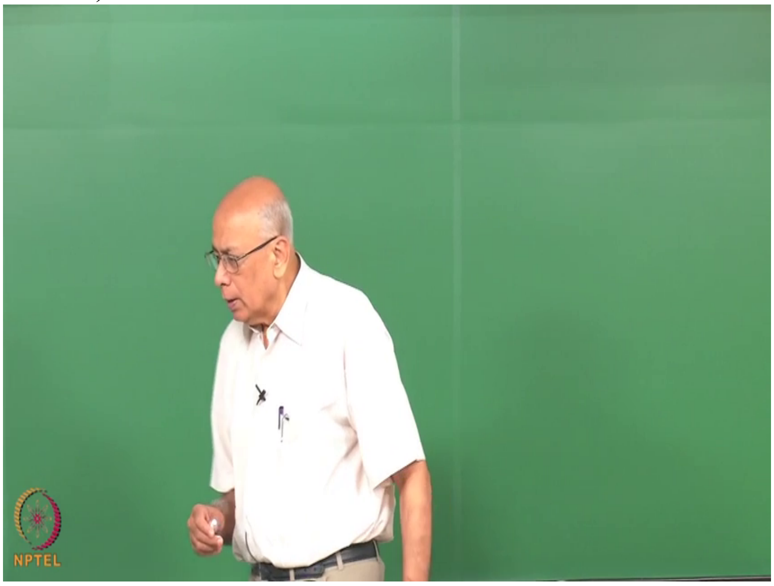
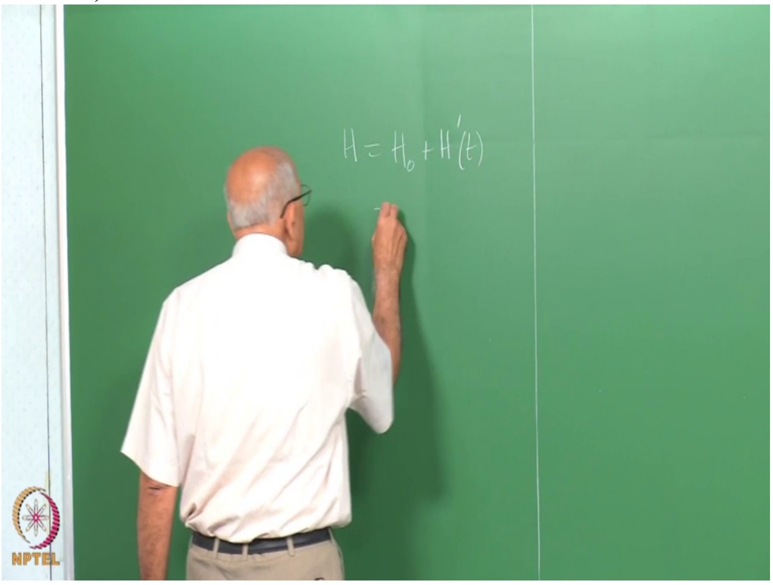
Nonequilibrium Statistical Mechanics
Professor V. Balakrishnan
Department of Physics
Indian Institute of Technology Madras
Lecture No 08
Linear response theory (Part 3)

(Refer Slide Time 00:17)



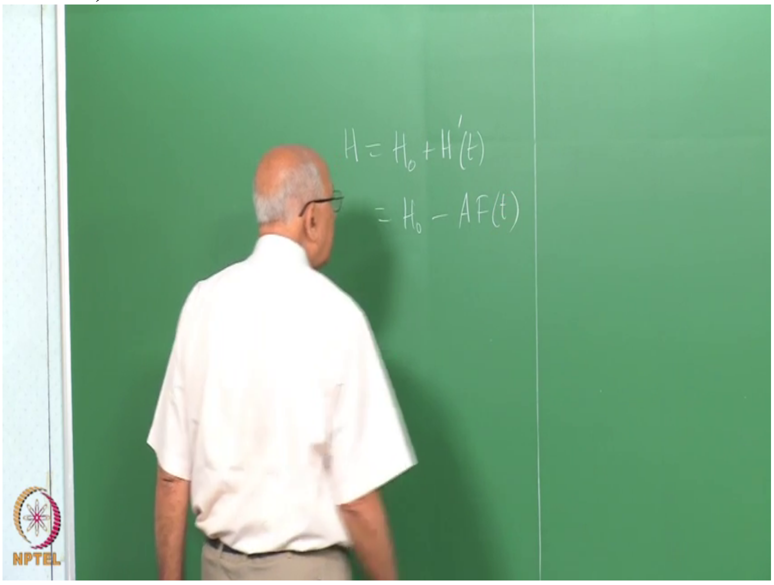
Right, so to recapitulate what I said the last time we have a situation where you have a system with a Hamiltonian which is this, a function of time

(Refer Slide Time 00:31)



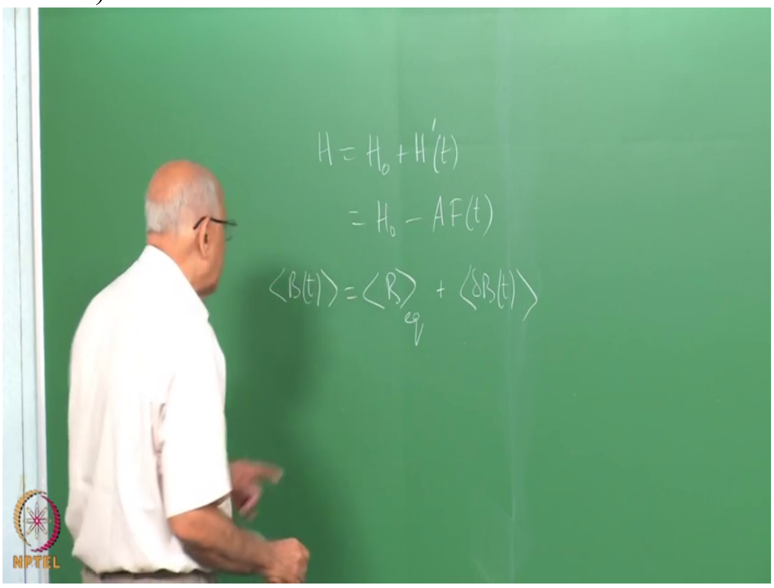
which we took to be H naught minus some A F of t,

(Refer Slide Time 00:37)



prescribed function here and then the question was what happens to thermal averages or average value observables, arbitrary observables and we found that if you took any observable B and ask what it's average was, it is B with respect to the equilibrium ensemble in the canonical ensemble for example, plus delta B of t and we got the formula for delta B of t

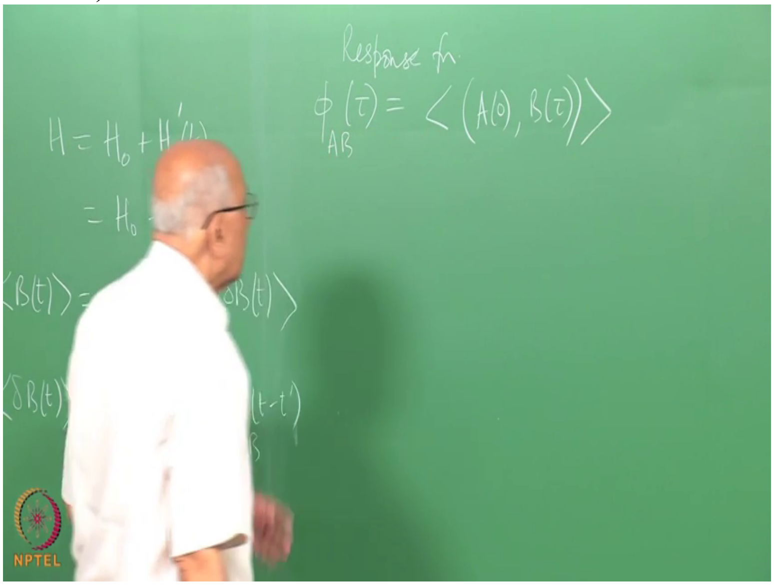
(Refer Slide Time 01:09)



which read average is equal to an integral from minus infinity to t d t prime the force integrated over the entire history of this force times the response function phi A B of t minus t prime.

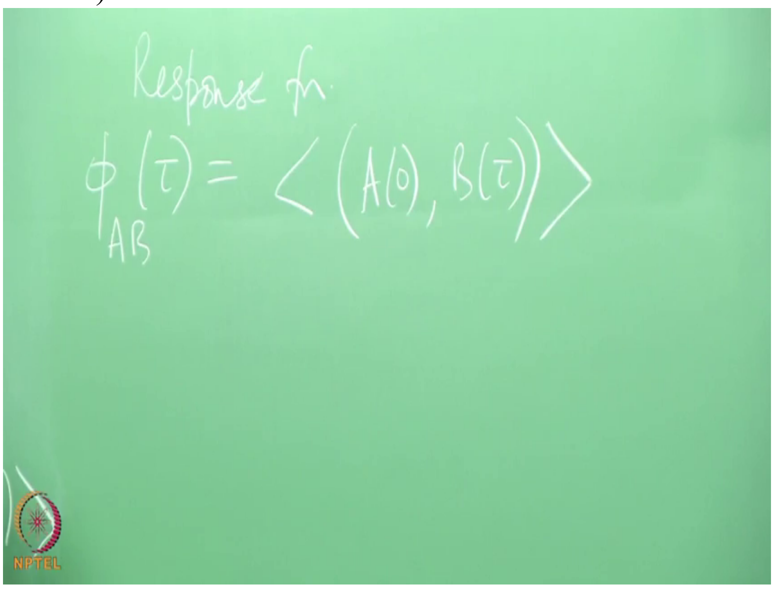
This response function is a certain correlation function in equilibrium so we discover that phi A B of tau for instance we have put t minus t prime equal to tau, this quantity, the response function was equal to the integral, was equal to the equilibrium expectation value of A of zero with B of tau, either the commutator or the Poisson bracket

(Refer Slide Time 02:16)



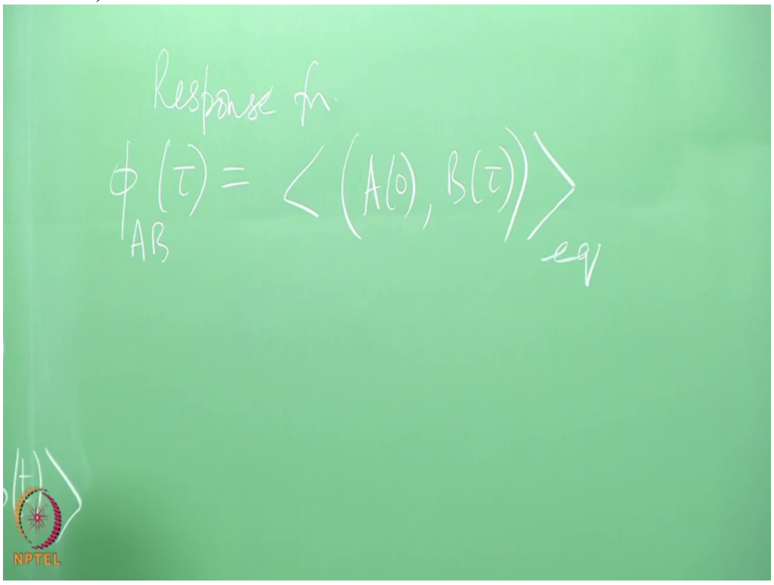
apart from some numerical factor

(Refer Slide Time 02:18)



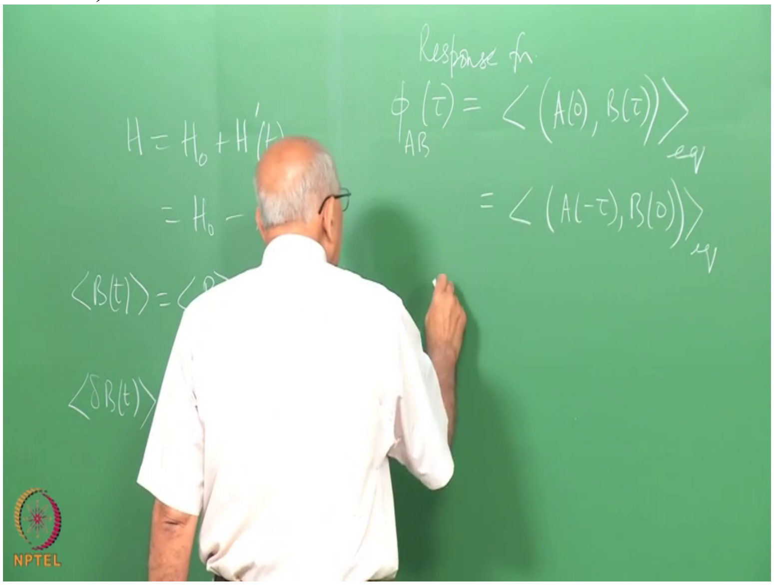
and that was what this was in equilibrium.

(Refer Slide Time 02:24)



So this average means something different. This is the average in the presence of the external force and if I write an equilibrium in here it means it is in the absence of the external force like this case here. We could also write this in several ways. We could write this as A of minus tau B of zero in equilibrium or if you like,

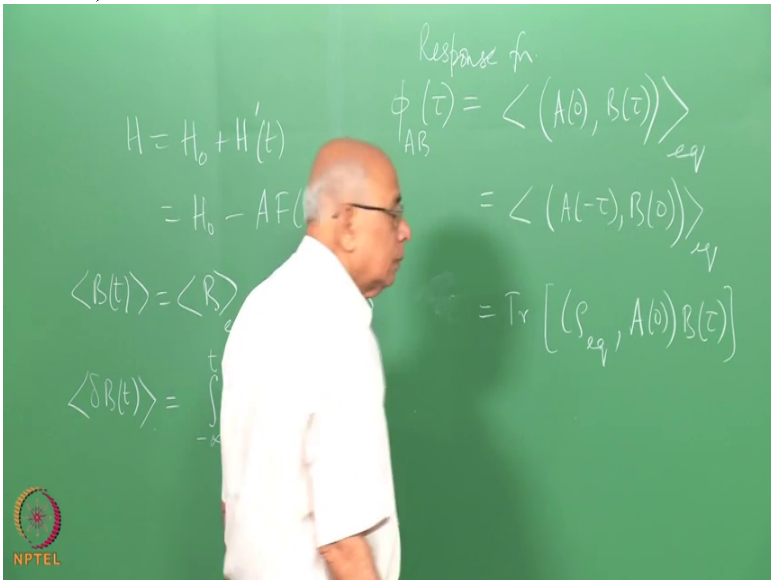
(Refer Slide Time 02:53)



you could also write it as equal to the trace.

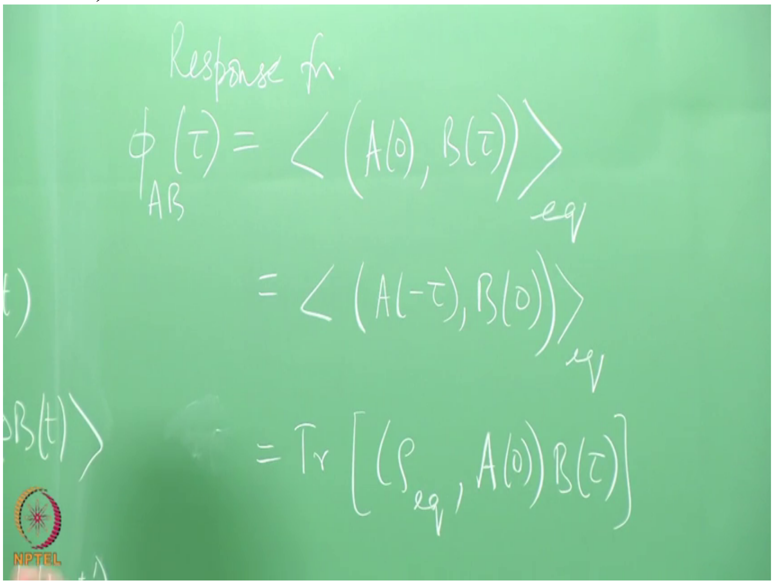
By the cyclic property of the trace, we could write in a number of ways, one of them is rho equilibrium with A of zero B of tau,

(Refer Slide Time 03:13)



just by the cyclic property of the trace. Or if you like rho equilibrium with A of minus tau B of zero and so on. Or this B could also come here because of the cyclic invariance of the trace. So we have a number of ways

(Refer Slide Time 03:27)



of writing or computing this quantity depending upon what is convenient.

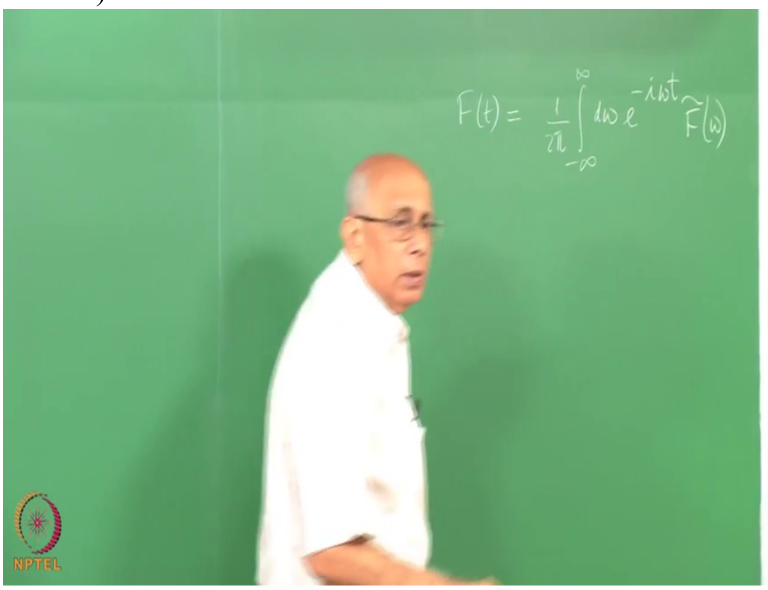
Now let us ask, what does it imply? What does this thing imply for us? Well, if you took a general, we already saw, we interpreted this to mean that the response is causal, linear first order in this course, causal because of this and retarded because the time argument depends on the elapsed time since the effect took, since the force acted at whatever time t prime. So given this closed formula, this formal expression here we could now proceed to analyze this in a little more depth.

The first thing you notice is while this is true for an arbitrary F of t, in arbitrary force history, because it is a linear response, the response to the sum of two forces is equal to the sum of the responses, individual responses because of the superposition principle. Now we know that any arbitrary force, any time dependent force can be resolved into its Fourier components, into frequency components. And then you find the response to a given frequency component and you can add up all those responses to get the full response. This is the whole point of Fourier analysis.

So it is very convenient to do that and let us see what happens if you did that, because it will give us a handle on what the system does for an arbitrary F of t in terms of what it does for various harmonics. We need a Fourier transform convention and I am going to stick to one because it is very easy to make numerical mistakes otherwise.

So let me write down Fourier transform convention here on this side. It doesn't matter which one you choose but we need a consistent one. So if I have a function F of t, I resolve into Fourier components then the Fourier components are resolved as minus infinity to infinity d omega e to the minus i omega t F tilde of omega.

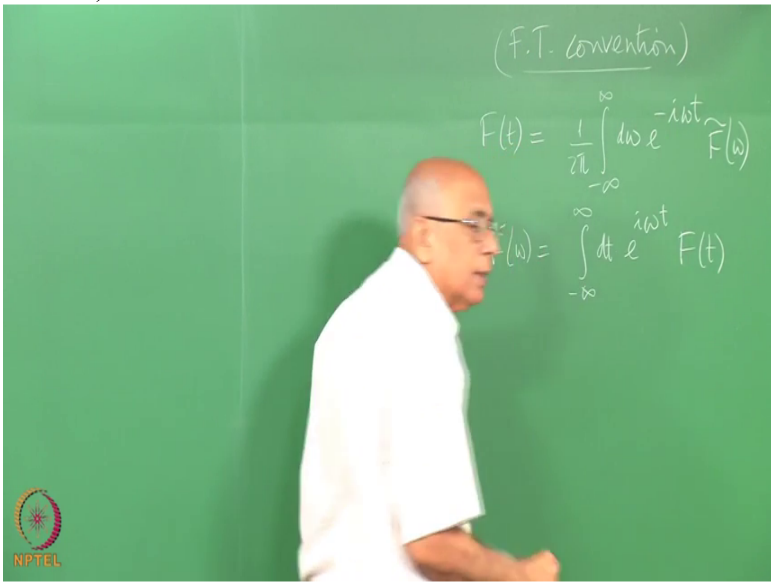
(Refer Slide Time 05:40)



And this implies that Ff tilde of omega equal to integral minus infinity to infinity d t e to the i omega t F of t 0:05:55.0.

So this is my Fourier transform convention once and for all.

(Refer Slide Time 06:06)

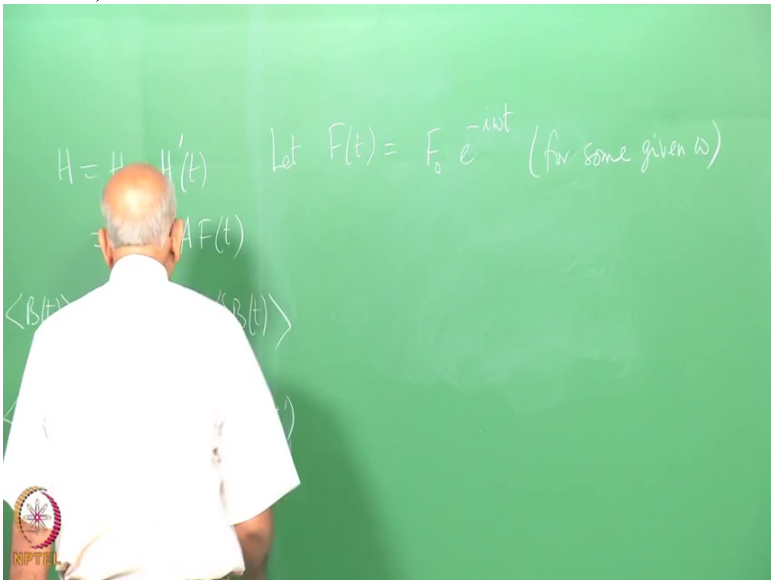


We will stick to this and if I make a mistake please point it out because we have to be careful with these signs. One appears with the minus, one with the plus, the 2 pi appears here rather than here and so on, now of course there are many other conventions, any one of them is just as good as the other, very often they use 1 over square root of 2 pi here, 1 over square root of 2 pi here to make it symmetric, this could be a plus and that could be a minus and so on. But we will stick to this convention.

So when I go from function, when I Fourier transform the function of time, it is 1 over 2 pi d omega is the measure and f tilde of omega is just d t, that is this. So we will try, I will try my best to stick to that convention. Then let's do the following.

Let's ask what happens if I apply a single harmonic and apply the force. So the force that I am going to apply is F of t equal to some amplitude F naught, later I will do with different amplitudes and that will be my F tilde of omega times e to the minus i omega t, some fixed omega, for some given omega. So let this be so and then

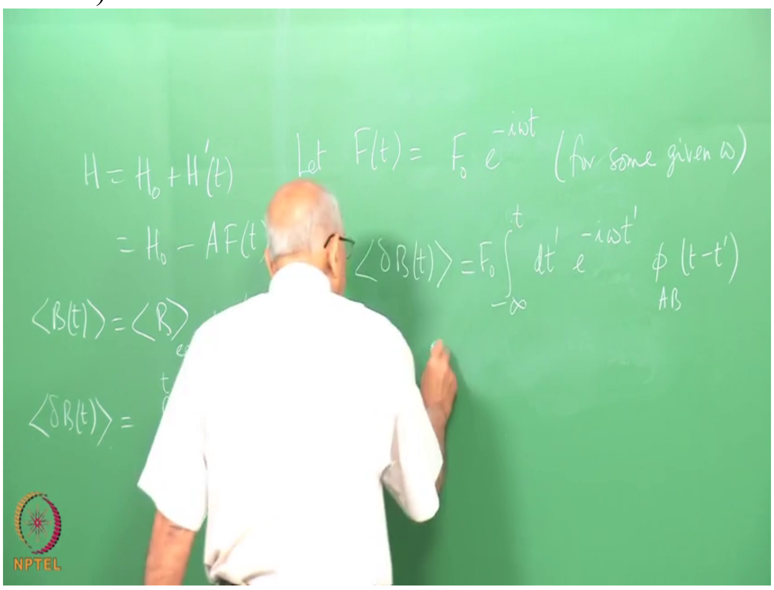
(Refer Slide Time 07:33)



we ask what the response is, this response is.

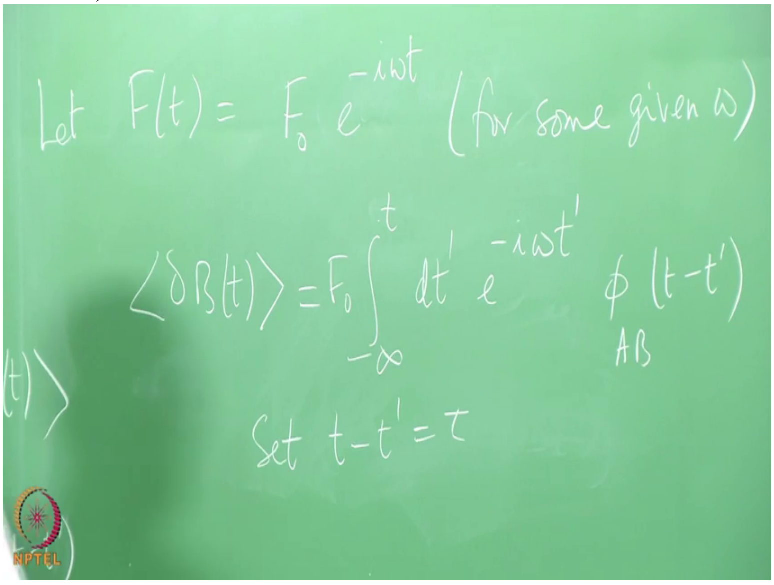
The corresponding response is delta B of t equal to an integral minus infinity to t and this is a F naught which comes out of the integral times d t prime e to the minus i omega t prime phi A B of t minus t prime and now let us set

(Refer Slide Time 08:06)



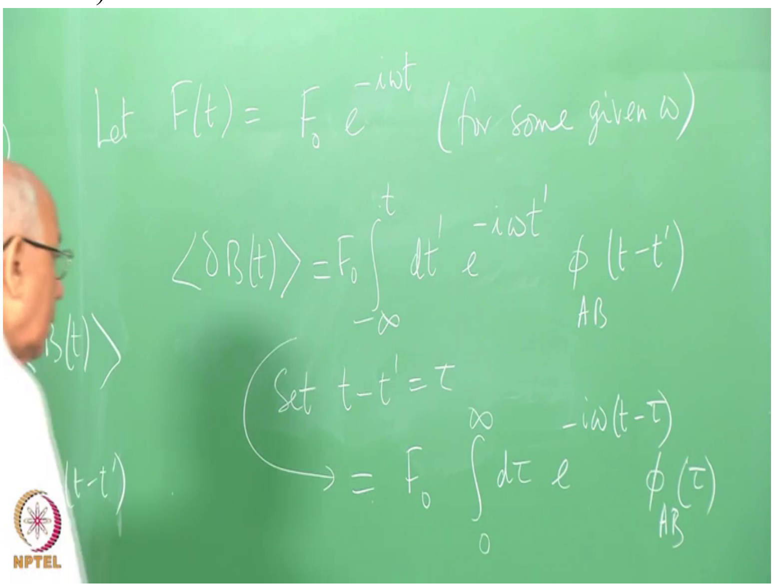
t minus t prime equal to tau. That's the obvious thing to do.

(Refer Slide Time 08:13)



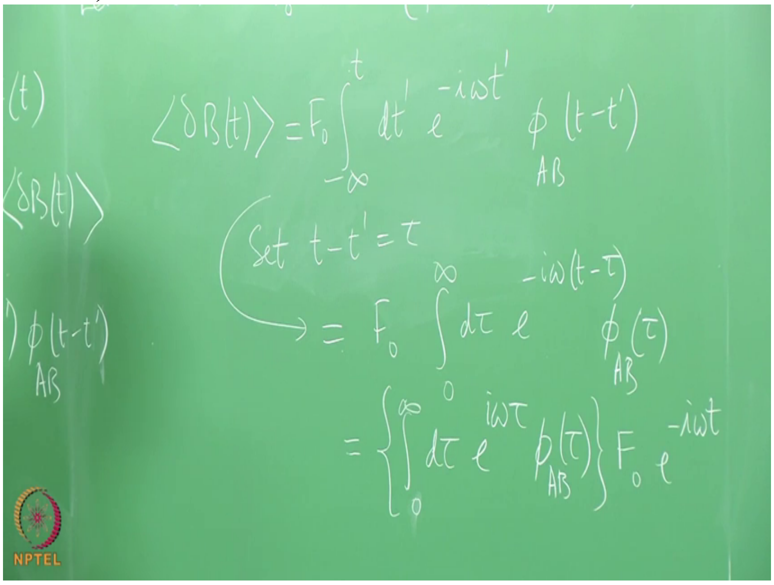
So this becomes equal to F naught integral, d t prime is minus d tau but this will run from infinity to zero here so I will switch that, zero to infinity d tau e to the minus i omega, t prime is t minus tau, phi A B of tau

(Refer Slide Time 08:48)



which is equal to, an integral from zero to infinity d tau e to the i omega tau 0:09:02.5 phi A B of tau, this whole thing multiplied by F naught e to the minus i omega t.

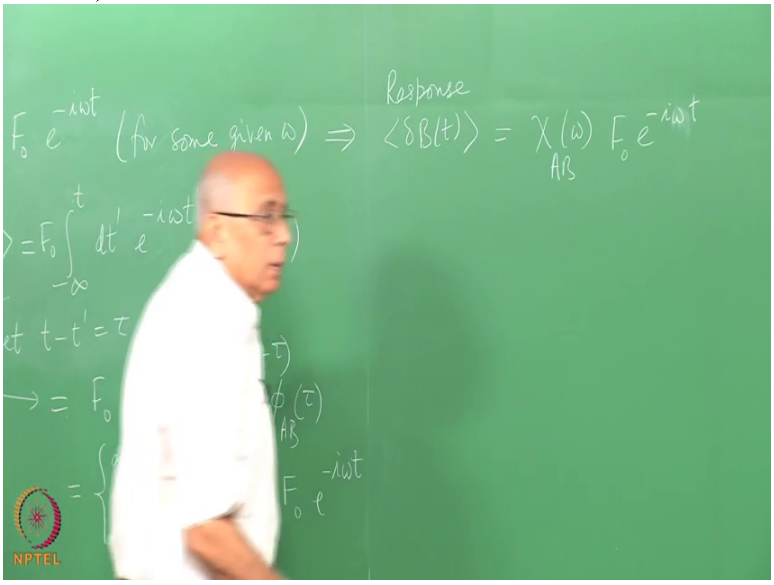
(Refer Slide Time 09:18)



So this immediately says that if I apply the force F naught e to the minus i omega t, in practice of course I apply a real force but technically it could have this as a complex number, F naught I don't have to say, I don't impose a reality on F naught, it could be complex so this is of the form cos plus sin or something like that, we will take real, imaginary parts later but if I write the force of this kind then the response is the same force multiplied by the function of just one variable. And what's that?

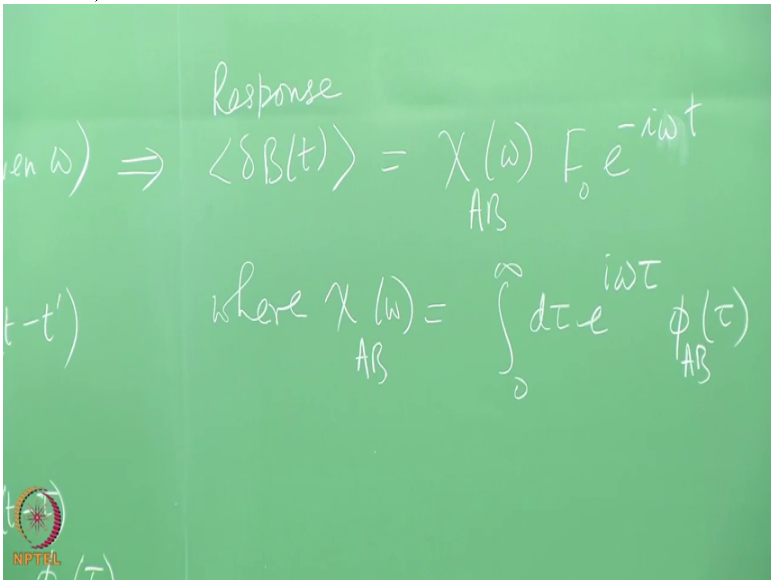
This depends on omega. Because tau is integrated over, it is a dummy variable so this is a function of omega. If of course depends on what is A, what is B but it is a function of omega. So this says, this implies that the response delta B of t, given this force, the response this is equal to some function kai A B of omega times the force.

(Refer Slide Time 10:35)



In other words, the response is just the same, is multi/multiplied, is the force multiplied by some function of omega depends on omega alone, some attenuating factor where kai A B of omega is this integral, zero to infinity d tau e to the i omega tau phi A B of tau, Ok.

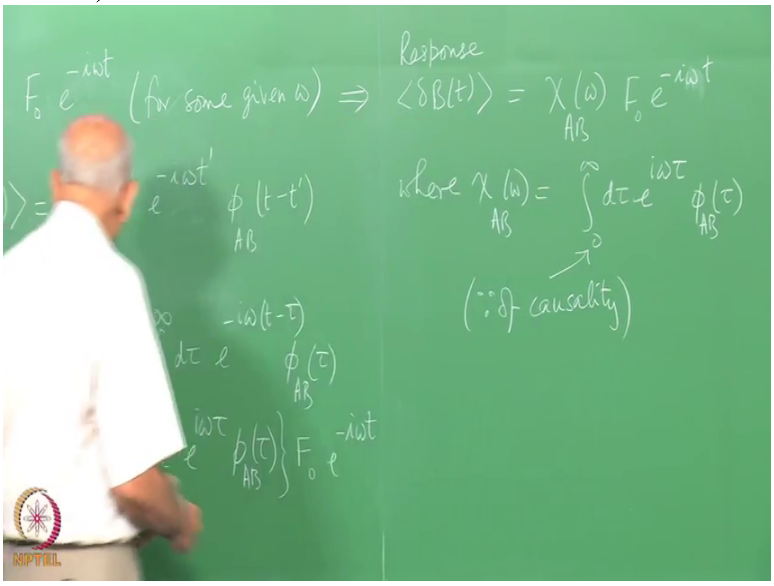
(Refer Slide Time 11:06)



This is the Fourier transform of the response function? No, it's not.

It’s the integral from zero to infinity. It is the one-sided, see we haven't even defined this quantity for negative tau. Formally we can do so but right now we are not interested in it. Because this integral is cut off at t. It is because it got cut off at t, that when I change variables the lower limit became zero. So this zero is a direct consequence of causality. This quantity here is because of causality.

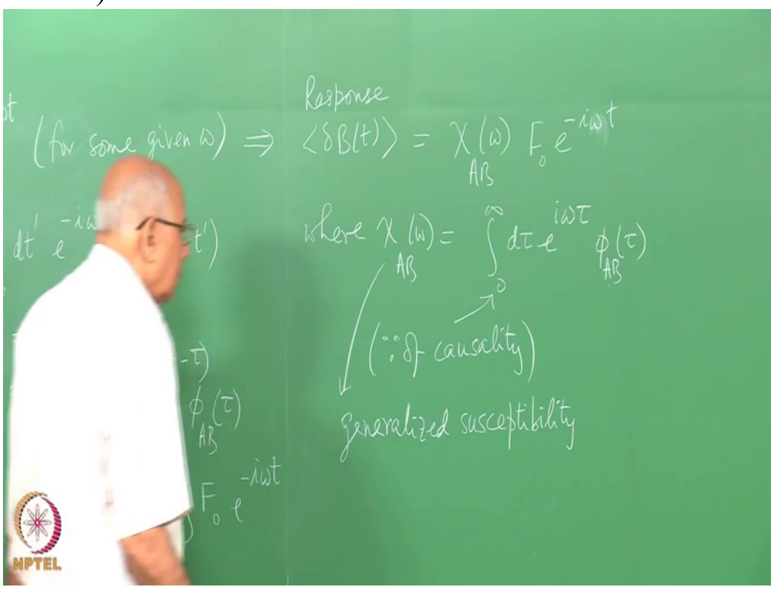
(Refer Slide Time 12:03)



The force at a later time cannot affect the effect at earlier time. So it is like the one-sided Fourier transform.

If this had been minus infinity, then you would have argued that by analogy with this formula I would have said it is the Fourier transform. But this fellow is just the one-sided Fourier transform. The integral is running from zero towards here. This thing here, just as this is called the response function, this is called the generalized susceptibility, Ok

(Refer Slide Time 12:48)

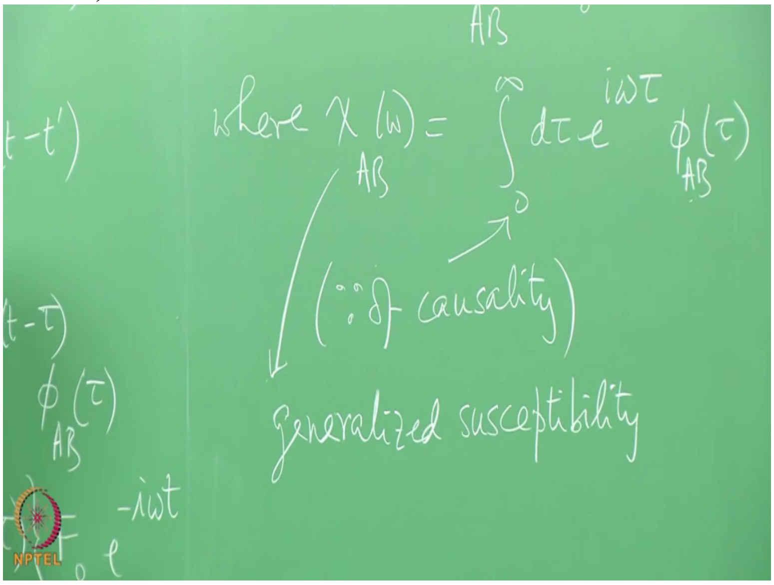


corresponding to the cause A and an effect B.

In other words you put up the system through A and you measure some other quantity B which could be A itself in some cases. So common examples are you apply a magnetic field, you measure the magnetization. You apply the electric field. You measure the polarization. You apply a stress; you measure the strain and so on. So this is a very, very general framework. We will look at many examples. But this is a very, very general framework and this quantity here carries all the information that is carried in this response function.

Once you give me

(Refer Slide Time 13:35)

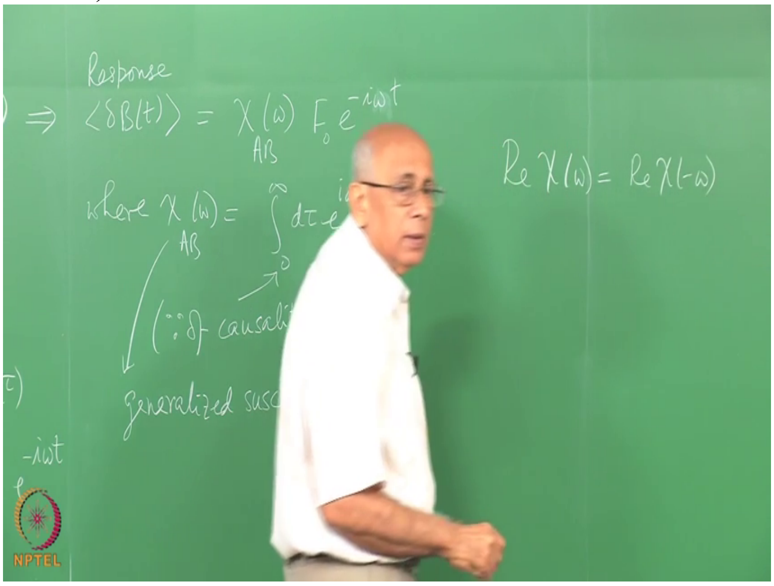


this kai of omega and I know what it does for a particular frequency, it looks like this. This is the response. For a general force all I have to do is to sum all these fellows with this rate factor as a function of frequency times F tilde of omega as the amplitude of frequency omega and I integrate over all the frequencies and that is the general response in principle. So the susceptibility carries all the information. But it is crucial to note that it is a one-sided Fourier transform. It is going to have important consequences, very crucial consequences.

Now the question is can we write this in terms of Fourier transform itself? Can we write this guy in some fashion as a Fourier transform itself? So let me do that but before that there is one more thing I want to point out which is that the real; there is no reason why this quantity is real at all. In general it is complex and we will see shortly that it cannot be either purely real or purely complex, purely imaginary. It has to be complex in general. Because we will attach physical meaning to the real part and the imaginary part.

Now if you take the real part of this, it is the real part of e to i omega tau provided this fellow is real and this guy here is in terms of physical quantity so these are all observable quantities, all the operators are Hermitian , then phi A B of tau is actually a real quantity. So the real part of this has a cosine and the imaginary part has a sine function and therefore the real part of this kai is a symmetric function of omega. So real kai of omega equal to real kai minus omega,

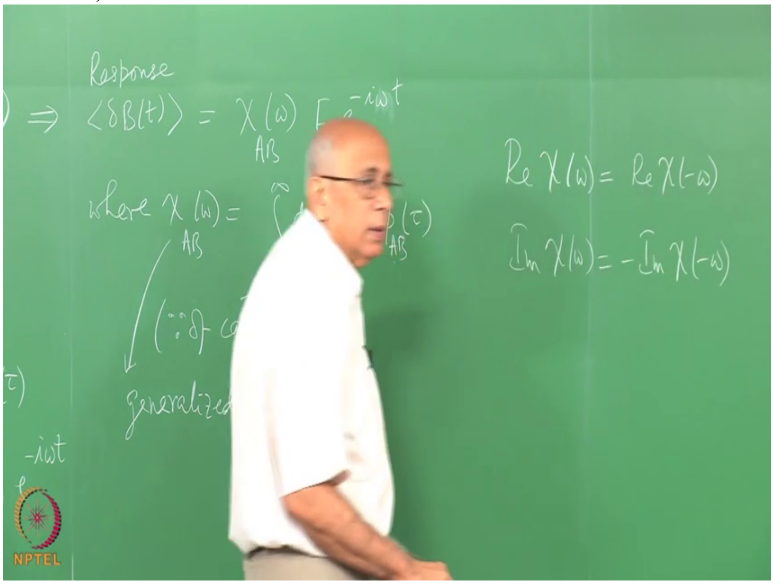
(Refer Slide Time 15:39)



symmetric function.

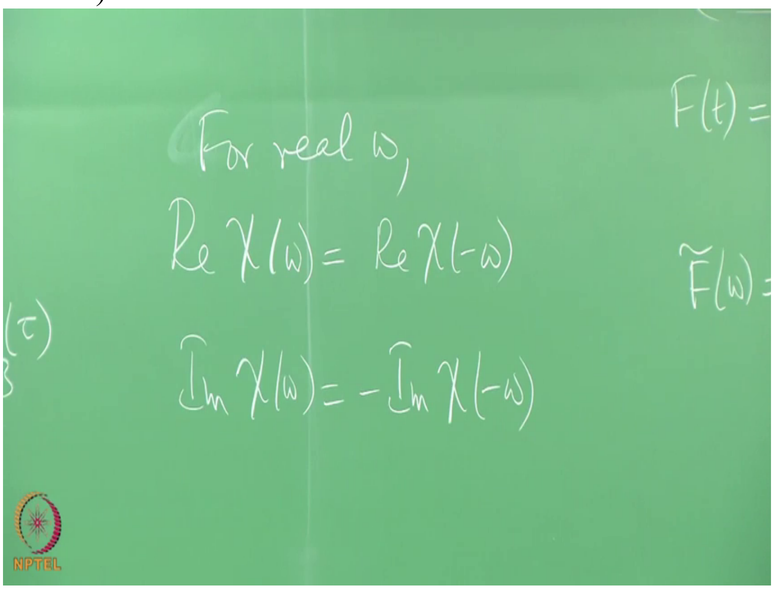
On the other hand, imaginary part, kai of omega, it is minus imaginary part kai of minus omega,

(Refer Slide Time 15:51)



for real omega. And so far our frequency is here, just like time, the frequency is here. Very soon we are going to make an excursion into the complex plane. We are going to go to complex frequencies and then come back for physical quantities to real frequencies but for real values of omega, for real omega, which are the, in fact the physical frequencies are not only real but positive,

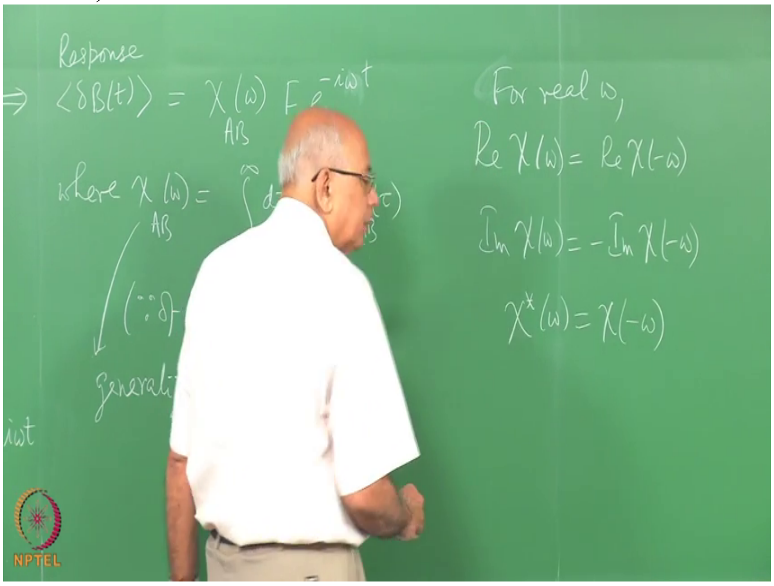
(Refer Slide Time 16:24)



non-negative. We will come to that but at the moment as a mathematical exercise, for real values of omega you see that the real part of kai is a symmetric function, the imaginary part is an anti-symmetric function.

You can combine both by saying kai star of omega equal to kai minus omega.

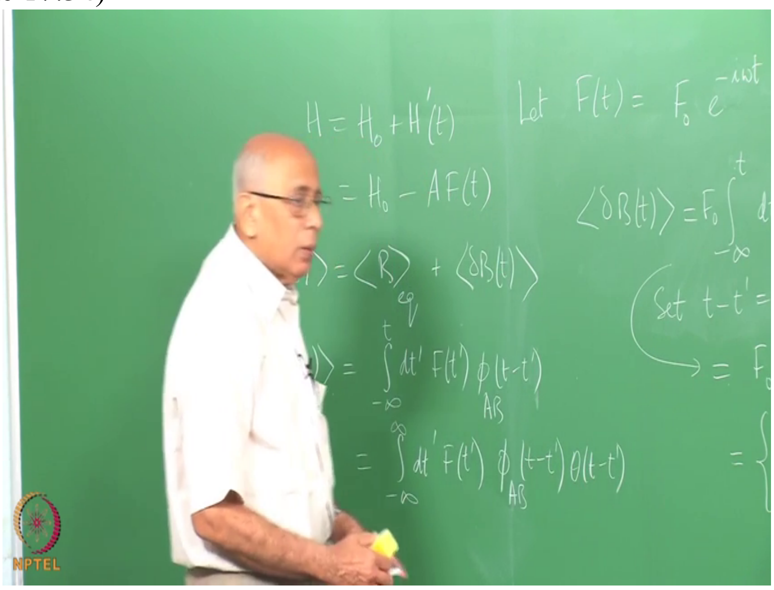
(Refer Slide Time 16:47)



Because if we take the complex conjugate here, this is real, this becomes minus; that is the same as kai of minus omega. That is a useful symmetric property. We will make use of it 0:17:01.8.

Now could I possibly write this in terms of this response, could I write it in terms of a Fourier transform itself? The answer is yes because you see you can always write this as minus infinity to infinity d t prime F of t prime phi A B of t minus t prime multiplied by a step function theta of t minus t prime where this is

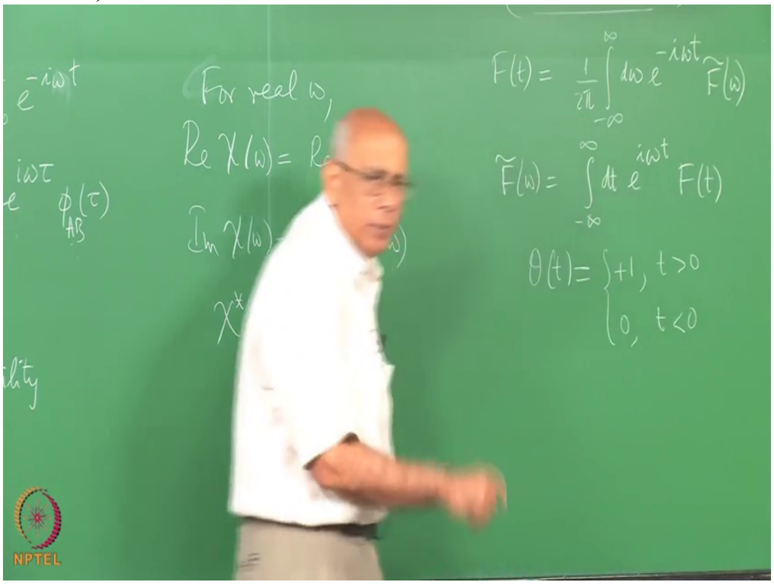
(Refer Slide Time 17:34)



the unit step function.

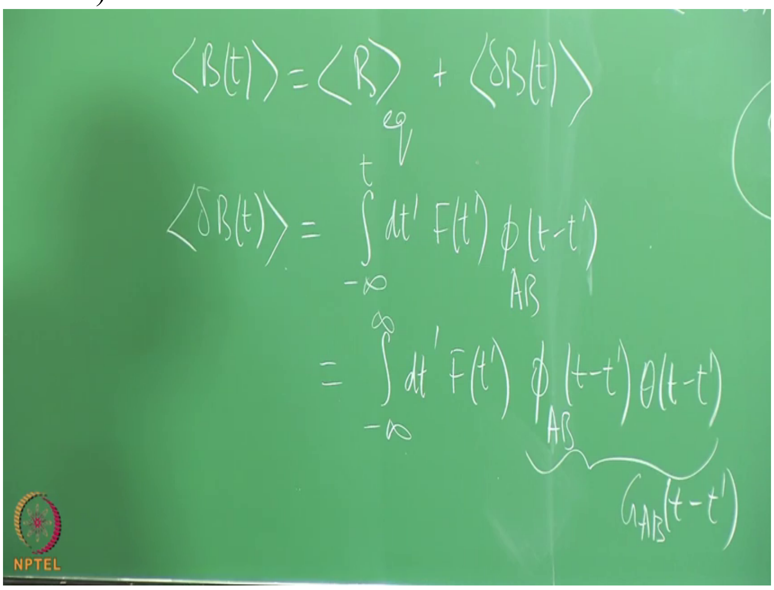
I presume, is this the notation you use for it or do you use any other notation? Sometimes people say I 0:17:46.9 write U or H or whatever but this is equal to plus 1, t greater than zero,

(Refer Slide Time 17:56)



so that's my definition of the theta function, the unit step function I will retain it. So if I put that in then this integral runs all the way to infinity because it gets cut off at t less than t prime. And I want to give it a name to this, so let me call it G A B of t minus t prime. G A B is the Green function. Because

(Refer Slide Time 18:24)

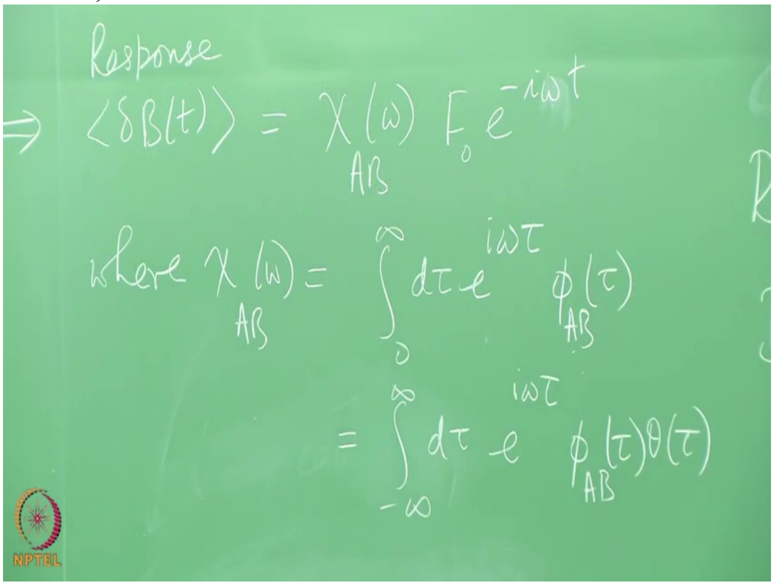


this is how you would write the thing in general.

You would say I apply a perturbation and I am looking for the response, whatever equation it satisfies we don't care, some dynamical equation. After I take averages the average value of this collection, the expectation of B is an integral over the force history for all of these times 0:18:44.4 Green function here. We will write a specific model down where we will see what G of t looks like, this fellow looks like.

So if we do that, then you could also write this formally, we could also write this as an integral from minus infinity to infinity d tau e to the i omega tau phi A B of tau theta of tau 0:19:16.1 just by

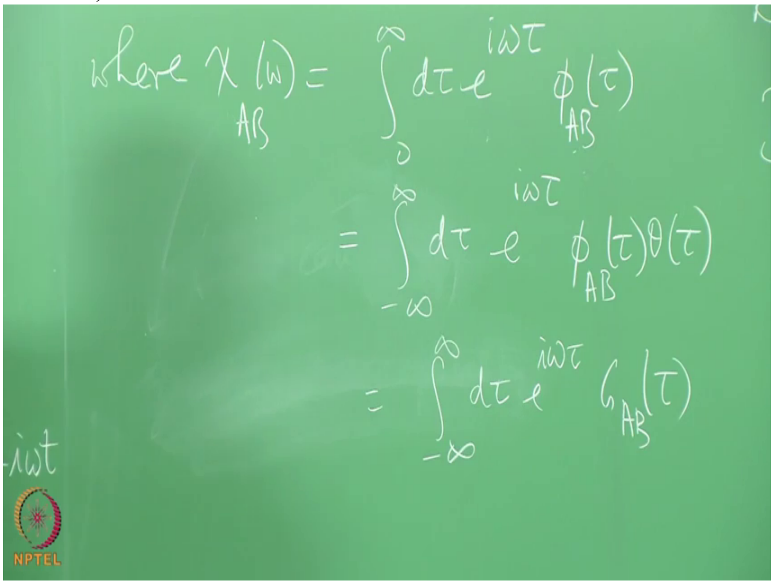
(Refer Slide Time 19:18)



putting in a theta function there. But this is what I have called the Green function, so this is equal to integral minus infinity to infinity d tau into the i omega tau G A B, Ok. And that is a Fourier transform.

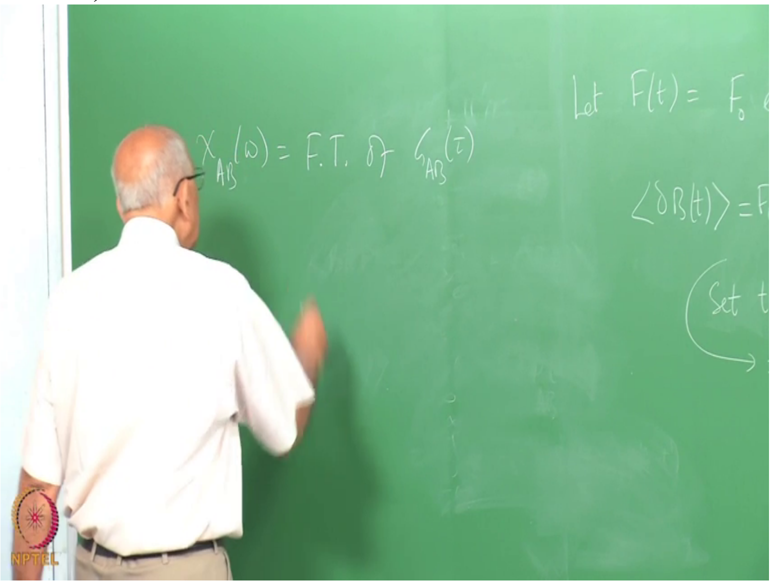
So it immediately says

(Refer Slide Time 19:46)



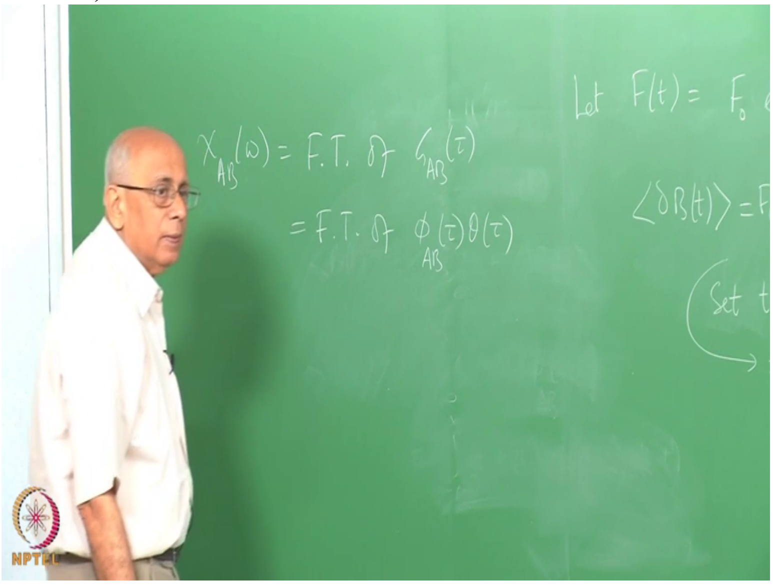
that this quantity is a Fourier transform of this G A B, tilde if you like. So where does that get us, right? Well it actually gives us some information because this guy Fourier transform of G A B of tau,

(Refer Slide Time 20:24)



which is the Fourier transform of phi A B of tau times theta of tau,

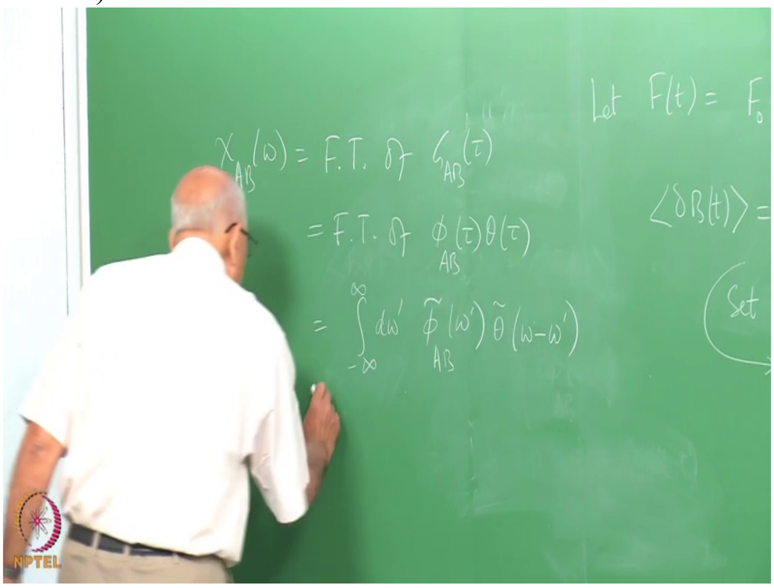
(Refer Slide Time 20:35)



right, by definition. But what's the formula for the, what theorem tells you, how to find the Fourier transform of the product of two functions of t? The convolution theorem.

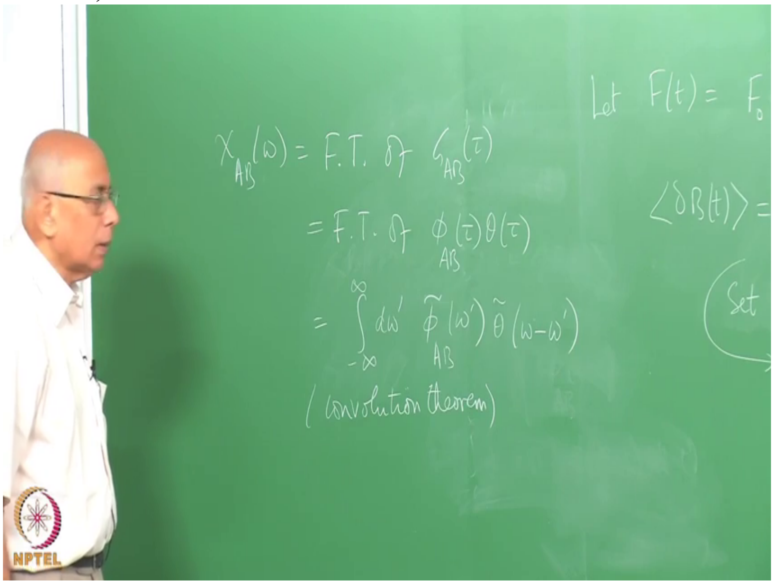
So it is clear that this must be equal to an integral from minus infinity to infinity d omega prime, the Fourier transforms of each of these. So phi A B tilde of omega theta tilde of omega, sorry of omega prime, theta omega of omega minus omega prime. This is the convolution theorem,

(Refer Slide Time 21:22)



right,

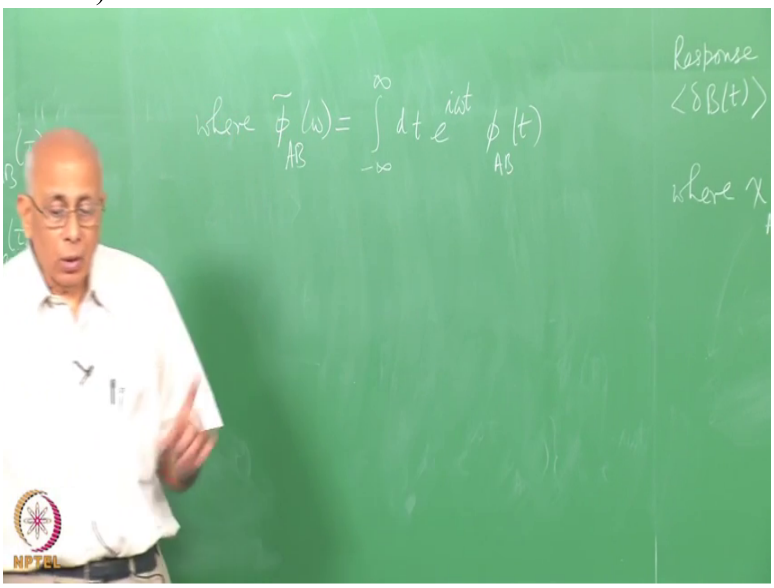
(Refer Slide Time 21:35)



where I have to define these quantities, where phi tilde A B of omega is the Fourier transform of phi A B.

Now phi is the one-sided Fourier transform but now we want the full-blown Fourier transform. So you go to this expression here, the Fourier transform is this, integral minus infinity to infinity d t e to the i omega t phi A B of t 0:22:14.5. Notice this requires now

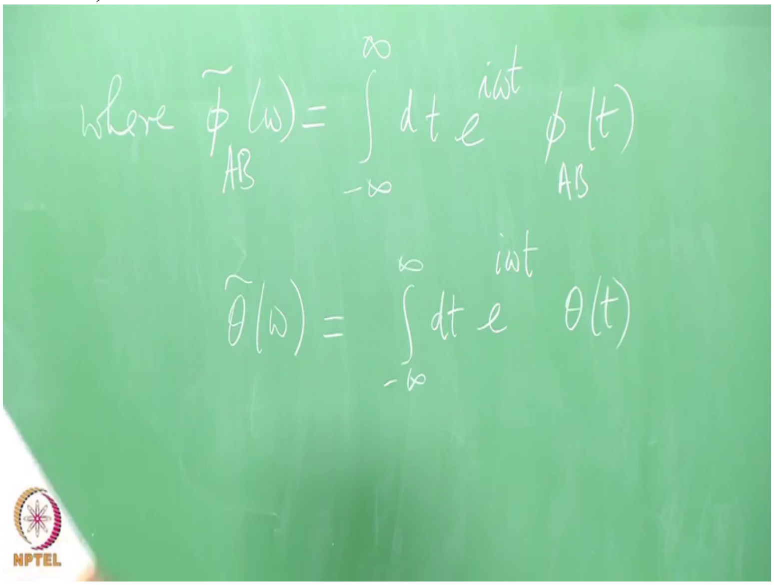
(Refer Slide Time 22:18)



a knowledge of phi A B of t for t less than zero. So we have to find that somehow.

So what we will do is to compute phi A B of t and ask what it does at reverse time, negative. So we will be able to define what phi A B of t is for all t. We will do that by 0:22:36.7. So this is equal to that and theta tilde of omega equal to an integral from minus infinity to infinity, at least formally d t e to the i omega t theta of, now you can write this fellow as zero to infinity d t, e to the i omega t which does not exist, it does not converge. Because e to the i omega t

(Refer Slide Time 23:07)



oscillates as t goes to infinity and as a Riemann integral, this does not exist.

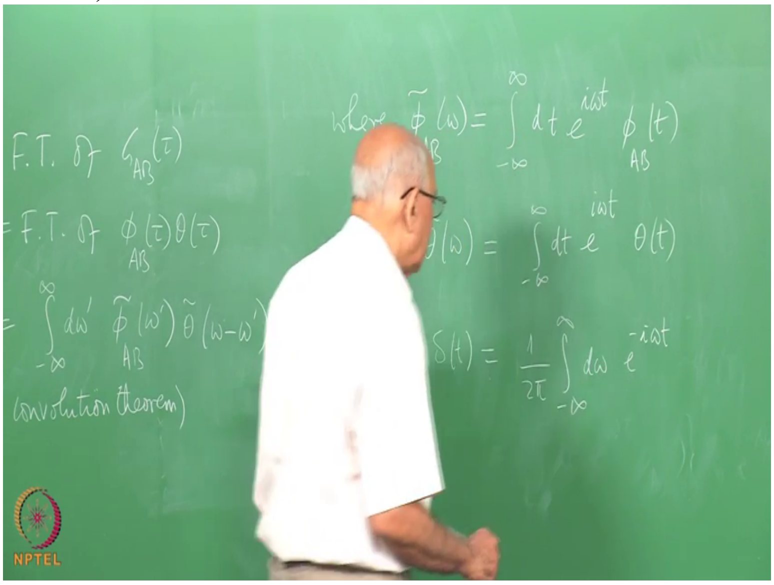
But this doesn't bother us because we know how to define Fourier transforms of distributions; theta of t, delta of t are not ordinary functions, they are distributions, right? So what I need is a Fourier transform, a Fourier representation for this quantity here. What would you do?

(Professor – student conversation starts)

Student: 0:23:33.2

Professor: I would like to find a representation as a contour integral of some kind, how do you do that? There are many representations. But we want something which looks like this representation here, what would you do? Well let's start with the statement that delta of t, and I want to keep a track of that kind of convention, e to the minus i omega t, so it is 1 over 2 pi integral minus infinity to infinity d t e to the minus i omega t, delta of d omega.

(Refer Slide Time 24:18)

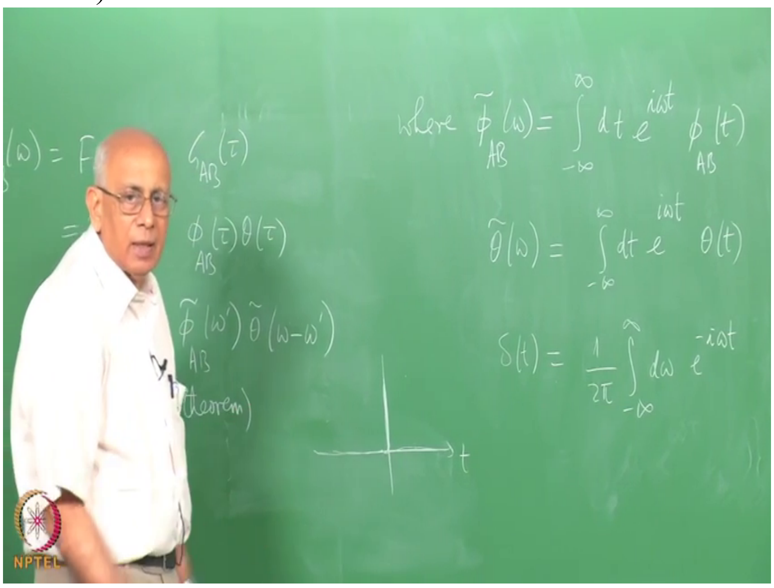


That is 0:24:19.8 the well-known representation, Fourier representation for a delta function, right? It also says delta tilde of omega is 1. That is what this is trying to tell us, Ok. Now given delta of t, how is the theta function related to the delta function?

Student: integral 0:24:35.1

Professor: It is the integral of it, and it is clear that if you got delta function in t at t equal to zero, if you integrate from minus infinity up to any point less than zero, the answer is zero. You integrate beyond t equal to zero and the answer is 1. So it is precisely the theta function,

(Refer Slide Time 24:54)

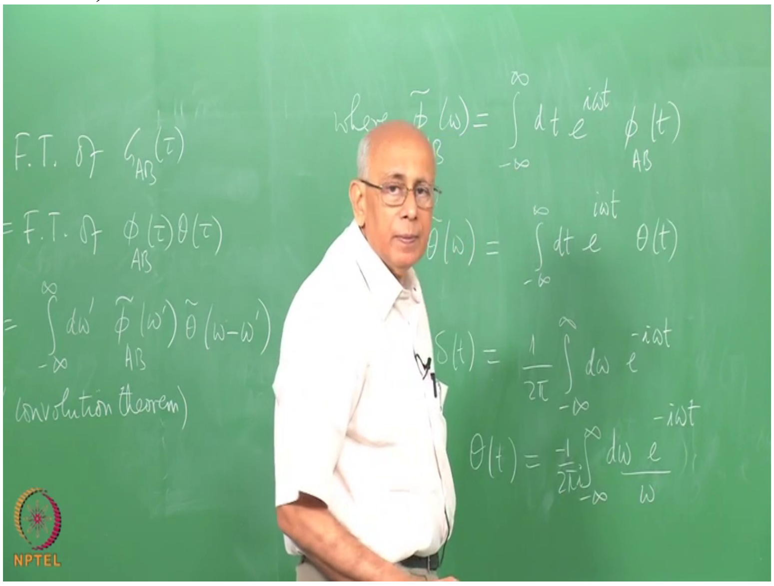


the integral of the delta function. If I differentiate, if I integrate this quantity, I must integrate this with respect to t.

(Professor – student conversation ends)

So the conjecture is that this quantity theta of t is equal to an integral 1 over 2 pi minus infinity to infinity d omega e to the minus i omega t divided by minus i omega, formally. This is the integral, right? So let me write it as i and put a minus sign here, over omega.

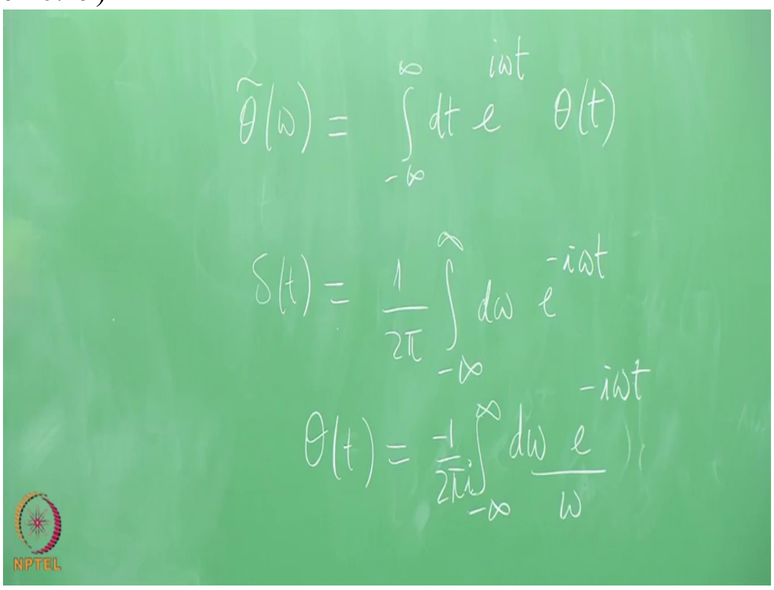
(Refer Slide Time 25:42)



That is not a great idea because this integral does not exist, it is singular. It passes through omega equal to zero and this fellow is singular. So it is not yet there. We have to fix this problem. What would you do?

You shift this pole at omega equal to zero away from the real axis and then you would find what the boundary value is in the limit, right? So we want an answer,

(Refer Slide Time 26:19)

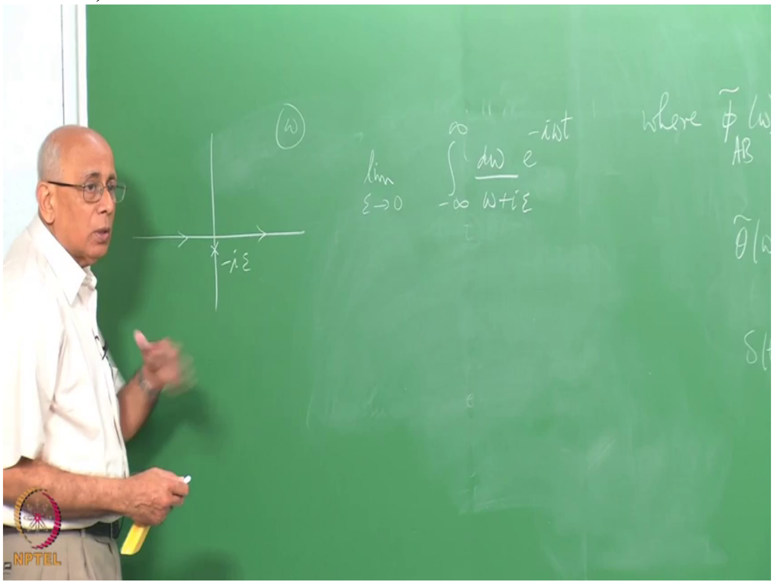


we want to fix it in such a way that theta of t must be equal to 1 for t greater than zero and zero for t less than zero, right? So let us look at this contour integral.

In the omega plane the integration runs from minus infinity to infinity. There is a polar t origin. If that pole is displaced downwards by i epsilon here instead of zero then we ask what happens to this integral? Well, let's ask what is limit epsilon goes to zero from above integral minus infinity to infinity d omega over omega plus i epsilon. So the pole is at minus i epsilon e to the minus i omega t. What is this fellow equal to?

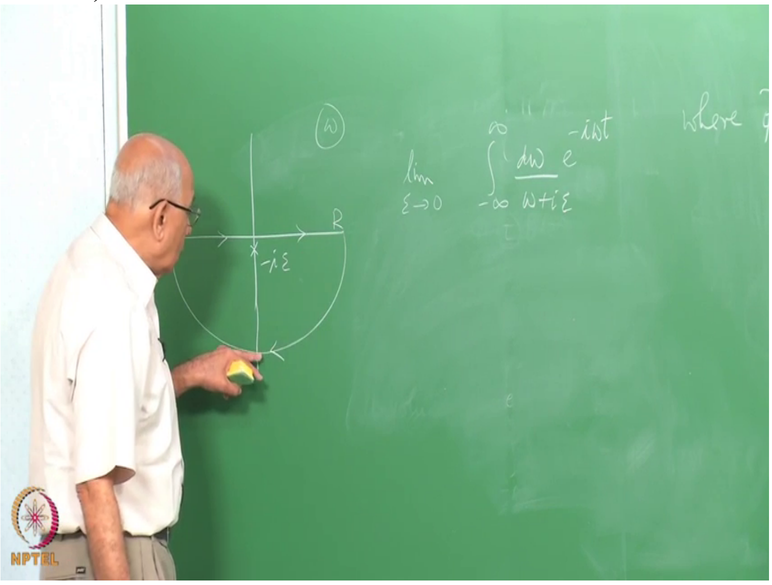
As a contour integral it is perfectly well-defined now because there is no singularity on the line, region of integration, on the contour

(Refer Slide Time 27:28)



of integration. But now the only way we know how to do contour integral is using Cauchy's theorem for a closed contour. So we need to close the contour. We must formally define it as running from minus r to r and take the limit r going to infinity. But we could close the contour with a semi-circle and if you do that in this fashion here then the contribution, if this is R, some radius R

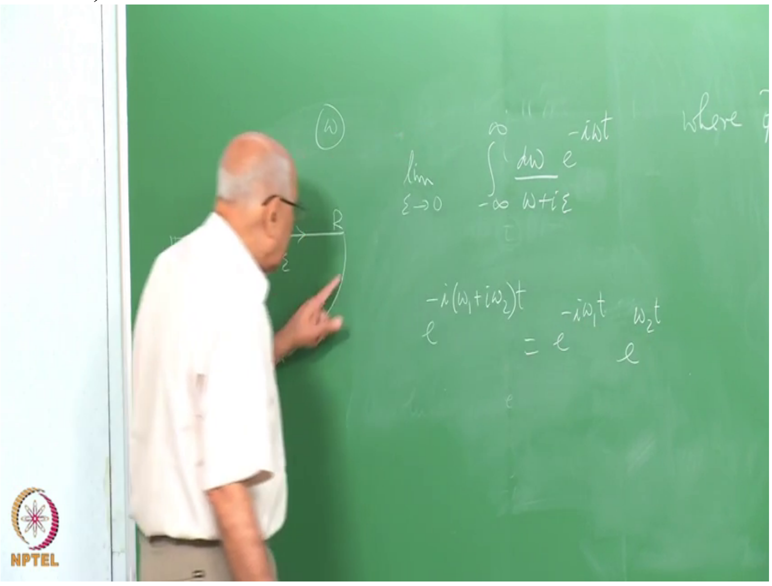
(Refer Slide Time 27:57)



on this circle, this variable omega is R e to the i theta. You can see that, if I have e to the minus i omega 1 plus omega 2 t, this is equal to e to the minus i omega 1 t if omega is complex like anywhere in this plane, and then plus omega 2 t, times e to the omega 2 t.

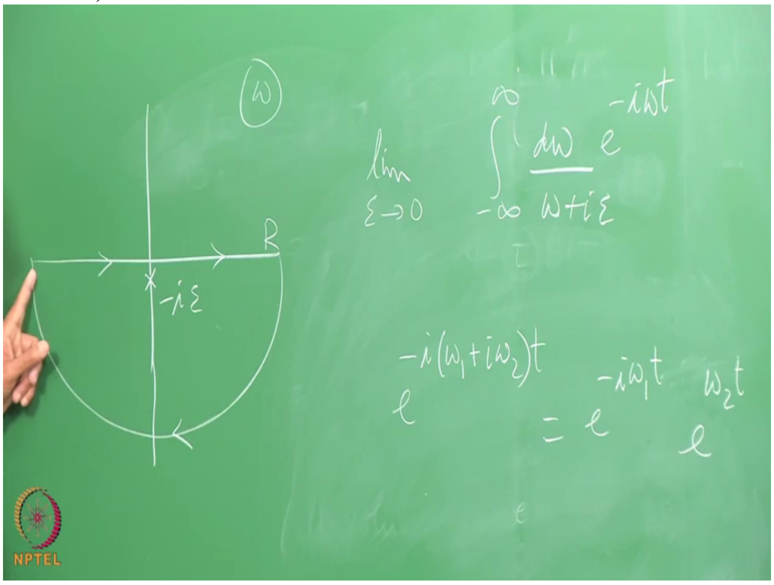
Now if t is bigger than zero, this is a positive number then this

(Refer Slide Time 28:34)



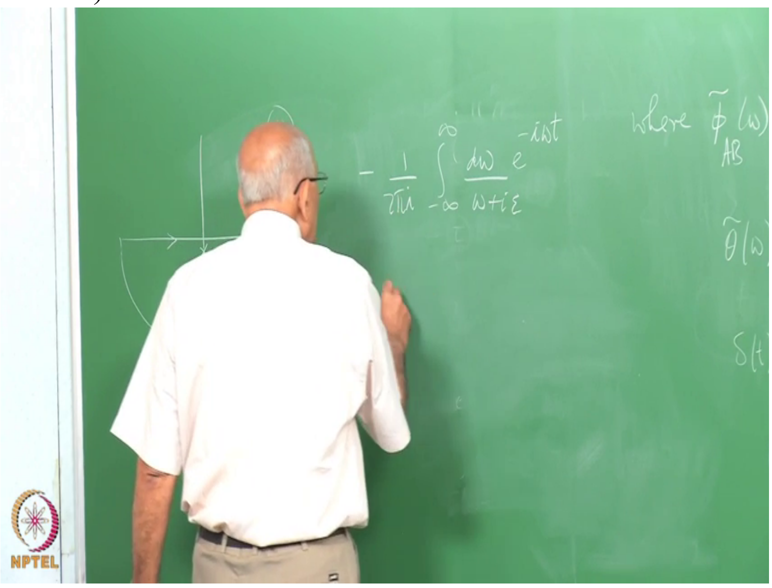
contribution vanishes as R goes to infinity provided this term is negative. This means the omega 2, the imaginary part of omega must be negative, which means the omega must be in the lower half plane. In other words this is the contour to choose,

(Refer Slide Time 28:55)



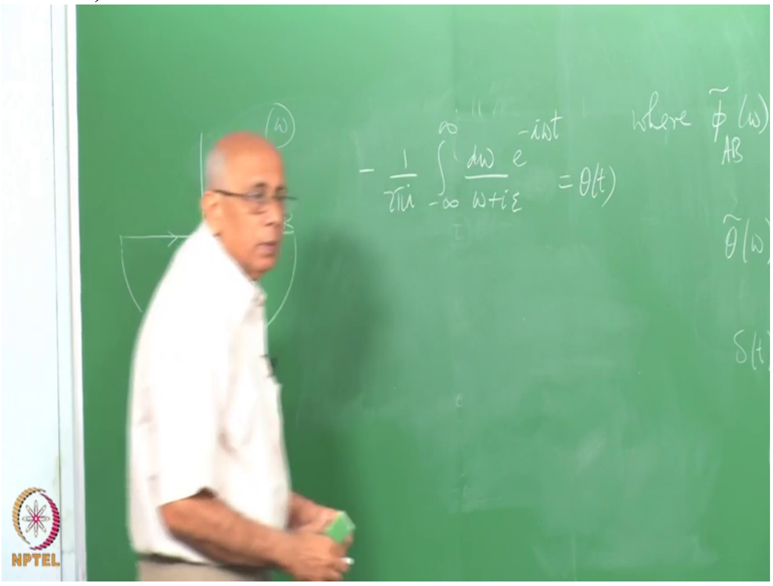
right? If t is negative you are forced to close it in the upper half plane. But there is no singularity in closing it in the upper half, when closed by the contour in the upper half plane. So this is going to give you 2 pi i whatever it is, if it is in the lower half plane, if t is positive, if t is positive it is going to give you zero. So this is equal to, so let's put in the minus 1 over 2 pi i as well, minus 1 over 2 pi i, this quantity

(Refer Slide Time 29:35)



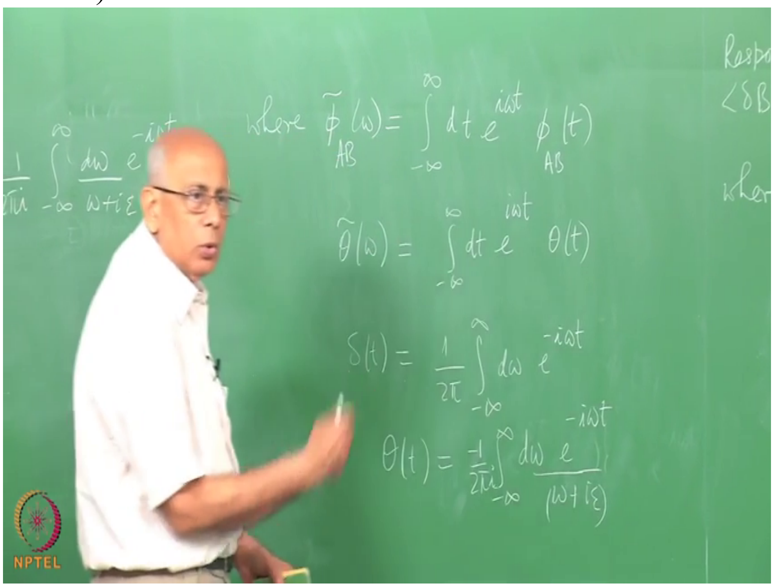
is equal to, there is a minus 2 pi i over here and when you close it here you are going in the clockwise direction so it is minus 2 pi i times the residue, the two minuses cancel each other and you get e to the minus i t times omega is minus i epsilon, and now take epsilon goes to zero, e to the zero is 1. And you end up with the theta function. So this is precisely equal to the theta function.

(Refer Slide Time 30:06)



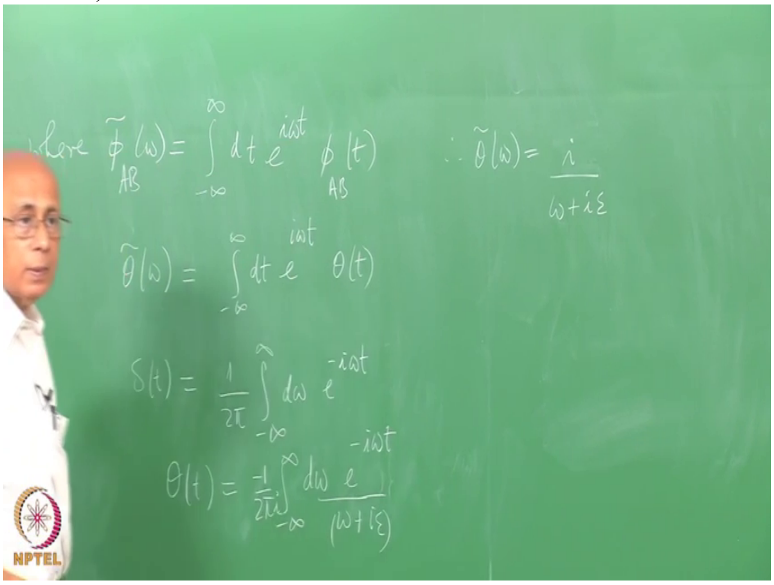
If I want a theta of minus t then I have to put plus i epsilon, move it in the upper half. So what we have done is to find a Fourier representation for the theta function. So theta of t is equal to this, the limit as epsilon goes to zero

(Refer Slide Time 30:27)



from positive values. So what is theta tilde of omega? We have a formula now. Therefore theta tilde of omega equal to limit, well I don't write this limit, it is understood, this sense, if you look at the Fourier transform definition, it is integral theta tilde of ome/omega, theta of t, look at its definition, 1 over 2 pi e to the minus i t times the Fourier transform and what is the coefficient of 1 over 2 pi e to the minus i omega t? So theta tilde of omega is equal to minus 1 over i, which is i divided by omega plus i epsilon,

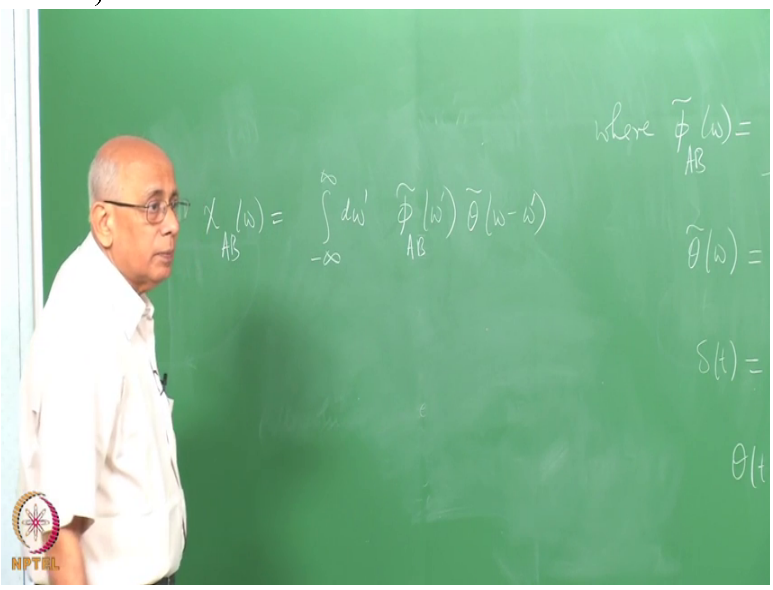
(Refer Slide Time 31:25)



Ok. That is the Fourier representation of the theta function.

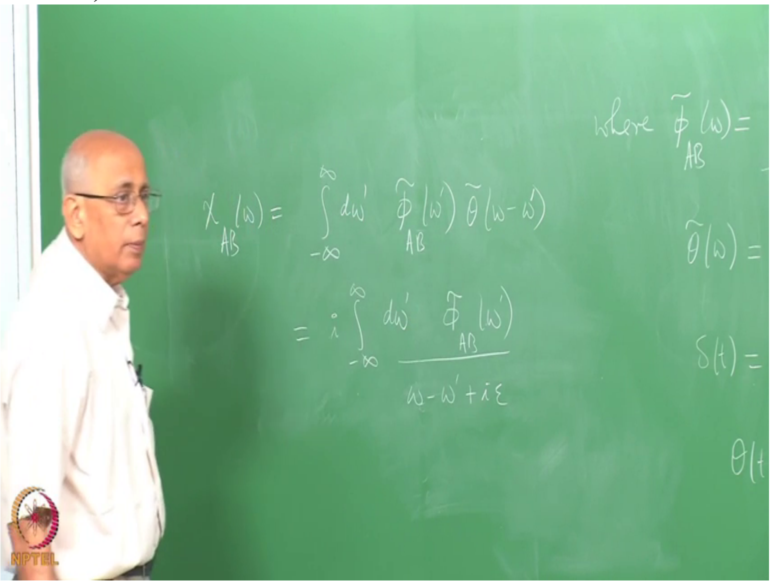
Now let's go back and we said that susceptibility kai A B of omega was equal to a convolution minus infinity to infinity t omega prime phi A B tilde of omega prime, theta tilde of omega prime minus omega, sorry omega minus omega prime. That was a convolution.

(Refer Slide Time 32:06)



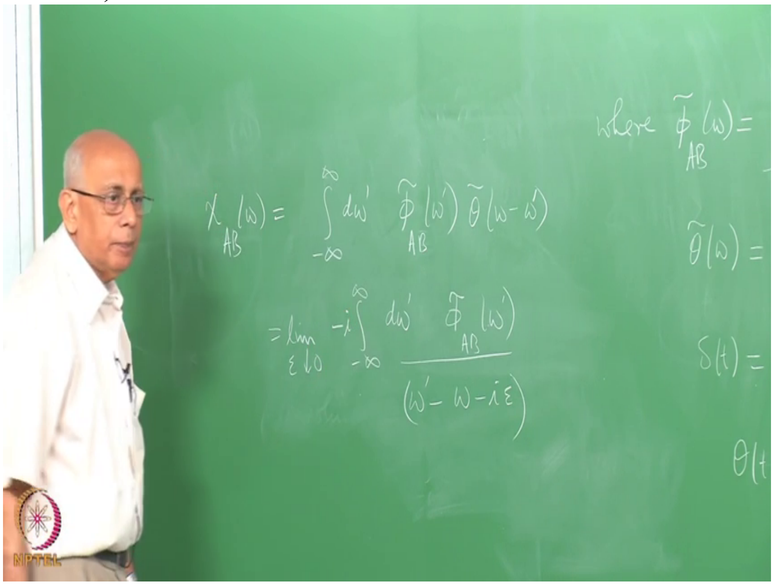
Therefore this is equal to minus infinity to infinity d omega prime phi A B tilde of omega prime divided by, there is an i outside, omega minus omega prime plus i epsilon, wherever omega appears I have to write omega minus omega prime.

(Refer Slide Time 32:42)



It is convenient to write this in order to do the integral as omega prime minus omega minus i epsilon, so let's write it as equal to limit epsilon goes to zero minus i times this guy.

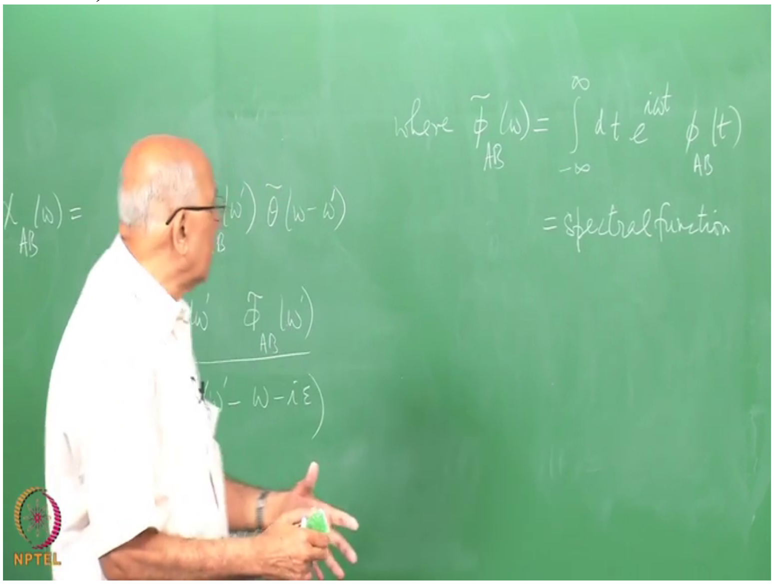
(Refer Slide Time 33:05)



So the susceptibility at any frequency omega has this Cauchy kernel out here, 1 over omega prime minus omega and the weight factor with which the given frequency omega prime appears is given by the Fourier transform of the response function. So this is like a spectral resolution with different frequencies of this function here. So not surprisingly this quantity is defined as the spectral function.

So we have introduced 3 different quantities, all related to each other.

(Refer Slide Time 33:54)

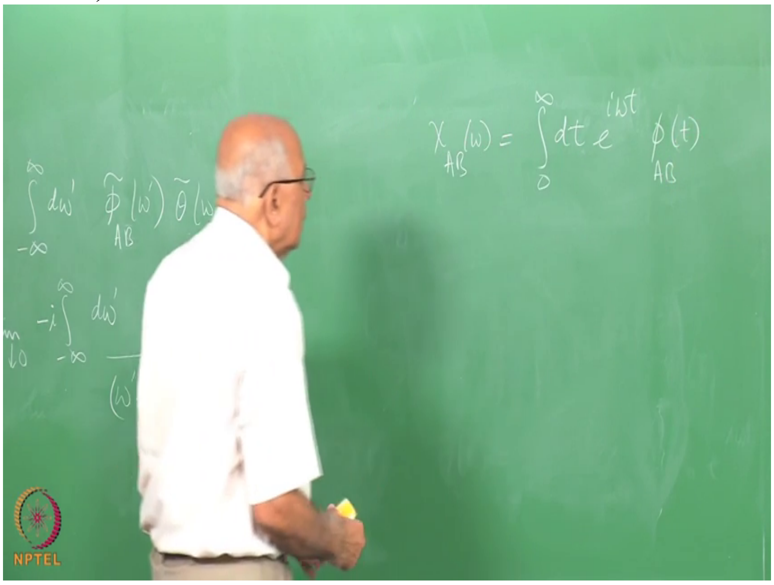


The first is the response function phi A B of t. The second is the one-sided Fourier transform which is the generalized susceptibility kai. And third is the Fourier transform of the response function which is the spectral function. And the weighted integral over the spectral function with this Cauchy kernel gives you this quantity here. So you see already, all we use is that the theta function has that spectral resolution. So the relation in abstract terms, the relation between the Fourier transform of the function and its one-sided Fourier transform is quite complicated. It is not an altogether trivial relationship at all.

We will use this fact, we will use this 0:34:45.1 when we write dispersal relations for this generalized susceptibility we will use this relation here, Ok. So to summarize what is gone on so far, we have a causal, linear, retarded response characterized by a certain equilibrium average of a correlation function, some commutator expectation value in equilibrium, its Fourier tran/transform, one-sided Fourier transform gives you the generalized susceptibility. Its two-sided ordinary Fourier transform gives you the spectral function and the later two are related by this thing here.

Now let's go further and ask what will this susceptibility actually do in practice? Well the first thing to do and I will come back to this point, is that kai A B of omega which is zero to infinity d tau e to the i omega tau phi A B of tau or let me just write t,

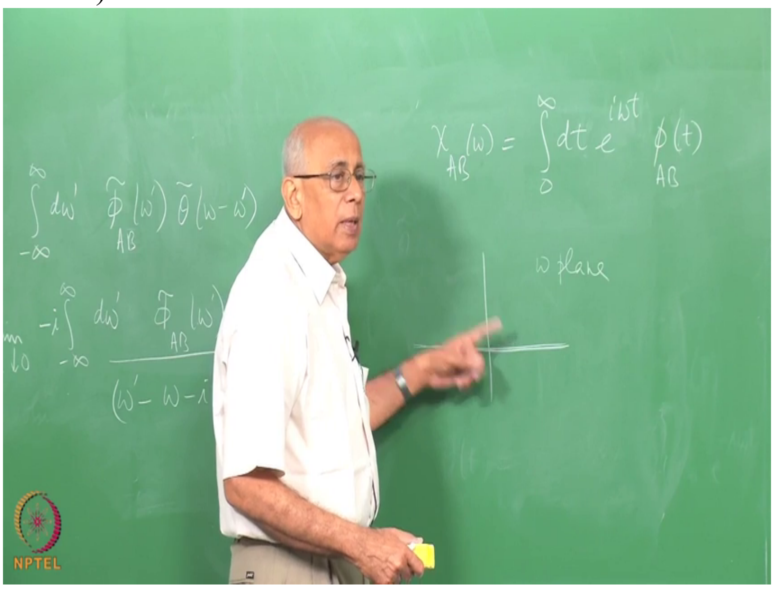
(Refer Slide Time 35:53)



this quantity here if it exists for real omega, then certainly it is going to exist if you multiply it by some function which is a decaying exponential of t. Because if this integral exists, then you multiply by number which is less than 1 and you integrate, especially if that thing goes to zero as t tends to infinity, it is going to converge even better.

Now if omega becomes a complex number, in other words you move off the real axis in the omega plane, so far we have defined it on the real axis, for real omega but if you give imaginary part to omega,

(Refer Slide Time 36:36)

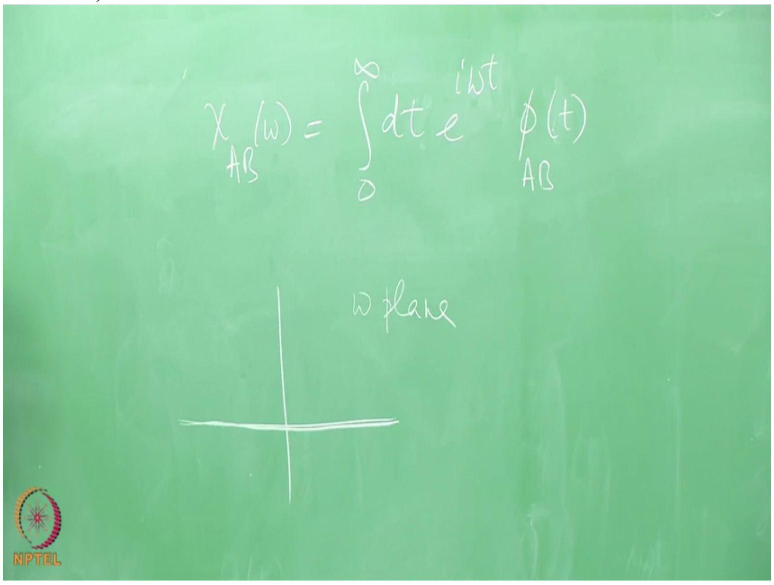


if that imaginary part is positive then this is going to have an i omega 2 multiplied by this which is going to be e to the minus omega 2 t and if omega 2 is positive as it is in the upper half plane the integral exists and converges. So this function as an purely mathematical device defines susceptibility not only for real values of omega but also for all complex values in the upper half plane. So this provides an analytic continuation of this function to the upper half plane, definitely. And the same representation is valid.

On the other hand if omega acquires a negative imaginary part, there is no guarantee this integral converges. In fact you will see that in that case you have an increasing exponential and this integral will not converge unless this dies down fastly. So in general it will not converge here. This representation is useless as far as the lower half plane is concerned. But it is analytic in the upper half plane. That's obvious by inspection. There are some further technical niceties but this heuristic argument is good enough for our purposes.

The upper half plane, this function is well-defined. We are going to make an excursion into the upper half plane and derive dispersion relation

(Refer Slide Time 38:02)

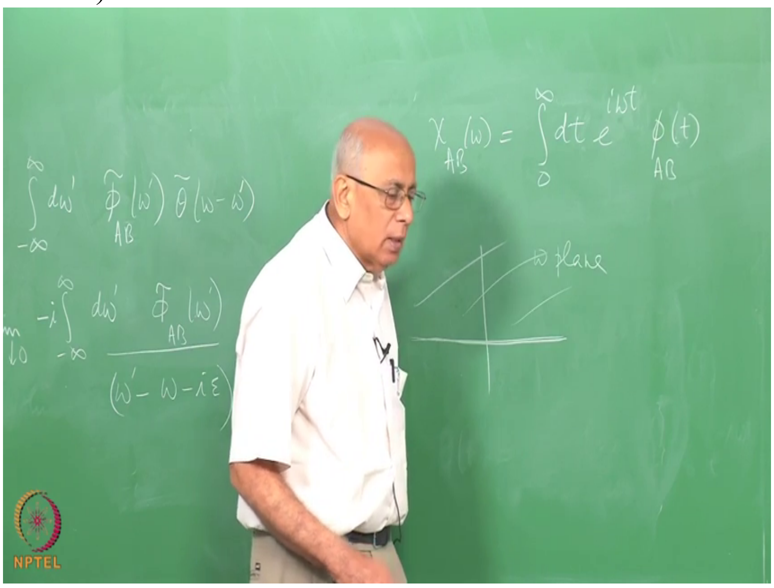


for this after we do some examples. What can you expect in the lower half plane? Well, you can't see much from here because this will be a representation that does not even converge any more. It is like saying, I give you the geometric series 1 plus z plus z squared all the way to infinity, this is equal to 1 over 1 minus z provided mod z is less than 1. But if mod z is greater than 1, substituting that value of z inside the series will just give you infinity. And if mod z is exactly equal to 1, then depending on what value of z you are actually choosing on the unit circle you can get all kinds of values from the infinite series.

For instance, if you choose z equal to plus 1, you get 1 plus 1 plus 1 which goes to infinity, if you choose z is minus 1, you get 1 minus 1 plus 1 minus 1 which oscillates between zero and 1, so you can get whatever you like depending on what the value of z you substituted is. But for all mod z less than 1, in the interior of inner circle, you can substitute a numerical value of z and you are guaranteed that the series converges to the correct value of the function, Ok. You may or may not be able to continue it outside the unit circle.

In this trivial case you can because the function 1 over 1 minus z makes perfect sense for all z except z equal to 1 where it is singular. So we are in that position. We have an integral which makes sense everywhere here and therefore defines an analytic function of this omega. We don't know what is going to go on downstairs

(Refer Slide Time 39:37)



but the point is that you know that if you have an analytic function of a complex variable, that's analytic everywhere, has no singularities whatsoever including the point at infinity, that function has to be a constant. There is no function which is analytic everywhere including the point at infinity, right?

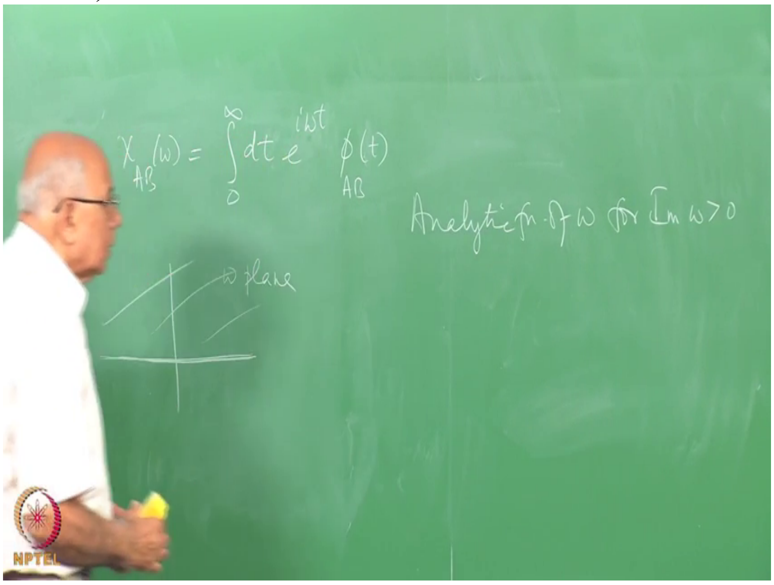
So in general I expect in physical problems and this is the lesson that you must bear in mind, I expect this quantity to have singularities in the lower half. Now you could ask why not the upper half plane. And what would you say? It's entirely the matter of the Fourier transform convention. Had I chosen the opposite convention, had I put a plus here and a minus here, then the generalized susceptibility would have been converg/convergent, would have been analytic in the lower half plane in omega and the upper half plane would be, may have singularities and so on. So this is the reason why we have to be careful. We choose a Fourier transform convention and I stick to it, Ok. So the one I have chosen is the conventional one and in this convention, with this plus sign here this is an analytic function in the upper half plane.

(Professor – student conversation starts)

Student: Sir?

Professor: Yeah

(Refer Slide Time 41:07)



Student: It is not converging; value of phi is not converging...

Professor: Yeah, this is now, this is entirely possible that for real values of omega also, phi may die down so slowly at infinity because this fellow is just an oscillatory function that this will not exist, may not exist at all. Now that is a careful case, we have to handle carefully. I made the implicit assumption that this exists, this integral exists as a Riemann integral for real values of omega. But this is an assumption, may not be valid. And we will give an example to show you that under physical conditions, this will always happen, this.

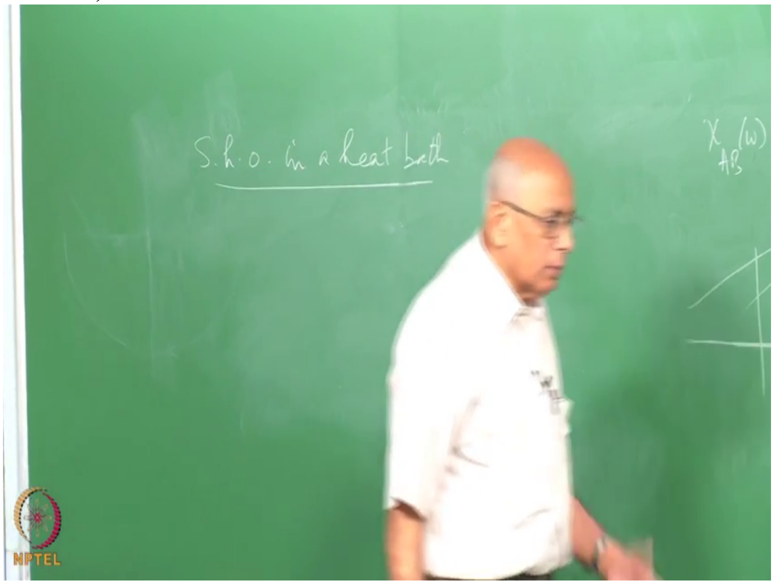
(Professor – student conversation ends)

The best way to do this, of course there are pathologies, there are cases where it is singular at the origin and things like that and then I will use a trick to define this. The trick used is, in general that you include a small e to the minus s t here and then analytically continue in s

0:42:03.4 to zero. So you find the Laplace transformation of this fellow which will converge even if i increases, doesn't increase, doesn't converge to zero at infinity. And then you make an analytic continuation. So in principle you can do analytical continuation to define the response function. But we will look at the specific cases to see what happens. Now quickly you can see that if you consider the following problem.

So let us consider a simple harmonic oscillator in a heat bath. So we have a single particle, a massive particle,

(Refer Slide Time 42:46)



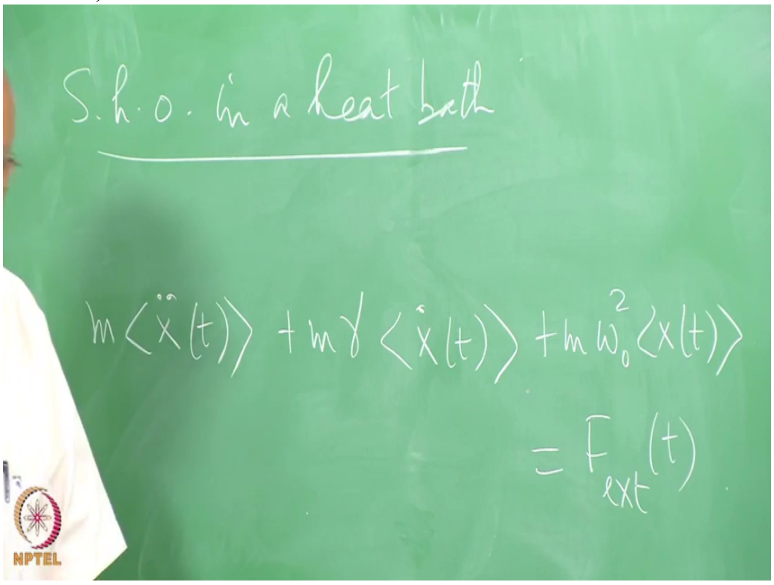
an oscillator. We already did Langevin dynamics for this, for a free particle but now we will assume that it is a simple harmonic oscillator in one dimension and this is immersed in a bath of particles and it drives fluctuations on this particle, right.

So what does one do in this case? Well, either I could write the Langevin equation down as a random equation, stochastic equation, make some assumptions about the noise or I don't do that. I simply say, look. Let's compute what this problem does in terms of thermal averages; which is attitude we have taken here, right? So the equation that I write down would be the following.

m times x double prime of e average value plus m omega naught squared x of t equal to, in the absence of an external force, this fellow would be equal to some internal force, which is provided by the friction in the problem, right, but I could add an external force to this whole thing. Then I need a model for this guy and let's take this approach that the average force on this particle depends on the average velocity of this particle, the usual friction term.

Then this term, this becomes exactly what the Langevin equation gives, it becomes plus m gamma x dot of t plus m omega naught squared x of t 0:44:29.0 is equal to whatever force you apply on the system, F external. So I am applying an external

(Refer Slide Time 44:36)

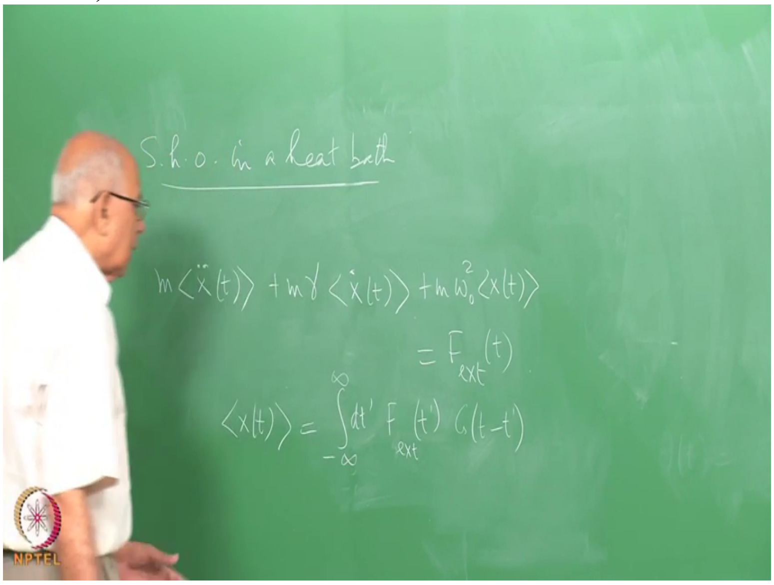


force, an applied force on the system and the system is in this heat bath, it is being buffeted around by the particles of the heat bath and because this force is present, this system has been disturbed from equilibrium. I want to know now what its response function is, what is the generalized susceptibility and so on, Ok.

Now given an equation like this, the way you would solve it is of course by using Green functions. So you immediately say x of t equal to an integral from minus infinity to infinity d t prime F external of t prime times the Green function, Ok. You could also write it in terms of generalized susceptibility and so on, we will compute that point.

Now the fact that you have t minus t prime here is the reflection of the fact that the system is time translation variant. It is the same parameters right from the beginning, so there is

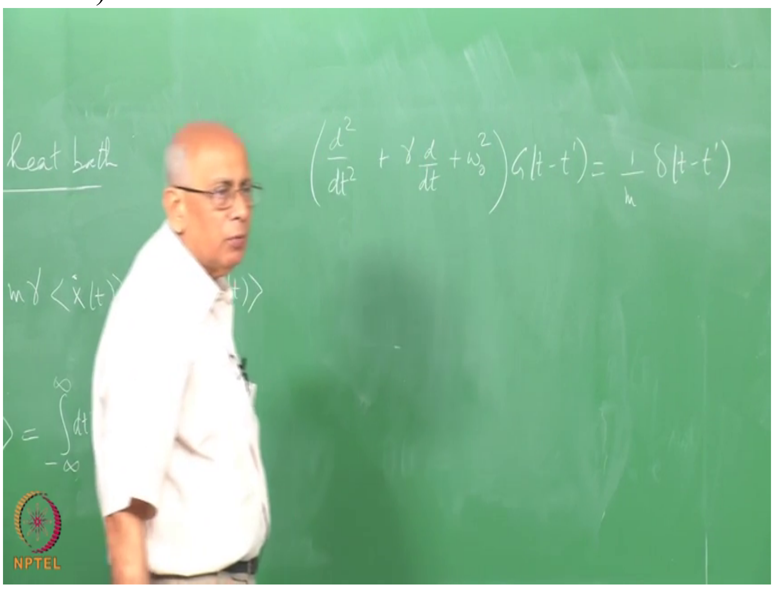
(Refer Slide Time 45:57)



time translation variance; this is G as a function of t minus t prime out here. Now what is the equation obeyed by G of t minus t prime?

Clearly you must apply the derivative operators, twice derivative, first derivative etc etc and that must give you on the right hand side F external of t which will happen only if this is the delta function on the right hand side. So it immediately follows that d 2 over d t 2 plus gamma d over d t plus omega naught squared on G of t minus t prime equal to 1 over m delta of t minus t prime. This will make it easy for us,

(Refer Slide Time 46:45)



right? That is the usual Green function.

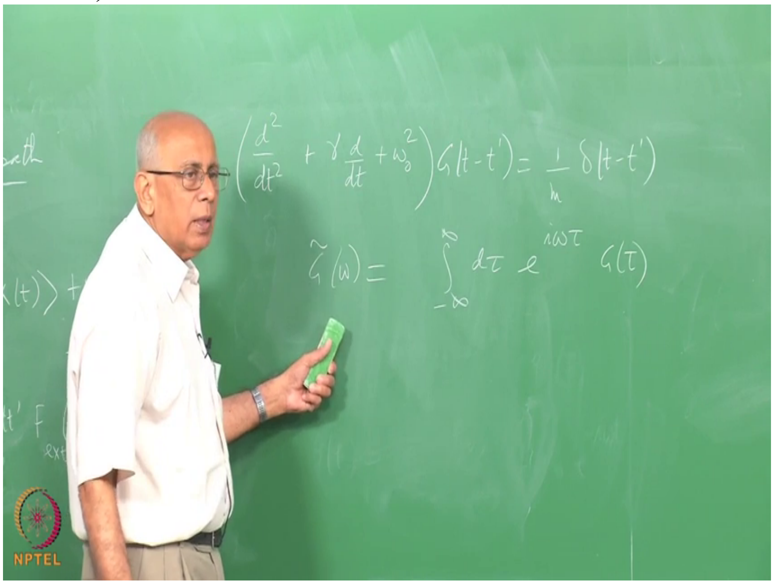
I have used a boundary condition here. And that has tacitly assumed that at t equal to minus infinity there was no external force. System was in thermal equilibrium. That is the condition we have been imposing all the way all the time. That is why I have only a particular integral here which depends only on the source and no complementary function here because this integral runs from minus infinity. I must pull out causal functions out of this. This must get cut off at t by causality. It must come out of this directly. What would one do to solve this equation?

(Professor – student conversation starts)

Student: Fourier transform 0:47:36.1

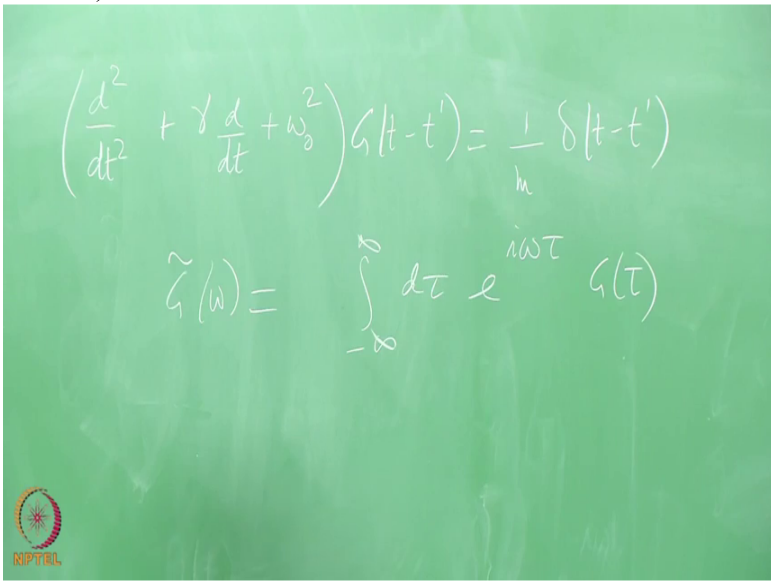
Professor: You would do Fourier transform because Fourier transform converts differentiation to multiplication, right? So if I define G tilde of omega is equal to by that equation here, integral minus infinity to infinity d tau e to the power i omega tau G of tau and use a similar representation for the delta function, then you get an equation for G tilde of omega.

(Refer Slide Time 48:08)



You put that back and do the inverse Fourier transform and you are going to get G. I leave that to you as an exercise when we meet again, give me the answer and we will start from that point.

(Refer Slide Time 48:20)

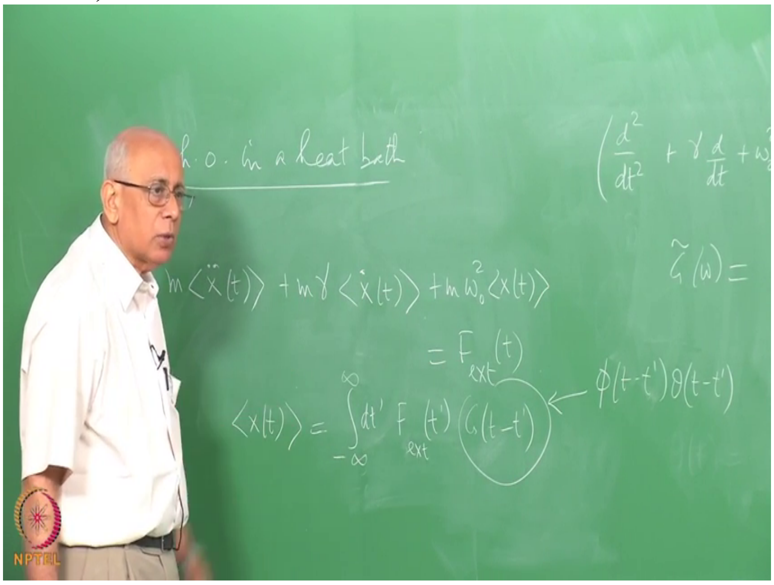


The time is over, but the theta function must appear naturally. This thing is physical, so it has got to cut off at t here. So remember this quantity here is phi of t minus t prime times theta of t minus t prime. That must appear when you solve the problem, automatically. By the way what phi is this? What is A and what is B in this problem?

Student: 0:48:53.7

Professor: We are finding the average value of X. So B is X that is for sure.

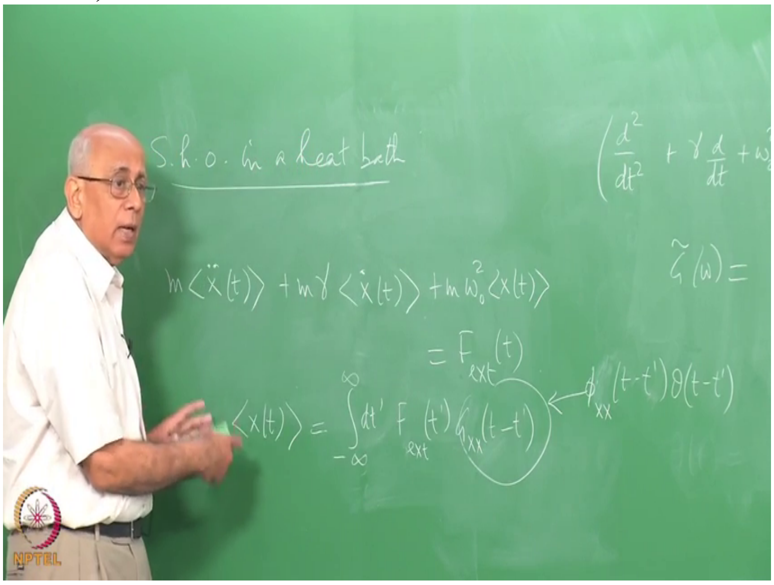
(Refer Slide Time 48:58)



Now the equation of motion said it is F external of A, so it is clear it would come from a potential which is minus x times F external of t. If you differentiate that with respect to x and put a minus sign you are going to get this fellow here. So in this problem this is really x x.

This is G x x. I haven't written it explicitly but that's what it is. I could have said what is the average velocity. Then

(Refer Slide Time 49:32)



I get the x v and so on. So now you see how to identify A and B in this simple example. It is the displacement we are asking for, so this Green function will be x x.
(Professor – student conversation ends)

But you can also see intuitively that there is going to be a relation between G A B or phi A B and phi A dot B or phi A dot B dot or phi A B dot depending on what you differentiate etc. So there are going to be relations between these functions as we will see, Ok. So compute this one and verify it has singularities only in the lower half plane and omega. Let us stop here.