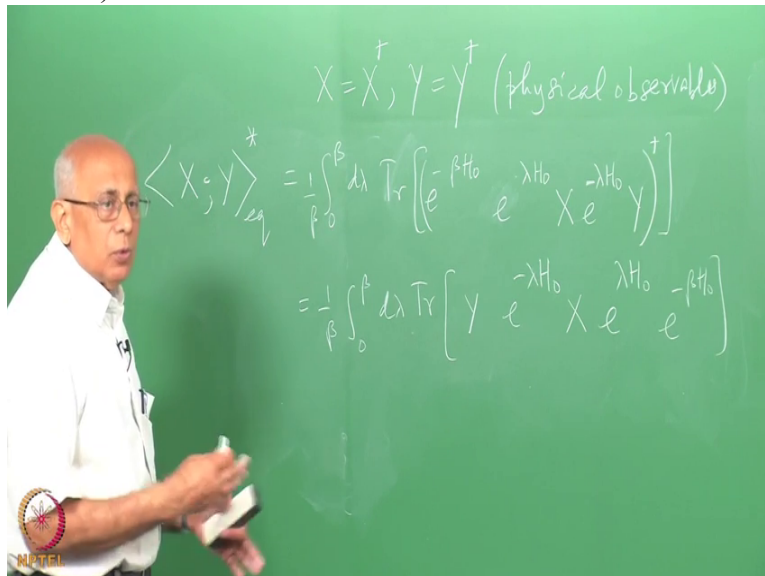
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all I have to do is to reverse the order. So it is equal to Y , Y dagger is the same as Y , H naught is Hermitian, the Hamiltonian, so e to the minus beta H naught is Hermitian, that is this fellow and then X and then this fellow and then this guy.

Now the same trick

(Refer Slide Time 18:37)



as before. We change variables of integration. So this is 1 over beta, integral zero to beta d lambda trace $Y e$ to the minus, so I am instead of lambda I am going to say lambda prime is beta minus lambda, so lambda is beta minus lambda prime.

(Refer Slide Time 19:10)

$X = X^\dagger, Y = Y^\dagger$ (physical observable)

(ii) $\langle X, Y \rangle_{eq}^* = \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[e^{-\beta H_0} e^{\lambda H_0} X e^{-\lambda H_0} Y \right]$

$\lambda' = \beta - \lambda$

$= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[Y e^{-\lambda H_0} X e^{\lambda H_0} e^{-\beta H_0} \right]$

$= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[Y e^{-\beta H_0} \right]$

(Refer Slide Time 19:15)

$X = X^\dagger, Y = Y^\dagger$ (physical observable)

(ii) $\langle X, Y \rangle_{eq}^* = \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[e^{-\beta H_0} e^{\lambda H_0} X e^{-\lambda H_0} Y \right]$

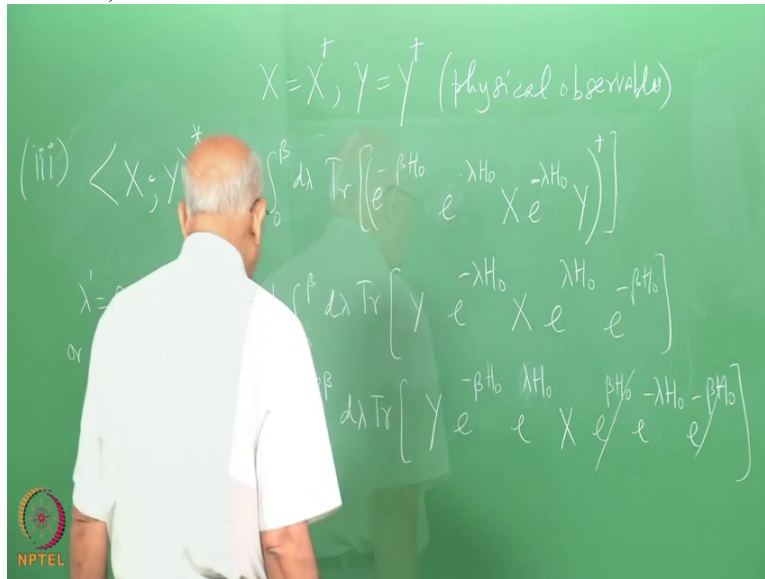
$\lambda' = \beta - \lambda$
 or $\lambda = \beta - \lambda'$

$= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[Y e^{-\lambda H_0} X e^{\lambda H_0} e^{-\beta H_0} \right]$

$= \frac{1}{\beta} \int_0^\beta d\lambda \text{Tr} \left[Y e^{-\beta H_0} \right]$

So minus lambda is minus beta plus lambda prime. And then this H is e to the beta H naught e to the minus lambda H naught, there is an extra beta H naught somewhere, yes that is Ok, it is Ok. Now this factor cancels against this 0:19:56.8, because it commutes through H naught here.

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So where are we now? Yes. Yes now it is a simple matter.

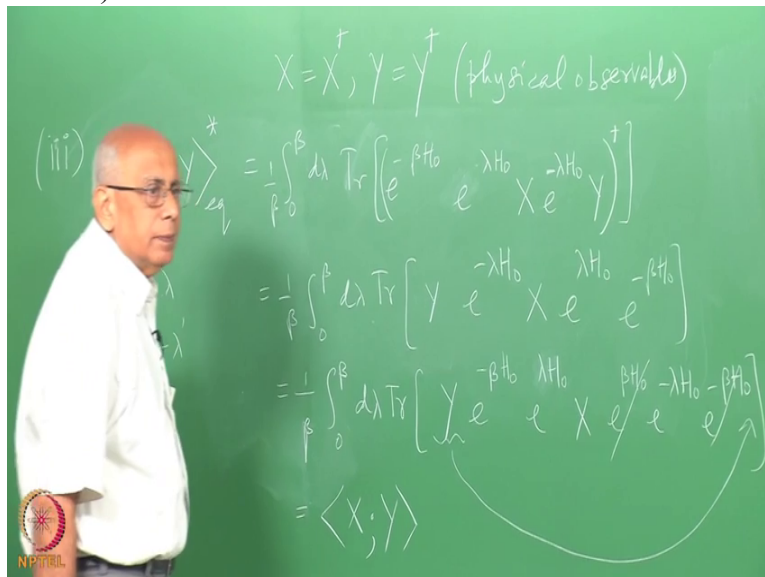
(Professor – student conversation starts)

Student: Take Y

Professor: Take Y to the end. We will take this fellow, integrate all the way 0:20:24.5. So this is equal to,

(Professor – student conversation ends)

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So the third property is reality. The response function therefore written in this form is stationary, symmetric and real, real for Hermitian operators. That immediately implies a certain symmetry property here. We will see what consequence of it is. The consequence

(Refer Slide Time 21:02)

$$\begin{aligned}
 X &= X^\dagger, Y = Y^\dagger \text{ (physical observable)} \\
 \text{(iii)} \quad \langle X; Y \rangle_{eq}^* &= \frac{1}{\beta} \int_0^\beta d\lambda \operatorname{Tr} \left[e^{-\beta H_0} e^{-\lambda H_0} X e^{-\lambda H_0} Y e^{-\lambda H_0} \right] \\
 \lambda' = \beta - \lambda & \\
 \text{or } \lambda = \beta - \lambda' & \\
 &= \frac{1}{\beta} \int_0^\beta d\lambda \operatorname{Tr} \left[Y e^{-\lambda H_0} X e^{-\lambda H_0} e^{-\beta H_0} \right] \\
 &= \frac{1}{\beta} \int_0^\beta d\lambda \operatorname{Tr} \left[Y e^{-\beta H_0} e^{-\lambda H_0} X e^{-\lambda H_0} e^{-\beta H_0} \right] \\
 &= \langle X; Y \rangle \text{ (Reality)}
 \end{aligned}$$

is that, so this quantity is real if A dot and B are Hermitian.

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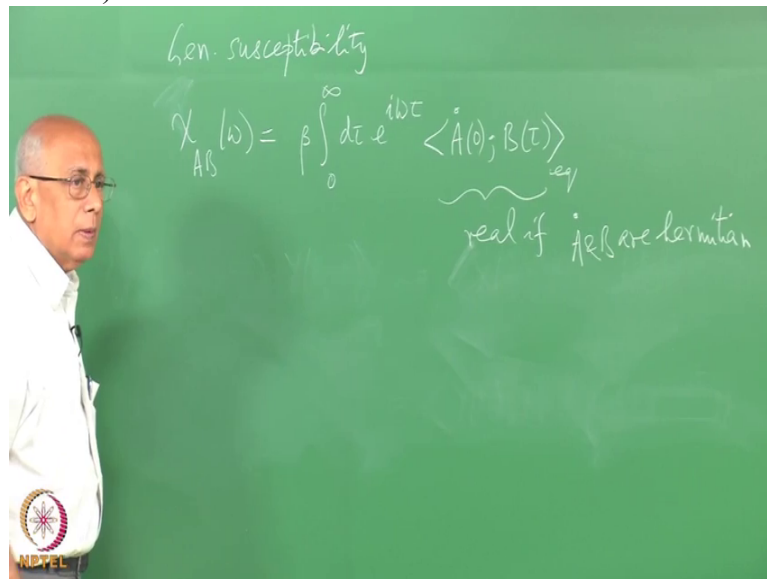
Gen. susceptibility

$$\chi_{AB}(\omega) = \beta \int_0^\infty d\tau e^{i\omega\tau} \langle \dot{A}(0); B(\tau) \rangle_{eq}$$

real if \dot{A}, B are hermitian

Instead of

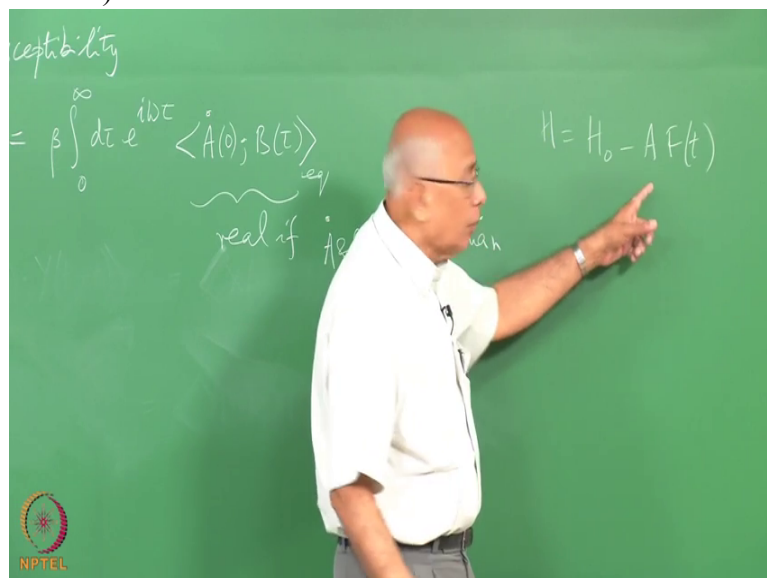
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X I call it A dot; instead of Y I call it B. We have just seen that it is real if A dot and B are Hermitian, Ok.

Now what appears in the Hamiltonian, if you recall, is this. If you remember perturbation or total Hamiltonian was equal to H was H naught minus A F of t. This was the operator

(Refer Slide Time 21:46)



that appeared, not A dot. A dot came because of manipulations in between, Ok. So A is certainly a Hermitian operator. I apply a real force to the system, H naught is the Hermitian operator, A is the physical observable and the Hamiltonian has to be Hermitian so this is Hermitian here but what is the guarantee that A dot is Hermitian? How do I know that if A is Hermitian, the operator A dot is also Hermitian?

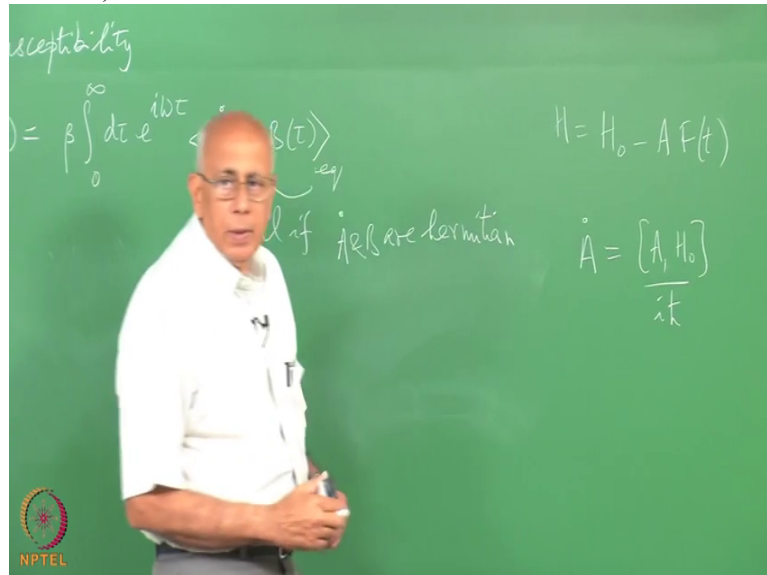
I mean this sounds like common sense, right because if, after all, if A is the position, \dot{A} is the velocity. And it is as real or as physical as the position itself. But what is the guarantee in general that for some arbitrary observable A which is Hermitian, represented by Hermitian operator, what is the guarantee that the operator \dot{A} is also a Hermitian operator?

(Professor – student conversation starts)

Student: 0:22:50.9 Commutative

Professor: Commutative, yeah exactly. So you would write \dot{A} , the operator \dot{A} at any time is equal to

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A right basically. This is Hermitian, that is Hermitian so is the commutator Hermitian?

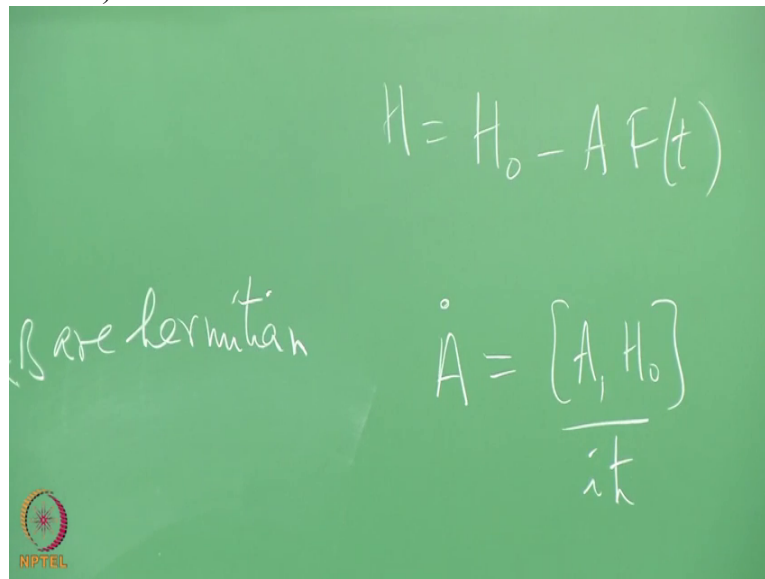
Student: 0:23:16.9

Professor: Pardon me?

Student: Anti-Hermitian

Professor: Anti-Hermitian, commutator of 2 Hermitian operators

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is anti-Hermitian, of course because $AB - BA$ becomes $BA - AB$ when you take the Hermitian conjugate, right? That is saved by this guy. That changes sign too. Therefore if A is Hermitian, \dot{A} is Hermitian, Ok. The commutator of two physical observables, represented by Hermitian operators has to be anti-Hermitian. And you put another i there, it becomes Hermitian, Ok.

(Professor – student conversation ends)

So we are in good shape. This says this is real if \dot{A} and A are Hermitian operators. Now if I apply a real force to a real system, I expect a real response. On the other hand I know that, I know the following. I know that if I apply the force $F \text{ naught } e$ to the minus $i \omega t$ to the system, this was my general force expression, for a particular frequency ω , right, so the force was this implies response $kai AB$ of $\omega F \text{ naught } e$ to the minus $i \omega t$.

That is the response; that is how we defined the generalized susceptibility.


(Refer Slide Time 24:49)

Gen. susceptibility

$$\chi_{AB}(\omega) = \beta \int_0^{\infty} dt e^{i\omega t} \langle \dot{A}(0); B(t) \rangle$$

real if A, B are hermitian

Force $F_0 e^{-i\omega t} \Rightarrow$ Response $\chi_{AB}(\omega) F_0 e^{-i\omega t}$



It was the quantity that attenuated, the force which was applied with one particular value of frequency. Any frequency component, if the force has an amplitude F naught, the response was the same thing multiplied by this, generalized susceptibility, right?

So if the force and it is the linear response, so if the force is F naught star e to the plus i omega t , if that is the force, then what should the response be? You can read it off from here. The force has got a term, sinusoidal oscillation e to the plus i omega t , right? So the response has to be $kai A B$ of minus omega, F naught star e to the i omega t .

It has to be so


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$$\chi_{AB}(\omega) = \beta \int_0^{\infty} dt e^{i\omega t} \langle \dot{A}(0); B(t) \rangle$$

real if A, B are hermitian

Force $F_0 e^{-i\omega t} \Rightarrow$ Response $\chi_{AB}(\omega) F_0 e^{-i\omega t}$

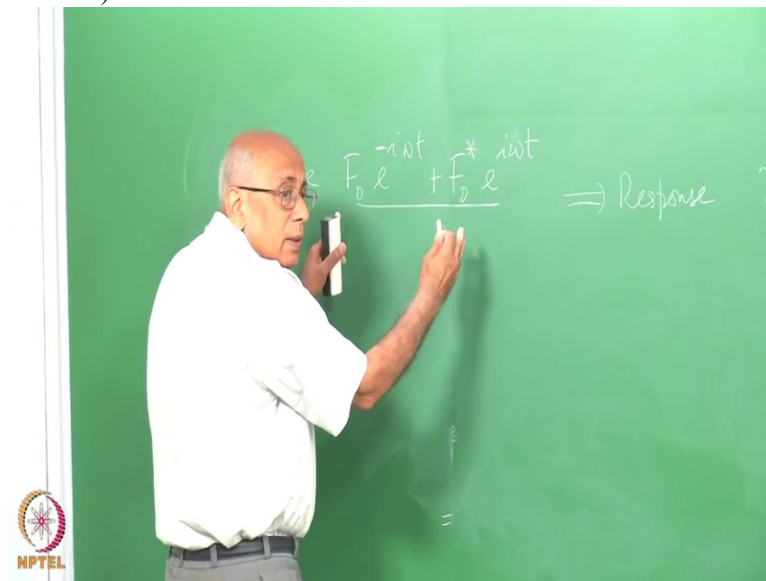
Force $F_0^* e^{i\omega t} \Rightarrow$ Response $\chi_{AB}^*(-\omega) F_0^* e^{i\omega t}$



because it is linear response. I can put whatever amplitude I like, whatever frequency I like and compare with this. If I add these 2 fellows, if I add these 2 forces, then what do I get? Immediately implies therefore if the force is $F_0 e^{i\omega t} + F_0 e^{-i\omega t}$, I take the half the amplitude in each case, must imply a response kAB of $\omega F_0 e^{-i\omega t} + kAB$ of $\omega F_0 e^{i\omega t}$ divided, over by t .

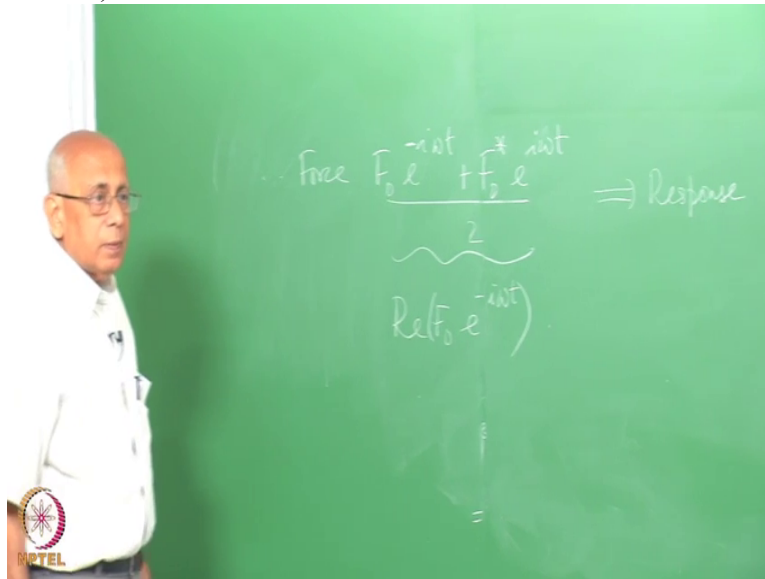
But this object here

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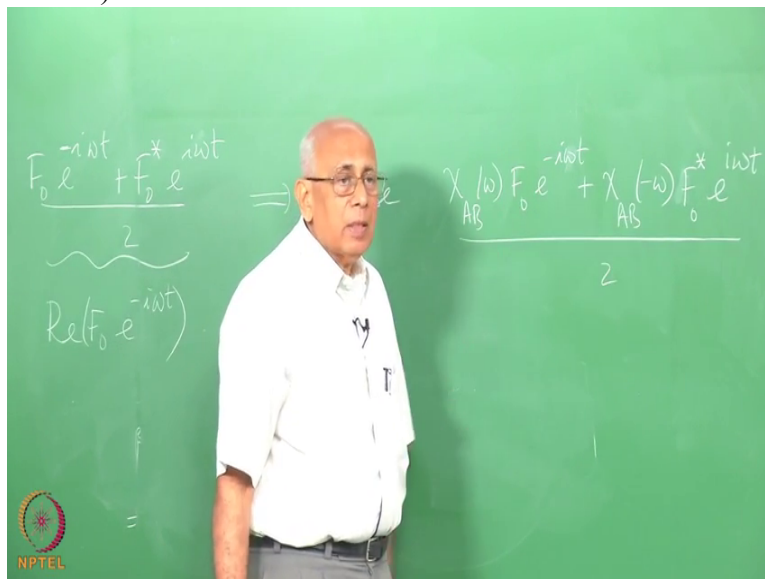
is real, it is a real part of, so this whole thing, it says the real part of $F_0 e^{-i\omega t}$ plus the real part of $F_0 e^{i\omega t}$.

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So that is the real force. The response has to be real. So this must be the real part of some

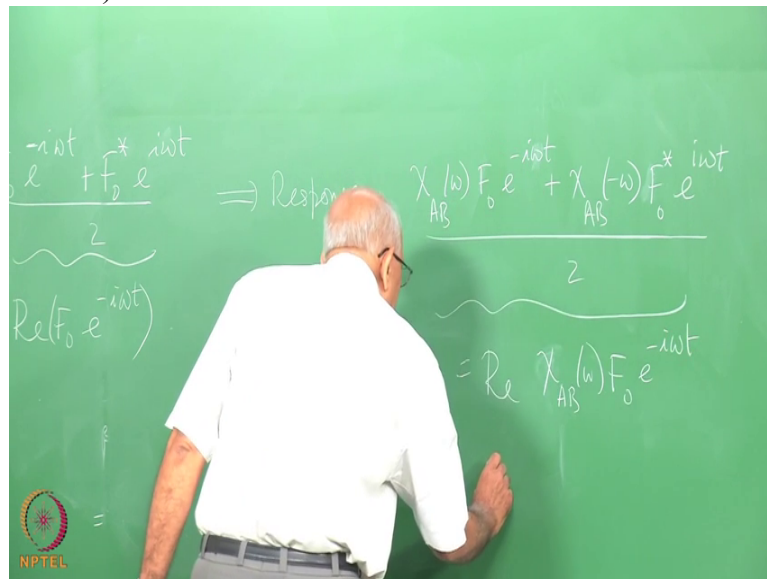
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complex number. We are almost there. Here is F_0 naught, here is F_0 naught star, here is $e^{-i\omega t}$ plus $e^{i\omega t}$ so this would be real. So this would be real

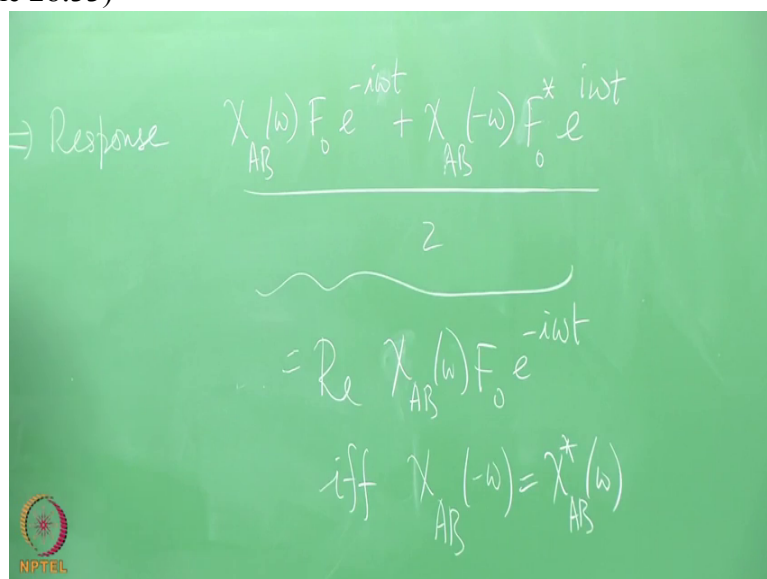
So this 0:27:54.5 part equal to the real part of $\frac{\chi_{AB}(\omega) F_0 e^{-i\omega t} + \chi_{AB}(-\omega) F_0^* e^{i\omega t}}{2}$ provided

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if and only if this part is the complex conjugate of this guy, there is no other way, if and only if $\chi_{AB}(-\omega) = \chi_{AB}^*(\omega)$,

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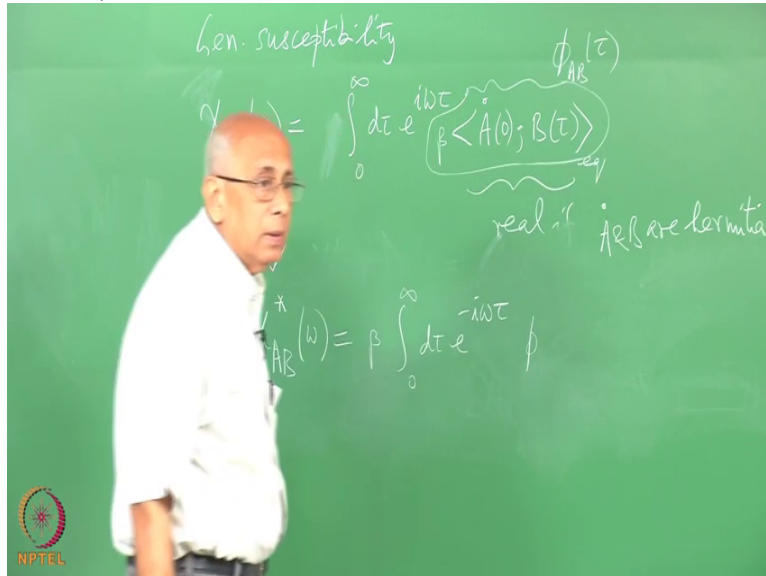


right? You see the argument. All I used is the superposition principle and the definition of the generalized susceptibility, Ok

That leads me to the conclusion that if I apply a real force, the physical force then the response is real if A and B are Hermitian if and only if this condition is satisfied for real ω . But let us look at what the complex conjugate is. This implies that $\chi_{AB}(-\omega) = \chi_{AB}^*(\omega)$, this quantity here, I take complex conjugate, this must be equal to β times integral

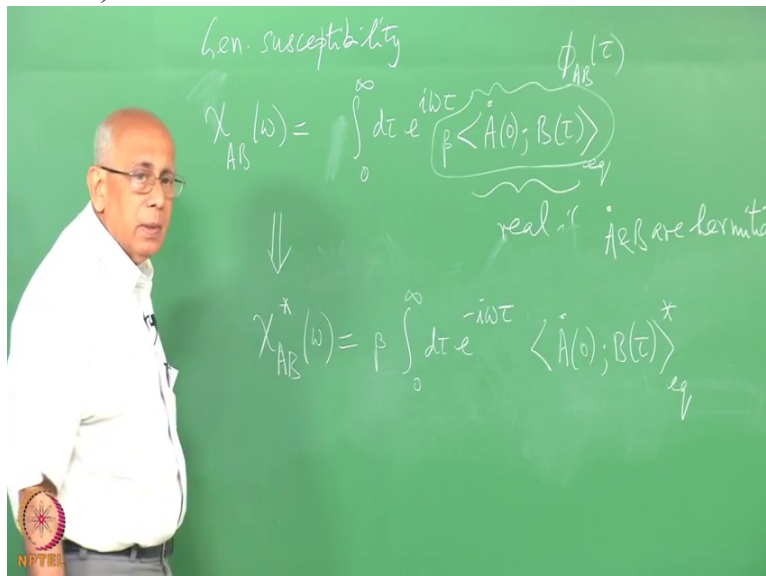
zero to infinity d tau e to the minus i omega tau, right times this quantity phi A B, this was equal to, apart from this beta, this fellow here was equal to phi A B of tau, right?

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So this is equal to out here, A dot of zero B of tau equilibrium complex conjugated, because I am taking the complex conjugate.

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So this however is equal to kai A B of minus omega provided this is equal to its own complex conjugate, provided that is real.

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Gen. susceptibility

$$\chi_{AB}(\omega) = \int_0^{\infty} dt e^{i\omega t} \frac{1}{\beta} \langle \dot{A}(0); B(t) \rangle_{eq}$$

$\phi_{AB}(t)$

real if \dot{A} & B are hermitian

$$\chi_{AB}^*(\omega) = \frac{1}{\beta} \int_0^{\infty} dt e^{-i\omega t} \langle \dot{A}(0); B(t) \rangle_{eq}^*$$

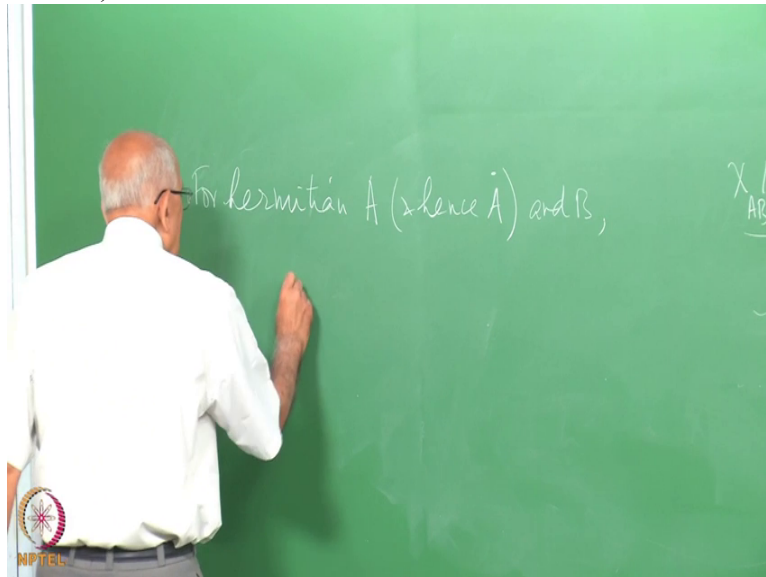
$$= \chi_{AB}(-\omega) \text{ provided } \langle \dot{A}(0); B(t) \rangle_{eq} \text{ is real.}$$


But we just saw for Hermitian operators that is real, Ok.

So the physical reason why you want that response function to be real is that it ensures that when you are dealing with the susceptibility involving Hermitian physical operators, you apply real perturbation, the response also is real. That is guaranteed by the fact that this correlation function even in the quantum case, we don't care, even there it is real, guaranteed to be real. Otherwise we will be in trouble. It would lead to an inconsistency.

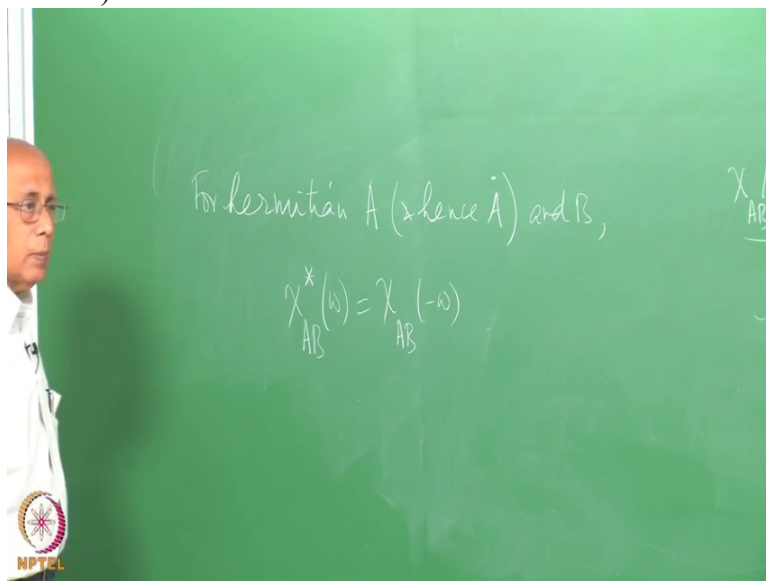
So that is good, that we have seen that the reality of this quantity, this response function ensures that the susceptibility has this symmetry property which is needed to ensure that the response to a real force is real. Now the consequence to this in turn is immediate. So again now we are specializing to A and B or \dot{A} and B , Hermitian, so and hence \dot{A} and B

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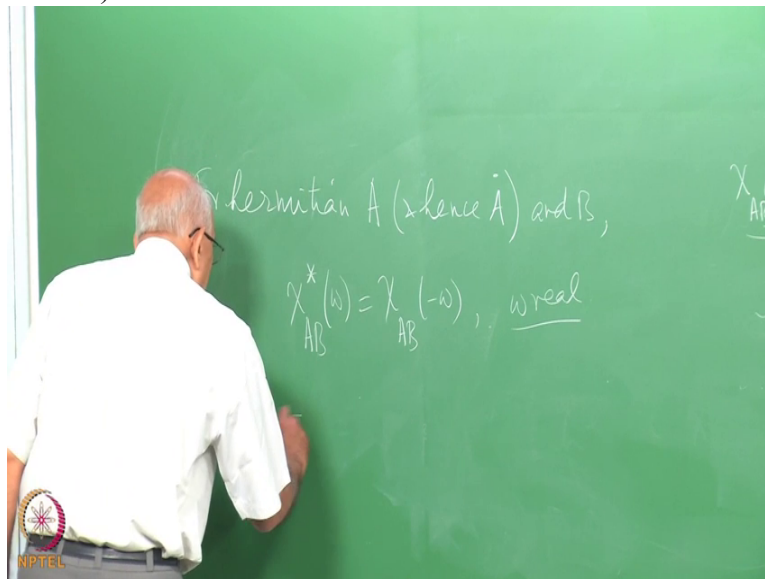
kai A B star of omega equal to kai A B of minus omega.

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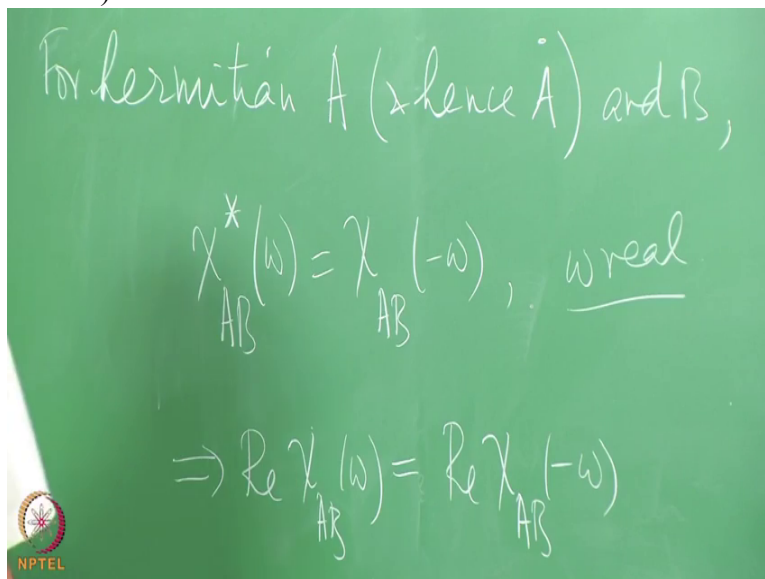
I want to emphasize that this, this of course we have assumed omega to be real. When I took the complex conjugate of this quantity, I just put e to the minus i omega tau which would only be true if omega is real, time of course is real, so there is no problem, tau is real but we want to make sure omega is also kept real. Because very soon, in a minute, we are going to talk about complex omega, Ok.

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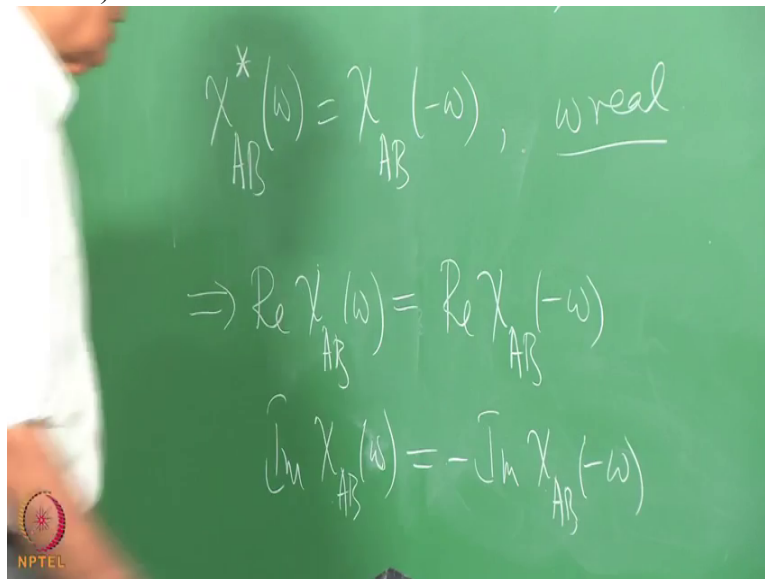
By the way this implies immediately that the real part of $X_{AB}(\omega)$ is equal to the real part of $X_{AB}(-\omega)$. Take real parts on both sides and you see that it is a symmetric function.

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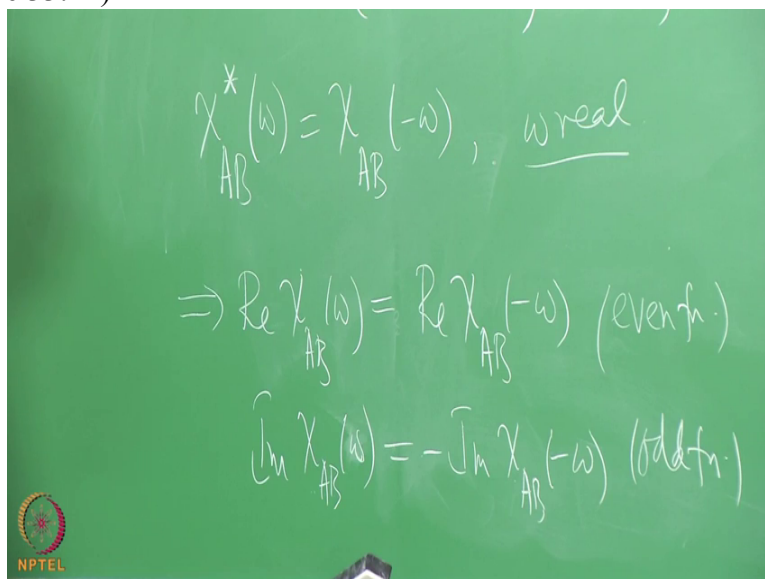
The imaginary part, $X_{AB}(\omega)$ equal to minus the imaginary part $X_{AB}(-\omega)$, it is an odd function. So

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$$X_{AB}^*(\omega) = X_{AB}(-\omega), \quad \omega \text{ real}$$
$$\Rightarrow \text{Re } X_{AB}(\omega) = \text{Re } X_{AB}(-\omega)$$
$$\text{Im } X_{AB}(\omega) = -\text{Im } X_{AB}(-\omega)$$

this is an even function and that is an odd function. It is going to be useful, right?

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$$X_{AB}^*(\omega) = X_{AB}(-\omega), \quad \omega \text{ real}$$
$$\Rightarrow \text{Re } X_{AB}(\omega) = \text{Re } X_{AB}(-\omega) \text{ (even fn.)}$$
$$\text{Im } X_{AB}(\omega) = -\text{Im } X_{AB}(-\omega) \text{ (odd fn.)}$$

So there are these symmetric properties. This is going to be useful because physically you talk of real values of omega which are also positive, non-negative. But we are going to talk about analytic properties in omega, in the omega plane which will involve integrals over negative values of omega. But they can be got rid of by using these properties. So you can fall things back on to the positive real axis, Ok. Now

(Professor – student conversation starts)

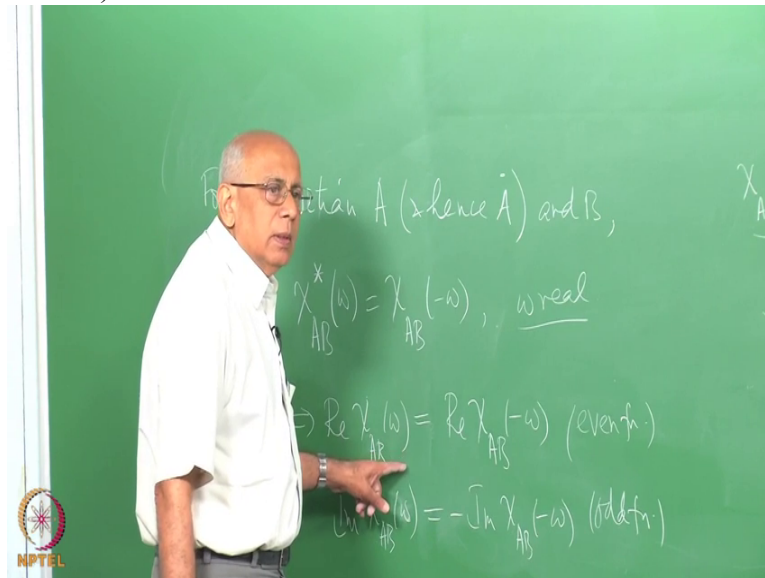
Student: 0:34:16.2

Professor: Yeah, a very often I do the opposite. I want to draw contour integrals and so on, so we will see, we will go back and forth.

(Professor – student conversation ends)

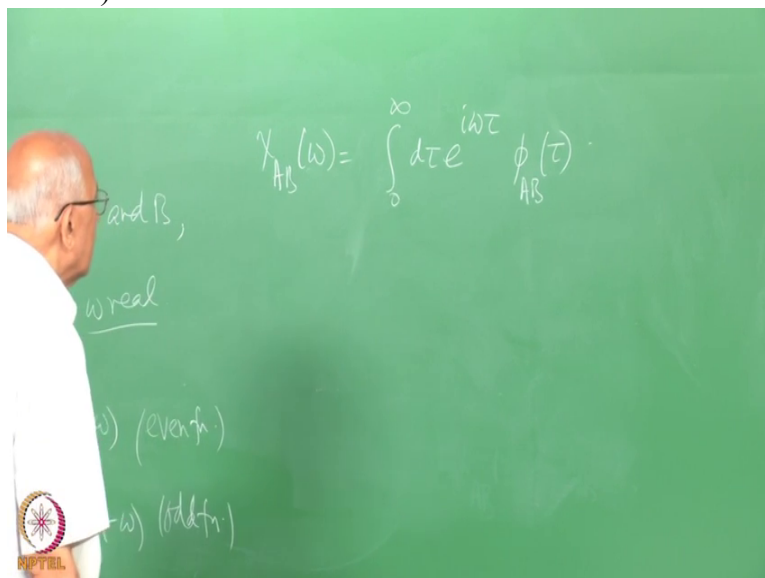
The point is that if you know this quantity

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for some positive omega you also know it for negative omega by this symmetric property. But now there is a very interesting property of analytic behavior and let me do this by motivating it, starting with this formula which is this one. So, sorry you don't have this.

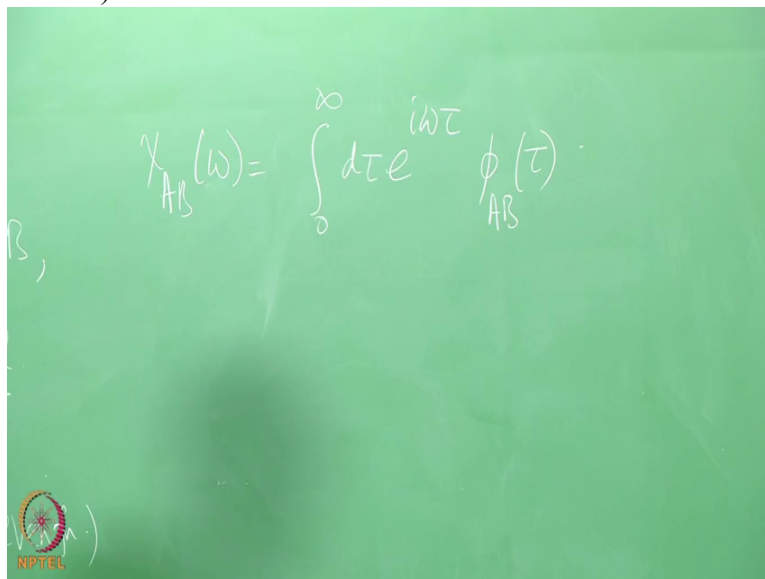
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And we have seen that this is real for Hermitian A and B, and therefore for A dot and B, and we have seen that it is symmetric in A and B exchange and we have seen that it is real, symmetric and stationary, Ok. Now if this integral exists for real values of omega, this is an oscillatory factor, then in general they should go to zero as tau goes to infinity. So that the integral converges, Ok.

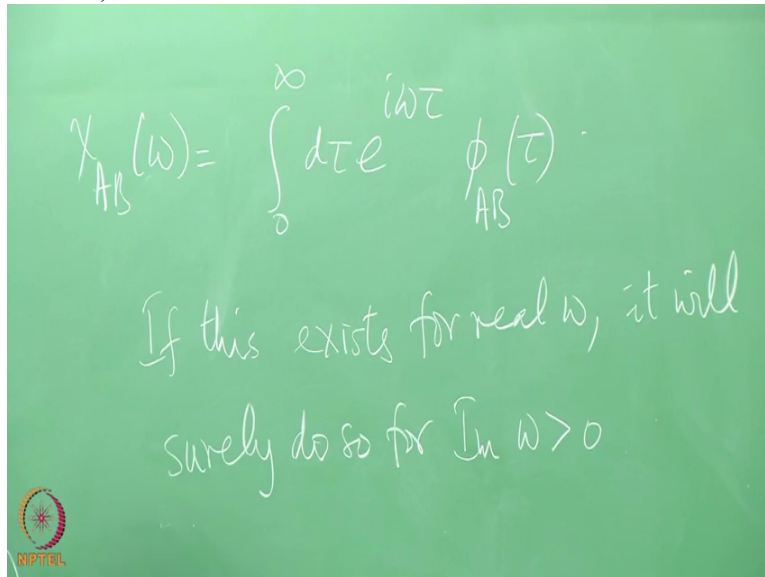
If that is so, if I add a convergent factor to it, then the integral gets more and more convergent.

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$$\chi_{AB}(\omega) = \int_0^{\infty} d\tau e^{i\omega\tau} \phi_{AB}(\tau)$$

So if this exists, if this exists, and that is by no means guaranteed, we don't know for sure, we got to look at it, if this exists for real omega, by exists I mean if it is convergent for real omega it will certainly do so for imaginary omega greater than zero. So I make omega complex purely as a mathematical exercise.

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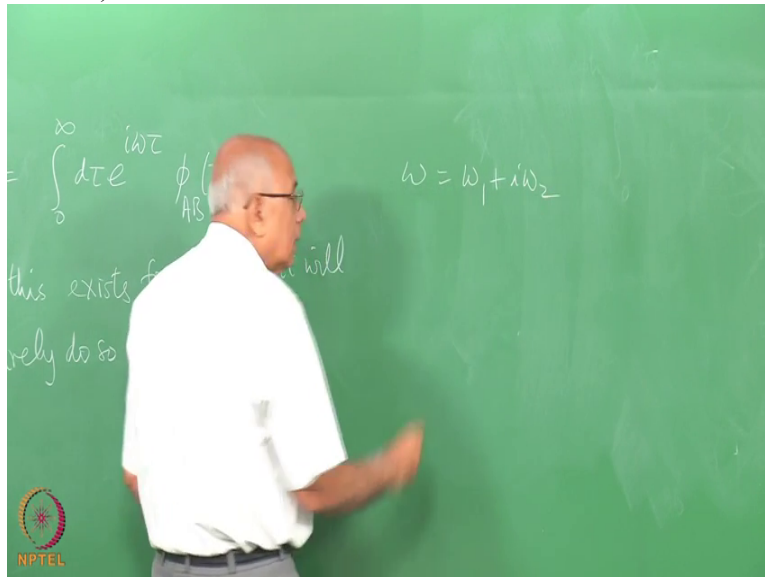
The image shows a green chalkboard with handwritten text. At the top, the formula $\chi_{AB}(\omega) = \int_0^{\infty} d\tau e^{i\omega\tau} \phi_{AB}(\tau)$ is written. Below it, the text reads: "If this exists for real ω , it will surely do so for $\text{Im } \omega > 0$ ". In the bottom left corner, there is a small circular logo with the word "NPTEL" underneath it.

I know physical frequencies are real but here is a formula which is a function of omega. And I say alright, very nice, let me talk; think about this in terms of the complex variable omega, purely as a mathematical excursion. There will be a reason for doing so. Then the question is does it exist, does it make sense?

Well in general, if you are familiar with the theory of analytic continuation then you know that if something is analytic in the complex variable sense on dense set then you actually have some continuous set of, some suitable kind of set in the complex plane, then you can define in general analytic continuations of this function to the rest of the complex plane or to some region of the complex plane called the domain of whatever holomorphy or something.

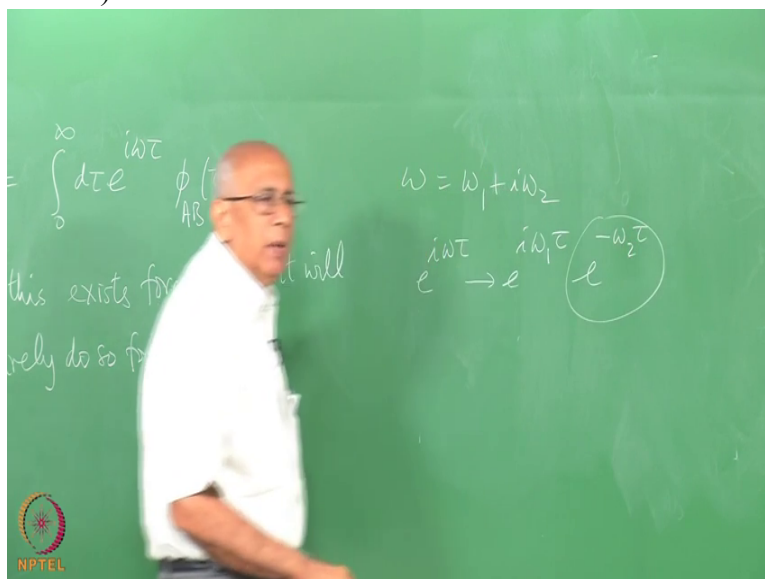
But now we will look at this very heuristically. If I put omega equal to omega 1 plus i omega 2

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then this factor e to the $i\omega\tau$ becomes e to the $i\omega_1\tau$ times e to the minus $\omega_2\tau$. So there is an extra

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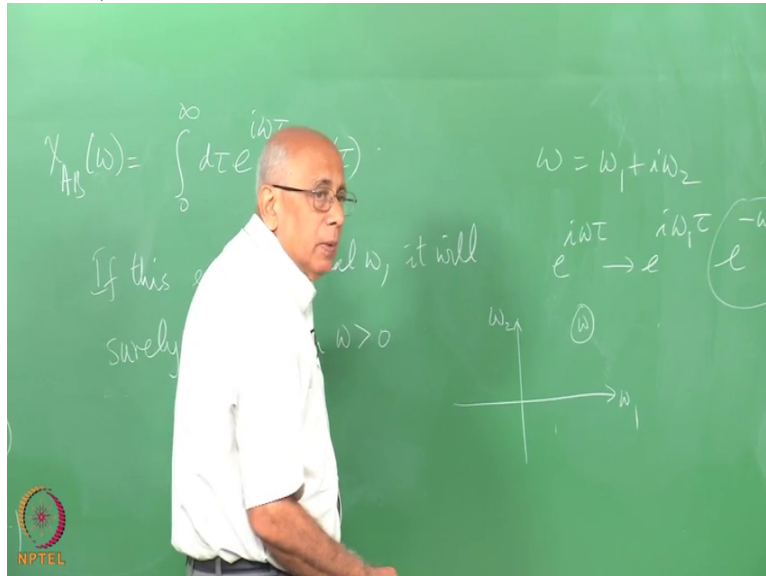


damping factor provided ω_2 is positive. ω_2 is the imaginary part of ω and if it is positive, then since τ runs only over positive values, you are guaranteed that this provides you with an extra convergence factor out here.

It is crucially dependent on the fact that τ runs only over positive values. If τ had gone to minus infinity then this is finished, you cannot do this, Ok. So this means that the formula as it stands makes sense even for complex ω as long as the real, imaginary part of ω is

positive, in other words as long as you move into the upper half plane. So what we have is a situation, in the complex omega plane this is omega 1 and that is omega 2, the imaginary part,

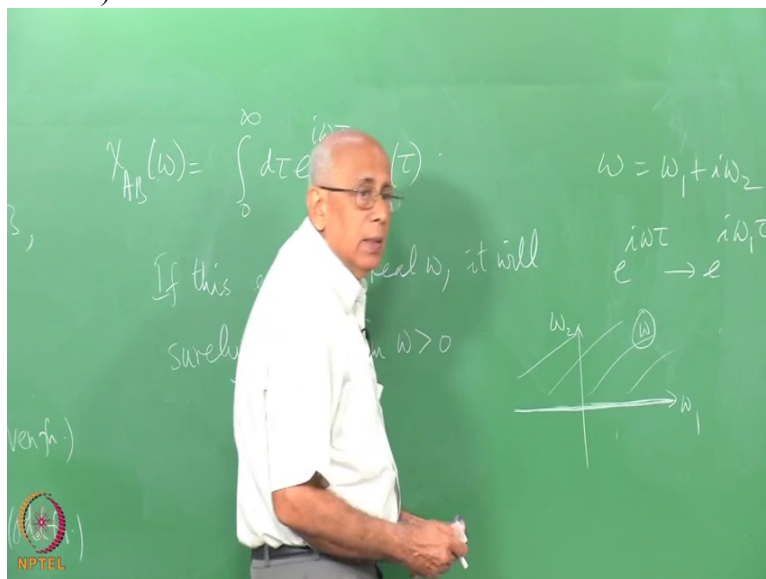
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you assume this formula all along the real axis and you set by assumption that this formula defines for your function of omega through this convergent integral for all real omega.

It follows as a consequence of that assumption that if you move up into the complex omega plane throughout up here

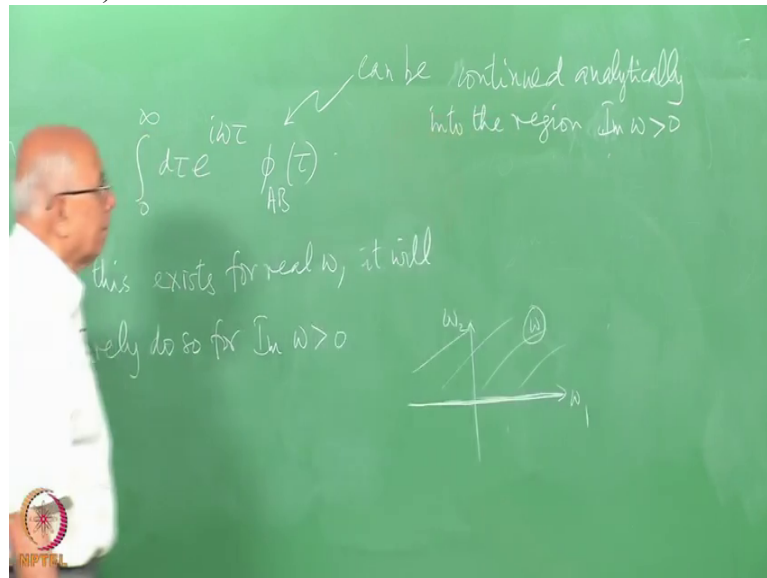
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at any value of omega to find the value of this function at that value of omega all you got to do is to substitute that value of omega in this formula and it makes sense. So the formula

provides an analytic continuation into the upper half plane. So this thing here can be analytically continued...

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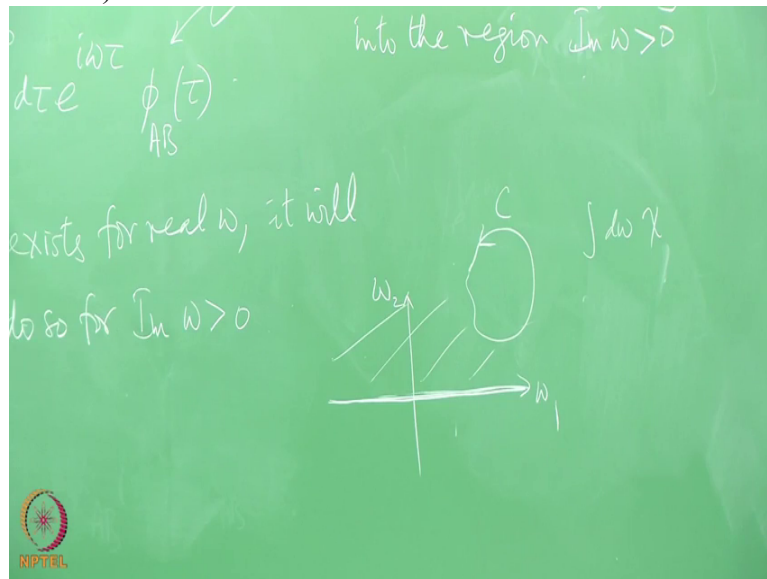


And moreover you are guaranteed it defines an analytic function there. You can therefore differentiate it any number of times as you know in analytic function of a complex variable is a very special kind of function. It means it satisfies the Cauchy Riemann conditions between the real and imaginary parts. It means that every derivative of this function exists and is also an analytic function satisfying the Cauchy Riemann condition.

There is a Cauchy integral formula for this and then you also know that the line integral of this function round any closed contour is, provided the contour stays entirely in the region of analyticity and does not enclose any singularities, the answer is zero. So is everybody familiar with these theorems? Ok. So once we have that in place then it provides a very powerful handle.

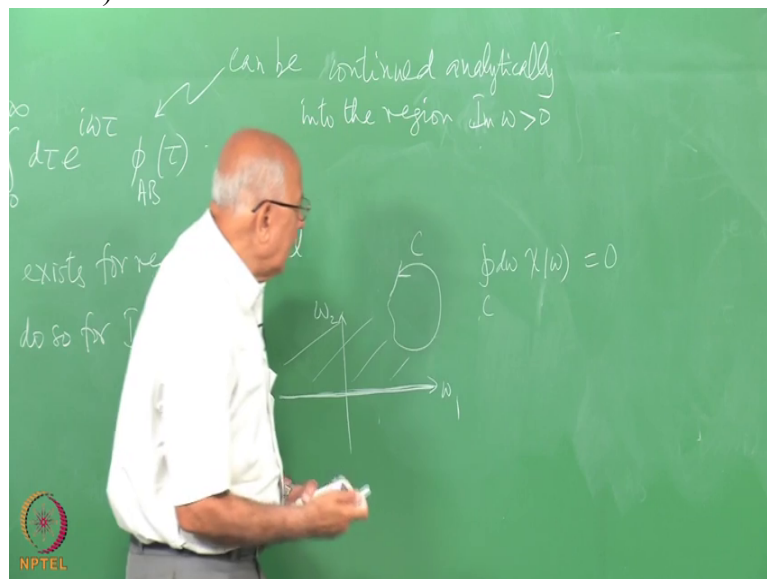
It says if you start anywhere and you draw closed contour like this C, the integral of $d\omega$, let me drop the subscript A B all the time because it is true for any A and B

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as long as whatever properties you established so far are true, so let us for convenience, simplicity in notation drop this and just call it γ of ω , this over this contour C is equal to zero, provided

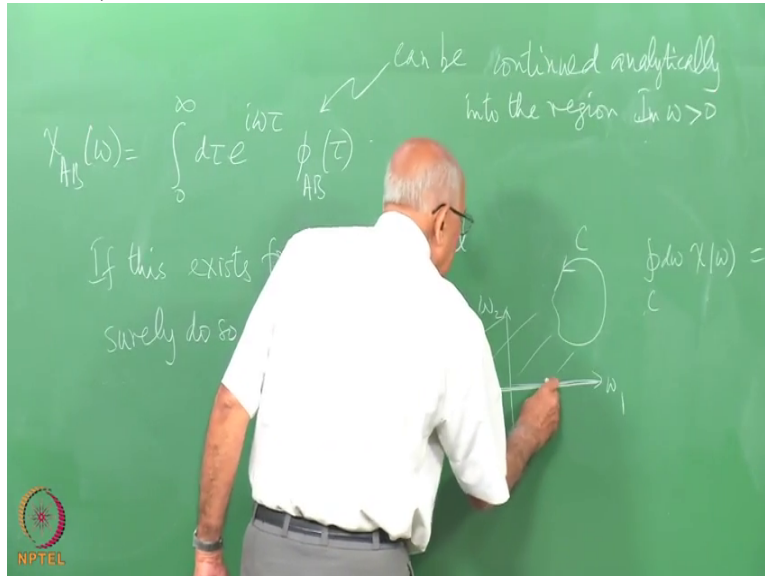
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C does not get anywhere into the lower half plane, provided it remains in the region of analyticity of this function which is the upper half plane and the real axis by assumption.

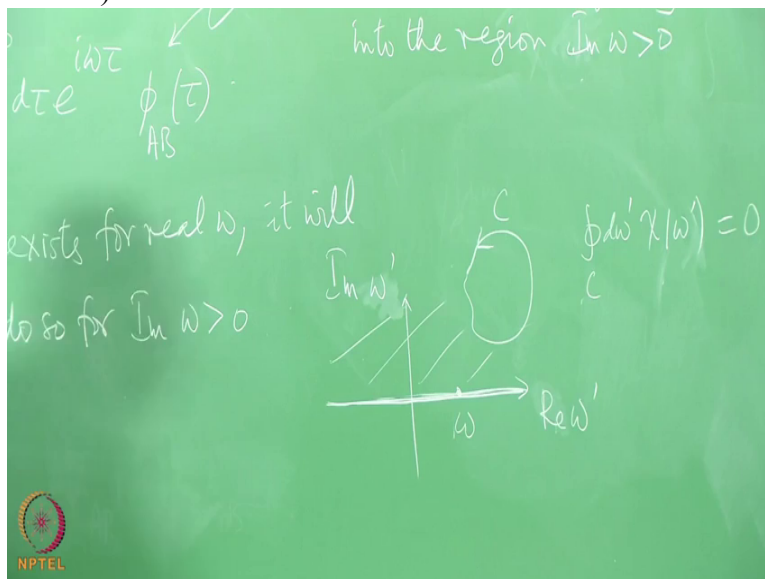
So that's the consequence of Cauchy's theorem, integral formula or whatever you call it. It is the consequence of the fact that this thing is a nice analytic function, Ok. So now suppose you start with some value of ω on the real axis which we are interested in. Let us suppose I start with some fixed value of ω here.

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And I want to choose another symbol for the integration symbol, so let me call this omega and let me call this real omega prime and this is imaginary omega prime.

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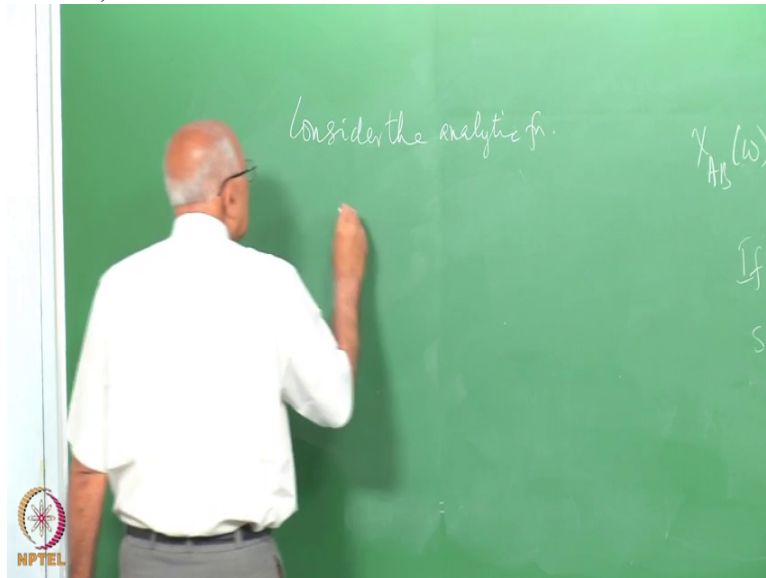


I want to make sure, and this is certainly true.

Now I can distort this contour as I please provided I never come down below here, right. And what I would like to do is to use this property to derive a formula, and that is the target for kai at this point, this physical point, in terms of an integral over kai over the rest of the real axis, Ok. And the way to do that is to single out this point here. How do I single it out?

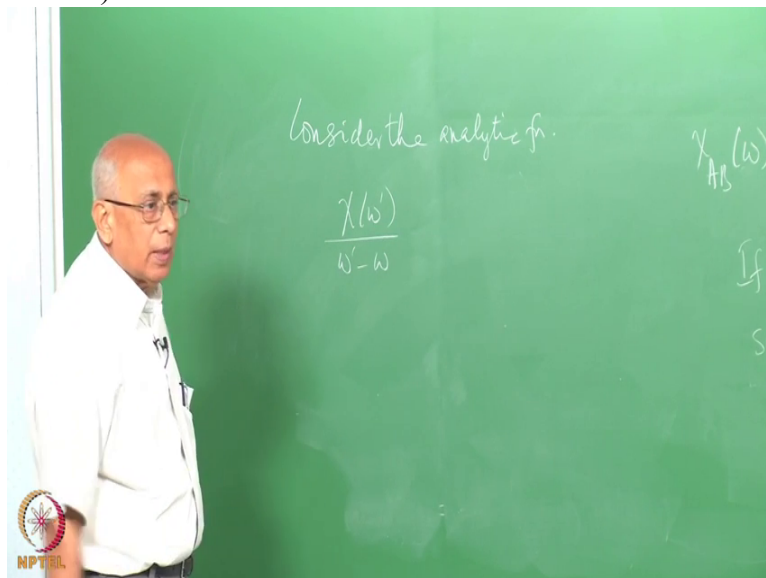
But I should ensure that $\text{Re}(s)$ of ω becomes a residue of some function of ω prime at this point. I should therefore divide by ω prime minus ω . So let us consider the analytic function

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$\text{Re}(s)$ of ω prime divided by ω prime minus ω in the ω prime plane as a function of ω prime.

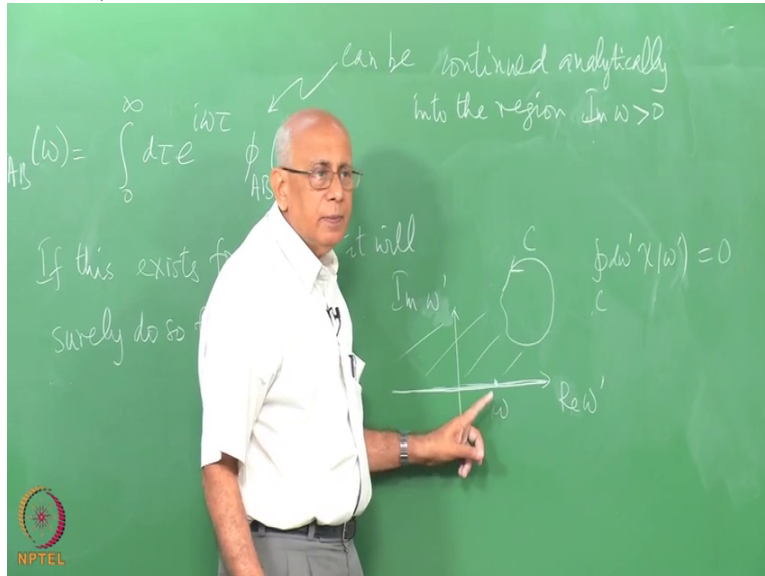
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This function is analytic on and above the real axis. This provides a simple pole at ω prime equal to ω .

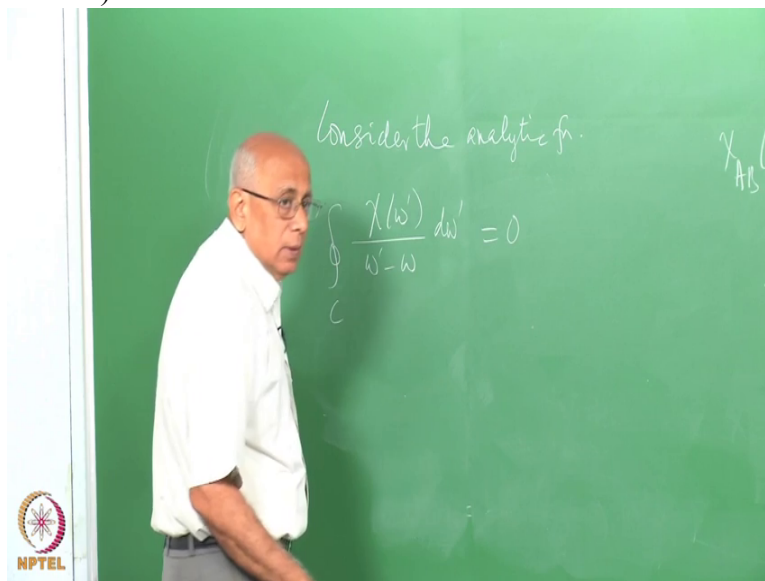
So this function itself is analytic everywhere in the upper half plane except for the pole at this point.

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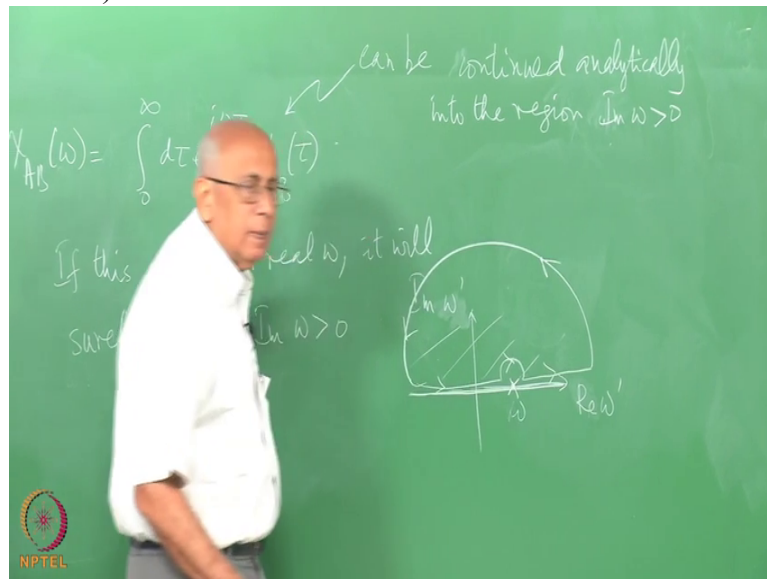
And it has a simple pole out here. As long as I don't cross that pole or hit that pole I can distort this contour as I please provided I don't go into the lower half plane. So let me start distorting it without changing the value of integral. So I start by saying, an integral over this contour C $d\omega'$ equal to zero

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to start with because it is an analytic function, if C looks like what I do earlier. But I can make that C look bigger by writing it like this,

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Ok.

I can make this go on the real axis because it is still analytic there but for clarity I have shown it a little above. I should avoid this pole so I go above it and stay in the region of holomorphy and I go to this side and this side. And the answer is still zero. I would like to do this till I extend this to infinity and I take an infinitely large semicircle, am I allowed to do that?

(Professor – student conversation starts)

Student:

Professor: How do you know? How do you know? Because I am going to have to argue that this contribution, I would like it to go to zero. Is that going to happen? Is that going to happen?

Student: You assume that 0:46:05.9 exists

Professor: I have assumed that it exists but I have not said anything about what it does as omega prime goes to infinity along any direction.

Student: 0:46:14.3

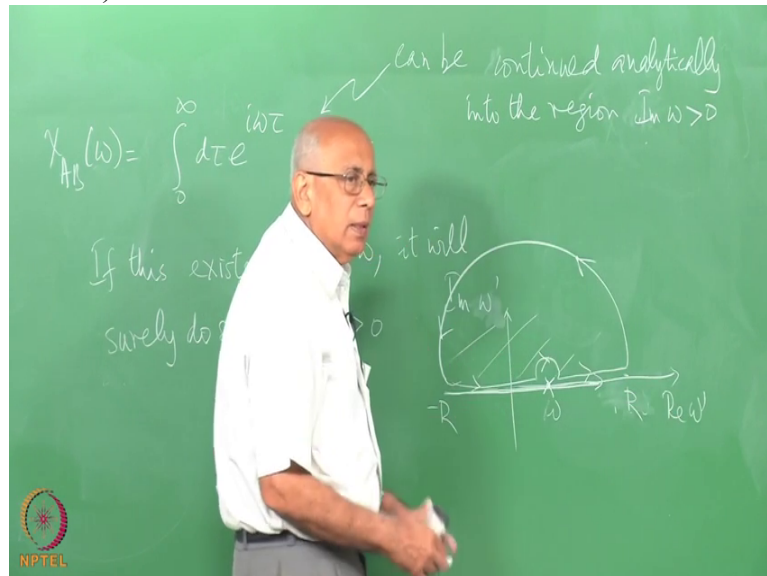
Professor: Pardon me? kai is independent of what?

Student: phi A B 0:46:20.2

Professor: There is no phi any more, right. I am saying this is an analytic function. I am only focusing on this function now as of, phi is gone, you know, it is represented by this, so I am just saying this is an analytic function of omega prime in the upper half plane with the pole at omega prime equal to omega on the real axis. Everywhere else in the upper half plane, it is

analytic. So am I allowed to say that if I write a contour integral from minus R to plus R, this is plus R and then this big semicircle,

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it is still valid, this is still true? Can I take R equal to infinity? Am I allowed to do that?

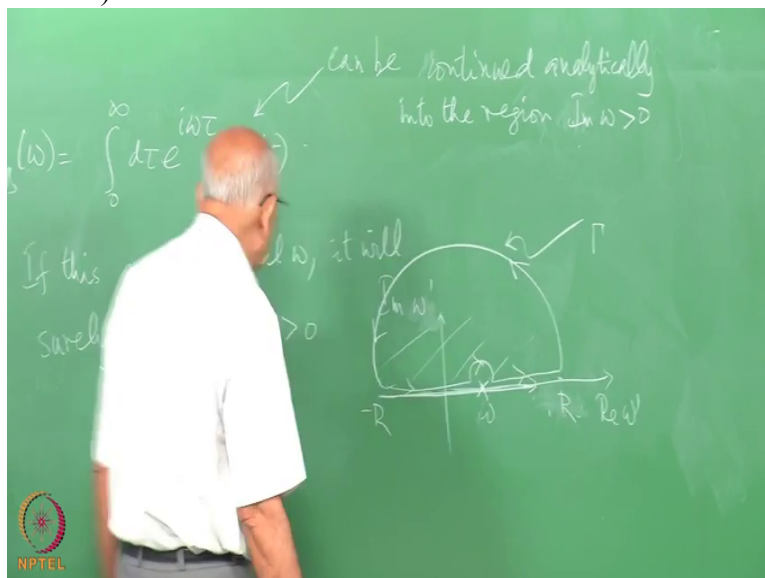
Student: 0:47:16.5 exponential factor

Professor: I have the exponential, where is the exponential factor? That has been used up in showing that this is analytic.

Student: 0:47:25.3

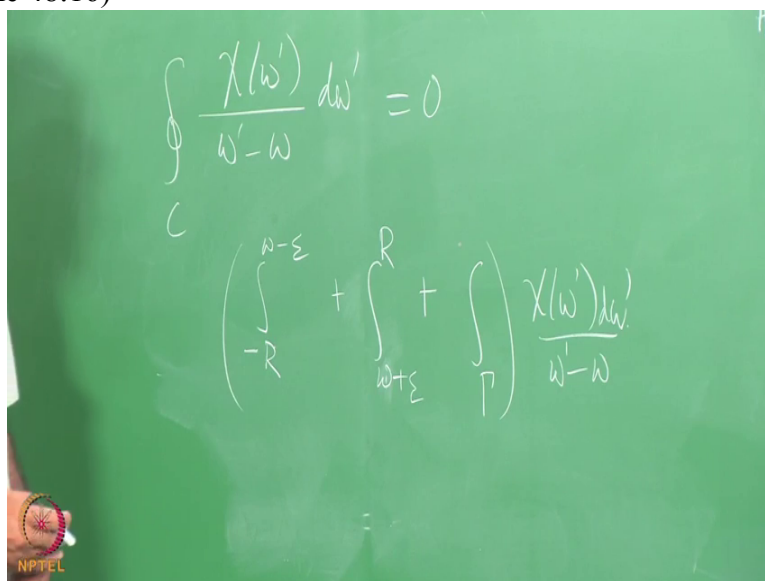
Professor: That has gone. Ok. So when is that contribution from semicircle, let us write it down, let us call this contribution from the semicircle, let us call this contour gamma, big gamma,

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so this quantity is integral minus R to omega minus epsilon plus an integral from, omega plus epsilon to R plus an integral over gamma of the same thing, $\oint_{\Gamma} f(\omega') d\omega'$

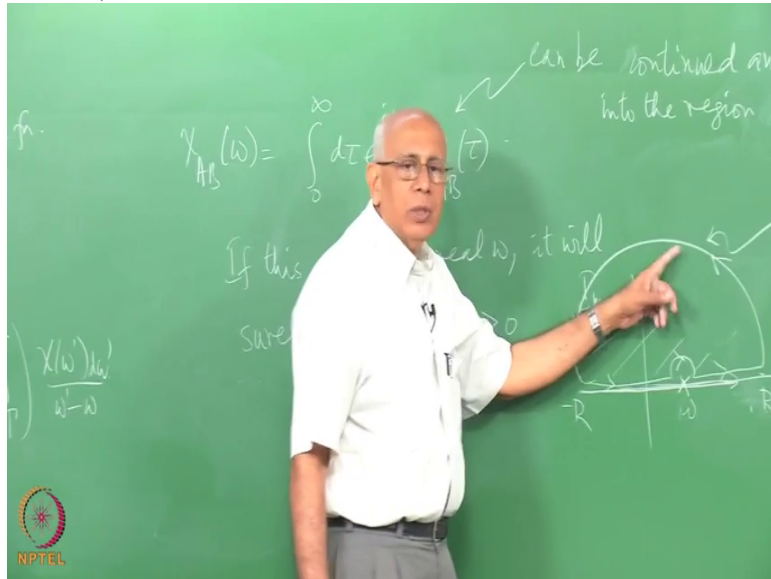
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(Professor – student conversation ends)

I am going to let R go to infinity, so this integral runs minus infinity to infinity except for that little integral around omega and then I would like this to be zero. Is that guaranteed? Think about it till tomorrow since we have run out of time, think about it. Otherwise it won't be useful. Because it would still involve integrals over some complex values of omega. I want to restrict it to real values, physical values of omega, right. So I want this contribution to vanish.

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And you have to tell me what further assumption is needed to do this. So we will take it from here tomorrow.