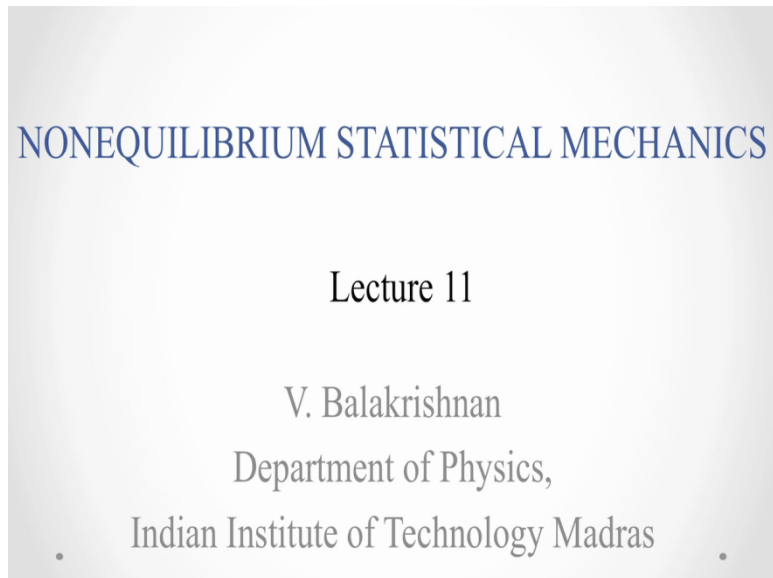
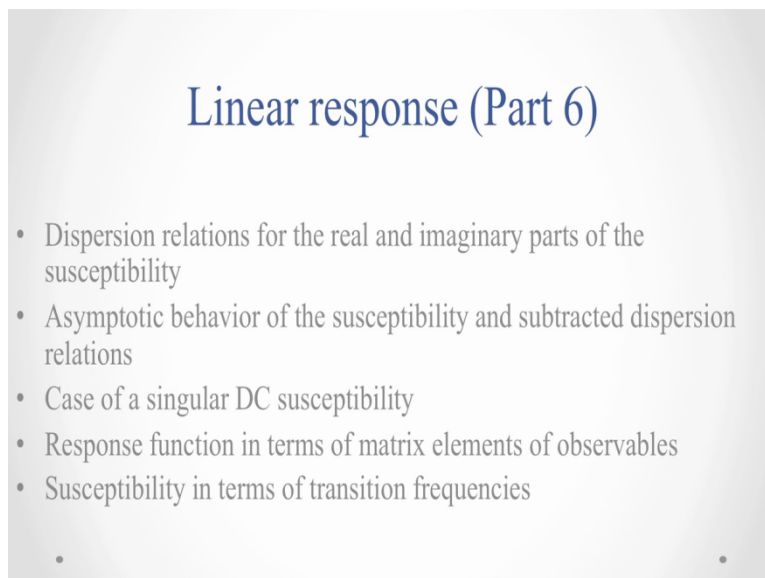


Non Equilibrium Statistical Mechanics
Prof. V Balakrishnan
Department of Physics
Indian Institute of Technology Madras
Lecture 11
Linear response (part 6)

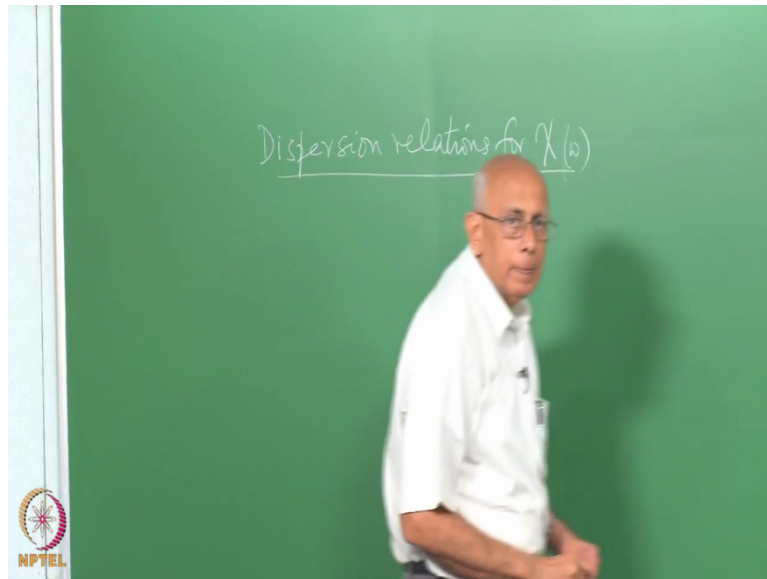
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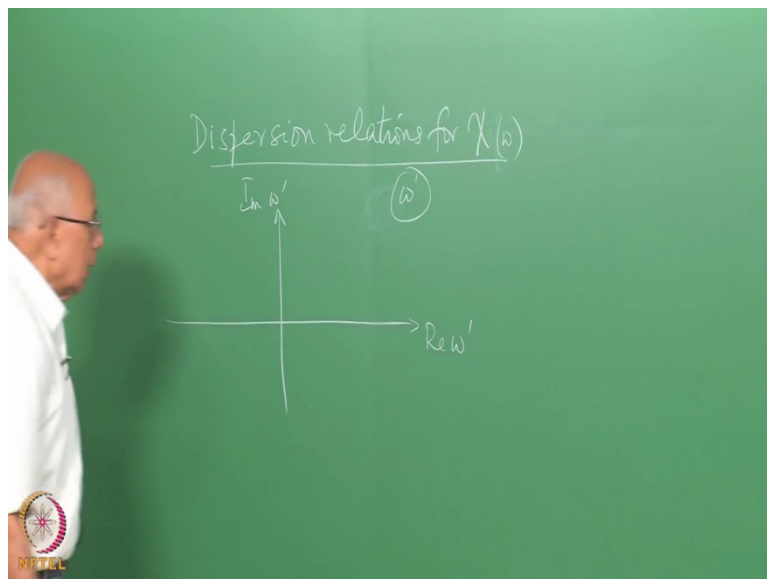


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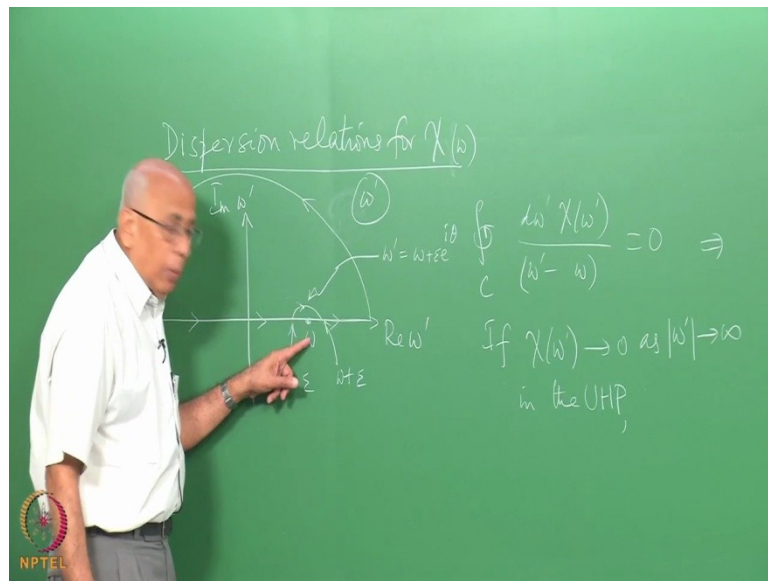
Right, so we were exploring the consequences of the fact that the generalized susceptibility $\chi(\omega)$ is analytic in the upper half plane in the frequency.

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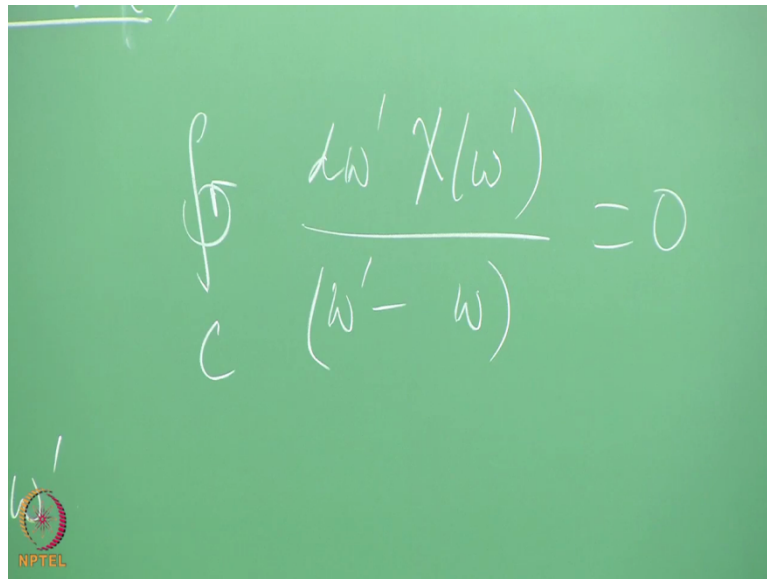
So if I draw the frequency plane this being the frequency with the real ω here and imaginary ω let us call it prime, so this is the ω prime plane out here. Then the point was that it will start with any fixed real frequency ω and we discovered that the integral over the close contour C of $d\omega$ prime $\chi(\omega$ prime over ω prime minus ω over this contour.

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So all the way from minus infinity coming in and then a little indentation, a semicircular indentation in the upper half plane through an radius Epsilon say and then back on the real axis and all the way down and closed in this fashion, this is equal to 0 and with the condition we needed for this was that this integral, the integral have to vanish as omega prime went to infinity anywhere in the upper half plane.

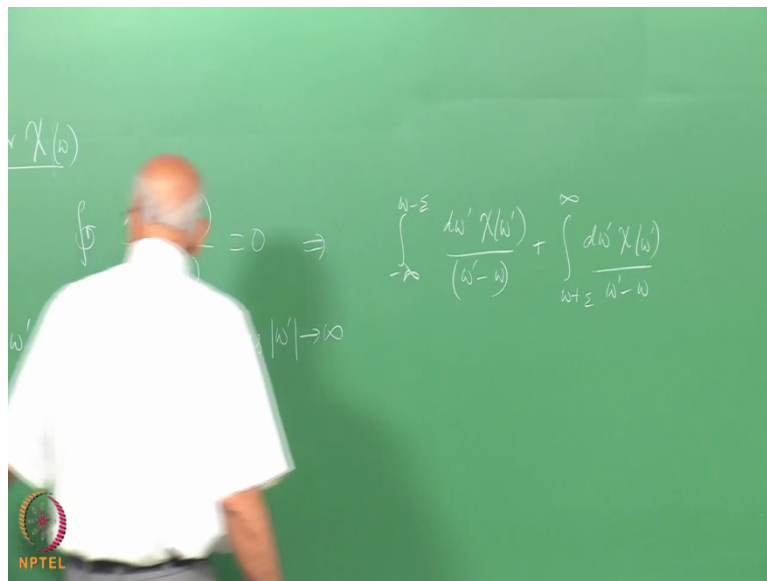
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$$\oint_C \frac{dw' \chi(w')}{(w' - w)} = 0$$

So if χ of ω prime goes to 0, if χ of ω prime goes to 0 as $\text{mod } \omega$ prime tends to infinity in the upper half plane then this contour C could be blown out all the way to infinity this contribution would then vanish because this is going to give you a capital R into the $i\theta$, this is going to give you a capital R they 2 cancel each other and then if this goes to 0 the answer goes to 0, okay.

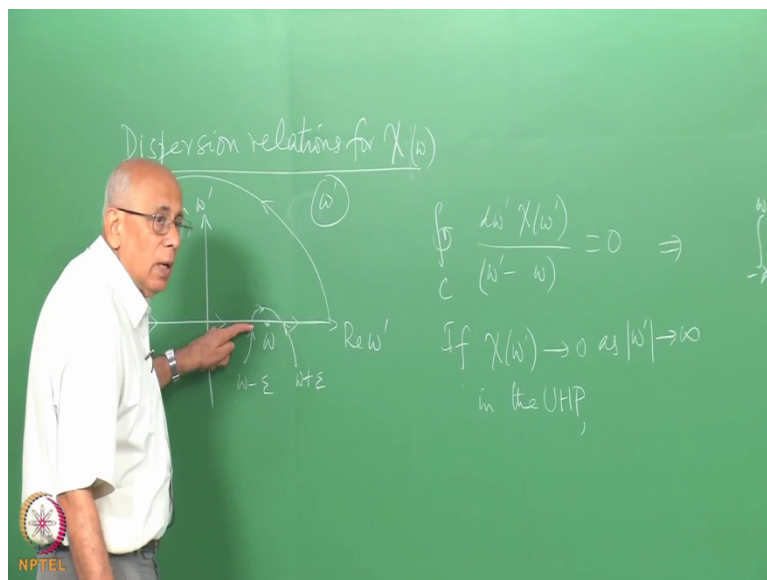
So a sufficient condition for this integral to converge and for this contribution goes to 0 is that this be true that χ vanish in the upper half plane. As you can see it suffices if χ vanishes along the real axis because on the imaginary axis you actually have extra convergence factors. So if this is true then this 0 implies that the integral from minus infinity up to this point which is ω minus ϵ and this is ω plus ϵ up to infinity plus this semicircle is 0.

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And since the arc integral from this in that contribution from the semicircle is 0 anyway you end up with this statement that integral from minus infinity to omega minus Epsilon d omega prime Kai of omega prime over omega prime minus omega plus an integral from omega plus Epsilon to infinity the same thing.

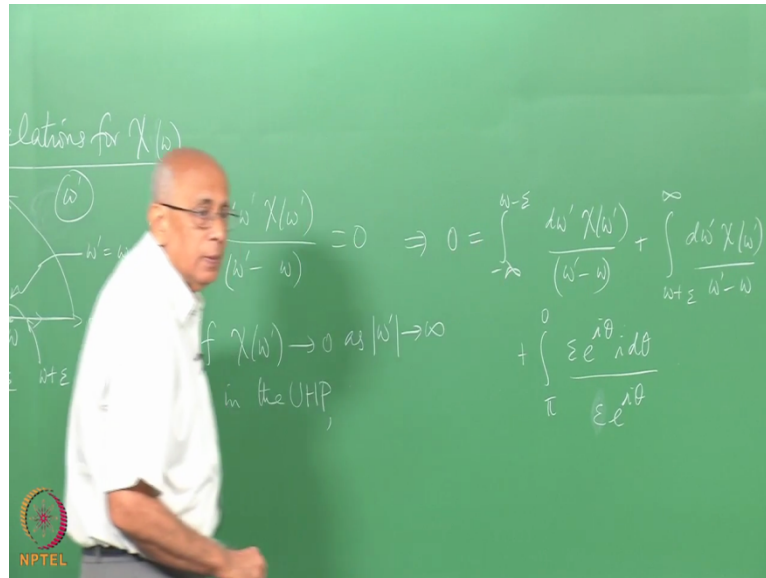
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These 2 plus this contribution this little contribution is as follows plus an integral from on this contour on this little contour here omega prime equal to omega plus Epsilon e to the i theta. So it is circle about the point omega, so omega prime is omega itself plus this little complex

number Epsilon ϵ to the i theta and the integration variable here is theta running from π to 0 it goes the other way.

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So this is equal to Epsilon ϵ to the i theta $i d$ theta that is what d omega prime is, I just differentiate this quantity and then the integral runs from π up to 0 divided by omega prime minus omega that is equal to Epsilon into the i theta and that is it. So 0 is equal to this whole thing, okay.

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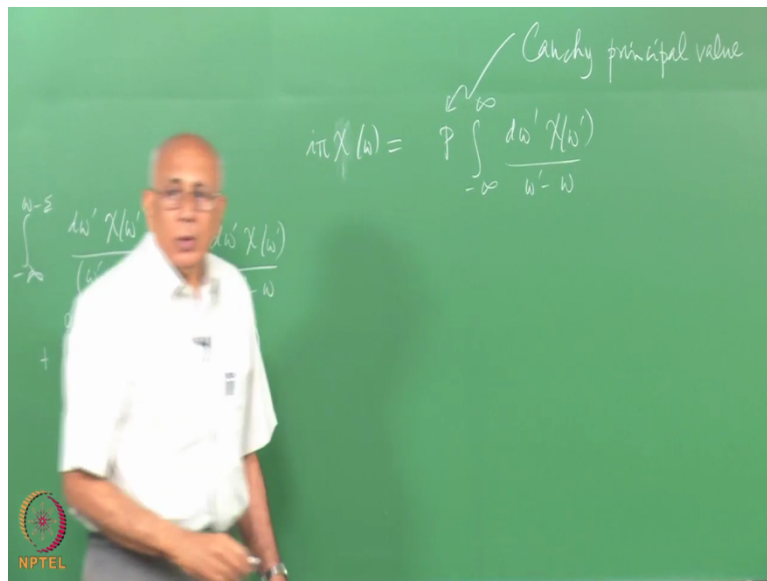
$$0 = \int_{-\infty}^{\omega - \epsilon} \frac{d\omega' \chi(\omega')}{(\omega' - \omega)} + \int_{\omega + \epsilon}^{\infty} \frac{d\omega' \chi(\omega')}{(\omega' - \omega)}$$

$$+ \int_0^{\pi} \frac{\epsilon e^{i\theta} i d\theta \chi(\omega + \epsilon e^{i\theta})}{\epsilon e^{i\theta}}$$

And this cancels, this term cancels here and the integral is minus $i\pi$ times $\chi(\omega)$. Sorry there is $\chi(\omega + \epsilon e^{i\theta})$ there is of course sitting inside there.

So in the limit in which ϵ goes to 0 this becomes the ϵ cancels the θ cancels and you are left with $i\pi$ times $\chi(\omega)$, right? Minus $i\pi$ because this is from π towards.

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So this finally says that $i\pi K(\omega)$ is equal to an integral from minus infinity to infinity $d\omega' K(\omega')$ over $\omega' - \omega$ leaving out a small portion which is symmetric about the point ω and this is called the principal value integral this is called the Cauchy principal value. So this is equal to, let me just write it as P and this stands for Cauchy principle value.

So this was an invention of Cauchy's, he discovered that in many cases when you have an integral with a singularity on the real axis on the axis of integration on the contour of integration in general the real axis then if you leave out a small symmetrical portion about this a little segment which is symmetrically situated about the singularity in this case at ω and take the limit as ϵ goes to 0 then that can be finite and it is called the Cauchy principal value.

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In this case it's finite and it's equal to this susceptibility at this point apart from this factor here. So if I bring the $i\pi$ to the right-hand side over $i\pi$. So look at what has happened? We did an excursion we met an excursion from real values of ω to complex values but we are back to the real axis because this contribution went away we are back to the real axis and what we have done is.

We have succeeded in expressing this susceptibility at any real frequency as an integral over all other frequencies except from (ω) (7:50) interval about that point that frequency, okay. This sort of thing is called a dispersion relation we will write a simpler form of this in a minute but notice that you are back on the real axis, so there are no complex frequencies here it is completely physical, right?

All we have to do, now is to take real and imaginary parts of this, so it follows that the real part of χ of ω is equal to it comes from the imaginary part this is real plus i times imaginary and the i cancels and you get P over π integral minus infinity to infinity by the way I have written this as P integral minus infinity to infinity. Sometimes it is written like this minus infinity to infinity with a slash over the integral that notation is also used just to show you that leave out a symmetrical portion about infinite decimal symmetrical segment about the singularity and take the limit, okay.

That limit is not always guaranteed to exist but in this case it does, okay. So this is equal to d ω prime imaginary part χ of ω prime over ω prime minus ω , the singularity of the integral integrant at the point ω prime equal to ω is avoided by the

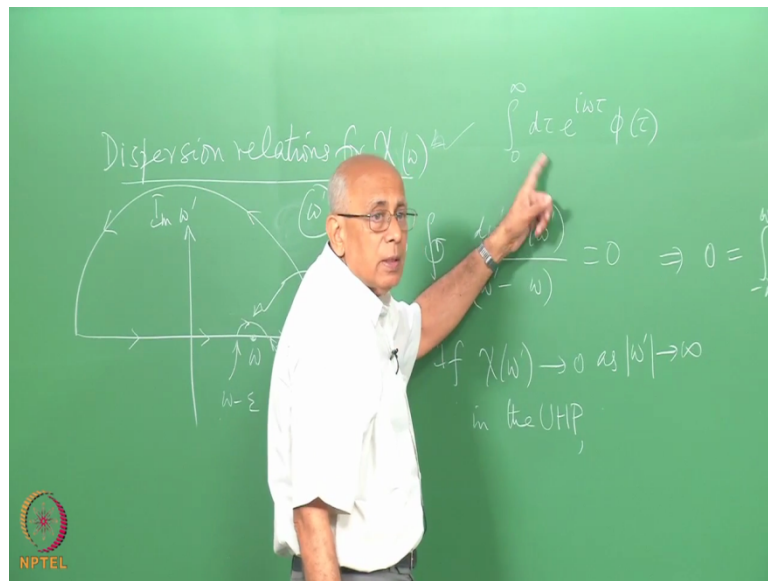
principle value supposed to be left out omitted and similarly imaginary part of K of ω equal to, that comes from the real part but there is a minus i here and you take this up, so it is equal to $-\frac{P}{\pi} \int_{-\infty}^{\infty} d\omega' \text{Re}[\chi(\omega')]$, so this is the reason why asserted in the beginning that this susceptibility cannot be purely real or purely imaginary.

Because if it were so then being an analytic function it would just vanish identically, you cannot have this to be identically 0 or this to be identically 0 because then the whole thing is 0, okay. These relations are called dispersion relations, they are also called occasionally for historical reasons these are the people who introduced these relations first into physics Kramers Kronig relations.

Dispersion because it was introduced by Kramers and Kronig first in the context of refractive index, it is an optical susceptibility if you like refractive index, the complex refractive index is just the optical susceptibility and they introduced within that connection. Now any 2 real function, any 2 functions real valued functions of a real variable such that you have supposed say 2 functions f and g then the fact if you have $f(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{g(x')}{x - x'} dx'$ and $g(x) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(x')}{x - x'} dx'$ principal value equal to g and g is the inverse relation they hold a pair of Hilbert transforms.

So the real and imaginary parts of a causal, linear retard susceptibility form a Hilbert transform pair, okay. So the real part is a Hilbert transform of the imaginary part and imaginary part is a Hilbert transform of a real part, notice there is a minus sign. So in principle if I substitute for imaginary K of ω from here in this, you will have one more integration to do, in principle you should get an identity, in other words that intermediate integral should turn out to be a Delta function, okay which it will, I am not going to show it over here but it will. So these 2 guys real K and imaginary K form of a pair of Hilbert transforms.

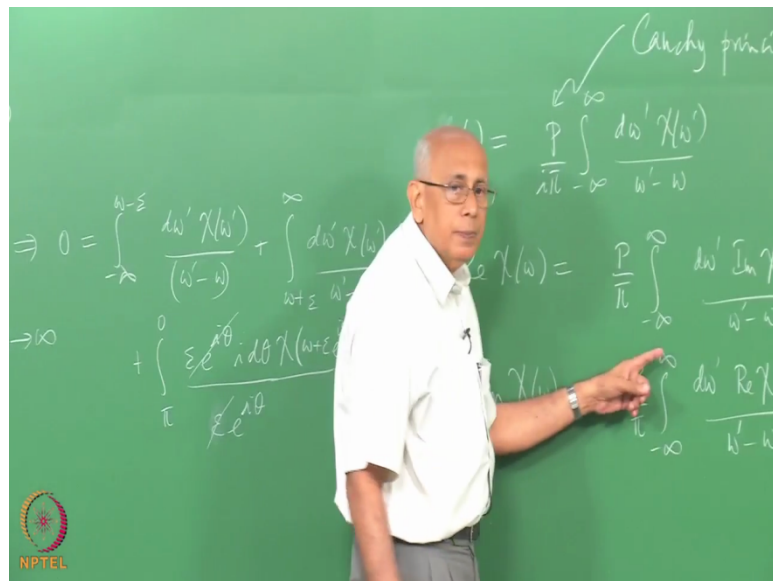
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Now what is the reason for this whole thing happening? Well it happened because this is an analytic function in the upper half plane and where did the analyticity come from? What is the origin of this business? Remember this got represented as an integral 0 to infinity $d\tau e^{i\omega\tau}$ of $\phi(\tau)$. So it got represented in terms of this one-sided Fourier transform and then the argument was if this is true for real ω then for ω with positive imaginary part? It is certainly true an analytic.

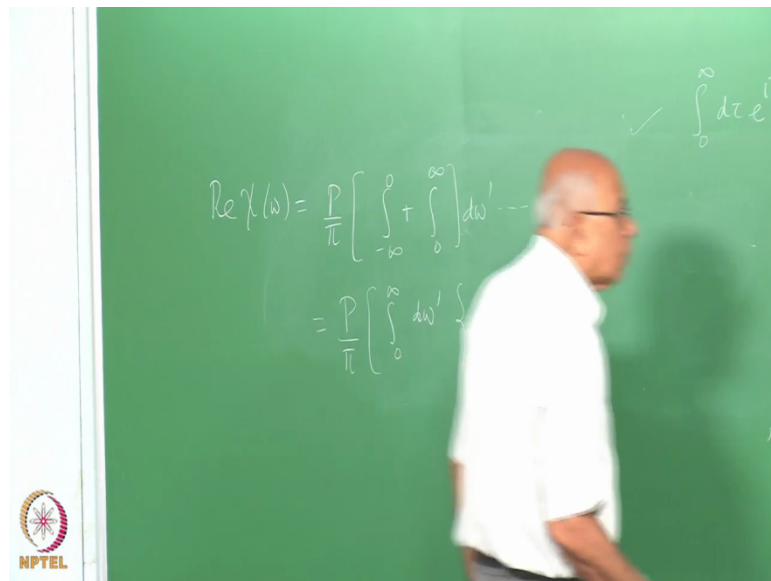
So it arose from this and where did this come from, why is this 0 and not minus infinity or anything else? Causality, so in all cases dispersion relations are a consequence of causality, finally that is what is doing it. So the physical reason why the generalize susceptibility satisfies dispersion relation is because it is a causal response, okay. And this has profound implications in other parts of physics especially in particle physics, Quantum field theory and so on anywhere where dispersion relations appear and they appear in the large number of places but finally it is traced down to causality, okay.

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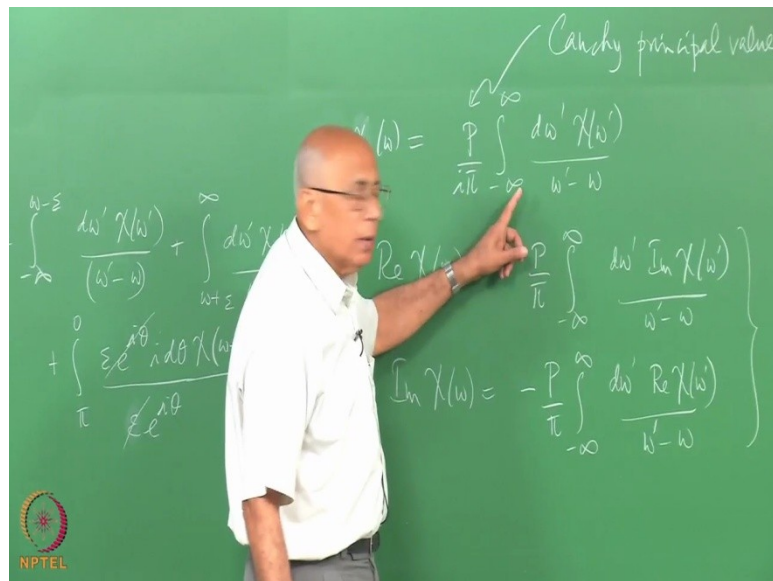
Now you might say look this is an integral over negative frequencies also whereas physical frequencies are positive but there the fact that this is an anti-Symmetric function comes to our aid. So we can convert this integral into something that runs over from 0 to infinity. So let us do that.

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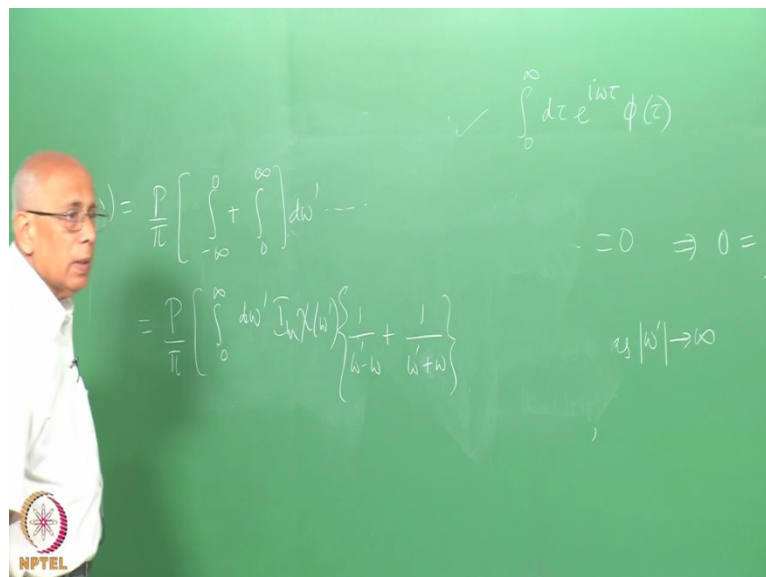
The real part therefore equal to P over pi there is an integral from 0 to infinity and then the portion from minus infinity to 0 I am going to write in this form, is minus infinity to 0 plus integral 0 to infinity times d omega time blah blah blah, in this term so I am going to write this as P over pi I am going to change variables to minus omega prime when I pull out a minus sign due to the Jacobian, this becomes infinity to 0 and those 2 minus signs cancel.

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So both integrals look like 0 to infinity d omega prime and then in the first integral I have Kai of omega prime over omega prime minus omega that is integral from 0 to infinity in this formula and then minus infinity to 0 remember I change variables to minus omega prime. So let us write that as, so this is imaginary plus imaginary Kai of minus omega prime divided by minus omega prime minus omega because I change variables.

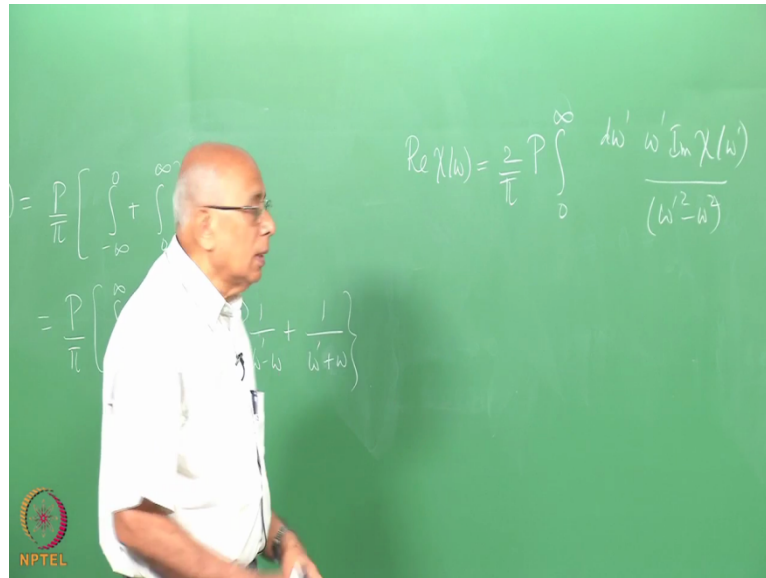
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But this fellow is an odd function, so it is equal to minus imaginary Kai of omega prime that minus sign cancels with this and you are left with the following, you are left with imaginary I

of ω' times one over ω' minus ω plus one over ω' plus ω but this ω cancels and just gives you $2\omega'$.

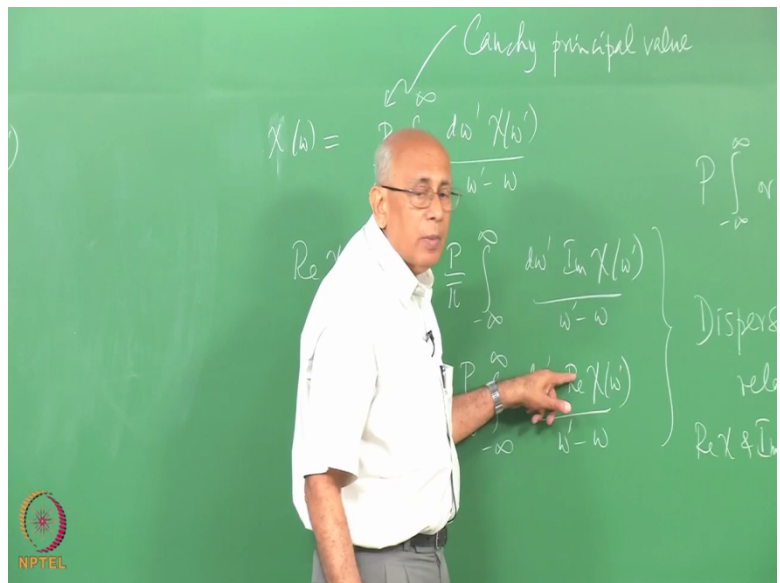
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So therefore I have a nice representation which says that in general we have useful representation which says real $\chi(\omega)$ equal to $\frac{2}{\pi}$ principle value $\int_0^{\infty} d\omega' \frac{\omega' \text{Im} \chi(\omega')}{(\omega'^2 - \omega^2)}$ because when I add these 2 I get $2\omega'$ divided by $\omega'^2 - \omega^2$. Now everything is physical it says this denominator has a simple pole at $\omega' = \omega$, the one at $\omega' = -\omega$ is outside the region of integration and you have to take the principal value in the pole at $\omega' = \omega$ and integrate this quantity, okay.

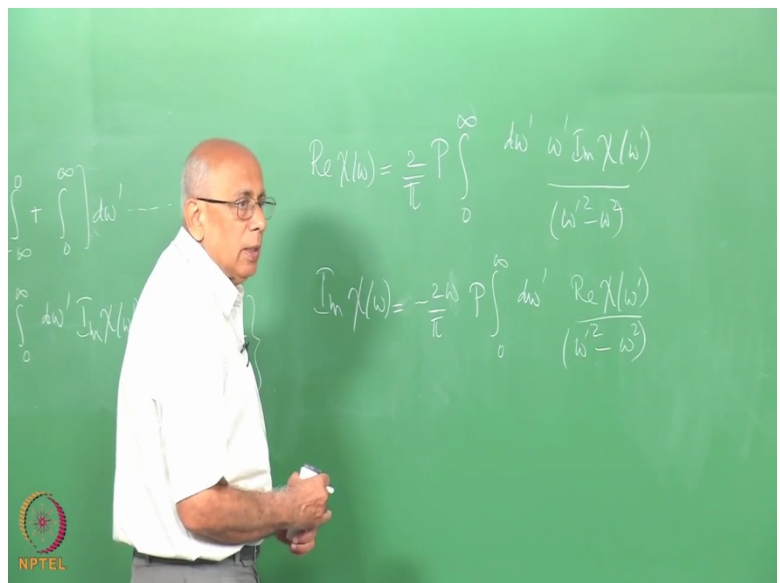
Its guarantee to converge, at infinity this is going to produce capital R, that is going to produce capital R, this is going to produce R square they cancel each other but this fellow goes to 0 and the integral exists. So this is a physical form of the dispersion relation. Similarly you do the same thing for imaginary for $\chi(\omega)$ equal to still be $\frac{2}{\pi}$ and there was a minus sign which is going to persist, so minus $\frac{2}{\pi}$ times principle value from 0 to infinity $d\omega'$.

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Now you are going to subtract one over omega prime minus omega minus one over the other because this fellow is symmetric, so it does not produce an extra minus sign.

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When you subtract that you get 2 omegas, so this becomes an omega which is outside the integral and then the real part Kai of omega prime, okay. That is a very useful form of the dispersion relation, so this is the one that you would use in practice, okay. In practice what happens is the physical use this is put to is, suppose you know the susceptibility or you have measured the susceptibility both the real and imaginary parts because they have physical meanings.

You measured it in some frequency range and you could approximate it by 0 or something like that outside this range then to find this susceptibility at any point outside the range you could use this formula to first order it will be correct even if you cut it off that sum up a limit here, okay.

“Professor -Student conversation starts”

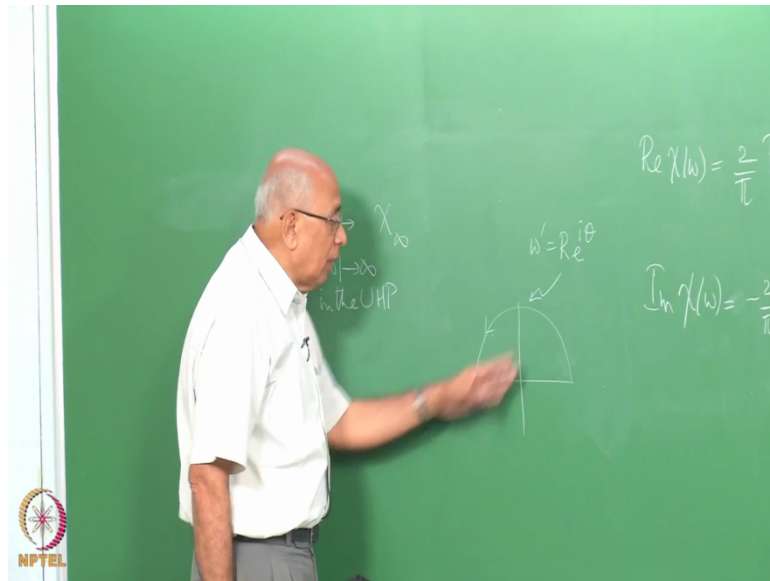
Student: How the second integer looks better than.

Professor: Yes that is the consequence of the fact that one the real and imaginary parts that is the reason, yes sure that is exactly true but it is not really better because these functions behave differently asymptotically, okay.

“Professor-Student conversation ends”

Now you could ask the other questions we slurred over some points we said Kai of omega must go to 0 at infinity, suppose it does not, you still have to deal with this situation because that can happen in many cases.

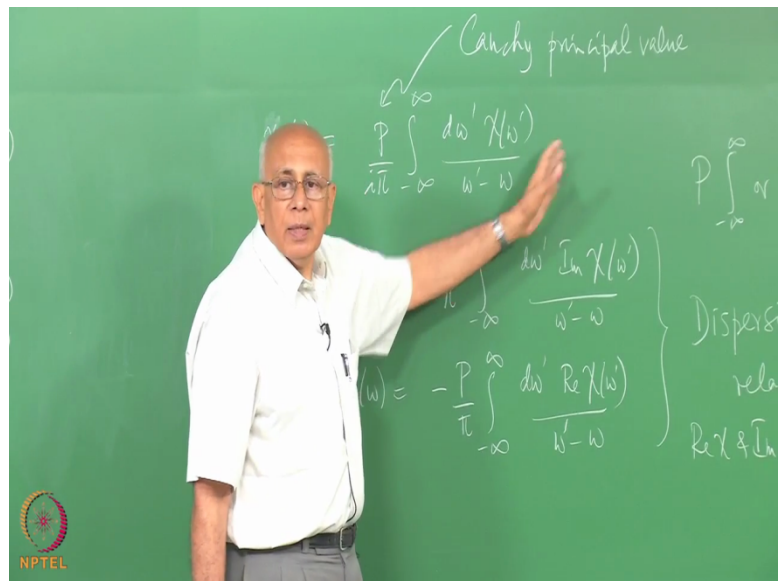
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Suppose it does not go to 0 but it goes let us say on the upper half plane suppose not K as ω goes to some number, some K as ω goes to infinity as ω goes to infinity in the upper half plane, suppose this were true then the contribution from the semicircle is not 0 that is all but you can still work out what the contribution is because now you notice that this infinite semicircle is here.

On the semicircle K goes to K as ω goes to infinity and then you have on this circle $\omega = R e^{i\theta}$, so $d\omega = i R e^{i\theta} d\theta$ and so on and in the denominator you have the same thing $\omega - i$ as ω is going to produce an R . So you will end up with a K as ω goes to infinity as a constant in integral so fine.

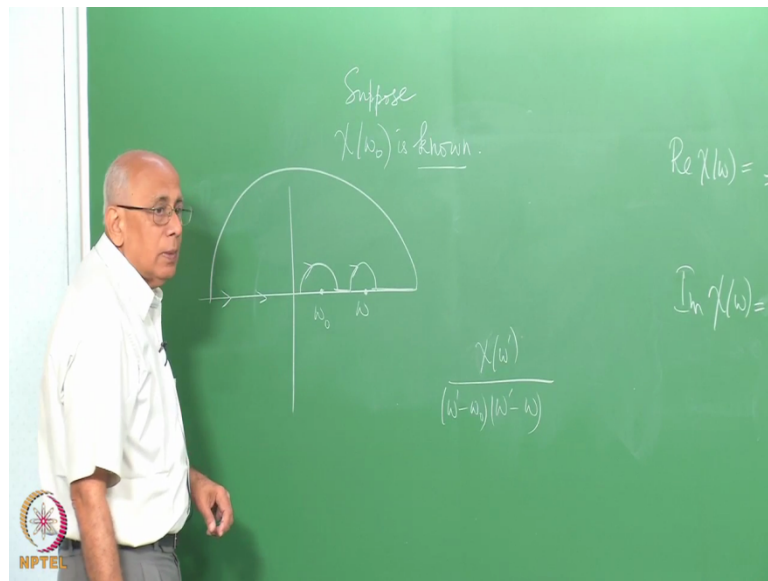
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You will still get dispersion relations but you get an extra contribution here plus something like π times K or something like that, so you can still write it down still compute but now suppose you say well I do not know K or infinity I just know that it does not go to 0 but I do not know or suppose it is a function of the angle. Suppose the limit that it goes to does not go to 0 but suppose it is a function of which way you go to infinity you know handle on that.

I have assumed here that all through uniformly it goes to the same constant but if it depends on the angles and you cannot do the angular interpretation, right?

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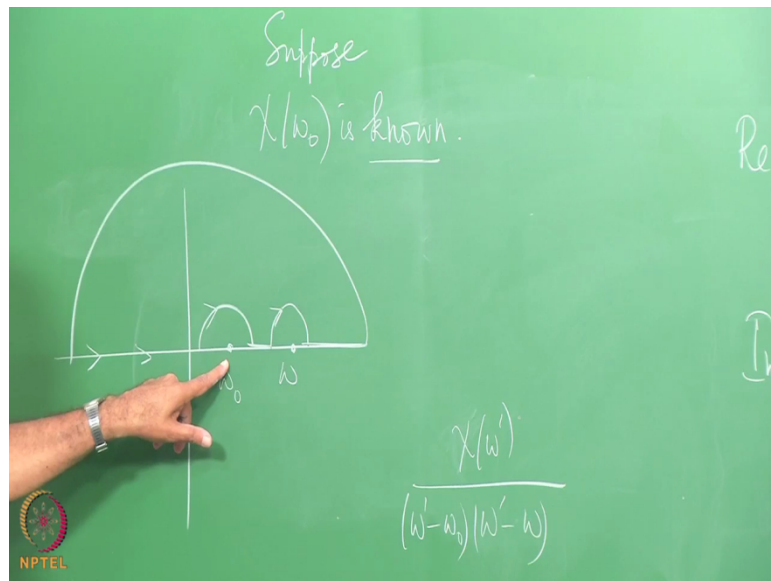


Then this is the trick you do in that case, what you do is to modify the function whose analytic behaviour you are looking at. So your omega prime plane here is omega choose some value of the frequency at which you know the value of the susceptibility. So let us suppose there is a point omega not and let us suppose that Kai of omega not is known or measured.

So suppose, so you know the value at this point and now I am trying to derive dispersion relations. So the function I am going to look at is not Kai of omega prime over omega minus omega prime minus omega this is not good enough because it does not converge fast enough but if I multiplied by this omega prime minus omega not then I am in good shape because there is an extra omega prime capital R sitting from here and the d omega prime will cancel against this.

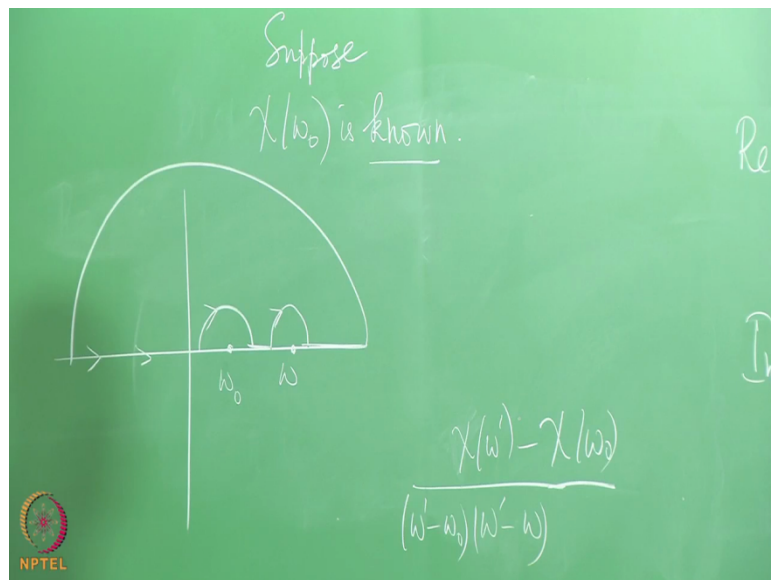
There is 1 over capital R here and there is this fellow who goes to a constant some constant at infinity, so there is 1 over R and this contribution will still vanish but now you will say that is not good because there is a singularity at this point now. So what you will have to do is to consider the contour this way and then the indentation here and then another indentation there and then all the way to infinity, okay.

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So that is one way to do this, another way to do this, so what would that amount doing? What would this contribution be finally? It would be $i\pi$ or $-i\pi$ whatever it is, Kai at that value sitting and then Ω not minus 1 would sit there.

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You can save yourself some trouble by considering not this function but this function this is a constant, this function if this is got a simple pole at ω_0 not than this function is well-behaved at ω_0 , okay.

So I write a dispersion relation for this function, keeping track of the fact that this is a complex number in general.

“Professor -Student conversation starts”

Student: Basically you are making it a reversible direction.

Professor: Yes I convert this singularity into a removable singularity by subtracting this one here.

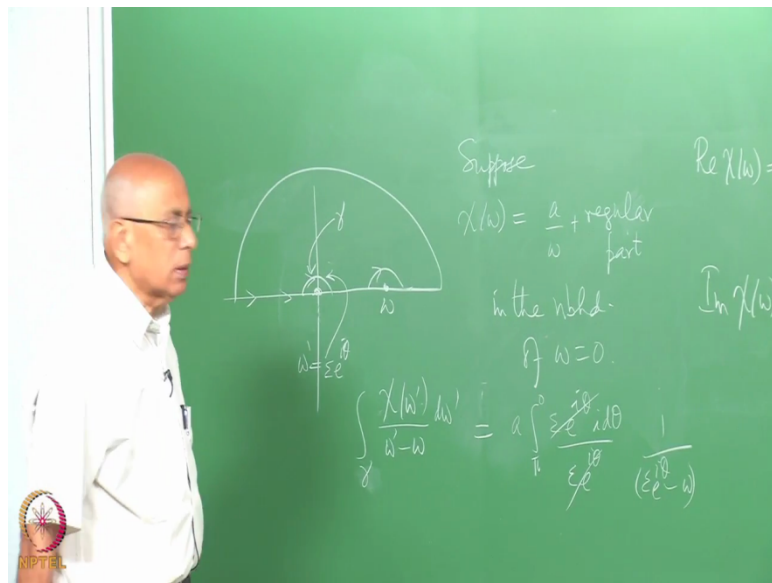
“Professor-Student conversation ends”

So since I have subtracted this, this is called subtracted dispersion relation and this is called the point of subtraction. So there are several ways of fixing this problem of Kai not going to 0 at infinity subtracted once, this assumes that Kai is such that it goes to ∞ , does not go to 0 at infinity but goes to a constant. Suppose it goes like ω' itself what would you do? Then I have to subtract at 2 points and so on.

So each time you add a denominator it improves the convergence, okay. And then it is a doubly subtracted dispersion relation and so on, as long as it does not have an essential singularity at that point at infinity you are in good shape, as of now there is no, so if it blows up like some polynomial like some power of ω' as ω' goes to infinity we are okay.

Blows up exponentially you cannot write dispersion relations, okay. So these are techniques just techniques for getting rid of singularities but this tells you what the basic idea is or there is one more very important case where you have to deal with this situation which is as I mentioned it happens so happens in many cases that the dc susceptibility is actually divergent that it blows up namely you apply steady force to the system forever and the response becomes exploit it divergences, okay.

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What you do then? That implies that Kai of ω has a pole or singularity at the origin and simplest case it has a simple pole, right? So suppose that happens, suppose so this part is taken care of.

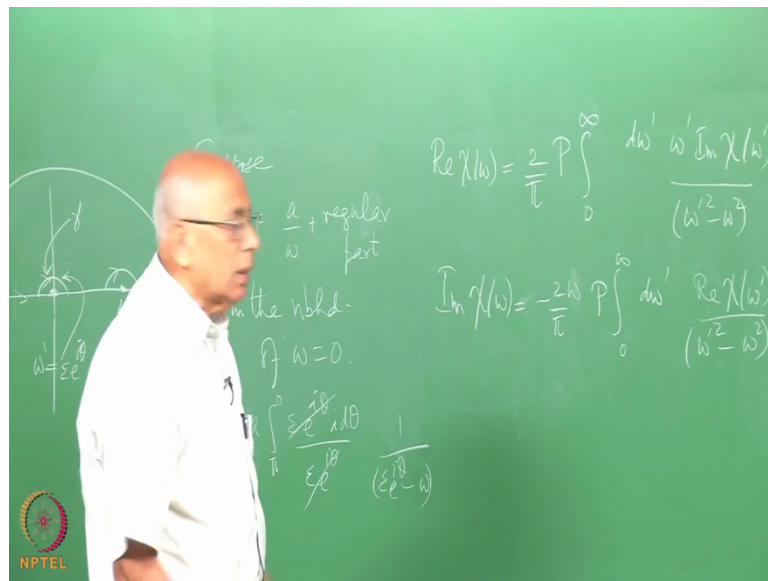
Now suppose Kai of ω has a simple pole at the origin, so it is of the form some residue a over ω plus regular part in the neighbourhood of ω equal to 0. So suppose it has a simple pole at this point at the origin, here is my ω then the thing do is to go back and consider this contour out here and consider the original function itself. So you have Kai of ω prime over ω prime minus ω and you look at it over this contour.

So indent this in the upper half plane, so as to avoid the pole and stay in the region of analytic behaviour of this function and include the contribution from here in the contour integral, this indentation is going to give you minus $i\pi$ Kai of ω , what is this going to give you? What is the contribution going to be? We are going to have to integrate remember that on this contour ω prime is just equal to $\epsilon e^{i\theta}$ plus 0 because it is at the origin.

So this thing here integral b ω prime over this little semicircle, so let me call this little semicircle little γ little γ this fellow here is going to become equal to this is going to go like a over ω prime plus the rest of it, right? So the leading term is going to be a and then an integral from π to 0 $\epsilon e^{i\theta}$, $i d\theta$ that is $d\omega$ prime divided by ω but ω is $\epsilon e^{i\theta}$. So $\epsilon e^{i\theta}$, that is the Kai the behaviour of Kai with an a here and then there is this factor which is harmless.

So that factor is $1/\epsilon^{i\theta - \omega}$, so the pole contributed $1/\omega'$ which cancels gives you this ϵ to cancel this, so this fellow goes away and this is $i\pi$ or $-i\pi$ times a and the rest of it will follow with a $-\omega$. So the whole integral will have a contribution which is essentially a/ω which it should because they are writing a representation for ζ and if it is got a singularity residue a at $\omega = 0$ there better be an explicit term a/ω that is what is happening here.

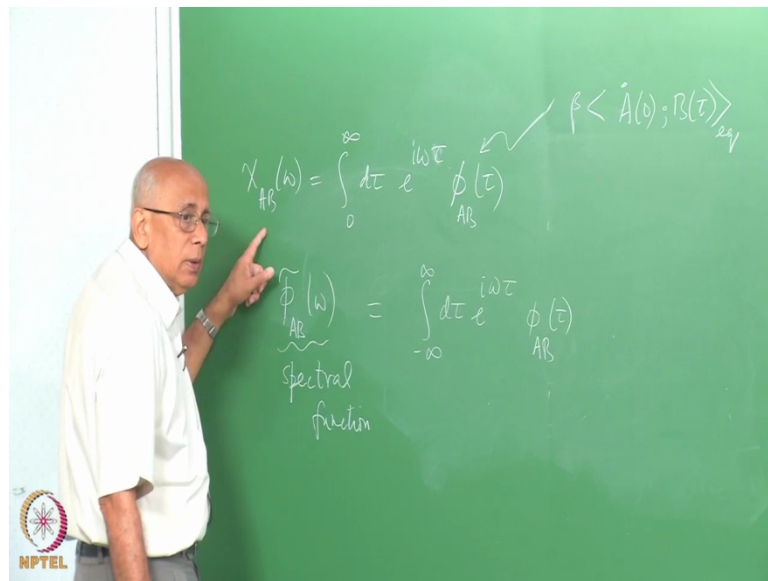
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So tacitly the point of subtraction has been the origin in that sense. So in all these cases we know how to deal with this situation but the physics of it is that causality leads to dispersion relations Kramers Kronig relation for that generalized susceptibility, okay. And that is a general statement and you can write it in terms of physical frequencies using this which is then usable for numerical evaluations.

Okay, now let us come to terms with what is this susceptibility actually is? We have to look at the response function a little more carefully, so let us do that, we want to attach some physics to the whole thing, so given for instance quantum mechanical system can I say what the structure of this response function is? What does it really look like etc? In particular I want to be able to write things in terms of this spectral function.

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If you recall I pointed out that just to write these formulas out again Kai AB of omega is integral 0 to infinity d tau e to the i omega tau phi AB at tau this guy here be showed was the canonical ensemble f is equal to beta times the equilibrium the canonical correlation between A dot of 0 and B of tau we already defined this quantity the classical case is subsumed in this as a special case and this was analytic in the upper half plane etc etc.

We also had defined a Fourier transform of this quantity of omega and I call this the spectral function for reasons which will become clear now, this was the Fourier transform of phi the response function, so this was equal to integral d tau minus infinity to infinity e to the i omega Tau phi AB of tau, this will talk not very much about what is this quantity for tau less than 0?

Because the susceptibility just involves this right here, I will come back to this we will deal with the question of how to define it for negative values of tau? But notice that this spectral function this Kai here was also related to the Green function, we found out what the Fourier transform of the Green function was and the Fourier transform of the Green function which is this multiplied by theta function of tau.

So I called it GAB of tau that quantity it is Fourier transform was the susceptibility, exactly the susceptibility. We also found the relation between this fellow and this fellow by writing a theta Fourier representation for the theta function and if you recall that was a pi AB of omega was equal to an integral for minus infinity to infinity d omega prime phi AB tilde of omega prime over omega prime minus omega minus i Epsilon in the limit in which Epsilon goes to 0 from above and there was some i factor somewhere here.

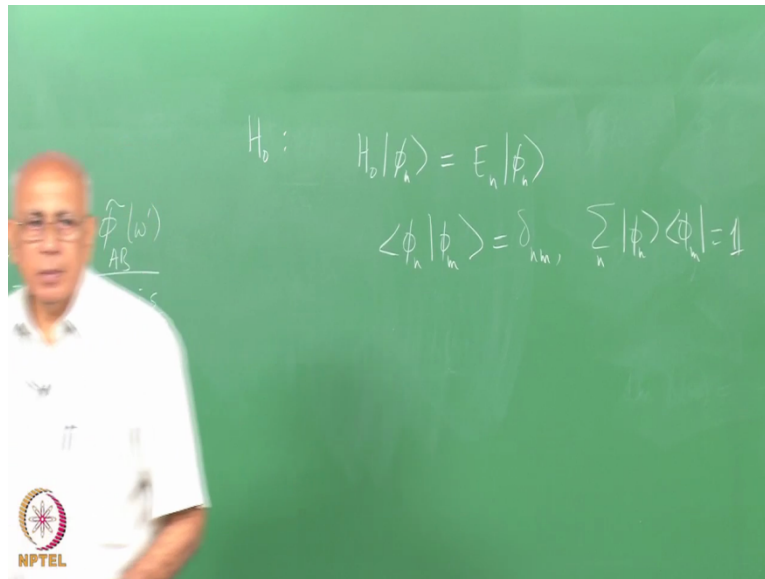
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The image shows a handwritten equation on a green chalkboard. The equation is:
$$\chi_{AB}(\omega) = -i \int_{-\infty}^{\infty} d\omega' \frac{\hat{\phi}_{AB}(\omega')}{\omega' - \omega - i\epsilon}$$
 In the bottom left corner of the chalkboard, there is a small circular logo with the text 'NPTEL' below it.

Would you check and let me know there was an i dependent on the Fourier transform Convention which I have fixed once and for all but I am pretty sure there was an i here somewhere, i or minus i or something like that. I just want to keep this straight, okay. So now let us see what the content of this response function is in general?

What would it imply? We will take a specific case and I will do this then the simplest notation possible and then we can add fields to it later. So we will look at the quantum mechanical system to start when and take A and B to be summation operators their physical observables or operators corresponding to physical observables and then I am going to assume that there is a discrete spectrum of the Hamilton in h not in this system, just so that the notation becomes simple.

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So let us suppose that this is Hamiltonian H_0 and it has a complete set of states labelled by a quantum number or set of quantum numbers let me call n for collectively, so I have H_0 not on normalised Eigen function ϕ_n is E_n on ϕ_n and n runs say 0, 1, 2, 3 whatever that discrete spectrum just for notational convenience and then this is an orthonormal basis, so let us say $\phi_n \phi_m$ equals to δ_{nm} and similarly $\sum_n \phi_n \phi_m$ equal to the identity operator.

So it is a complete set of states and it satisfies orthonormality, okay. Are you familiar with the terms completeness in orthonormality, okay. So given any state vector of this system you can always write it as an expansion in terms of these ϕ_n 's here, this summation here is supposed to sum over states labelled by this set of quantum numbers n and not the energy levels because there could be degeneracy in general.

So every time I write a sum like this it is not over the energy levels per se but over the states of the system, okay. Then this response function $\chi_{AB}(\omega)$ of τ , if you recall this quantity was equal to the equilibrium expectation value of A of τ , B of τ equilibrium that was one of the formulas we had for the response function and in the quantum case this stands for 1 over $i\hbar$ cross A of τ , B of τ stands for this.

So let us calculate this in this basis, we need to compute trace that is what this thing here means, so let us calculate that in the basis ϕ_n , you can compute a trace in any basis you like but let us do it in the basis of Eigen states of the unperturbed Hamiltonian H_0 .

“Professor -Student conversation starts”

Professor: Pardon me, no it is still a commutator.

Student: Yes but I mean it is A dot intervention.

Professor: No, no, no the response function is not a dot, after I compute, right? Then it becomes dot and so on, what happens then you get rid of the commutator and you get this Kubo transform or whatever it is and then it becomes a dot but before that it is just a commutator.

“Professor-Student conversation ends”

So let us calculate this, let us calculate $\langle A(0)B(\tau) \rangle$ at equilibrium this is equal to that the first in the commutator we will just compute this number this is equal to trace which means a summation over n $\langle \phi_n | e^{-\beta H} A(0)B(\tau) | \phi_n \rangle$ which is equal to a summation over n $e^{-\beta E_n} \langle \phi_n | A(0)B(\tau) | \phi_n \rangle$ because it is an Eigen state.

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$$\langle A(0)B(\tau) \rangle = \sum_n \langle \phi_n | e^{-\beta H_0} A(0)B(\tau) | \phi_n \rangle$$

$$= \sum_n e^{-\beta E_n} \langle \phi_n | A(0)B(\tau) | \phi_n \rangle$$

$e^{\frac{iH_0\tau}{\hbar}} B(0) e^{-\frac{iH_0\tau}{\hbar}}$

So $e^{-\beta E_n} \langle \phi_n | A(0)B(\tau) | \phi_n \rangle$ and now for this $B(\tau)$, let us write this as $e^{-\frac{iH_0\tau}{\hbar}} B(0) e^{\frac{iH_0\tau}{\hbar}}$ that is the meaning of $B(\tau)$, so that is the Heisenberg picture operator but that $B(0)$ is the Schrodinger picture operator because that is at $t=0$, that is the way we define the Schrodinger picture, okay.

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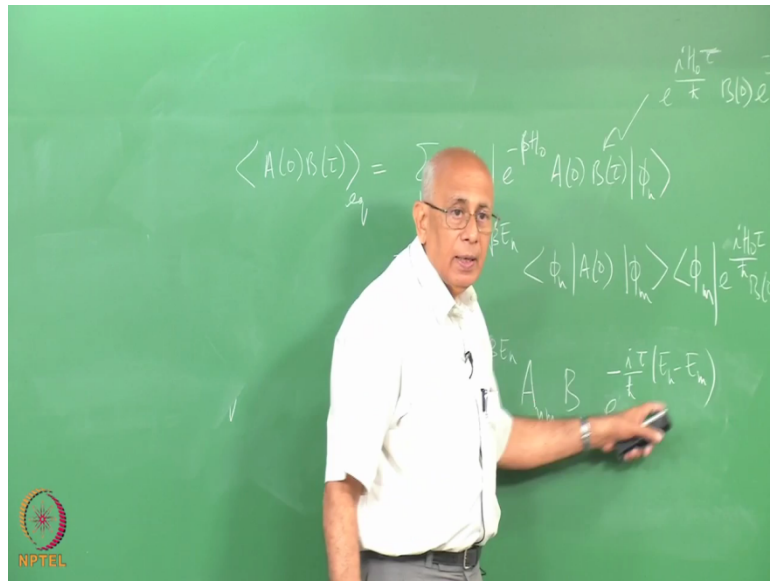
$$\begin{aligned}
 \langle A(t)B(t) \rangle &= \sum_n \langle \phi_n | e^{-\beta H_0} A(t) B(t) | \phi_n \rangle \\
 &= \sum_n \sum_m e^{-\beta E_n} \langle \phi_n | A(t) | \phi_m \rangle \langle \phi_m | e^{\frac{iH_0 t}{\hbar}} B(t) e^{-\frac{iH_0 t}{\hbar}} | \phi_n \rangle \\
 &= \sum_n \sum_m e^{-\beta E_n} A_{nm} B_{mn} e^{\frac{i t}{\hbar} (E_n - E_m)}
 \end{aligned}$$

So this fellow here I have to put this in but what I could do is in between I put $\phi_n \phi_m$ and sum over m that is the identity operator and then I put this in e to the minus $i \hbar \tau$ over \hbar cross B of 0 , e to the of plus i and minus $i \hbar \tau$ over \hbar cross times ϕ_n . This is equal to a summation over n , a summation over m , e to the minus βE_n on this side, what would you call this?

This is Schrodinger a picture operator the time independent Schrodinger a picture operator and if I represented in the basis on by the Eigen states of the Hamiltonian unperturbed Hamiltonian that is the n m th matrix element, okay. So this is just A_{nm} there is no time dependence that is just a number, okay. Some complex number in general, does it have to be a real number?

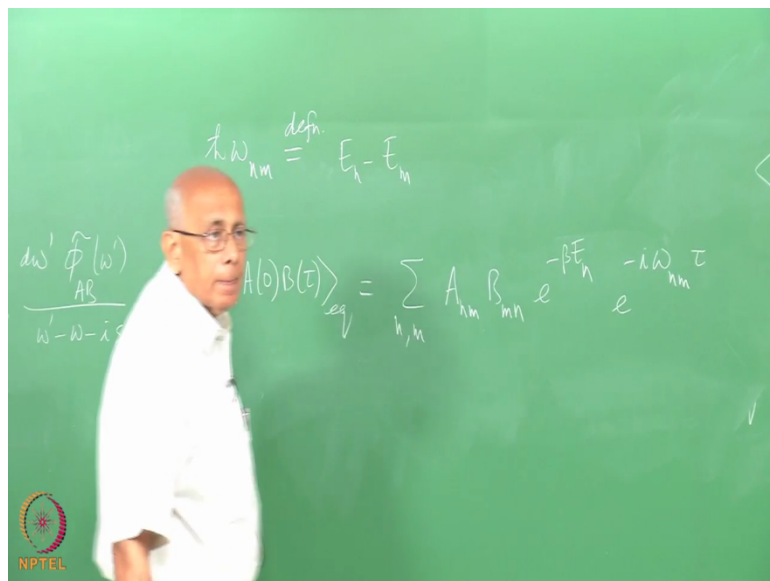
A is the hermitian operator does this have to be a real number? No, not true in general, does the diagonal element of A have to be a real number? Okay, alright. So this thing here A_{nm} and then here I can pull out an e to the i this becomes e sub m and this fellow becomes e sub n when you take it outside and what is left is B ? In n and then in e to the power i over \hbar cross τ and then you have an E_m minus E_n and that is it. So let us give this a name, let us write this as e to the power minus E_n minus E_m , what does that give you?

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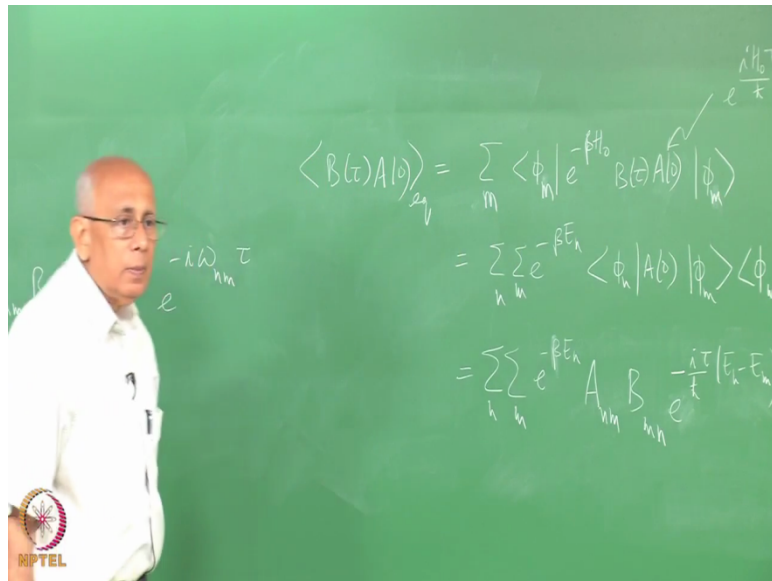
That says, let us now it is natural to do the following this is the energy difference between the n and the states its call that ω_{nm} times \hbar cross.

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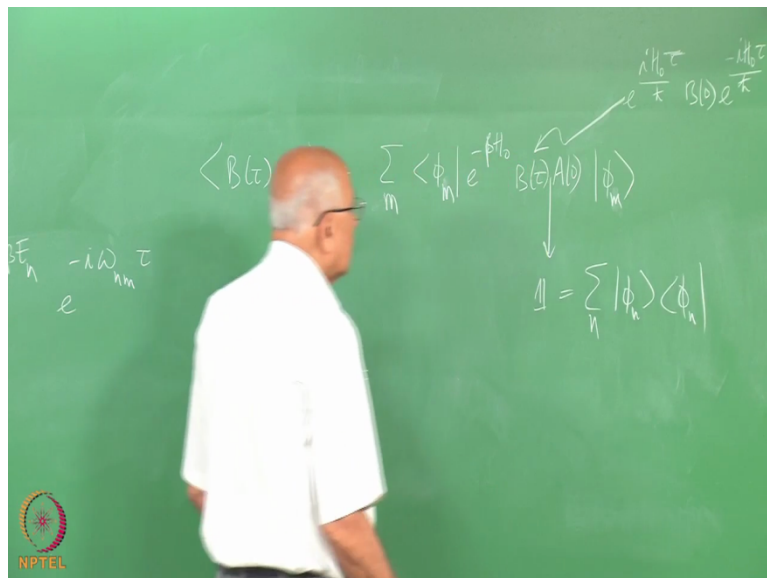
So I define $\hbar\omega_{nm}$ by definition equal to $E_n - E_m$ it says $A(0)B(\tau)$ in equilibrium can be written in compact form summation n, m $A_{nm} B_{mn}$ times $e^{-\beta E_n}$ and then $e^{-i\omega_{nm}\tau}$. So it can be written in quite a compact form.

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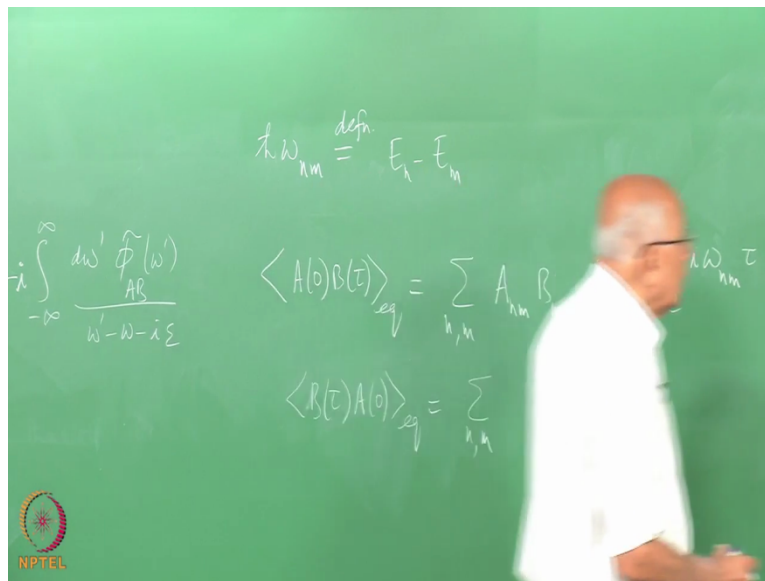


Next up is to wait for the other part of the commutator, right? So let us write the other way point B of tau A of 0 and this is now going to have B of tau A of 0 and since I want to match with that let us take the sum here to be over m and sum here in between to be over n and this fellow becomes B out here we have to work this out properly.

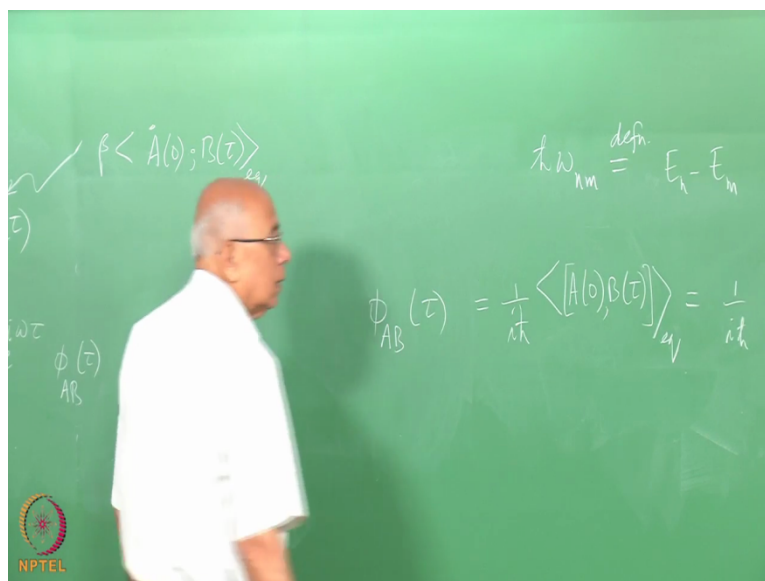
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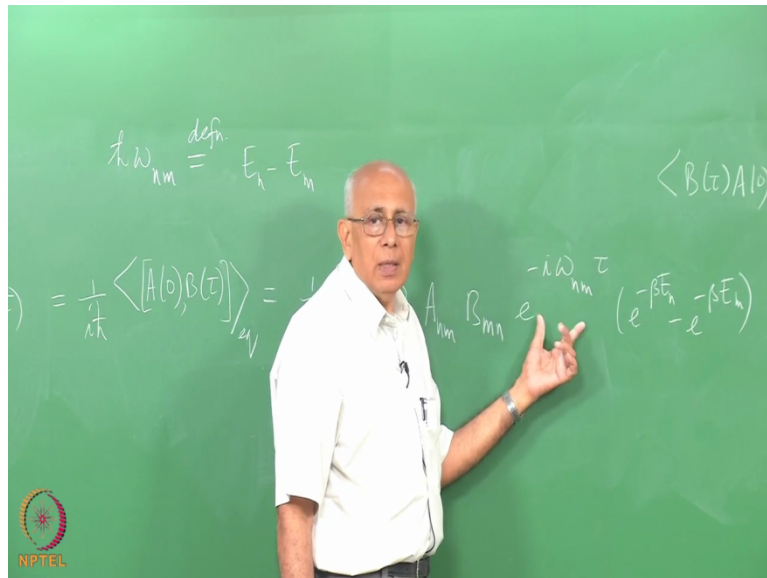


So this is just A of 0, this fellow here is that now introduce a complete set of states your by putting i into the summation over n phi n phi n therefore you can write-down directly, what this quantity is? B of tau A of 0 equilibrium equal to summation over n, m you are still going to get Bmn and then you going to get Anm which is the same as this, so this is still Anm Bmn but now this is going to hit this and give you e to the minus beta Em.

So this is going to be e to the minus beta En and the rest is going to be exactly the same as before. So therefore what does the commutator do? Let us divide by 1 over ih cross because that is what the response function is, all these portions are common but this becomes e to the

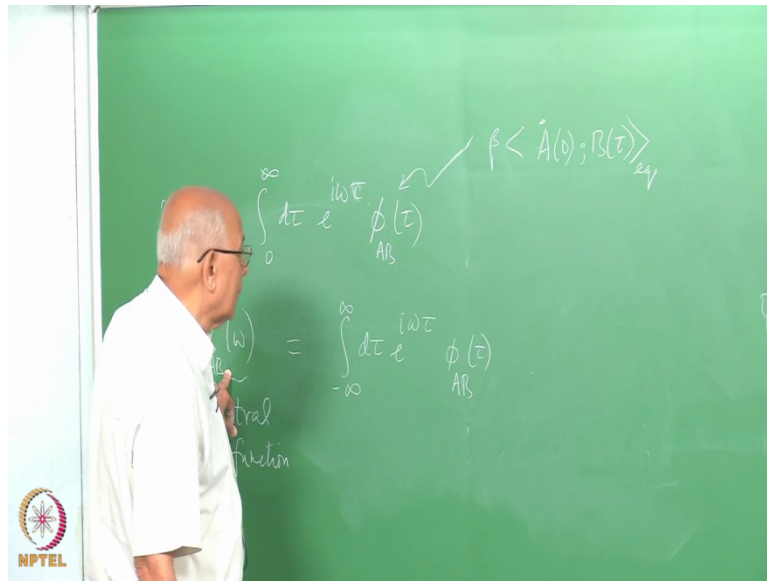
minus beta E_n minus e to the minus beta E_m and this goes away. So this is equal to 1 over $i\hbar$ cross summation over n summation over m $A_{nm} B_{mn}$ times this product that is it, Right? And this is equal to ϕ AB of τ .

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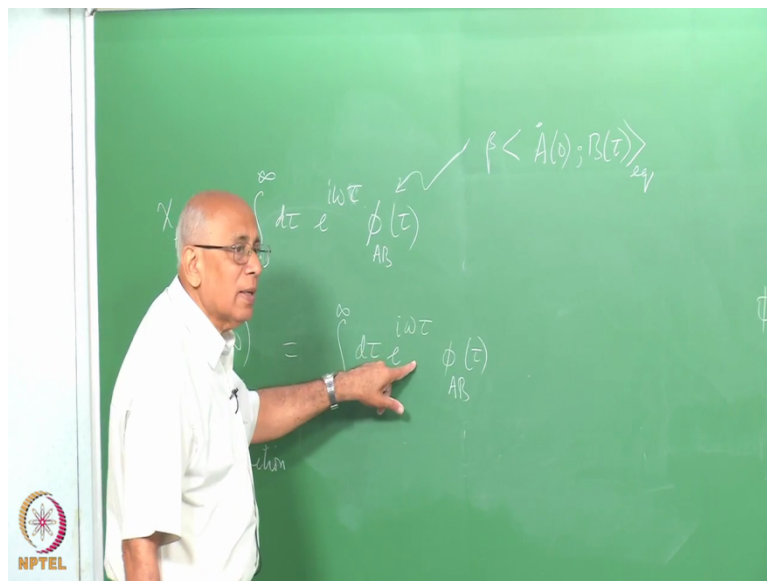


So we have now explicit equations in terms of physical quantities the matrix elements of these operators, you have representation for these operators then all that rigmarole about going to the interaction picture and so on and so on, finally ended up with just these quantities the τ dependence is sitting here and the temperature dependence is sitting here and this is a set of exponentials that is it.

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Now it is trivial to calculate what the correlation function is? What the spectral function is? What is going to happen? You want to do this integral and there is a minus out there, exactly. So what will this be? I am going to stop with that today, $\chi_{AB}(\omega)$ therefore equal to $\frac{1}{i\hbar} \sum_n \sum_m A_{nm} B_{mn} E_n - \beta E_n - e^{-\beta E_n} e^{i\omega t - \omega t} \int_{-\infty}^{\infty} dt e^{i\omega\tau} \delta(\tau)$.

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$$\hbar\omega_{nm} \stackrel{\text{defn}}{=} E_n - E_m$$

$$\frac{1}{i\hbar} \langle [A(t), B(t)] \rangle = \frac{1}{i\hbar} \sum_n \sum_m A_{nm} B_{mn} e^{-i\omega_{nm}t} (e^{-\beta E_n} - e^{-\beta E_m})$$

$$\Phi_{AB}(\omega) \equiv \frac{2\pi}{i\hbar} \sum_n \sum_m A_{nm} B_{mn} (e^{-\beta E_n} - e^{-\beta E_m}) \delta(\omega - \omega_{nm})$$

So this is 2π , so the spectral function is a function of frequency has peaks at all these points, okay. If the number of the levels are very close to each other it has a large system at many levels then it is going to look like a continuous spectrum, okay but these are the characteristic frequencies the next thing we will do is write down the susceptibility based on this representation.

So it will give you all explicit ω dependent thing involving the transition frequencies of the system these are the transitional frequencies of the system between which transitions another due to a perturbation, okay. So and then we will interpret this further and so let me stop here today.