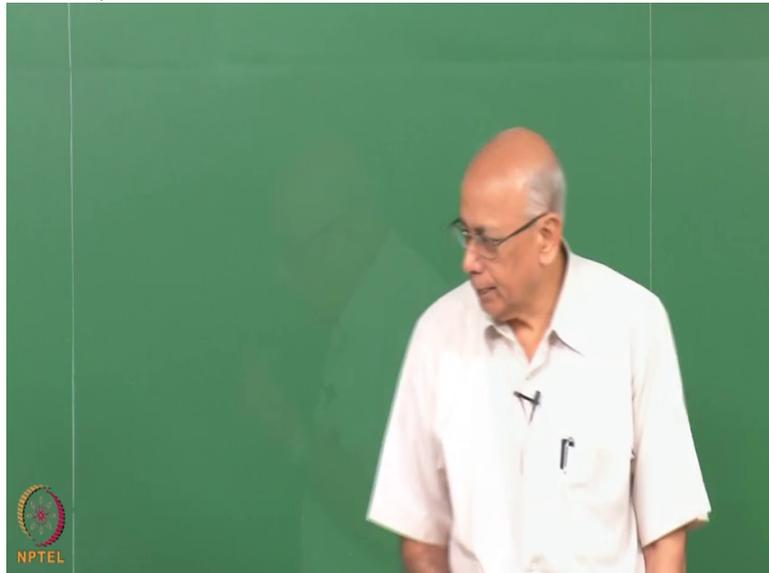


**Nonequilibrium Statistical Mechanics**  
**Professor V. Balakrishnan**  
**Department of Physics**  
**Indian Institute of Technology Madras**  
**Lecture No 09**  
**Linear response theory (Part 4)**

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So yesterday we started with a simple model and I was, I had just begun looking at this model where you have an oscillator in a fluid, so basically it is the model of an oscillator in a fluid which satisfies the following equation

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this  $x$  double dot of  $t$  for any coordinate, any Cartesian coordinate  $x$  say, plus  $m$  gamma  $x$  dot of  $t$  plus  $\omega_0$  squared  $x$  of  $t$  equal to the ensemble average on the right hand side in the presence of some external force.

The random force averages to zero and what is left is  $1$  over  $m$   $F$  external of  $t$  in this fashion. And the question we were asking is what's the average value of  $x$  of  $t$  equal to under these circumstances

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Osc. in a fluid

$$\langle \ddot{x}(t) \rangle + \gamma \langle \dot{x}(t) \rangle + \omega_0^2 \langle x(t) \rangle = \frac{1}{m} F_{ext}(t)$$

in general? And we were trying to do this by linear response theory, so that was the idea. Of course this is an inhomogenous equation for  $x$  of  $t$  and therefore you can solve it by the Green function method.

The Green function method says that  $x$  of  $t$  is an integral over whatever this inhomogenous term is up to time  $t$  multiplied by the Green function and that's all you need. So the Green function  $G$  satisfies,  $G$  of  $t$  minus  $t$  prime satisfies the differential equation  $d^2$  over  $d t^2$  plus gamma  $d$  over  $d t$  plus  $\omega_0$  square acting on  $G$  of  $t$  minus  $t$  prime equal to  $1$  over  $m$  times the delta function of  $t$  minus  $t$  prime.

It satisfies this differential equation,

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$$m \ddot{x}(t) + \gamma \dot{x}(t) + \omega_0^2 x(t) = \frac{1}{m} F_x(t)$$

$G(t-t')$  satisfies the d.e.

$$\left( \frac{d^2}{dt^2} + \gamma \frac{d}{dt} + \omega_0^2 \right) G(t-t') = \frac{1}{m} \delta(t-t')$$

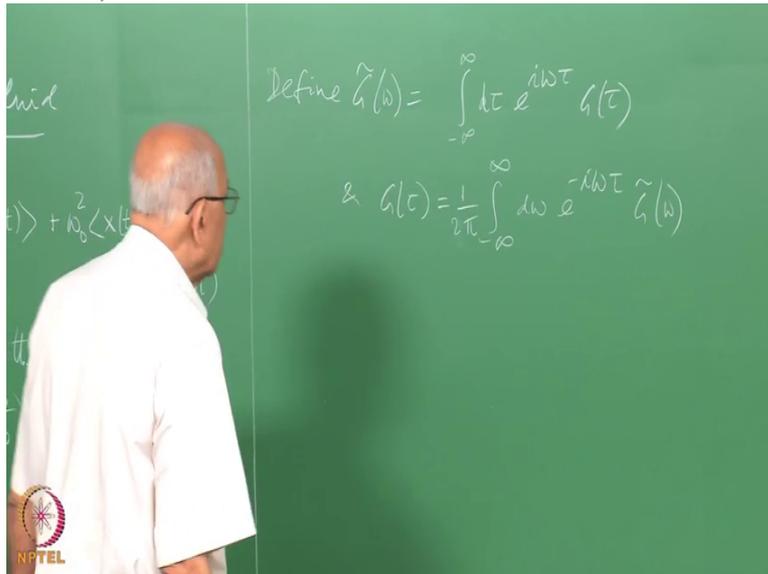
the same thing as I operate on the left hand side and then you have a delta function instead, 0:02:38.1. Ok. So we can solve this and the simplest way to do this is by Fourier transforms here, right? So let us define, define  $\tilde{G}$  or let us define  $G$  of  $t$  equal to, we must be careful about our Fourier transform convention, the convention I use was this is an integral from minus infinity to infinity  $d\tau$ , it will be  $i\omega\tau G$  of  $\tau$  and

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Define  $\tilde{G}(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G(\tau)$

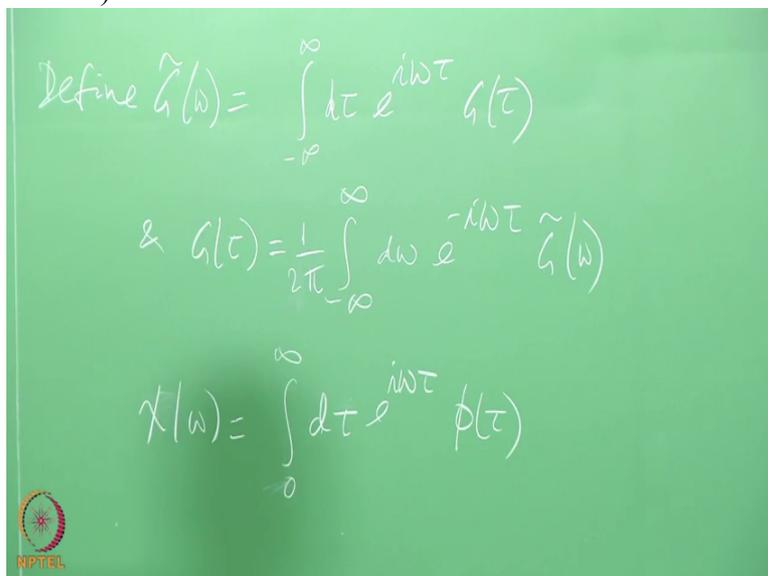
of course  $G$  of  $\tau$  is  $\frac{1}{2\pi}$  minus infinity to infinity  $d\omega e^{-i\omega\tau} \tilde{G}$  of  $\omega$ .

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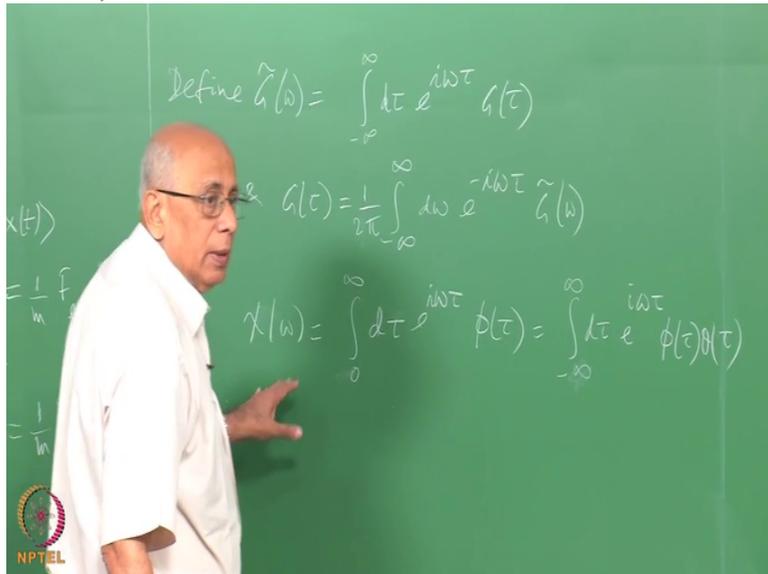
Now remember that the response function itself, the response function that we had was phi of tau, so we know that the generalized susceptibility  $\chi$  of omega in this problem, which I have not introduced for this problem, this we know in general is zero to infinity d tau e to the i omega tau phi of tau, Ok

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which can also be written as equal to integral minus infinity to infinity d tau e to the i omega tau phi of tau theta of tau, the step function theta of tau which is any way zero for tau less than zero so I could write it in this fashion here. That is the generalized susceptibility.

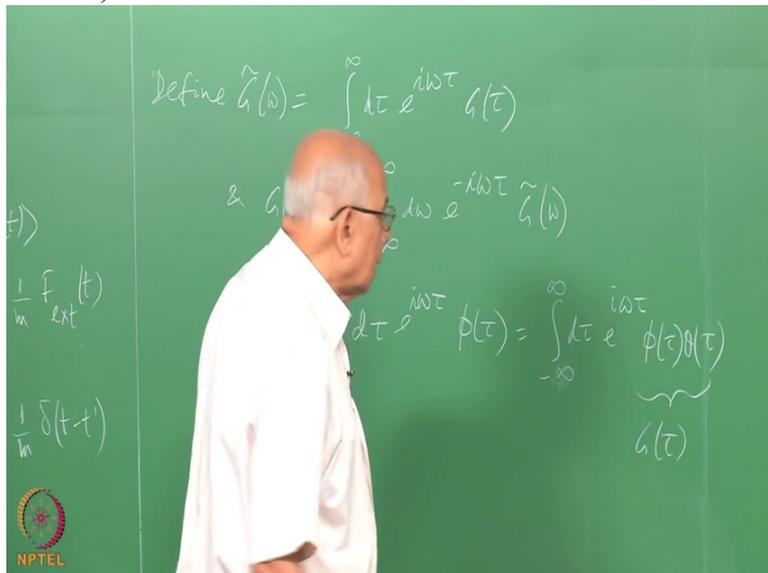
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This is the Green function.

We already have seen that this is G of tau. We have seen that already earlier that you

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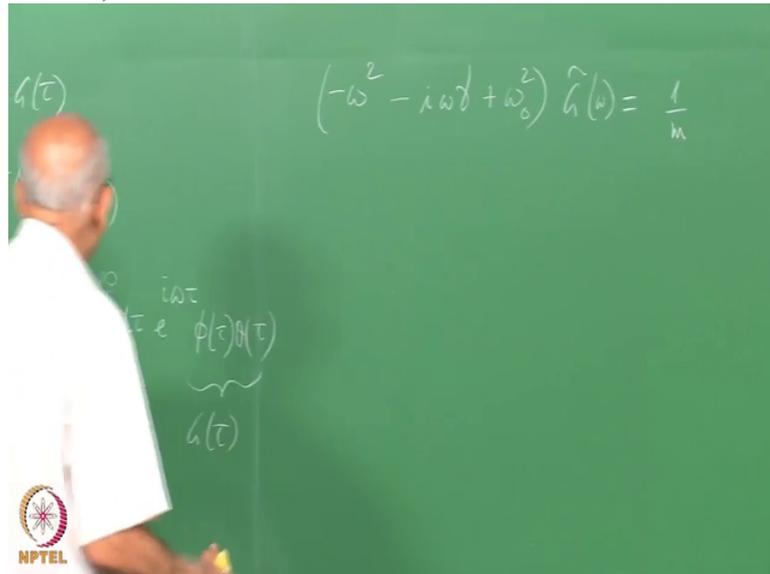
multiply the response function by this to maintain causality and you get the retarded Green function here. So it is clear from this formula that  $k(\omega)$  is the same as  $G$  tilde of  $\omega$ , it is just the Fourier transform, Ok. So it immediately follows that  $k(\omega)$  is the same as  $G$  tilde of  $\omega$ .

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So  $\chi(\omega)$  is the one-sided Fourier transform of the response function but it is actual Fourier transform of the Green function. So if I compute the Green function here by whatever means, I have actually found  $\chi(\omega)$  of  $\omega$ . And then I invert the transform in order to write down what the solution itself is. And after that I superpose all these harmonics to find what the solution is for the general frequency. It is a very simple problem but just to show you how this proceeds, let me do this, let us do this explicitly, Ok.

So let us try to solve this using Fourier transforms and I define the Fourier transform according to this equation, if I differentiate this once with respect to  $\tau$ , I pull down a minus  $i\omega$  inside. So derivative with respect to  $\tau$  is same as multiplication of the Fourier transform by minus  $i\omega$ . Therefore it follows from this that minus  $\omega^2$  minus  $i\gamma\omega$ , that takes care of these two terms, this is minus  $i\omega$  whole square, this is minus  $\omega^2$ , minus  $i\gamma\omega$  plus  $\omega^2$  square of course, this quantity acting on  $\tilde{G}$  of  $\omega$  is equal to  $1/m$  because

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delta function has Fourier representation  $\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} dt$ .

So the  $2\pi$  cancels out on both sides and you just end up with this expression. Or  $\tilde{G}(\omega)$ , that is the same as  $\tilde{G}$  of  $\omega$ , this is the same as this, is equal to  $\frac{1}{m(-\omega^2 - i\gamma\omega + \omega_0^2)}$ . So that is our expression for the Fourier transform of the Green function or the generalized susceptibility in this problem.

It is clearly an analytical function of  $\omega$ . You can define this for arbitrary complex  $\omega$ . It is an explicit analytic function but it has singularities when the denominator goes to zero and the singularities because

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$$(-\omega^2 - i\omega\gamma + \omega_0^2) \hat{X}(\omega) = \frac{1}{m}$$
$$\text{or } \hat{X}(\omega) = \frac{1}{m(\omega^2 + i\omega\gamma - \omega_0^2)}$$


this is quadratic in omega. It is just the product of 2 simple factors and therefore the singularities are 2 simple poles, Ok. So this can be written as equal to minus 1 over m times omega minus omega minus times omega minus omega plus where, and now the locations are of course the roots of this quadratic equation

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$$(-\omega^2 - i\omega\gamma + \omega_0^2) \hat{X}(\omega) = \frac{1}{m}$$
$$\text{or } \hat{X}(\omega) = \frac{1}{m(\omega^2 + i\omega\gamma - \omega_0^2)} = \frac{-1}{m(\omega - \omega_-)(\omega - \omega_+)}$$

where



and therefore, omega plus minus equal to minus i gamma over 2, that takes care of this portion.

So if you have an underdamped oscillator you can write this as plus square root of omega naught square, I pull out the half that cancels with 2, minus gamma square over 4.

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$$(-\omega^2 - i\omega\gamma + \omega_0^2) \hat{G}(\omega) = \frac{1}{m}$$

$$\text{or } \chi(\omega) = \frac{1}{m(\omega^2 + i\gamma\omega - \omega_0^2)} = \frac{-1}{m(\omega - \omega_-)(\omega - \omega_+)}$$

where  $\omega_{\pm} = -\frac{i\gamma}{2} \pm \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$

So there are 2 singularities at these 2 roots and they are simple poles in the omega plane. Now as long as omega naught is bigger than gamma over 2

(Professor – student conversation starts)

Student: plus or minus 0:09:01.8

Professor: plus or minus, those are the two roots for this quadratic, Ok.

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$$(-\omega^2 - i\omega\gamma + \omega_0^2) \hat{G}(\omega) = \frac{1}{m}$$

$$\text{or } \chi(\omega) = \frac{1}{m(\omega^2 + i\gamma\omega - \omega_0^2)} = \frac{-1}{m(\omega - \omega_-)(\omega - \omega_+)}$$

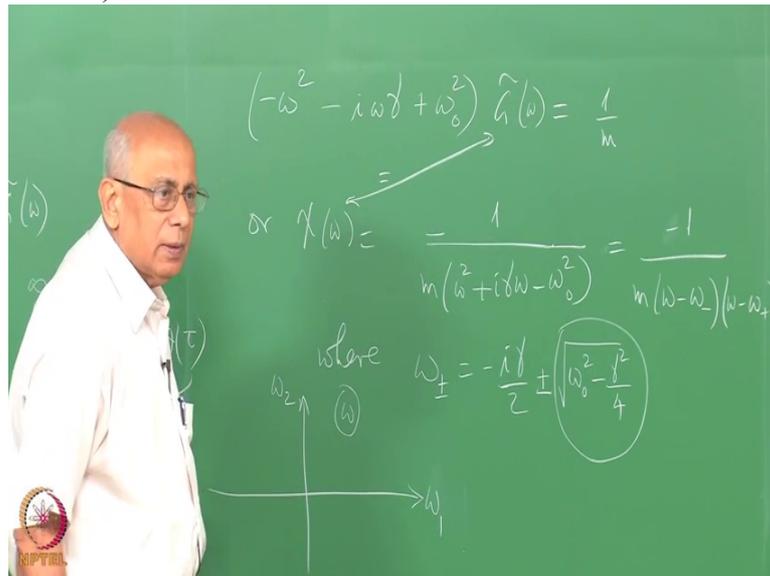
where  $\omega_{\pm} = -\frac{i\gamma}{2} \pm \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$

As long as omega naught is greater than gamma over 2, this is a real number here and therefore the imaginary part is negative. But we already know that the singularities of this Green function with this convention of Fourier transforms have to lie in the lower half plane in omega, the upper half plane it has got to be analytic, right?

(Professor – student conversation ends)

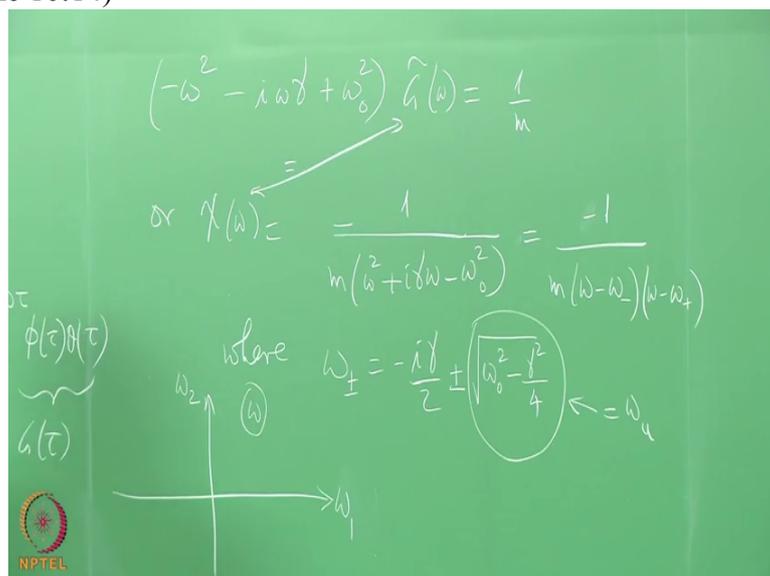
So you have two poles in the omega plane, this is real omega, let me just call it omega 1 and omega 2. And the two poles, let us give this a name. This is just the shifted frequency of the damped oscillator,

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right? So it has got physical dimensions of frequency. This is equal to omega undamped. Let me put a u there to show that it is undamped because only then is this omega, this is a real number. So the, sorry, the underdamped,

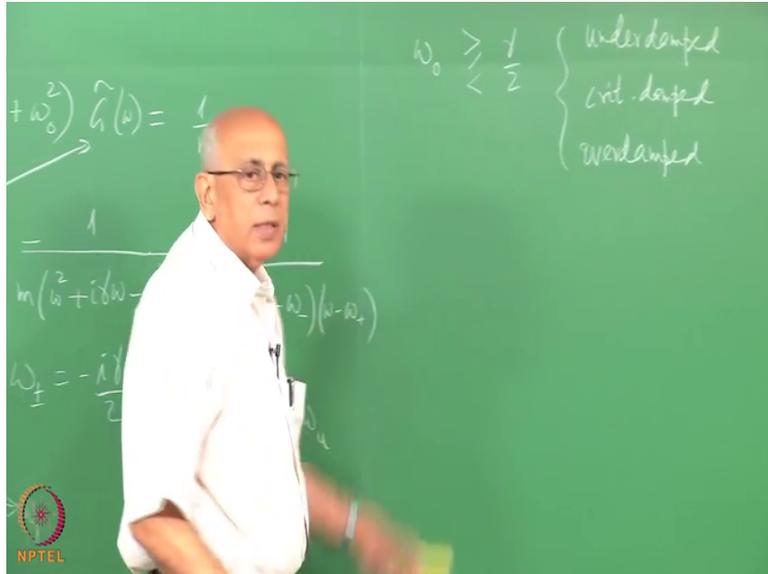
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when you have the underdamped oscillator equilibrium is reached in oscillatory fashion. If it is overdamped, it will just damped out exponentially.

So at least in the underdamped case, let us write this  $\omega_0$  greater equal to less than  $\gamma/2$  corresponds to underdamped, critically damped and overdamped. These 3 signs respectively

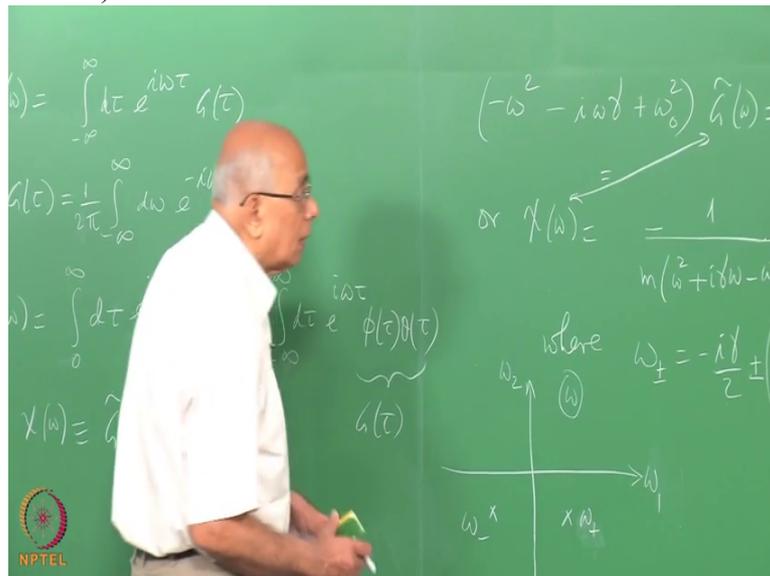
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relate, as you know very well from very elementary treatment of a damped harmonic oscillator or an L C R series circuit, you know that if  $\omega_0$  is sufficiently large and the friction is sufficiently small, then you have an underdamped case.

So let us first look at that case here. Where are these poles then located? Well, it is  $-i\gamma/2 \pm \omega_u$  which is some real number. So there is one pole here and there is another pole here and this is  $\omega_u$ , sorry this is  $\omega_u$  plus and this is  $\omega_u$  minus. By the way what happens to these poles if you start going

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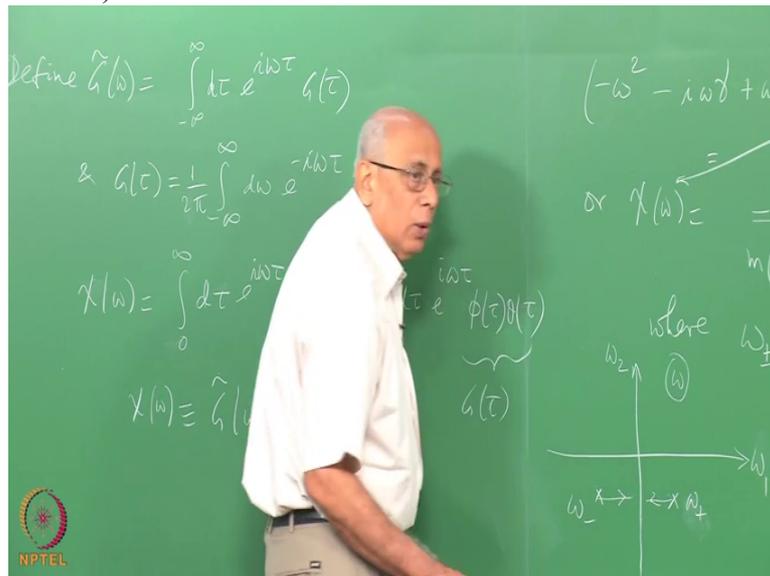


from the underdamped case to the overdamped case?

You can do that in 2 ways. You can either fix a gamma and change omega naught or you can fix an omega naught and change gamma in general. So the path of these poles will depend on what you are varying, what parameter you are changing. For definiteness let us say I fix a gamma, damping is fixed and I change this omega naught. So I start with very high omega naught, frequency much bigger than gamma over 2 and then it is like this, symmetric about the imaginary axis.

And then I start decreasing omega naught towards gamma over 2. This pole will move down like this and this other fellow will move down like this. Because gamma is fixed,

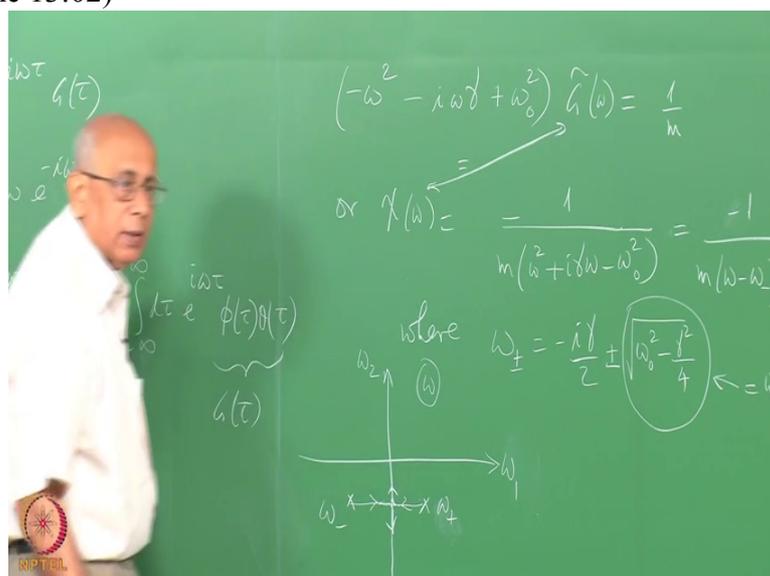
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all that is happening is that omega u is getting smaller towards gamma over 2. At omega naught equal to gamma over 2, the two coincide at this point and then beyond that this quantity becomes imaginary. So you have minus i gamma over 2 plus the small imaginary part or minus the small imaginary part.

The plus sign therefore will go upwards in this fashion along the imaginary axis and the minus sign will go downwards along this imaginary axis.

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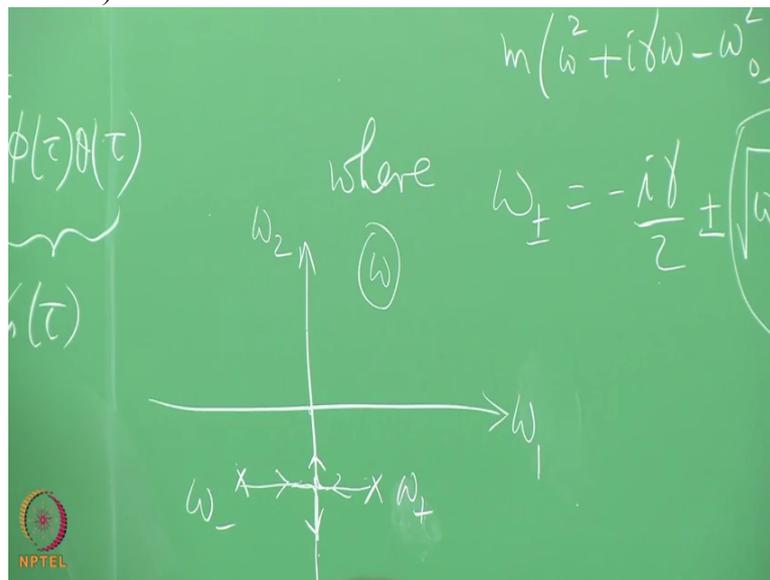


And finally as omega naught reaches the value zero, this goes away and you have plus or minus i gamma over 2. So this pole goes and hits the origin here. It is still approaching it

from below, from the lower half plane and the other fellow goes and sticks at gamma, minus i gamma, Ok.

So even in the other 2 cases, the overdamped and the critically damped, it is easy to see; it is very trivial to see that no singularity ever crosses this and goes up in the upper half plane. In fact they approach the real axis even asymptotically. There is really no singularity for any finite, non-zero value omega,

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Ok. So this justifies our assertion that will turn out, when I said, that the lower half, that the singularities of the generalized susceptibility would not lie in the upper half plane, it is completely analytic there, Ok.

What would happen if gamma were zero, no damping? What would that correspond to? Then you have undamped oscillator. This goes away. We saw there were problems with the undamped Langevin particle when you did not have friction term, things were not in equilibrium and so on, some such things should show up here too. Suppose you don't have this at all and you have just this oscillator, the plain undamped oscillator, then exactly the same thing will go through except you have omega squared minus omega naught squared without this term, which would mean you actually had a pole here and a pole here, out there on the real axis.

Now what does that physically correspond to? It says that this generalized susceptibility becomes singular at 2 real frequencies, plus or minus omega naught and what it actually, physically means is that if you do not have damping and you apply an external force with exactly the same frequency as the natural frequency of the system, then in the absence of damping the amplitude will become arbitrarily large, it will just diverge, as we know.

If you push a swing at exactly at its natural frequency, you go on kicking it and there is no damping, in principle the amplitude will become unbounded, right? So that is what happens here in the trivial example, right. But in all physical cases and this is a lesson for us in general, we will see why this should be so, in all physical cases the generalized susceptibility will have both the real and an imaginary part. It did not have gamma at all. It is pure real; we are in trouble as we will see. So system can never be either, this susceptibility can never be either purely real or purely imaginary for reasons which will become clear as we go along.

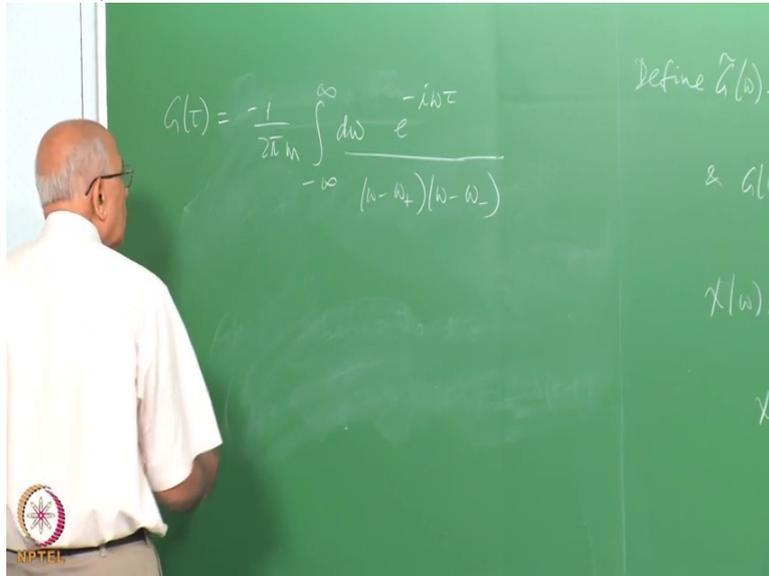
All the physical examples of susceptibility that we know of will have this property. For instance you put light through a medium. What would the corresponding susceptibility be? It is either the dielectric function of the medium or the refractive index if it is a transparent medium. Now in general the refractive index is a complex number. The real part of the refractive index will measure the amount of dispersion. But the imaginary part will measure the amount of absorption. And you can't have pure dispersion without any absorption at all.

Just as if you give me a piece of resistance, just a resistor, it has got a self-inductance. So there have, or you give me an inductor it has got a resistance. So it has got to have a reactive part as well as a resistive part always. And that is exactly what we are seeing here in this simple example.

Alright now back to how to compute this quantity. So let us try to calculate what the response does although it is fairly straight-forward here. We got till here and now let us compute it. So what we have is  $\chi(\omega)$  or  $G(\omega)$ , therefore I use this formula. Now I have to find  $G(\tau)$  equal to  $\frac{1}{2\pi}$  and there is a  $m$  there in  $\chi$  so this is equal to  $\frac{-1}{2\pi m}$  and integral from minus infinity to infinity  $d\omega e^{-i\omega\tau}$  divided by  $\omega^2 - \omega_0^2 + i\gamma\omega$ , in this fashion. That is the integral you have to do.

Now this sort of integral is fairly, this is the straightforward integral to do. But here is where the power of contour integral comes in. Because this kind of integral where you have a trigonometric function here and a rational function down here, it is geared, contour integration is tailored to do these integrations very easily. Now what would one do?

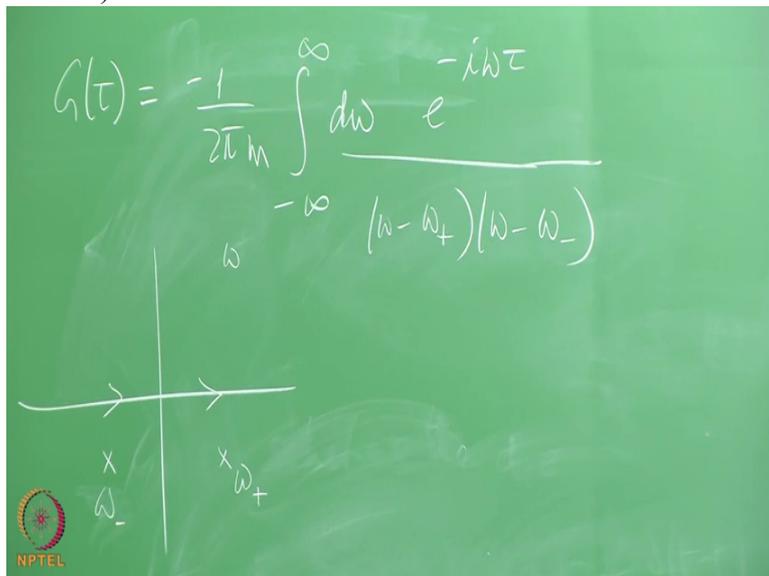
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Notice if I write omega as, well the contour of integration to start with, in the omega plane is minus infinity to infinity there and there is a pole here at omega plus, there is another pole at omega minus.

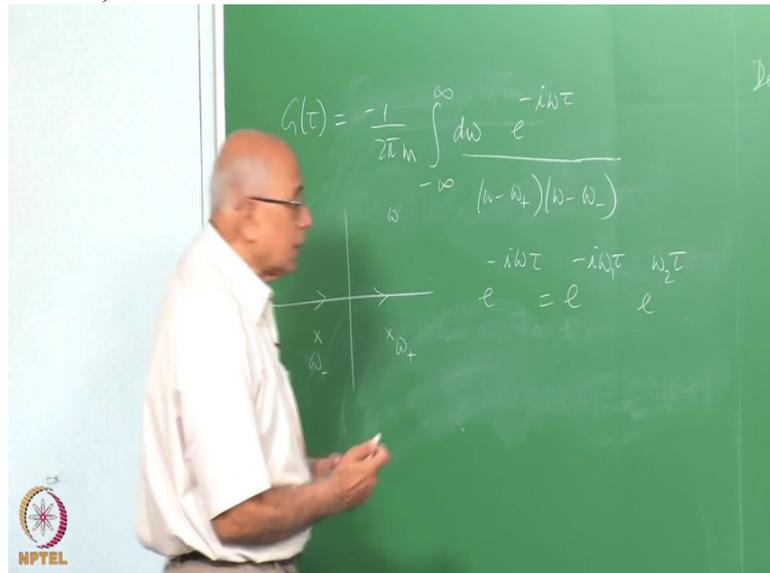
To do this

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as a contour integral, you have to close the contour. Remember this is minus R to R and the limit in which R goes to infinity. That is what is meant by this integration. So you keep R finite and then you close the contour and then let R go to infinity. Now if you write, if you go into, take an excursion into the complex plane and you write omega as omega 1 plus i omega 2, then e to the minus i omega tau becomes e to the minus i omega 1 tau and then minus i times i omega 2 so it becomes e to the omega 2 tau. This is an

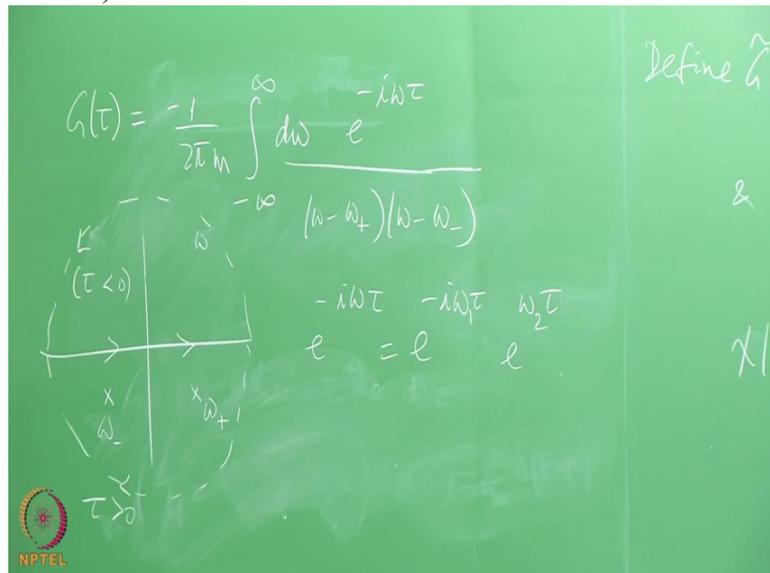
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oscillatory term but this fellow blows up for positive tau if omega 2 is positive. So for positive tau you cannot close it in the upper half plane because this contribution would be non-zero.

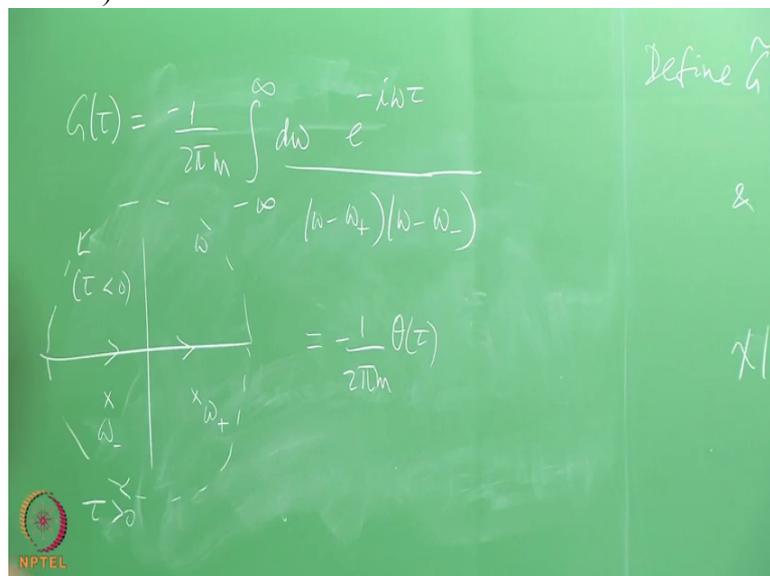
But you close it in the lower half plane, because this contribution from the semi-circle is zero in the limit in which the radius goes to infinity. So you can add a well-chosen zero to do the integral provided you keep track of the fact that when tau is positive you have to do it in the lower half plane and when tau is negative, you do it in the upper half plane, Ok. So you need to do this in this fashion, for tau less than zero and you need to do this for tau greater than zero.

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But you see if tau is less than zero, this contour does not enclose any singularity at all. So you can shrink it down to a point and it disappears. Therefore this integral has got to be equal to minus 1 over 2 pi m times the theta of tau because we know it is zero when tau is less than zero.

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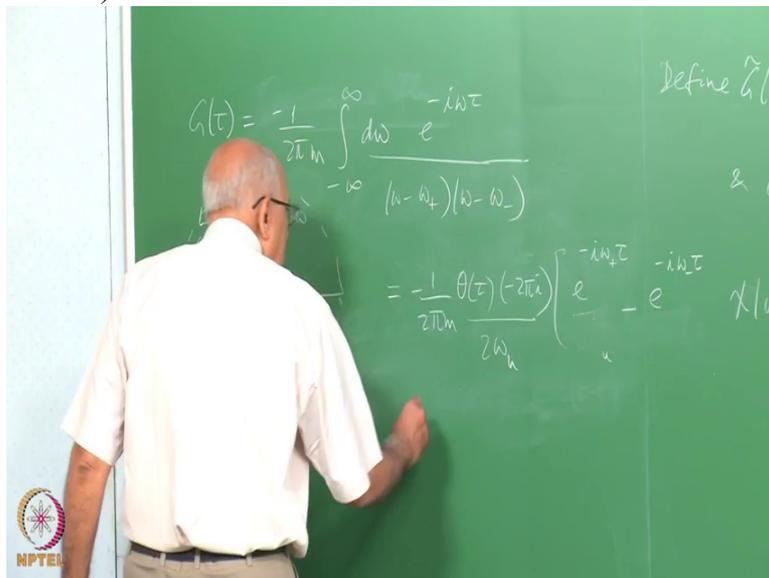
So that factor has emerged automatically as you can see, the Green function must have that theta function and whatever multiplies this is the response function, right? So theta of tau and then what?

Now in the lower half plane when you close the contour, you pick up contributions from the poles with a minus 2 pi. It is in the clockwise direction. So it is minus 2 pi i times p to the

power minus  $i\omega$  plus  $\tau$  from the  $\omega$  plus part, so you multiply by  $\omega$  minus  $\omega$  plus and take the limit as  $\omega$  goes to  $\omega$  plus. So you got  $\omega$  plus minus  $\omega$  minus which is twice  $\omega$  u, Ok. So there is a twice  $\omega$  u. Plus  $e$  to the minus  $i\omega$  minus  $\tau$  and now you multiply by minus  $\omega$  minus and take the limit, you got  $\omega$  minus, minus  $\omega$  plus which is minus 2  $\omega$  u, so you get a minus sign and then 2  $\omega$  u, so let us pull that out and you have this.

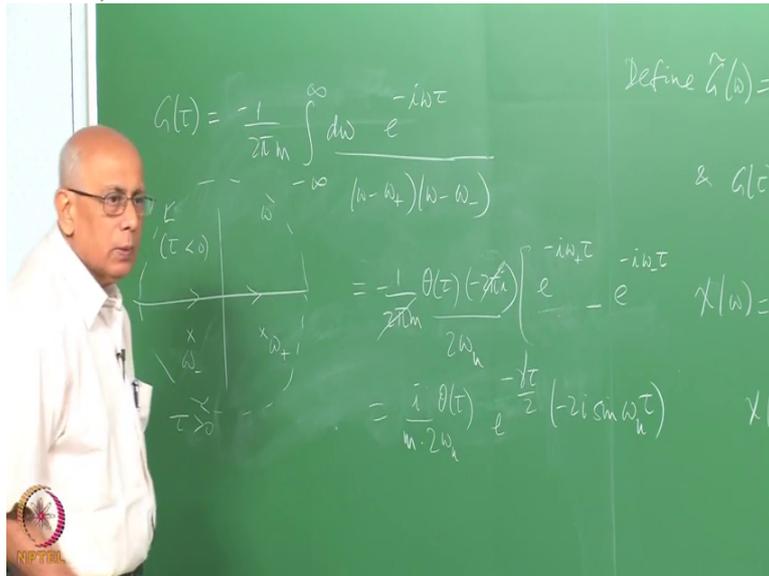
So this is,

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this 2 pi goes against this 2 pi so this is equal to  $i$  over  $m$  times 2  $\omega$  u eta of tau times this guy here, so this  $e$  to the power minus  $i$  times  $\omega$  plus or minus is another minus  $i$  gamma over 2, so the minus signs kill and the  $i$  square gives you a minus 1, so this is minus gamma tau over 2 times either the minus  $i\omega$  u minus  $e$  to the minus  $\omega$  u, that is equal to minus 2  $i$  sin  $\omega$  u tau, Ok.

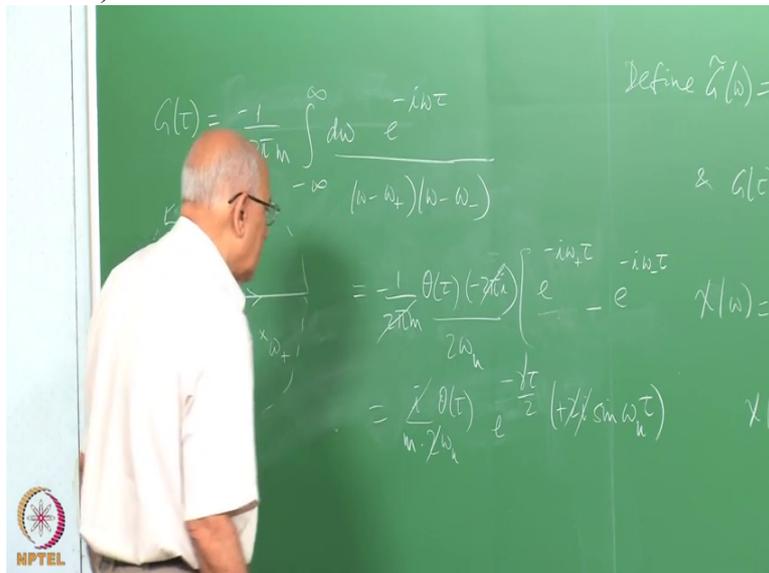
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So now we are in good shape.

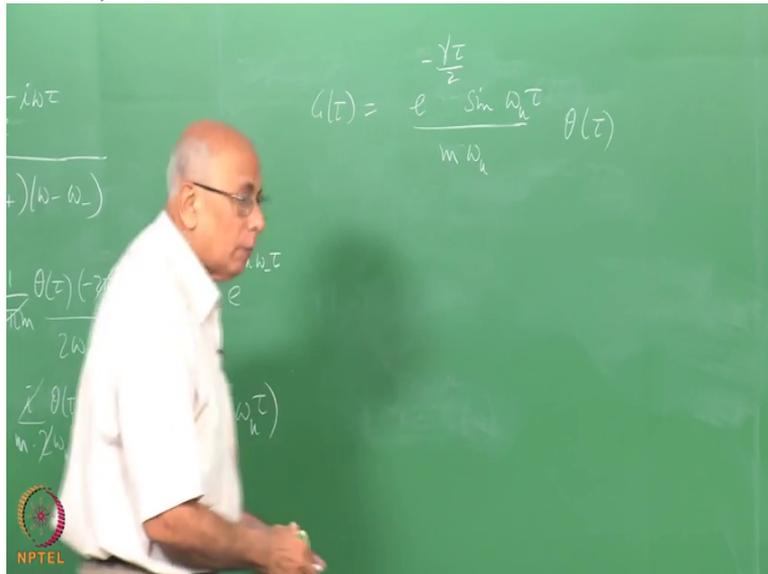
The i cancels against this, this cancels, the 2 cancels and you are left with

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just that. So we have our final answer which says that G of tau equal to e to the minus gamma tau over 2 sin omega u tau divided by m omega u multiplied by theta of tau,

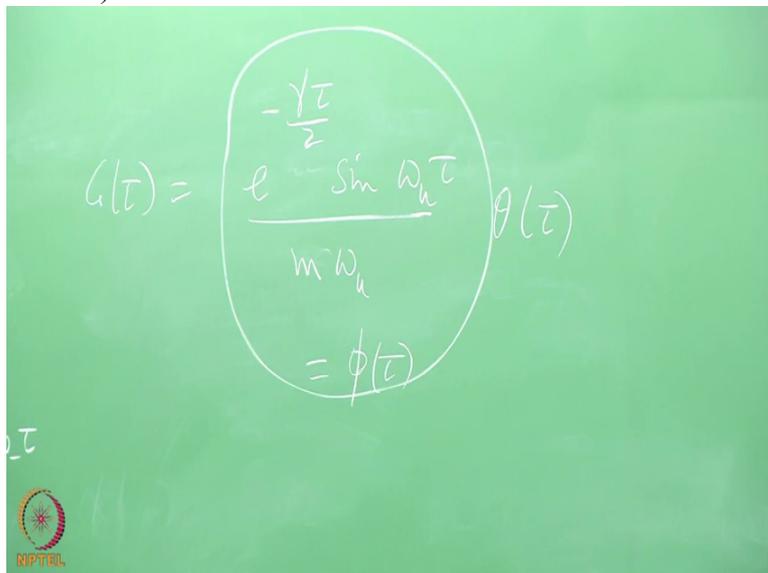
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from this factor.

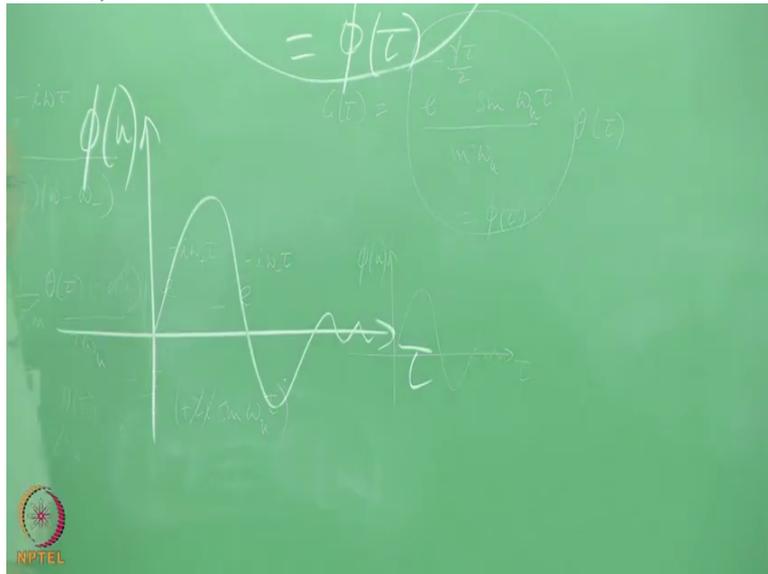
So we have a closed expression in this case. Therefore this part of it is equal to phi of tau.  
The response function,

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Ok and you can see in the underdamped case, the response reaches the value zero, the response function reaches the value zero so if you plot as a function of tau, you plot phi of u, this will start at, because this is linear in tau, it is going to start at zero, no instantaneous response as you will expect and then it is going up to a peak and then go down in this fashion.

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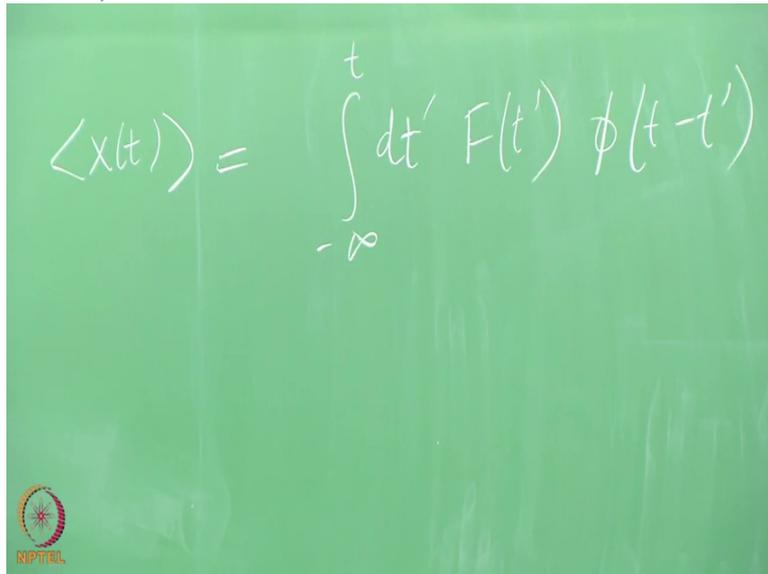
And the envelope goes like  $e$  to the minus  $\gamma$  over 2. So it is exponentially damped but there is an oscillatory tendency here because it is underdamped, Ok.

What would you do if it is overdamped? Well if it is overdamped,  $\omega_d$  becomes imaginary and  $\sin$  of  $i$  theta is related to  $\sinh$  theta apart from the  $i$  etc so you can actually write down, it will be exponentially damped, it will just die down exponentially without the oscillatory behavior. I leave you to work out the critically damped case etc; they are all trivial extensions of this.

So we have closed answer, in this case completely closed answer. In fact there is one more step and that is to write down what the actual average value is, it is easy to write down now. So you can write what is  $x$  of  $t$  equal to, this is an integral from minus infinity to infinity into  $t$   $d t$  prime times  $F$  of  $t$  prime  $\phi$  of  $t$  minus  $t$  prime. We have an expression for  $\phi$  of  $\tau$ , this is  $\phi$  of  $\tau$ , so we can plug it in and that's it.

For arbitrary force history, you can write down what the exact displacement is, average displacement is at any time, Ok. So this was the toy problem, a baby problem

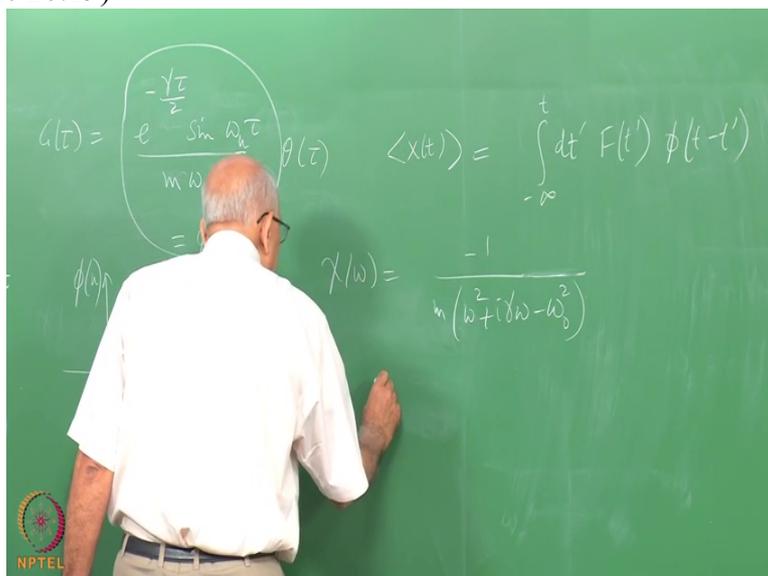
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$$\langle x(t) \rangle = \int_{-\infty}^t dt' F(t') \phi(t-t')$$

because it was just the harmonic oscillator damped but it gives us a lot of valuable lessons.

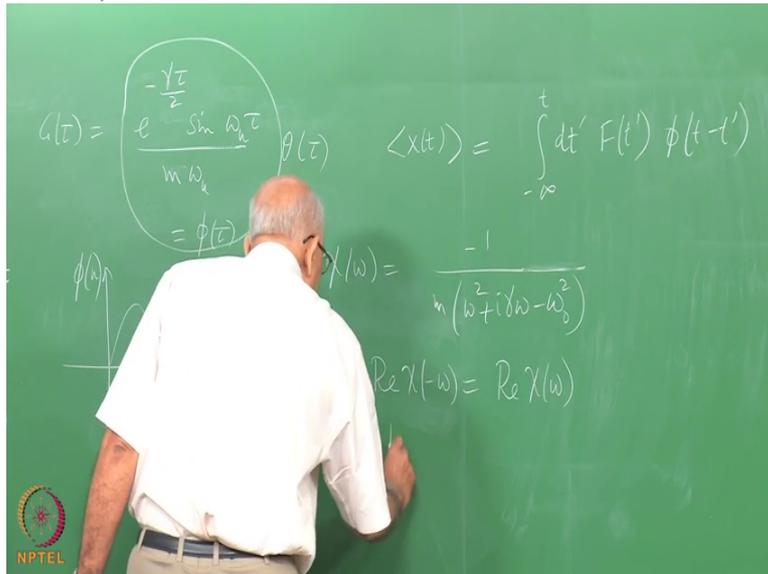
It corroborates the fact that susceptibility is analytic in the upper half plane. It also shows certain symmetry properties of this thing, of this  $\chi(\omega)$  because I leave you to find out, to check that if you took this, we know that  $\chi(\omega)$  in this problem is equal to minus 1 over  $m(\omega^2 + i\gamma\omega - \omega_0^2)$  and it is a trivial thing to verify

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$$G(z) = \frac{-\frac{\gamma z}{2}}{m\omega} \frac{e^{-\frac{\gamma z}{2}} \sin \omega_0 z}{\omega} \theta(z)$$
$$\langle x(t) \rangle = \int_{-\infty}^t dt' F(t') \phi(t-t')$$
$$\chi(\omega) = \frac{-1}{m(\omega^2 + i\gamma\omega - \omega_0^2)}$$

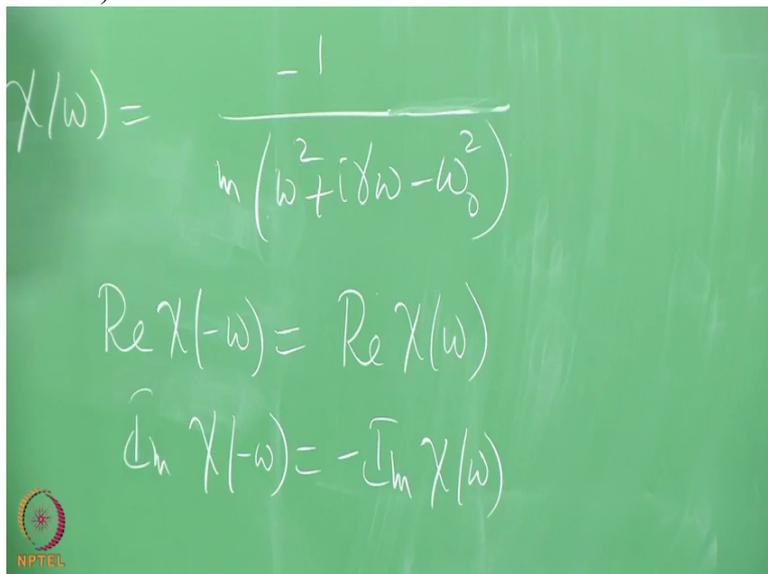
real  $\chi(\omega)$  of minus  $\omega$  is,

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that is immediately obvious.

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Because this goes up on top and the real part is going to involve this on top, the imaginary part is going to involve this with the mod squared of these fellows, so it is immediately obvious. The real part is symmetric and the imaginary part is anti-symmetric in omega.

(Professor – student conversation starts)

Student: We can do it directly 0:26:56.6 complex thing, no, like the kai star of..

Professor: Yeah, exactly. So together these two correspond to saying kai of omega, kai star of omega equal to kai of minus omega which is obvious here. So from this relation these two follow,

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$$X(\omega) = \frac{-1}{m(\omega^2 + i\delta\omega - \omega_0^2)}$$

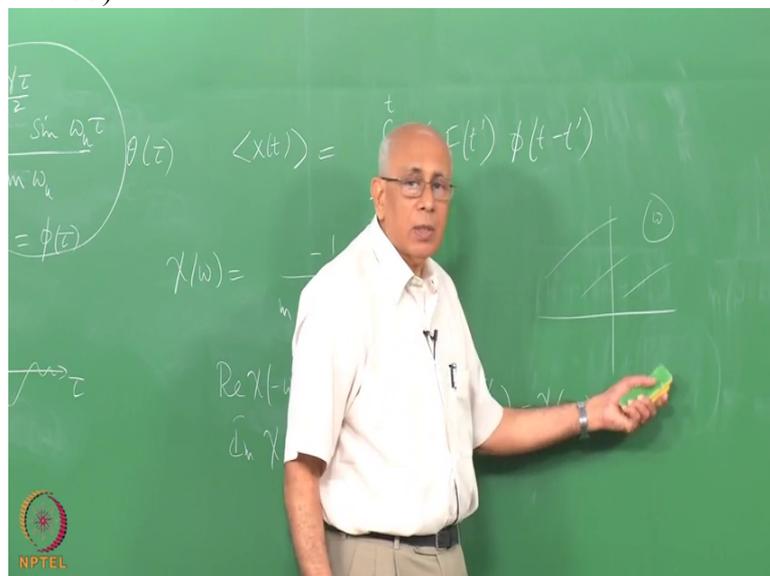
$$\left. \begin{aligned} \operatorname{Re} X(-\omega) &= \operatorname{Re} X(\omega) \\ \operatorname{Im} X(-\omega) &= -\operatorname{Im} X(\omega) \end{aligned} \right\} X^*(\omega) = X(-\omega)$$

for real omega, for real omega. Actually there is a symmetric property for complex omega as well. What is that property?

(Professor – student conversation ends)

You will have to put an omega star here, out here. Does it mean you know kai in the lower half plane? You have to be careful here because she is saying that kai of minus omega is related to kai star of omega star. We have an explicit expression for kai here. So there is no problem. But in general, in the more complicated problems we would know in the omega plane, you would know that it is an analytic function here and we may not be even be able to discover

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what is the singularity structure here.

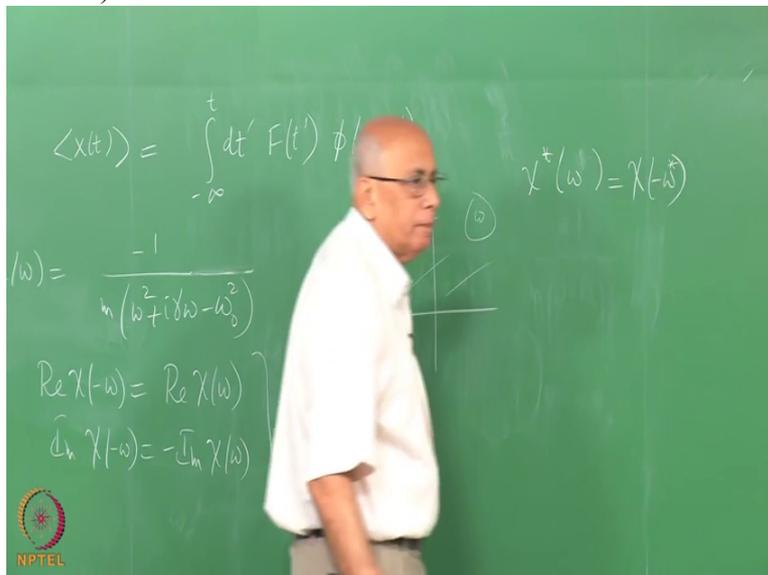
Because it won't be anything as simple as this in general. So all manner of beasts could lurk there and we don't know. So we do know that it is analytic up here. Now what would you say, if omega were complex and you had symmetry like  $\chi^*(\omega^*) = \chi(-\omega)$ ?

(Professor – student conversation starts)

Student: Exchange the role of omega star.

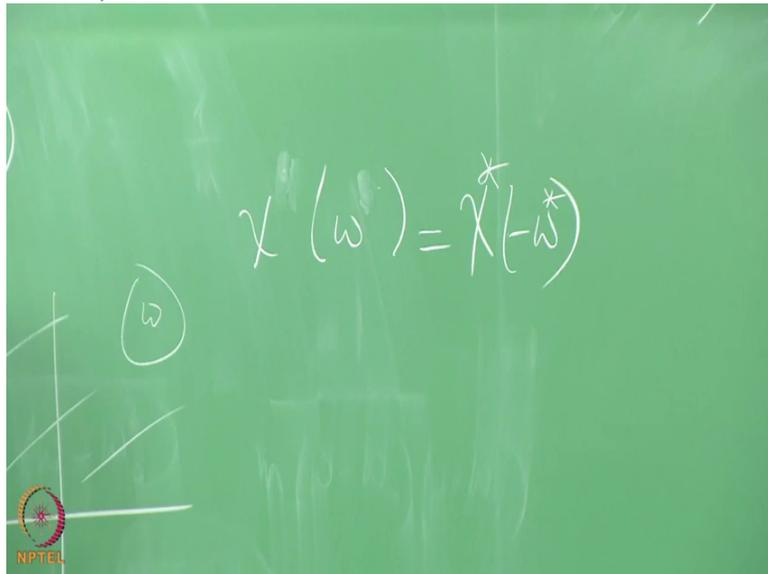
Professor: Yeah we should,

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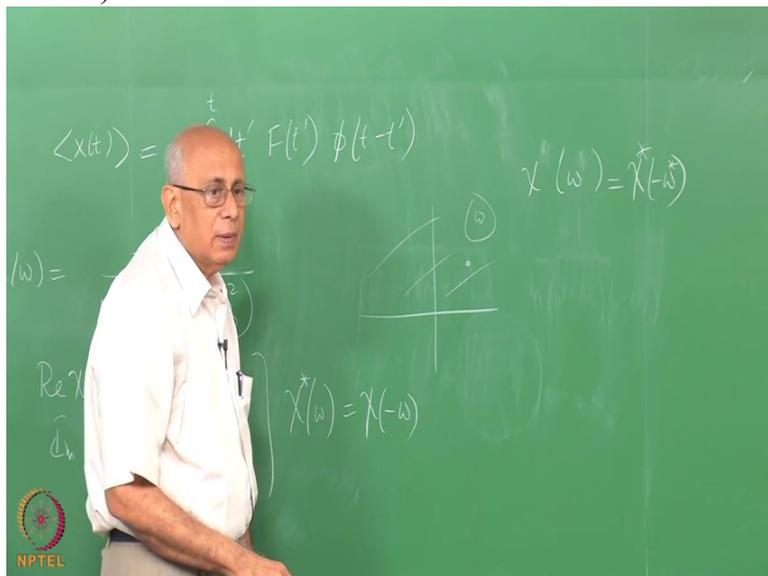
Ok. Now what is the symmetry property? What is it saying? If you start with some omega, we could put a star here as well, doesn't matter.

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If you start with some omega here, where is omega star?

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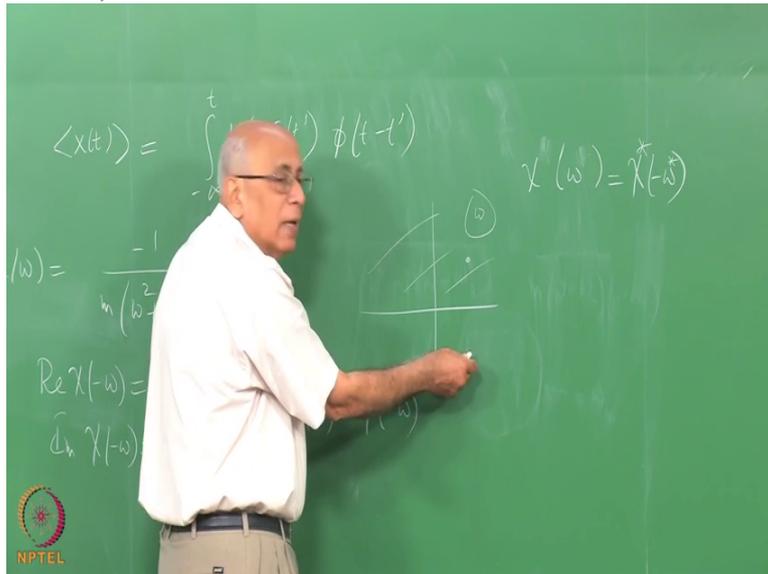
Student: It is there. 0:28:50.0

Professor: It is down here. But where is minus omega star?

Student: In there

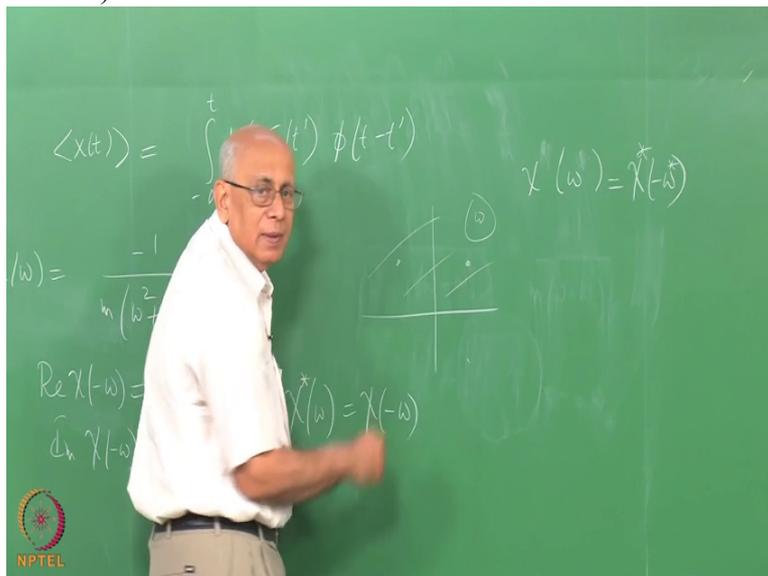
Professor: Both the real and imaginary

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parts have to be flipped. So it is here.

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And you are safe, you are really safe. Because it is not going into the lower half plane at all. We do not know anything about it in general. So it is relating a kai here with a kai here, this one and everything is Ok in general. So one has to be careful to check this all the time, that it is not giving you information. This representation alone is not giving you more information in this, Ok.

(Professor – student conversation ends)

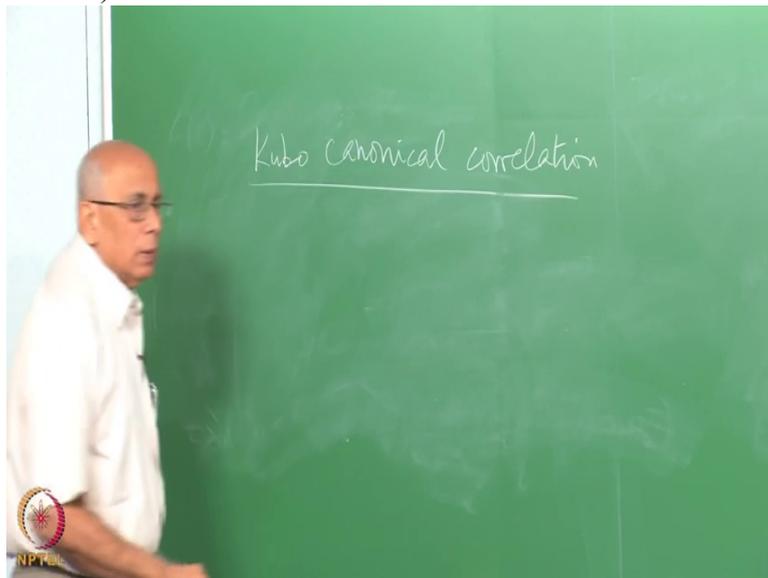
We will see what the implication of this is. The implication of the fact that the kai is well-behaved everywhere in the upper half plane and in general on the real axis as well has serious

implications, important implications and we will see what this means. In, in a nutshell what it will mean and we will derive this is that the value of  $\chi$  at any point is determined in a self-consistent way as an integral over  $\chi$  over the rest of the real axis.

So it is trying to say that an analytic function does not sit in isolation at every point. Because you say this function has derivatives of all orders, this function is highly constrained. You cannot really arbitrarily specify this function as you please. Once you have specified in the small region then you have specified it everywhere, Ok. We will get back to that issue.

But now at the moment let's go back to the general representation for  $\chi$  and see whether we can simplify the expression. So let us go now to a canonical, what is called the canonical, well actually it should be called the Kubo because the Japanese

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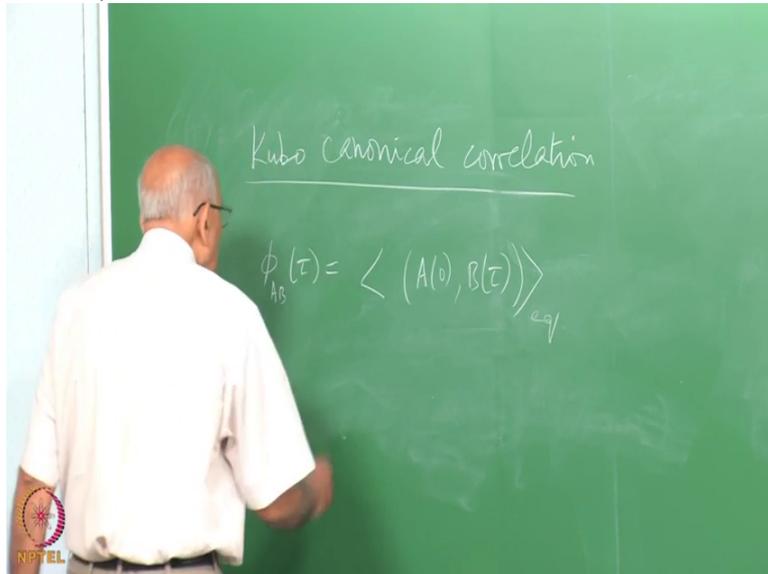


physicist Kubo first pointed out that you could write a representation for this correlation function valid for both the classical and quantum cases and it involves a certain specific operation that we need to do to simplify the correlation function.

So recall where we had started. We started by saying  $\langle A B(\tau) \rangle$  was equal to, in general, the equilibrium expectation value of  $A$  of zero then  $B$  of  $\tau$ , where this bracket stood for either the Poisson bracket or commutator divided by  $i\hbar$  cross depending on whether it was classical or quantum in equilibrium.

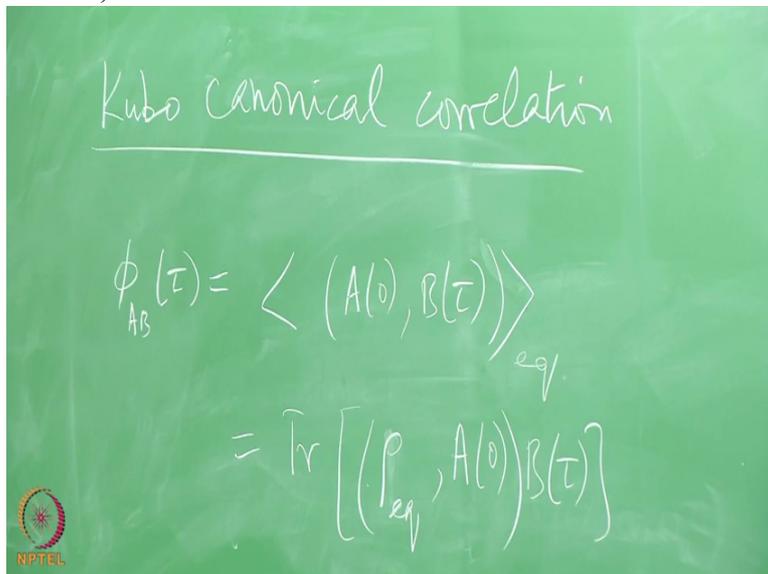
But you could also

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write this as the trace over the equilibrium density matrix of rho equilibrium with A of zero times B of tau. We could also write it like this. By the cyclic invariance of the trace. Now notice that I am using the cyclic

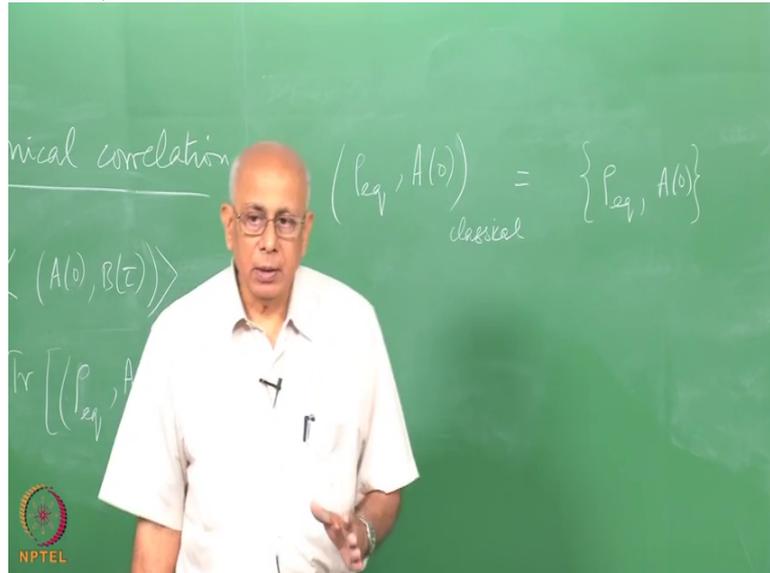
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invariance of the trace and it requires certain assumptions on the operators, Ok. We will assume that, till we trip up that these conditions are met actually, but remember that trace A B is equal to trace B A but under these circumstances but it does not mean A B is equal to B A. The operators themselves won't commute and we must be very careful about that in general. So we have this equilibrium.

Let us look at it classically and see what this actually means, whether we can make it a little simpler or whatever. Now if you go here, this actually means  $A$  of zero classical is equal to Poisson bracket of rho equilibrium with  $A$  of zero. What I mean by  $A$  of zero is that the time argument in the dynamical variables, the  $q$ s and  $p$ s is at  $t$  equal to zero, Ok and that, and the values of  $q$ s and  $p$ s at any time  $t$  is found by nominally solving the Hamiltonian equations of motion,

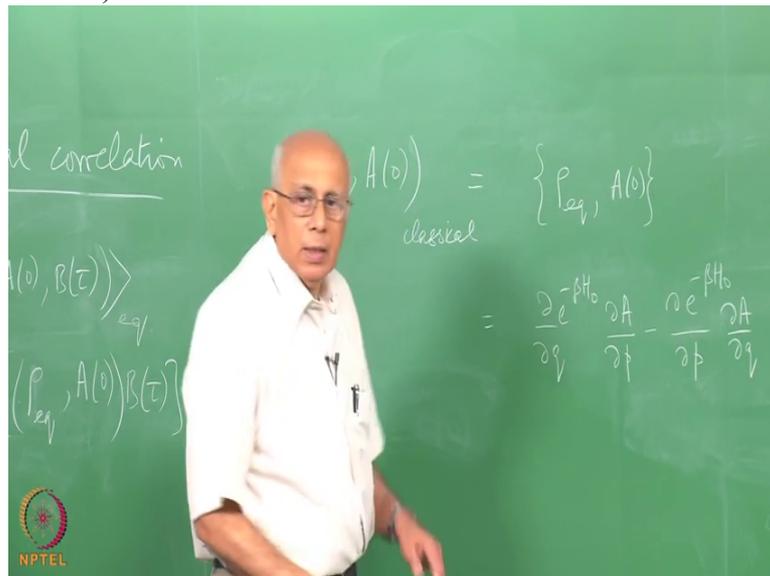
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Hamilton's equations of motion and since we are talking it in equilibrium there is no external force here to start with, the whole thing is done in the canonical ensemble, rho equilibrium is  $e^{-\beta H}$  naught, the unperturbed Hamiltonian and this refers to time evolution under the unperturbed Hamiltonian, all this. That is what appears in this 0:34:03.3 here, Ok.

Now this is equal to, if I wrote this out in terms of  $p$ s and  $q$ s this is equal to  $\frac{\delta}{\delta q} e^{-\beta H}$  naught,  $\frac{\delta A}{\delta p}$  at zero, let me just drop that argument for a minute,  $\frac{\delta}{\delta p} e^{-\beta H}$  naught over  $\frac{\delta A}{\delta q}$ . It stands for this,

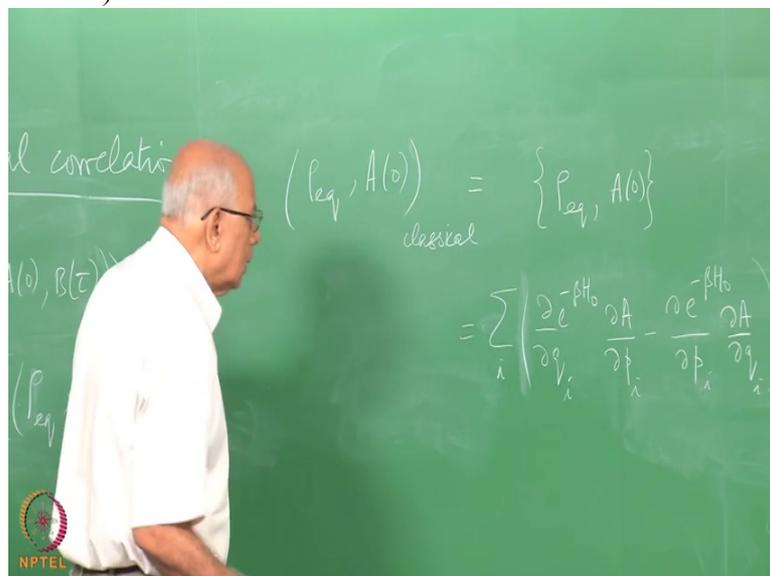
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summed over all degrees of freedom in the system.

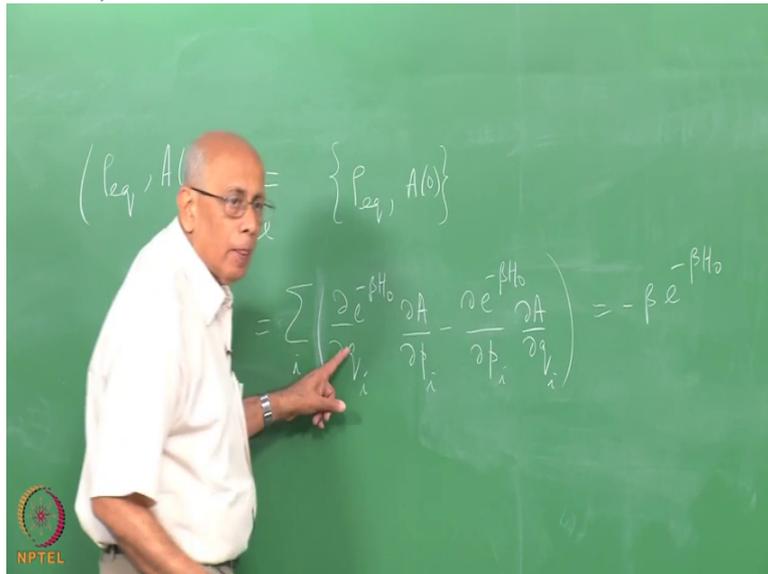
So there is, I should put  $q$  sub  $i$ ,  $p$  sub  $i$  and sum over  $i$ , this is understood. So if you like, let us write it as summation over  $i$ , I should use this bracket in this fashion.

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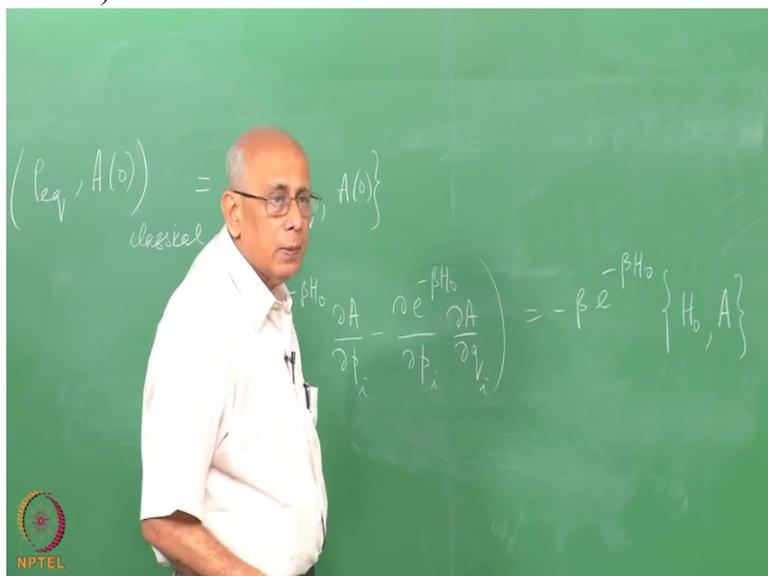
But if I differentiate this, this is the same as differentiating  $e$  to the minus, same as differentiating  $H$  naught pulling out a minus beta times  $e$  to the minus beta  $H$  naught. So this can be written as equal to 0:35:21.8 beta times  $e$  to the 0:35:25.7 minus beta times that

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and then I have a delta H naught over delta q i, delta A over p i and similarly H naught over p i, this but that is equal to the Poisson bracket of H naught with A

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which is equal to beta times e to the minus beta H naught the Poisson bracket of A with H naught. This is A at zero always.

Let us even put this here, Ok. But in

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$$\begin{aligned}
 (p_{eq}, A(t)) &= \{p_{eq}, A(t)\} \\
 &= \sum_i \left( \frac{\partial e^{-\beta H_0}}{\partial q_i} \frac{\partial A(t)}{\partial p_i} - \frac{\partial e^{-\beta H_0}}{\partial p_i} \frac{\partial A(t)}{\partial q_i} \right) = -\beta e^{-\beta H_0} \{H_0, A(t)\} \\
 &= \beta e^{-\beta H_0} \{A(t), H_0\} \\
 &= \beta e^{-\beta H_0} \dot{A}(t)
 \end{aligned}$$

classical mechanics I know that A, Poisson bracket of A with zero, A at zero H naught is just A naught. It is time derivative of this dynamical variable at t equal to zero. So if that A is the position, this stands for the velocity. If it is the velocity, it stands for the acceleration and so on.

So this is equal to beta e to the minus beta H naught A dot of zero, supposed to differentiate

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$$\begin{aligned}
 (p_{eq}, A(t)) &= \{p_{eq}, A(t)\} \\
 &= \sum_i \left( \frac{\partial e^{-\beta H_0}}{\partial q_i} \frac{\partial A(t)}{\partial p_i} - \frac{\partial e^{-\beta H_0}}{\partial p_i} \frac{\partial A(t)}{\partial q_i} \right) = -\beta e^{-\beta H_0} \{H_0, A(t)\} \\
 &= \beta e^{-\beta H_0} \{A(t), H_0\} \\
 &= \beta e^{-\beta H_0} \dot{A}(t)
 \end{aligned}$$

and then put t equal to zero. And we put that back here. So this fellow has turned out to be equal to beta times trace e to the minus beta H naught A dot of zero B of tau.

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$$\begin{aligned}
 (P_{eq}, A(0)) &= \{P_{eq}, A(0)\}_{\text{classical}} \\
 [e^{-\beta H_0}, A(0)] B(\tau) &= \sum_i \left( \frac{\partial e^{-\beta H_0}}{\partial q_i} \frac{\partial A(0)}{\partial p_i} - \frac{\partial e^{-\beta H_0}}{\partial p_i} \frac{\partial A(0)}{\partial q_i} \right) = -\beta e^{-\beta H_0} \{H_0, A(0)\} \\
 &= \beta e^{-\beta H_0} \{A(0), H_0\} \\
 &= \beta e^{-\beta H_0} \dot{A}(0)
 \end{aligned}$$

I restore this and I have written this. But what is this equal to?

This is the equilibrium auto-correlation function, correlation of A dot of zero with B of tau. So we have an extremely compact formula that tells you what to do in this case. This has become equal to, so I want to retain this, equal to, in the classical case beta times A dot of zero B of tau equal, no comma, no comma

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Kubo canonical correlation

$$\begin{aligned}
 \chi_{AB}(\tau) &= \langle (A(0), B(\tau)) \rangle_{eq} = \beta \langle \dot{A}(0), B(\tau) \rangle_{eq} \\
 &= \text{Tr} [(P_{eq}, A(0)) B(\tau)] = \beta \text{Tr} [e^{-\beta H_0} \dot{A}(0) B(\tau)]
 \end{aligned}$$

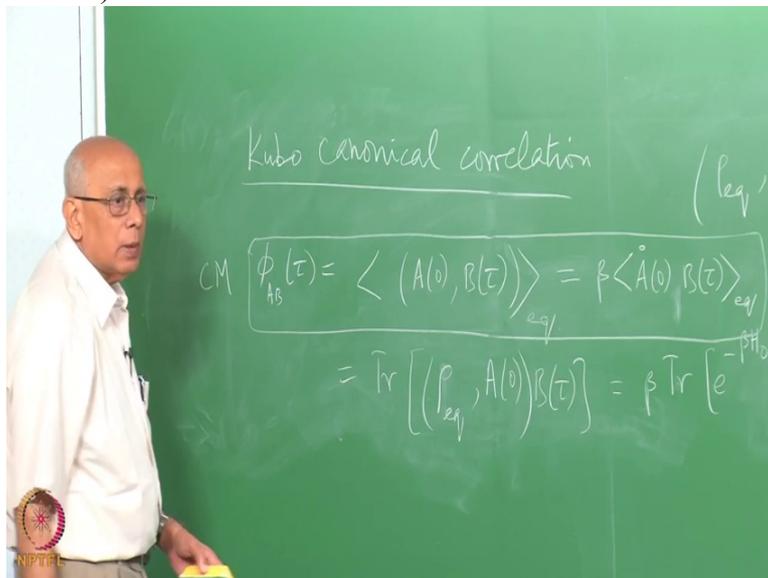
Ok?

So what has happened is that the average value, the equilibrium statistical average value of a commutator or Poisson bracket has become just beta times this 1 over k T times the average

value of  $\dot{A}$  with  $B$  of  $\tau$ , Ok. If this is a mechanical force,  $A$  is  $x$  for in one dimensional motion for example, and we have been computing the susceptibility, the position at some time later on. So  $B$  is also  $x$ . So it says if we want to find the response function to find  $x$  at a later time, you need to know how the velocity at an earlier time is correlated with the position at the later time, of course because the velocity at the later time will tell you what the position is at little later time. So it is not surprising that you ended up with this expression, Ok.

So this is one crucial result, classically.

(Refer Slide Time 39:10)



But quantum mechanically is another story. So now let us see what happens. This won't work; this is not equal to this, so I again start with this fellow here. So in the quantum case Q M,  $A$  and  $B$  need not commute and they need not commute with  $H$  naught itself in general. When they commute things become very trivial. But in general these three operators need not commute with each other at all and we have to be very careful about preserving orders. So let us write this out, this thing out. This is still true, this is a general formula. So now we have  $\phi_{AB}$  of  $\tau$  to be equal to trace, the commutator of this fellow with  $B$  of  $\tau$  on the right hand side, right?

So first we got to find what is this guy equal to. Let us do that. So this is equal to  $1$  over  $i$  h cross, the commutator trace  $e$  to the minus beta  $H$  naught  $A$  of zero  $B$  of  $\tau$  of course, minus  $B$  of  $\tau$ , well, alright let us leave it here that,  $B$  of  $\tau$ , sorry, let us do on right hand side, minus  $A$  of zero  $e$  to the minus beta  $H$  naught  $B$  of  $\tau$ , this way. I have just written this out,

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$$\text{QM}$$
$$\phi_{AB}(\tau) = \frac{1}{i\hbar} \text{Tr} \left[ e^{-\beta H_0} A(0) B(\tau) - A(0) e^{-\beta H_0} B(\tau) \right]$$


explicitly in two terms.

My target is to pull out this  $e$  to the minus  $\beta H$  naught, because then I will argue that whatever is left is the equilibrium average value and I take the trace with respect to it. I am stopped from doing so because this factor is sitting in the middle here, doesn't commute with this. So one solution is put plus or minus the same factor here.

So let us write this,  $\rho = \frac{1}{Z} e^{-\beta H}$  cross trace  $e^{-\beta H} A(0) B(\tau) - A(0) e^{-\beta H} B(\tau)$ . The whole thing is inside the trace, Ok.

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$$\text{QM}$$
$$\phi_{AB}(\tau) = \frac{1}{i\hbar} \text{Tr} \left[ e^{-\beta H_0} A(0) B(\tau) - A(0) e^{-\beta H_0} B(\tau) \right]$$
$$= \frac{1}{i\hbar} \text{Tr} \left( e^{-\beta H_0} \left[ A(0) - e^{\beta H_0} A(0) e^{-\beta H_0} \right] B(\tau) \right)$$


This may not commute with that, this may not commute with that. These two fellows may not commute at all, in general this is all, this is, you are stuck at this point.

But now

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$$\begin{aligned} \phi_{AB}(\tau) &= \frac{1}{i\hbar} \text{Tr} [e^{-\beta H_0} A(\tau) B(\tau) - A(0) e^{-\beta H_0} B(\tau)] \\ &= \frac{1}{i\hbar} \text{Tr} (e^{-\beta H_0} [A(\tau) - e^{\beta H_0} A(0) e^{-\beta H_0}] B(\tau)) \end{aligned}$$

Kubo had a very clever way of resolving this paradox. What do you do with this term here? Recall we are working in the Heisenberg picture and I put a time dependence as governed by the Hamiltonian  $H$  naught. So I say that any operator, let us call any operator  $M$ ,  $M$  of  $t$  is equal to  $e$  to the  $i H$  naught  $t$  over  $\hbar$  cross  $M$  of zero  $e$  to the minus  $i H$  naught  $t$  over  $\hbar$  cross.

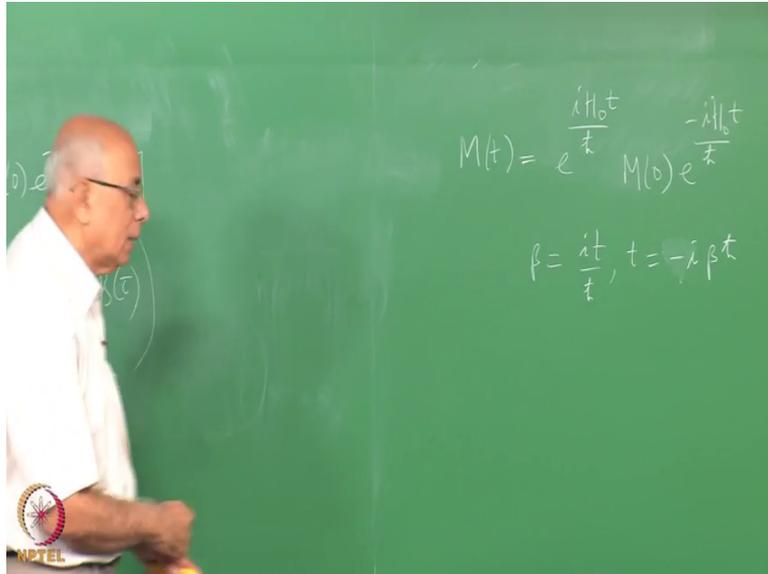
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$$M(t) = e^{\frac{iH_0 t}{\hbar}} M(0) e^{-\frac{iH_0 t}{\hbar}}$$

That is my definition of the time argument inside operators in the Heisenberg picture.

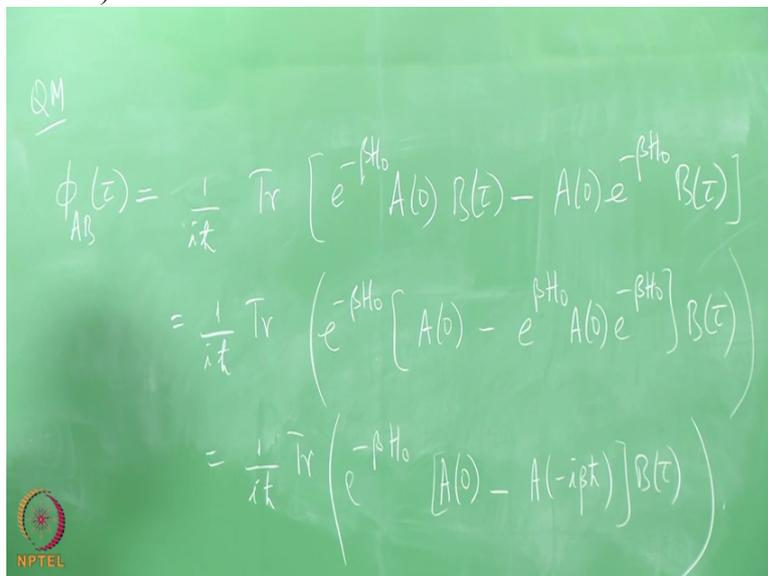
I can do this formally, formally, purely formally without affecting all orders of operators etc by identifying beta with a time. So essentially if I say beta is equal to i t over h cross, t equal to minus i beta h cross, Ok.

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So purely formally, I can write this whole thing as equal to 1 over i h cross trace e to the minus beta H naught A of zero minus A of minus i beta h cross, little bracket here, B of tau,

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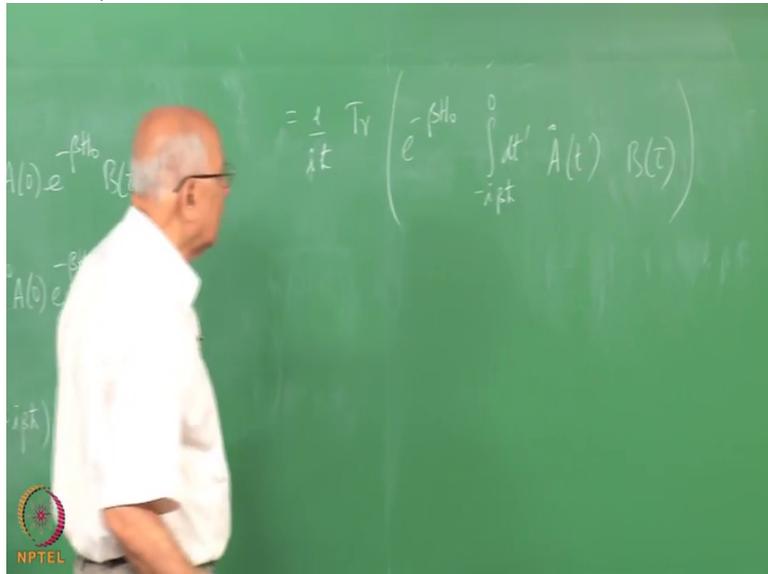


Ok.

But this is now looking more and more like the difference between two time arguments, looks at the integral of the derivative between these limits. So I could actually write this as equal to 1 over i h cross trace e to the minus beta H naught and integral d t prime from minus i beta h

cross to zero  $A$  dot of  $t$  prime, well that is the dynamical variable which when integrated will give you  $A$  of  $t$  times  $B$  of  $\tau$

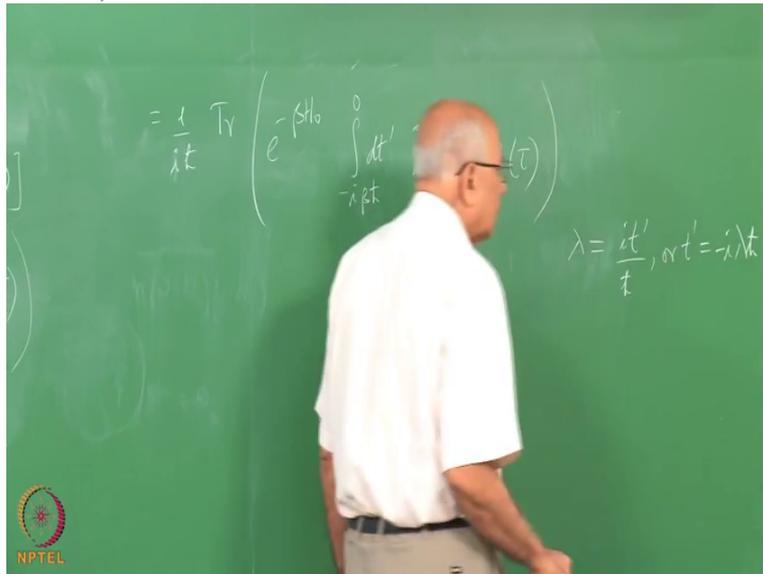
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and it is precisely this difference.

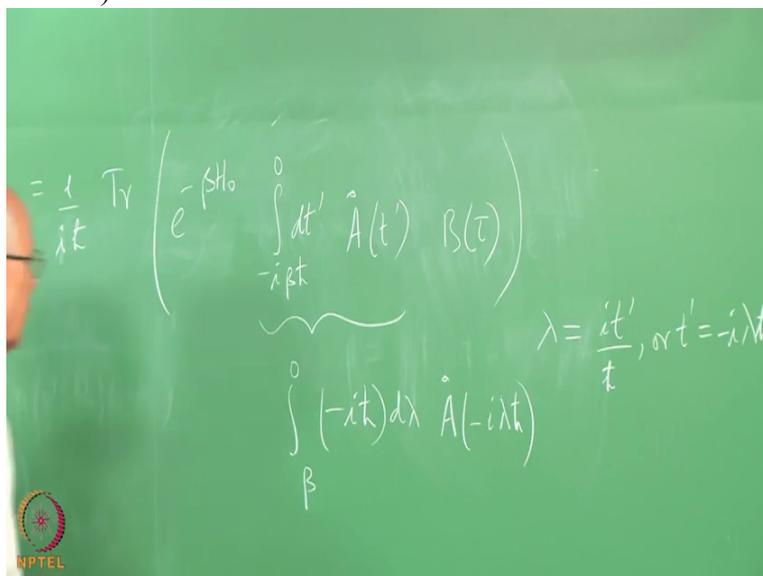
But now you have to get to specify a contour of integration. That is along the imaginary axis, from zero to minus  $i$  beta  $\hbar$  cross, that is uncomfortable, this fellow is uncomfortable. So let us change variables. Let us put minus  $i$   $\hbar$  cross, let us put  $\lambda$  equal to, I want to convert this to a real integral, and I would like  $\lambda$  to be, when  $t$  prime is equal to this, I would like  $\lambda$  to be beta. So how do I fix it?  $i t$  prime over  $\hbar$  cross, will that do the trick? Or  $t$  prime equal to minus  $i$   $\lambda$   $\hbar$  cross.

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Then this quantity here is integral to zero and when  $t$  prime, I have put, when  $t$  prime is minus  $i$  beta  $\hbar$  cross lambda is equal to beta, so beta and then minus  $i$   $\hbar$  cross  $\lambda$  A dot of, and now I have to put in what is going on, A dot of  $t$  prime is minus  $i$  lambda  $\hbar$  cross. So that is what this integral is, Ok which if I am

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little careful, I write it as zero to beta, I get rid of the minus  $i$   $\hbar$  cross sign and that will cancel against this.

So you will permit me to write this as integral zero to beta  $d$  lambda A dot of minus  $i$  lambda  $\hbar$  cross B of tau and this  $i$   $\hbar$  cross goes. These were intermediate steps.

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$$= \text{Tr} \left( e^{-\beta H_0} \int_0^\beta d\lambda \dot{A}(-i\lambda\tau) B(\tau) \right)$$

$$\lambda = \frac{i\tau'}{\tau}, \text{ or } \tau' = -i\lambda\tau$$

These were intermediate steps. But what is this fellow equal to? This guy here, now we are back to the real thing, it is equal to e to the power i over h cross H naught times minus i lambda h cross,

(Refer Slide Time 47:48)

$$= \text{Tr} \left( e^{-\beta H_0} \int_0^\beta d\lambda \dot{A}(-i\lambda\tau) B(\tau) \right)$$

$$\lambda = \frac{i\tau'}{\tau}$$

$$\frac{i H_0 (-i\lambda\tau)}{\tau} e$$

so the i and minus i cancels, the h cross cancels, it is e to the lambda H naught.

So this stands for, therefore this is equal to trace, e to the minus beta H naught integral zero to beta d lambda e to the lambda H naught A dot of zero e to the minus lambda H naught B of tau and it is the trace of the whole guy.

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$$= \text{Tr} \left( e^{-\beta H_0} \int_0^\beta d\lambda \dot{A}(-i\lambda t) B(t) \right)$$
$$= \text{Tr} \left( e^{-\beta H_0} \int_0^\beta d\lambda e^{\lambda H_0} A(0) e^{-\lambda H_0} B(t) \right) \quad \lambda = \frac{it'}{t}, \text{ or } t' = -i\lambda t$$

So it is the equilibrium expectation value, not of  $A$  dot of zero with  $B$  but an integral from zero to beta of this guy with these factors put in.

(Professor – student conversation starts)

Student: Are we allowed to pull that integration outside?

Professor: Yes, yes, yes you can pull the integral outside because the trace is over only the operators, Ok. This is going to be something called the Kubo canonical correlation. It is more complicated than the classical case. In the classical case, everything commutes. So this fellow cancels against this and that is it, and things would exactly the same thing that you got before.

(Professor – student conversation ends)

So let me stop here. Even the beta factor will come out. Because you got to do zero to beta  $d\lambda$  and that will give you beta factor which is sitting here, over here. So I will start at this point and show you what this does, what this quantum correction, we will do a calculation of a specific case and you will see why this thing is an extremely interesting quantity, Ok. Let me stop here now.