Non Equilibrium Statistical Mechanics
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Lecture 12
Linear response theory (part 7)

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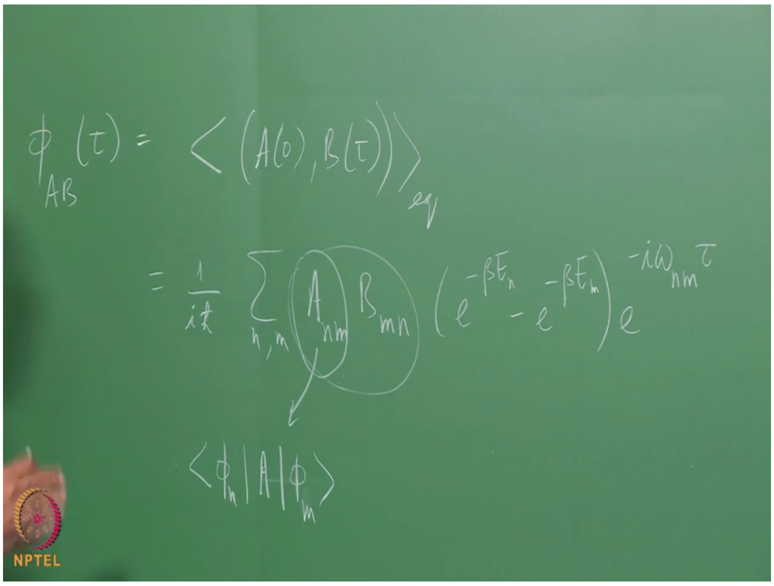

How do the area is the congenital tendency to this magic word adjust? We saw last time that the general response function phi AB of tau which is of course defined as the commutator of or some bracket as the case may be in the canonical ensemble we saw that this quantity here could be written in terms of the matrix elements of the individual operators A and B.

For instance in the quantum mechanical case we assume that there is a complete set of states given by the Eigen states of the unperturbed Hamiltonian in h not and in that basis this quantity at written as 1 over ih cross a summation over n and m if I recall right it was Annm Bmn the matrix elements of these operators multiplied by (()) (1:31) factors is times the actual time dependence which was e to the minus i omega mn tau expansion.

Check if these all the factors are there I am writing this down from memory from what we did last time but I believe it is okay as it stands these were actual matrix elements this quantity for instance Anm was phi n A in the Schrodinger of picture if you like phi m and likewise for B, so that immediately leads to a representation for this fundamental quantity spectral function.

So we are going to regard this spectral function the Fourier transform of this response function to be a fundamental quantity and then everything we expressed in terms of that spectral function. So spectral function phi AB tilde of omega is of course defined as an integral for minus infinity to infinity d tau e to the minus i omega tau phi AB of tau and this if you use the fact that this quantity here is where the tau dependence is sitting then this is equal to d tau e to the I use e to the plus i omega tau that was my Fourier transform convention.

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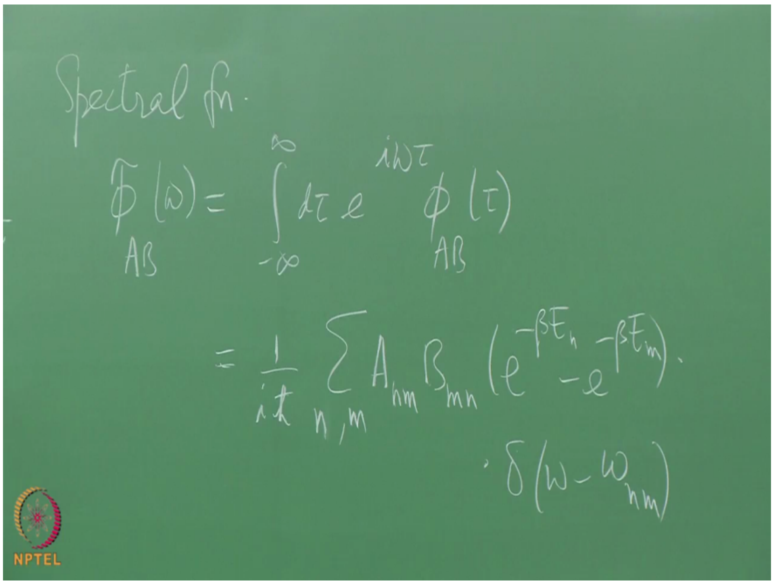

So this is equal to 1 over ih cross summation n, m Amn Bmn times a set of delta functions in the expansion. So it just consist of whole lot of Delta function spikes that is what this spectral function is and we know already what the representation from here they follows a spectral resolution of the susceptibility itself.

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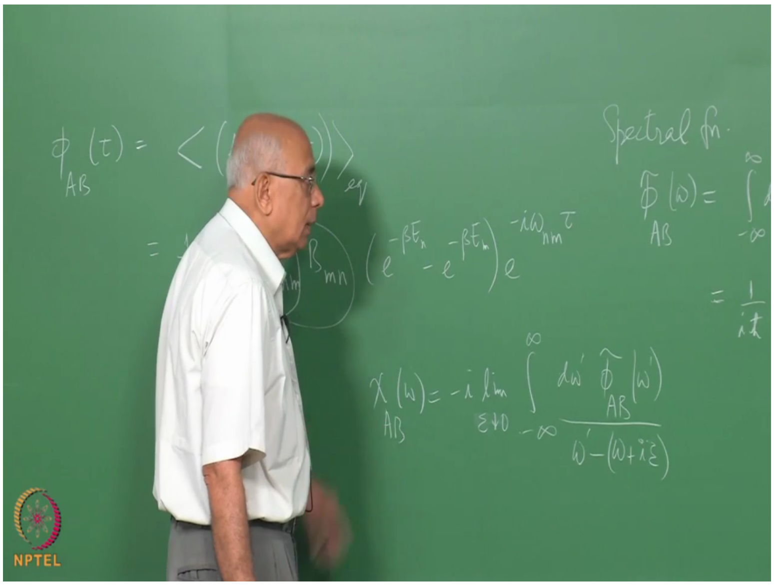

So that implies that kai AB of Omega equal to minus i limit Epsilon goes to 0 from above, so Epsilon goes to 0 and integral from minus infinity to infinity d Omega prime phi AB tilde of omega prime divided by Omega prime minus Omega plus i Epsilon, we had this relation between the Fourier transform of the response function and the generalized susceptibility.

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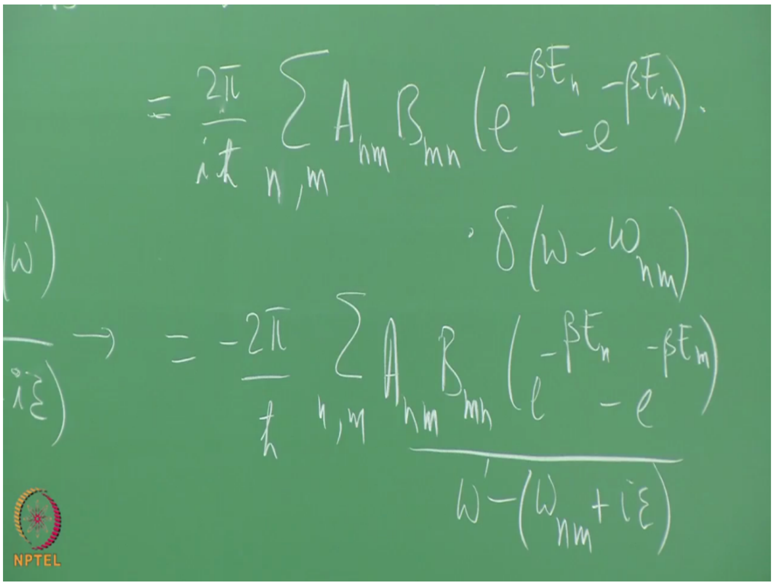

So this will imply then this quantity here is equal to the i and minus i will cancel, so if I put this in then it is equal to, yes when I do this I have to be careful because I did this integral d tau e to the i tau times omega minus omega mn that is 2pi times a Delta function 1 over 2 pi is times e to the i whatever you said delta functions, so there was a 2pi there, so this fellow is minus 2 pi over h cross the i cancels out summation n, m Anm Bmn e to the minus beta En divided by omega prime minus omega nm n is i Epsilon.

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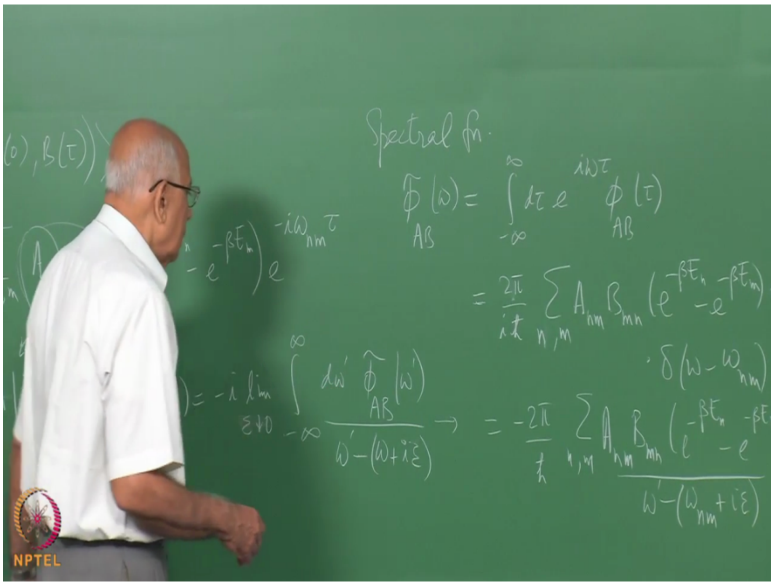

So wherever omega appears I just replace it using the Delta function I replace it by omega nm and that is it. So this is the representation for the susceptibility itself, okay. So again everything is expressible either in terms of Kai or in terms of this quantity phi we will use this preferentially because there are going to be various conditions put on this and that is the simplest way of expressing those conditions is to use the spectral function.

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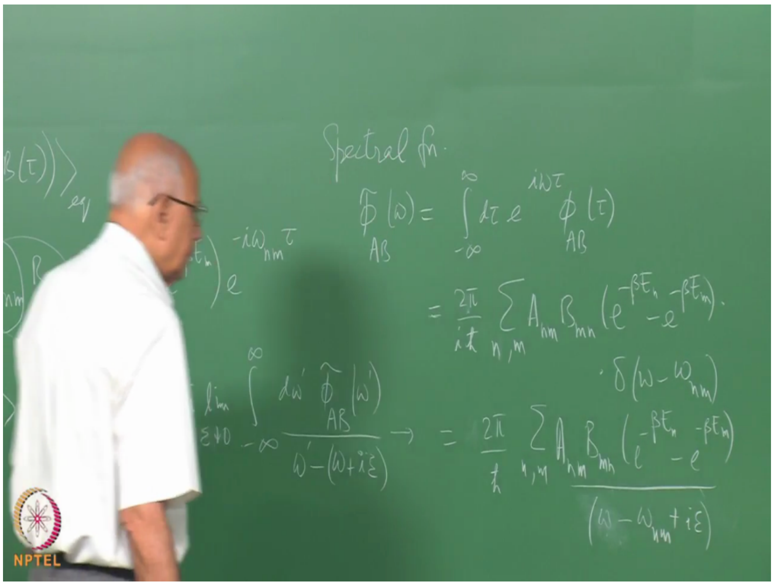

Now the first question what kind of function is this Kai as a function of omega? Yes, oh! Yes of course I is function of omega, you are right, thank you. Yes absolutely thank you absolutely it has got to be a function of omega, so omega nm, yes the minus sign can go away, so let us remove this and write it as omega minus omega nm plis i Epsilon, right thank you.

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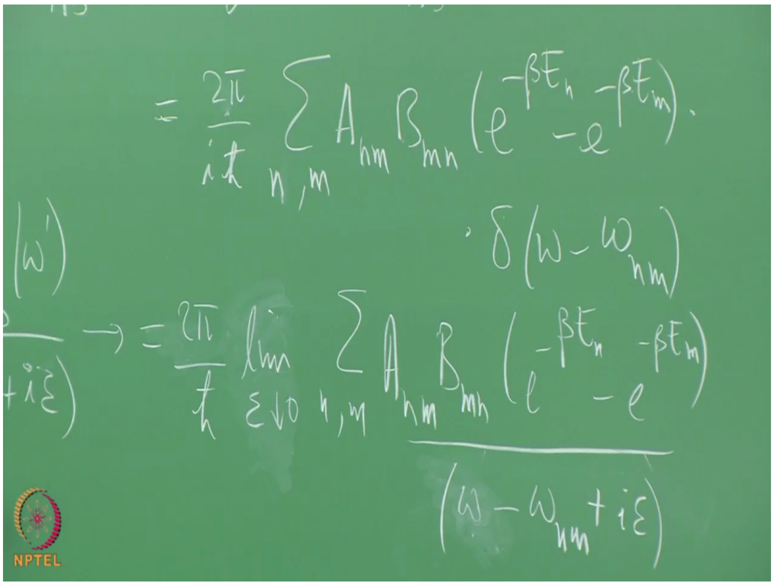

So it has got poles the susceptibility has poles at all that transition sequences but this representation tells you explicitly what kind of analytic function this quantity is. You see it is a function of omega which is analytic in the upper half plane explicitly, the physical susceptibility for real frequencies is the boundary value from above because as Epsilon goes to 0 you should first year put the limit equal to 2pi over h cross limit Epsilon goes to 0 of this guy.

For real omega this is the representator but if I remove this i Epsilon than it defines an analytic function in the upper half plane and what is happening is at the physical susceptibility in the omega plane is the boundary value of this function without the i Epsilon as you come down from above as you can see you give a small positive imaginary part to it and then let it go to 0, so it is really the boundary value from above, okay.

So what 1 can do is to define a function of omega for complex omega, okay. Using this so we could define some function let me use some other symbol for it, I want to do it in the lower half plane as well at the same time.

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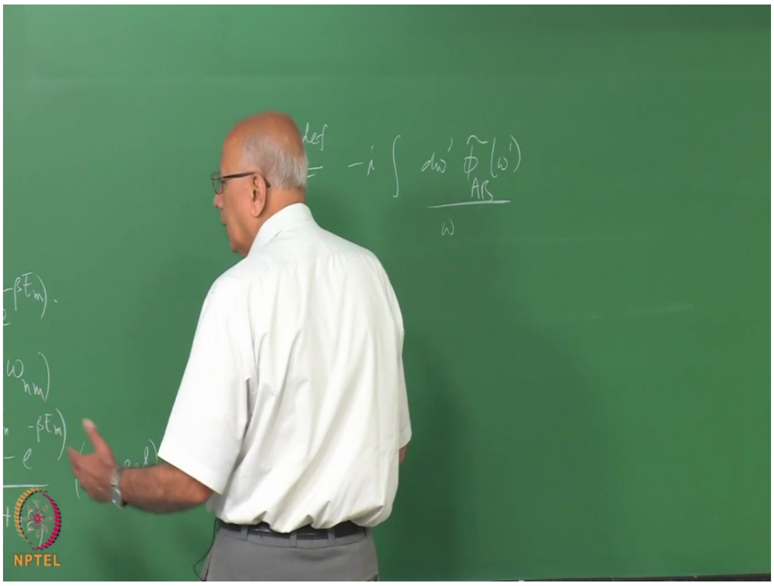

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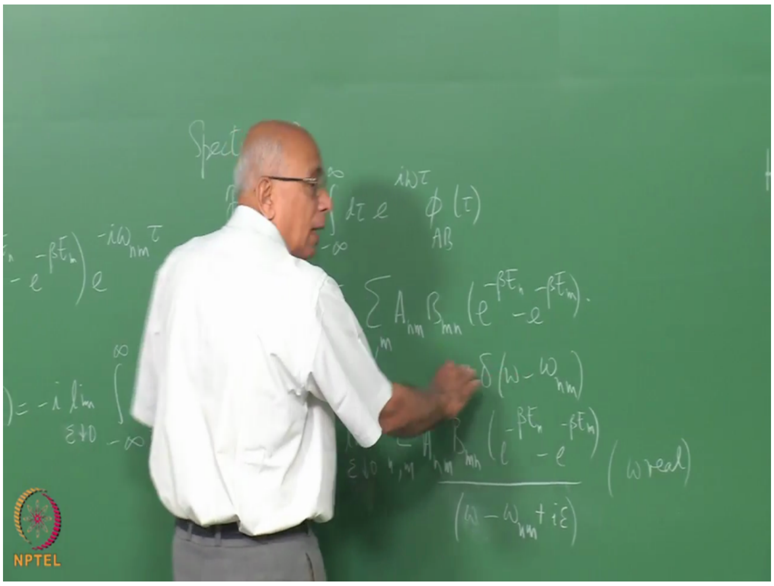

So I want to argue that let us let us recall this K for want of a better symbol, K AB of omega let us define this to be minus i integral d Omega prime phi AB tilde of omega prime over again write it as   minus i is still there, so omega prime minus omega, omega complex let me define such a function this quantity is defined for all real values of Omega prime through this into through this kind perfectly well-defined.

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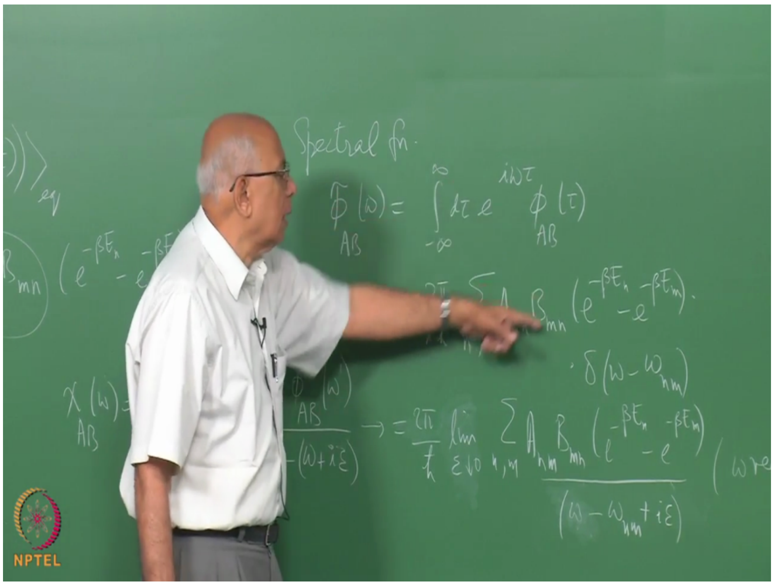

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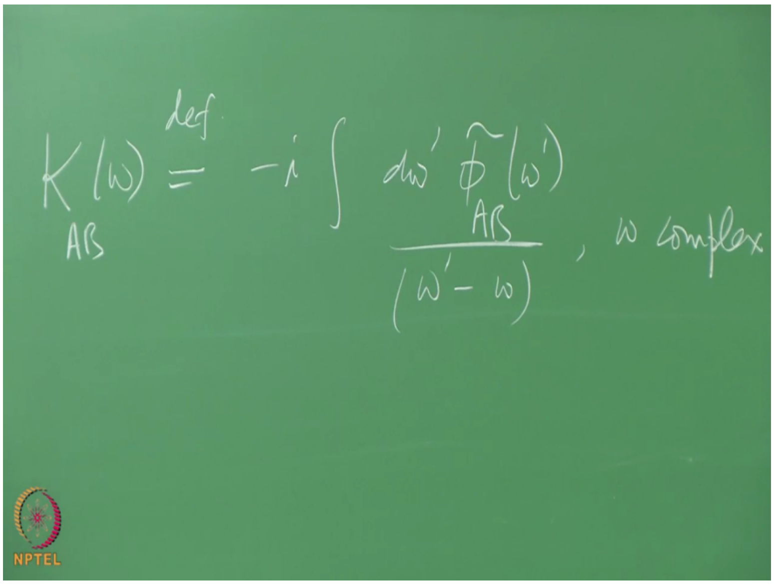

After all the argument of Delta function has to be real otherwise it makes no sense, so all this is for real omega, having got to this stage at this stage I say here is a function of omega real function integrate that function overall omega prime or real omega prime with the weight factor 1over Omega prime minus omega, okay. It makes sense as an integral for all Blacks values of omega but not real values because as soon as omega hits a real value there is going to be a singularity in the path of the integration along the path of integration. So it is defined as long as omega is not real there is some imaginary part.

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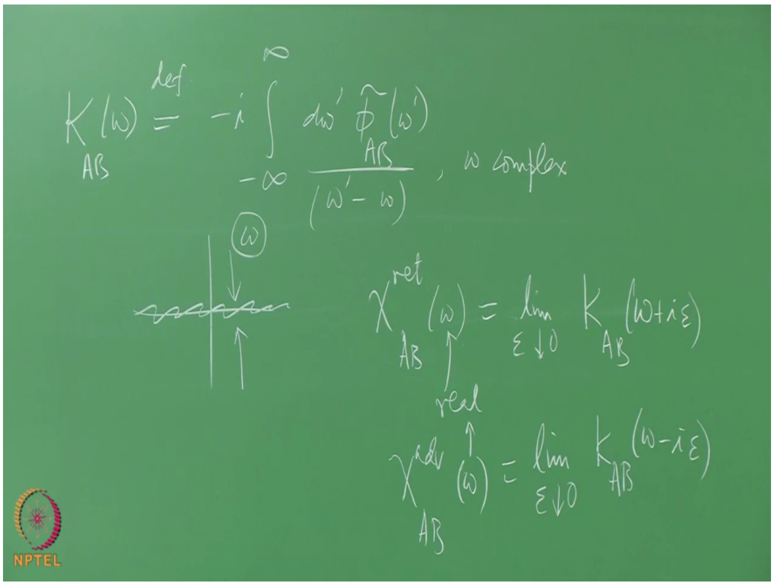

So in the omega plane this quantity defines an analytic function, okay. Makes sense everywhere except on this, so there is some kind of cut here in the omega plane.

“Professor -Student conversation starts”

Professor: No, no, no, for every real omega there is going to be, it is going to hit it, right?

“Professor-Student conversation ends”

It is another matter what he is says is right because ultimately phi itself has support only at these points. So even though you are integrating overall omega prime phi itself vanishes in between those delta functions if you like but you see it takes a very large system with a very large number of energy levels. So close to each other that is practically a continuum then practically everywhere in omega you are going to hit a singularity.

But now this analytic function here this master function if you like has a boundary value as you come down from above, it also has a boundary value as you go down from below and there is no reason why these 2 should be the same at all. What is happened is that Kai retarded, this is our retarded susceptibility Kai AB of omega real omega, this quantity is real that is the physical susceptibility is equal to limit from Epsilon goes to 0 from above of this guy, okay.

So instead of omega you see omega plus i Epsilon positive imaginary part and then you take the limit as down from above and the physical retarded susceptibility is the boundary value of that function from above, this thing here defines an analytic function for all complex omega but because you cannot the cross real axis there is no guarantee that the function get from above and the function you get from below are the same in fact they are not, they are not the same.

So similarly Kai advanced we look at the retarded green function but mathematically you can also about the advanced green function AB at omega and that is real to is the limit as Epsilon goes from above KAB of omega minus i Epsilon. So now you are approaching from below, this guy is guaranteed to be an analytic function of omega holomarphic in the lower half plane this fellow is analytic in the upper half plane the physical retarded response for real frequencies is a boundary value from above of this master function K and the other one you may want it for some other applications generally you would do actually that case is when you do then it's none of their analytic function it comes from below.

And whenever you have an integral like this you can ask what is the difference between this and that? So you really have to ask what is the discontinuity of this function as you are across this cut and what would you say?

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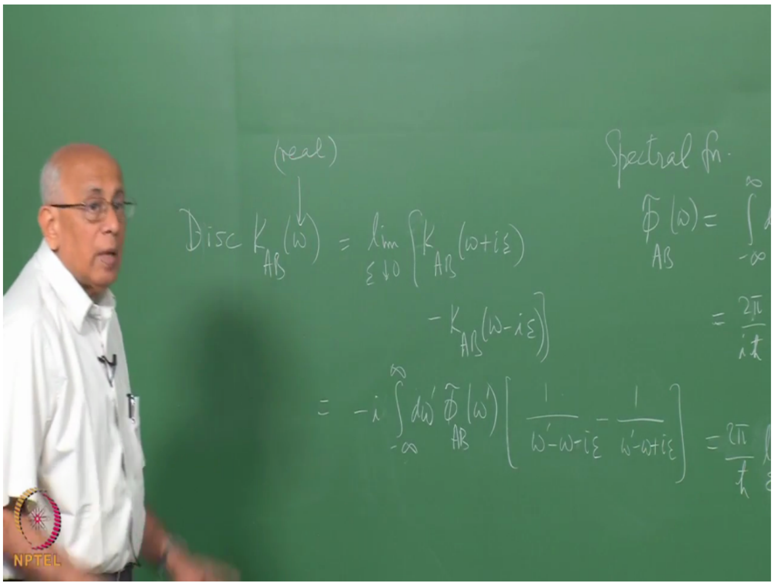

Well, the discontinuity let us do that just for fun although that is not what I am interested in right now but just as an exercise in analytic functions if you see that discontinuity KAB of omega and this is real by the way equal to limit Epsilon goes to 0 from above KAB of omega plus i Epsilon minus KAB of omega minus i Epsilon and now the only place where this i Epsilon appears is in the denominator, right?

So in one case you have, so this thing is equal to let us write it out minus i integral minus infinity to infinity d Omega prime phi AB tilde of omega prime and then inside you have 1 over Omega prime minus omega minus i Epsilon minus 1 over Omega prime minus omega plus i Epsilon, omega is real and omega prime of course is real as well, what is this equal to? This is the famous formula involving these i Epsilon's and so on.

You see if I live out this i Epsilon and on the region of integration in the omega prime plane here is the point omega in the omega prime plane, if I leave out this portion of it I get the principal value and then the meaning of this omega minus i Epsilon means the pole is at this point.

In the first-term the pole is at omega prime as omega plus i Epsilon, in the second case the pole is out here. So as I do this having the pole here is equivalent to putting the pole on the real axis and indenting the contour from below and taking half the contribution from that pole, right? Or equivalently close the contour or whatever and you are going to get 2 pi i times the value at this point, right?

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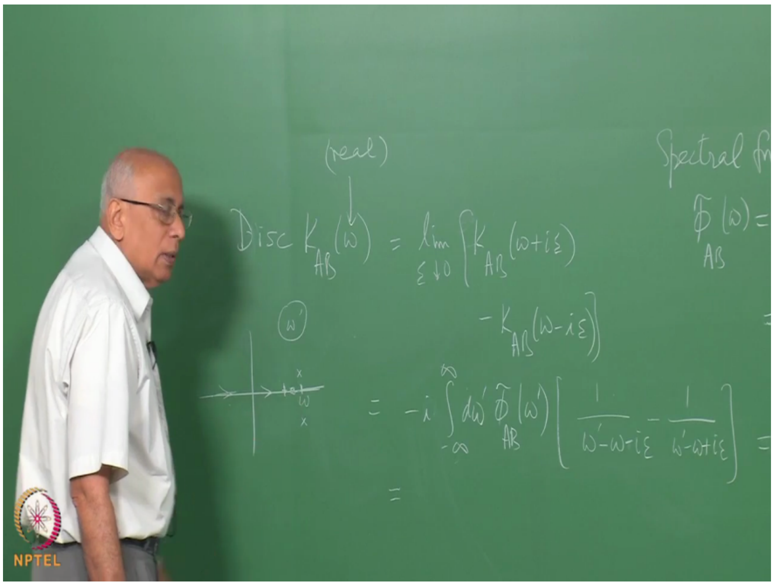

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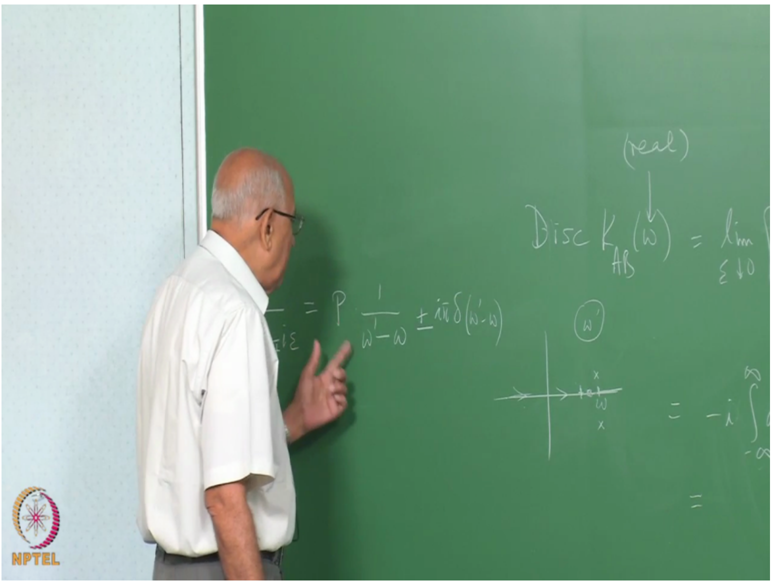

So from above you are going to get principle value 1 over omega prime minus omega, so 1 over Omega prime minus Omega minus i Epsilon is equal to symbolically it's this principle value plus i pi delta plus i pi because you want to go around anti-clock wise direction from 0 to pi, i pi dealt of omega prime minus omega and if you put a plus here then it becomes a minus here.

Now we want the difference of the 2, so you want P plus i pi delta minus P plus i pi delta, so you get 2pi i times at Delta function, so the discontinuity is straight away equal to minus i minus infinity to infinity d Omega prime phi AB tilde of omega prime times 2pi i delta of omega prime minus omega but that integral can be done just says replace omega prime by omega and the i cancels with minus i and we have 2pi.

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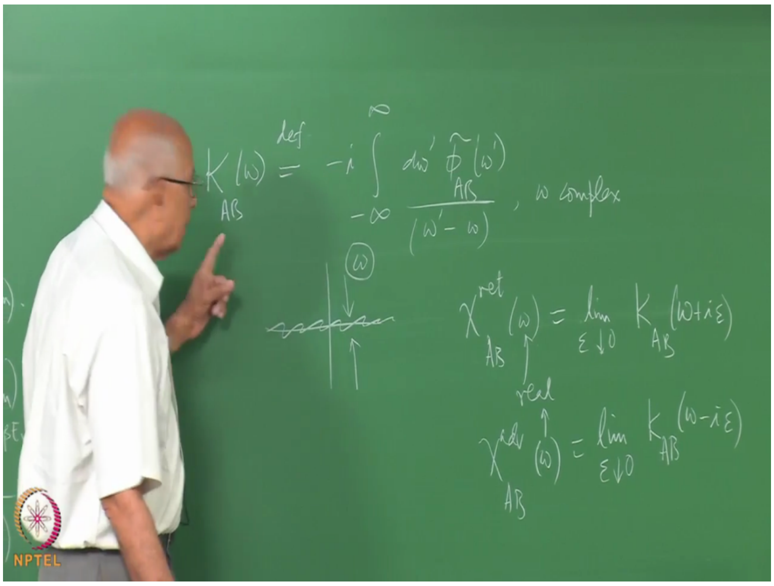

So we have a very interesting result which says that this is equal to 2 pi phi AB tilde of omega, so what you are really been doing is to be written at dispersion relation for this K. Not a Hilbert transform but a dispersion relation for this K with this Cauchy this kernel here and the meaning of the whatever is sitting up there the spectral function is that it is the discontinuity of this analytic function this is a general statement.

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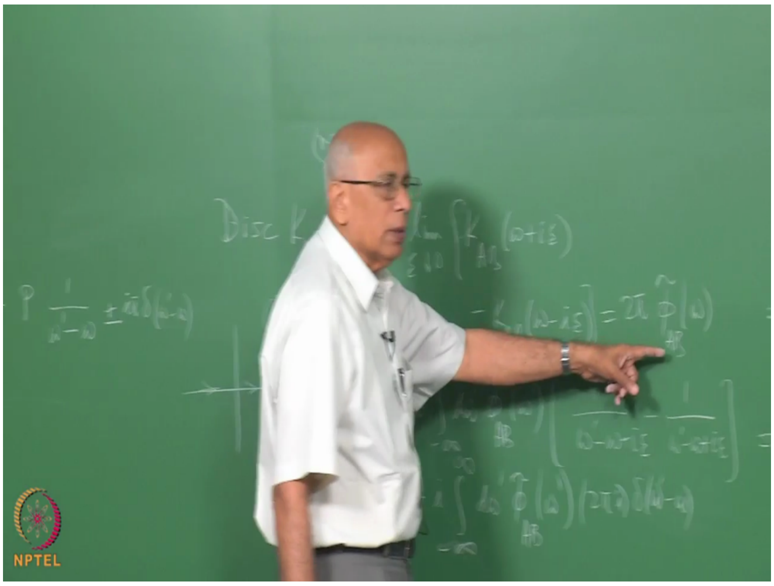

So again even this master function it is directly to this fellow here. A little later I will show that this fellow here the spectral function here is related to either the real on the imaginary part one of that too depending on the situation of the susceptibility itself. So what we are trying to do is get several relations, we know one relation between the susceptibility and the spectral function.

But you can invert this and ask what is the spectral function equal to in terms of the susceptibility? It will turn out to be either the real part or the imaginary part, okay. And we will see how? But for the moment this is how you show that A the physical retarded susceptibility is a boundary value from above in the omega plane of a certain analytic function of omega master function which has the spectral representation.

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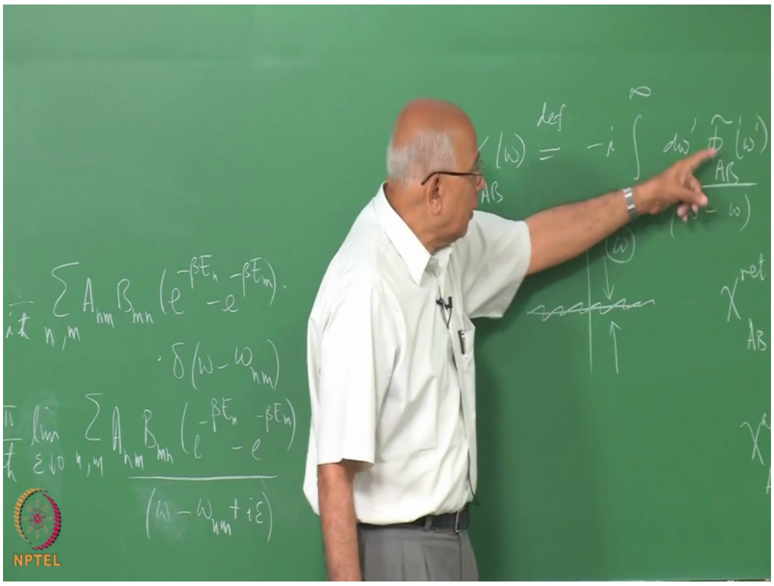

Spectral function itself is the discontinuity of this across the real axis, the retarded the advanced green function is the boundary value from below of this same master function here, okay. So it actually for the price of 1 you solve 2 different kinds of problems, 2 different boundary conditions but we are not going to get into that at the moment.

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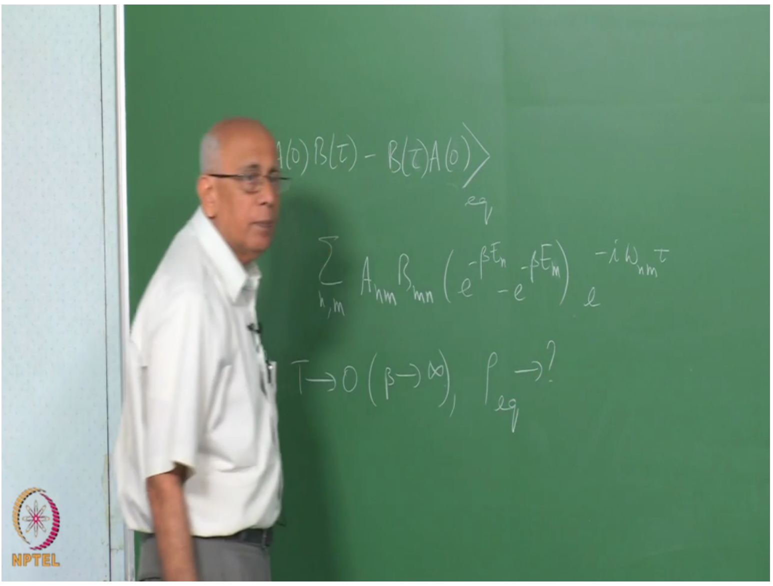

Let us come back here to this and ask the following question where do these formulas what do they reduce to if you had for instance we have seen there is temperature dependence let see what we can do say about that. So I need to again write down expectation value of let us write this commutator down explicitly d of tau minus B of 0,   B of tau A of 0 in equilibrium.

This was equal to, left hand side was the response function and we had a representation for it and you have to tell me what was the factors? This is equal to ih cross I divided by h cross so let us put that back n, m Anm Bmn, e to the minus beta En En e to the minus i omega nm tau we are writing all these representations for tau greater than 0, okay. Generally for tau less than 0 you will have a certain symmetry property which we will come to in a short while.

But for the moment let us keep Tau positive, pardon me. 1 over ih cross times the commutator was the response function and that is equal to this fellow. So in it's the commutator divided by ih cross that is the response function at was equal to this (()) (22:36), so I just brought this across from this side. What happens at absolute 0 of temperature? As you go to 0 temperature what you think should happen?

This would correspond to beta going to infinity, other words you switch of thermal fluctuation and then you should be back to quantum mechanics at 0 temperature there is no ih bar on the right-hand side.

"Professor -Student conversation starts"

Student: There is no ih bar.

Student: There is one icon ih bar that is okay, so if we do that it could be wrong also.

Professor: Yes.

Student: There is no ih bar.

Student: Dimensionally both should be AB.

Professor: Oh! What should be AB, right?

Student: Dimensionally.

Professor: oh! Yes, it is okay. Because I wrote the response function as 1 over ih bar times this I multiply by that ih cross this goes away, you are right. Absolutely, dimensional in as she says it should be just A perfect, okay.

"Professor-Student conversation ends"

Now what happens to this as t goes to 0 beta goes to infinity, what happens to rho equilibrium? Remember the density operator the canonical and sample was e to the minus beta h not but normalise such that trace e to the minus beta not was 1 normalise to that always. So what would you say is the density operator? What is the spectral representation of the density operator itself?

We are now assuming that the system is describable by a complete set of states in some Hilbert's space. So it is really not the formalism as written down here is really not the most general one because I have made a specific representation I have said that this system has a Hilbert space there are systems where you cannot talk about them and describe them in terms of (()) (25:06) and Hilbert space there is some density matrix and that is the end of it.

But we have made this assumption that year we actually have a Hamiltonian system it has got a nice Hilbert space complete set of states and it is slightly perturbed from equilibrium. So what is rho equilibrium equal to?

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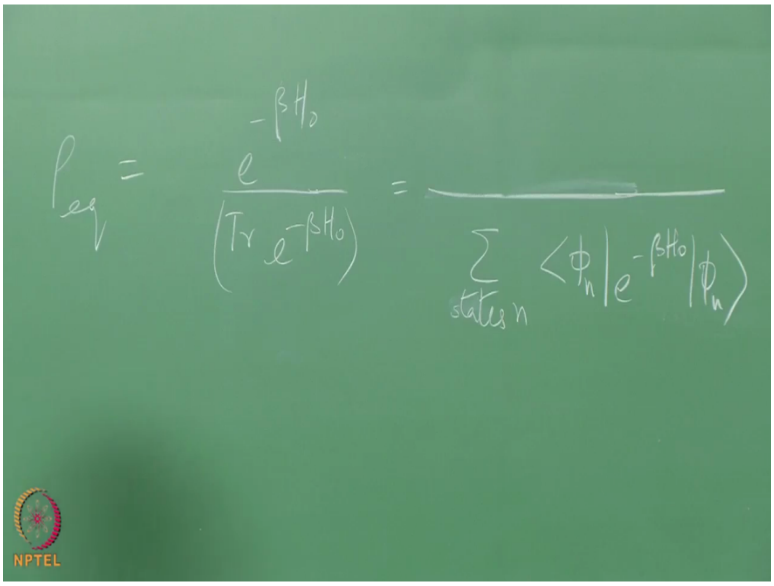

As an operator as an operator it is e to the minus beta h but now I am saying let us represent the operator in terms of ket vectors phi n in terms of basis formed by the Eigen states of Richmond, so it is clear what you must do is write e to the minus beta h divided by trace e to the minus beta h not that is what that is what the density operator is in (()) (26:11) form. On trace rho equilibrium is guaranteed to be equal to 1 because I have divided by this quantity.

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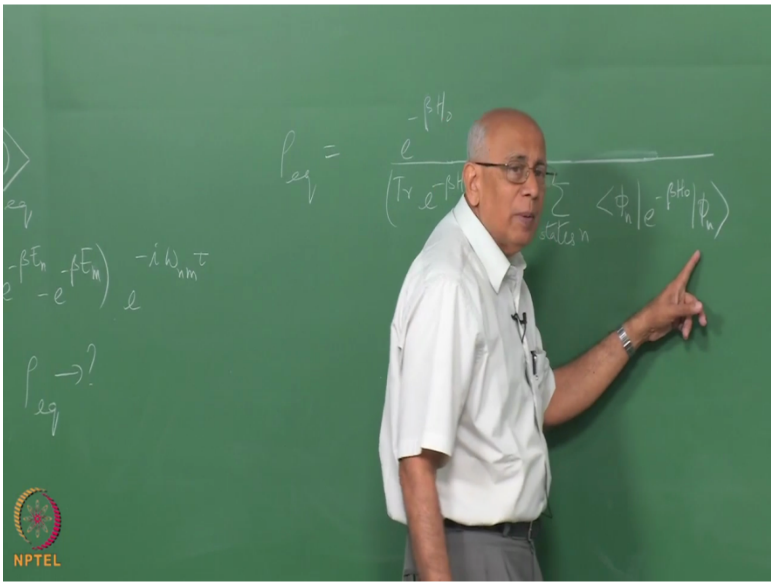

Now let us write this out in the basis on by the phi n's, so this is equal to in the denominator it is clearly equal to summation over states n states labelled by n or the collection of quantum numbers times trace, so this is phi n into the minus beta h not phi n that is the denominator obviously. What is the numerator? What is the numerator? Numerator is got to be an operator, so if this fellow, yes, if this fellow was former basis for all states in the Hilbert space there is also a basis for all operators, right?

For instance the unit operator is just sum over n phi n k phi n (()) (27:23), so every operator should be writable in that form. If the operator commutes with the Hamiltonian h not then you will have only the diagonal terms, right?

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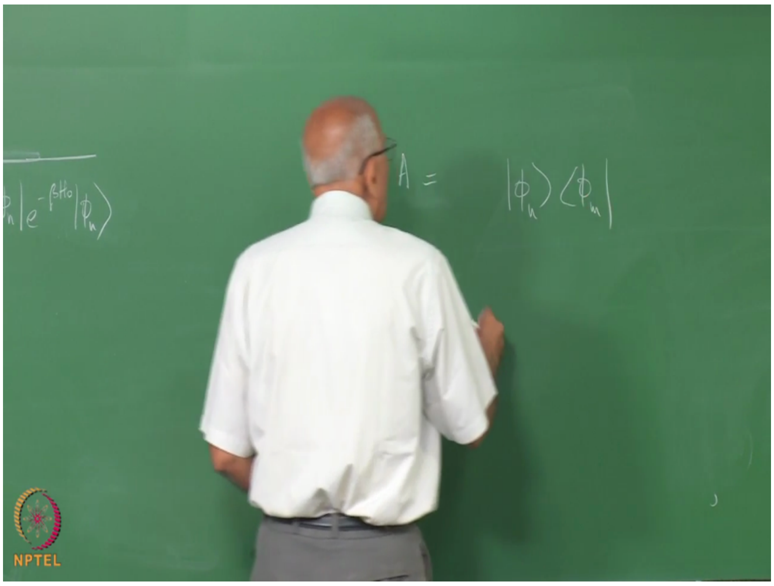

Otherwise in general if you have an abstract operator A you should be able to write this as phi n phi m and then some matrix elements here, what matrix element you have here? That is what you call Anm and there is a summation over n, m, right? That is what you mean by this operator, okay.

Just as when I write it to by 2 matrix A, B, C, D I mean a times 1 0 0 0 plus B times etc and that is the outer product, right? So it is just the same thing over again and therefore what is this equal to? It will have only these projections it will not have phi n phi m here it has got to be diagonal and then a summation over n of course and this state this projection is weighted by the corresponding energy, okay.

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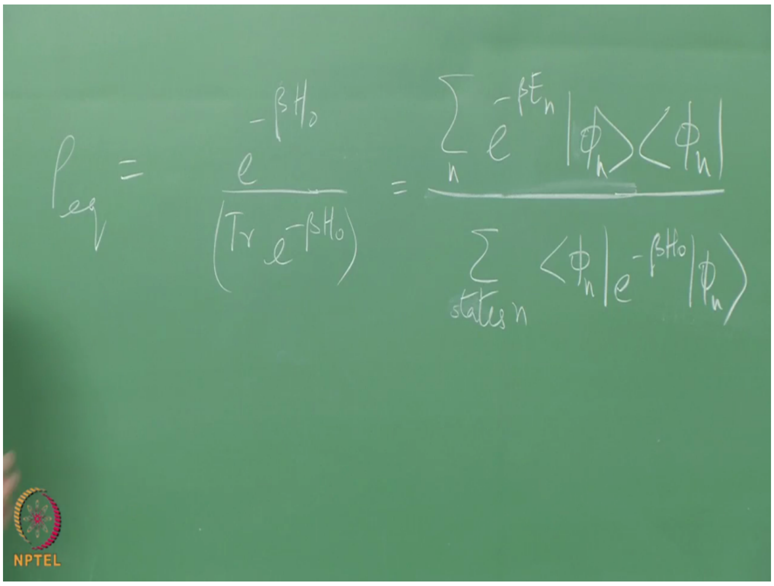

That is of course the representation of the density matrix in the basis formed by the Eigen states of H not. So notice these are operators this is just a number, okay. So that is what my rho equilibrium is, okay. What happens to this as t goes to 0 or beta goes to infinity? So let us suppose that all your, yes, so you can see, yes what does it do? Why should it be only the ground state?

But I am not assuming that the ground state energy is 0, why should I assume that it is 0? Is bounded from below, so we have assumed here tacitly that we have a respectable system whose ground state energy is bounded from below, if it is not grounded from below and goes to minus infinity then everything will sit there and take infinity (()) (29:54) to get it up out of that.

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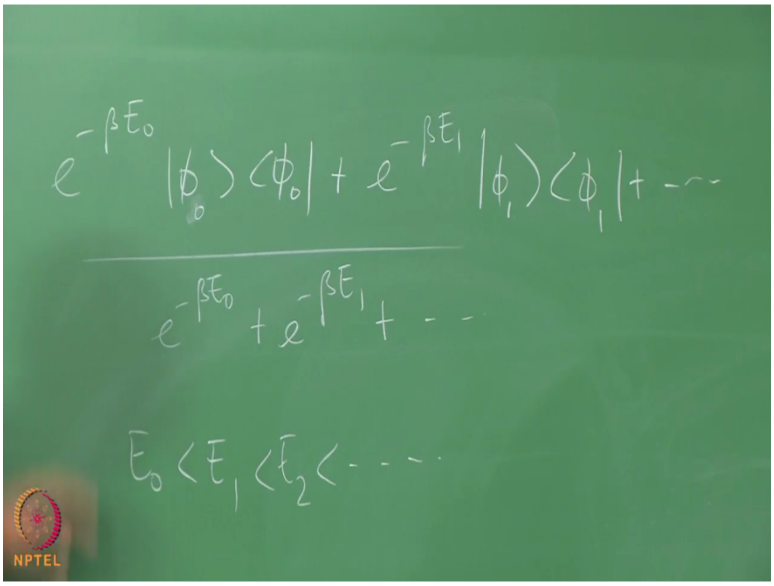

So what happens now? You see notice that this thing here can be written as e to the minus beta E not phi not phi not plus e minus beta E1 phi 1 phi 1 plus etc, yes divided by this fellow here and these guys they are all orthonormal, so it is e to the minus beta e not plus e to the minus beta E1. Now if E not is less than E1 less then E2 less than… Which it is because it is the ground state then you pull out the factor e to the minus beta E not, all these factors are going to go to 0 as beta tends to infinity As long as E not is greater than 0.

But whatever it is you can see that you can pull out this factor which is the biggest of the lot and these fellows will have even minus E not etc which are positive quantities and therefore as beta goes to infinity they will all go away, this e to the minus beta E not will cancel against this. So it is obvious that this will go to just the projection the ground state as it should.

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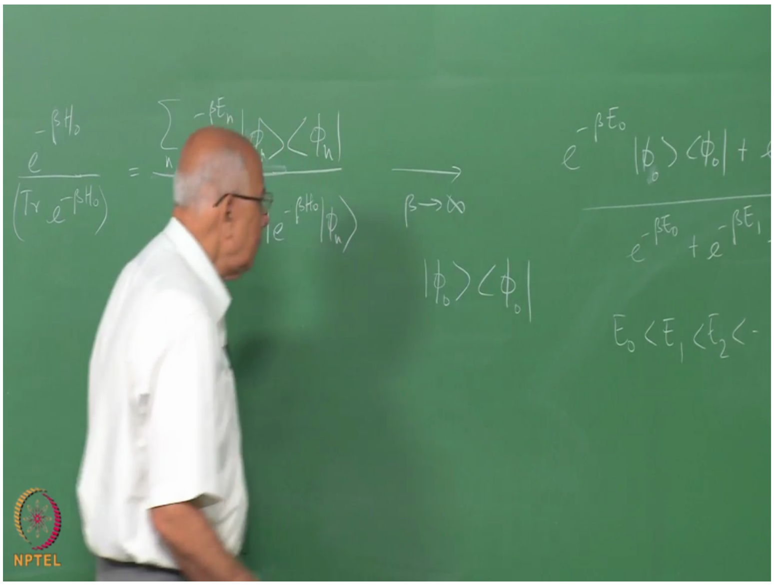

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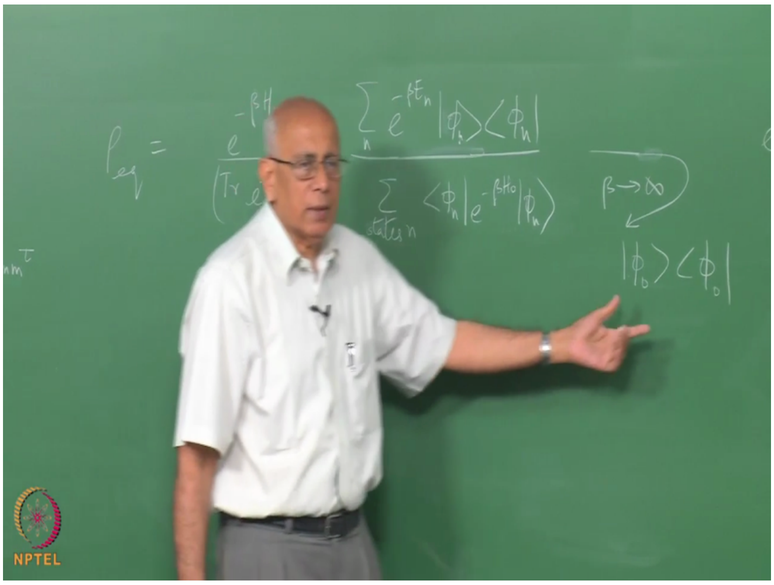

So as beta goes to infinity this thing goes to just the projector of the ground state. That is what is meant by saying that at 0 temperature things are at the ground state cause it says that all the (()) (31:31) factors go away and only thing that the density matrix has left in it is a project of the ground state.

There is no need to assume that E not is 0 or anything like that, E not is the smaller than all the other E's and of course we have assumed that the system has got a spectrum bounded from below. So what we have to do here in this case is precisely that go back to the calculation and this equilibrium now is just replace by a phi not phi not.

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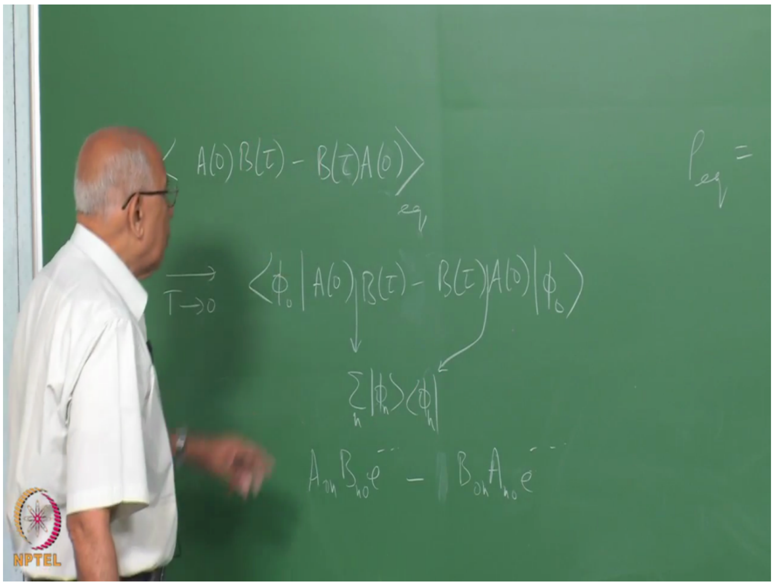

So at t equal to 0 and the limit of T goes to 0, it goes to this there can be no reference to temperature anymore it is gone to 0 that is it and this is it in this quantity Phi not phi not is normalised one, so that is automatically down that, it is gone. Now what you do is insert complete set somewhere here. So insert here summation n phi n phi n and ditto here, insert those fellows here.

And you are going to get the matrix element A0n and then Bn0 times e to the i omega n0 or whatever it is and we are going to get the opposite here. So the first term will have A0n Bn0 times e to the whatever it is and there will be a term which is of the form B0n An0 e to the whatever it is and the frequencies here would be just the frequencies would be omega n 0 plus and minus signs. So I leave you to complete this and figure out what this and just check that it goes to what you expect from ordinary quantum mechanics and you can write down the response function at 0 temperature, alright.

Now let us look at something more interesting which is got to do with the properties of this spectral function. What I had like to do is to exploit what we have for the commutator, to write out expressions for quantities which do not involve the commutator but any product of 2 operator's arbitrary operators.

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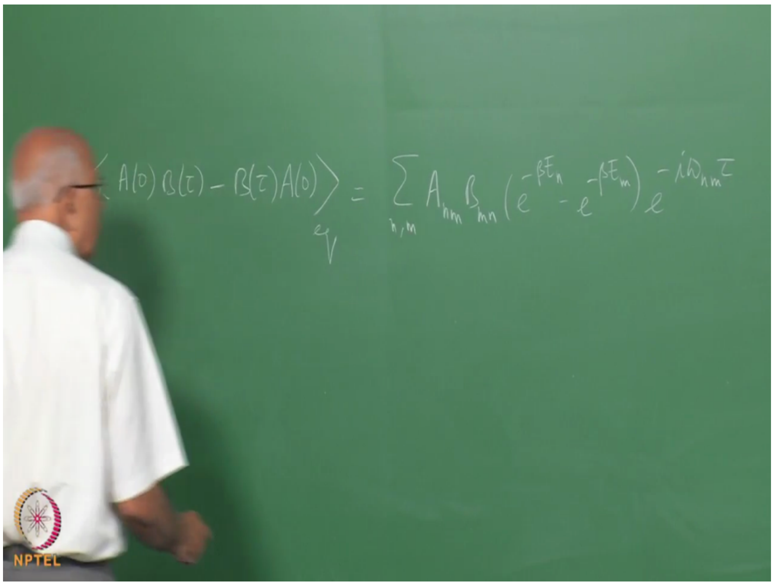

So recall that we have found that A of 0 B of tau minus B of tau A of 0 in equilibrium this quantity was equal to summation n, m Anm Bmn times what? e to the minus beta En m times e to the minus i omega nm tau. So this immediately led to the fact that phi AB tilde of omega was equal to a summation over n,m Anm Bmn small, there is 1 over ih cross in the phi and then we wanted to take Fourier transform of the response function.

So there was a 2pi and then a delta function of omega minus omega nm, right? So let us take this quantity to be a known quantity when I want to read various things in terms of this, various spectral representations of various time-dependent quantities giving this. So what should I do? The first thing to do is to write this as equal to 2pi over ih cross summation n, m Anm Bmn e to the minus beta En times 1 minus e to the beta h cross omega nm because that puts a plus e to the beta En minus e to the minus beta n, so that is okay, times delta of omega minus omega n.

Now since I am always going to integrate over omega in this I have a Delta function here which fires only when omega is equal to omega nm, so I can replace this omega nm by omega itself.

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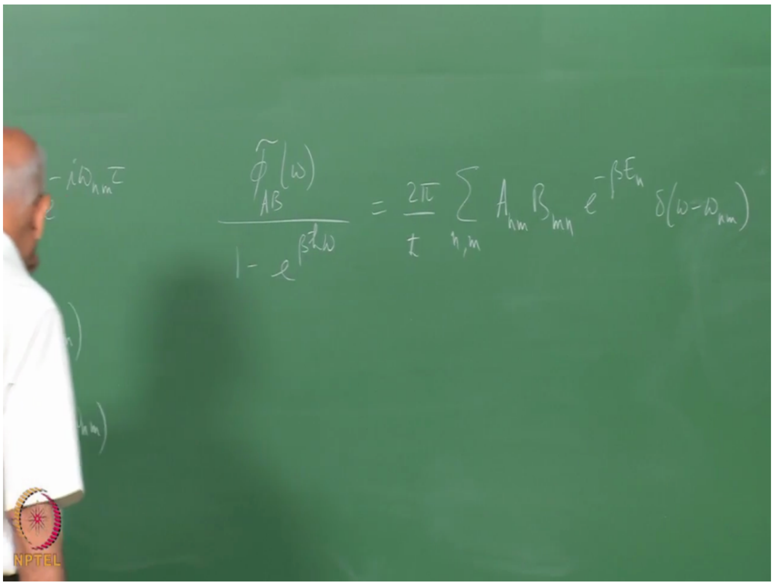

So I end up with phi AB tilde of omega divided by then I pull it out of the bracket to the left hand side, this guy here is equal to 2 pi over h cross summation n, m Anm Bmn e to the minus beta En, okay. So what I have got is the first part of this fellow, that is this, so now I can claim, pardon me, with an i factor? 2pi over ih cross, yes, okay. Now I want to be little careful with the algebra here.

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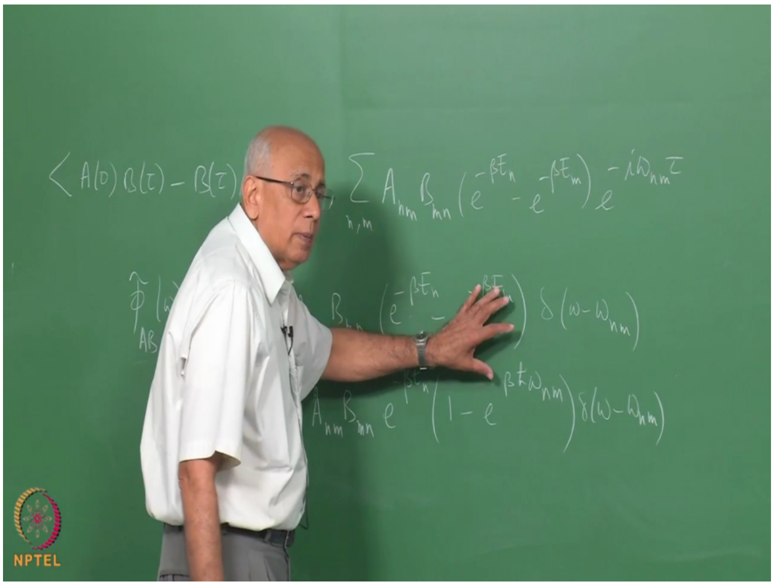

So I remove this portion, if I now take its Fourier transform, so I do integral from minus infinity to infinity d omega 1 over 2pi this guy, e to the power minus i omega tau phi AB tilde of omega divided by 1 minus e to the minus beta h cross omega this is equal to 1 over ih cross summation n, m Anm Bmn e to the minus beta En, an integral over omega times e to the minus i omega tau times that fellow. So e to the minus nm tau but what is that equal to? Apart from that ih cross factor it is equal to the first term here came from A of 0 B of tau.

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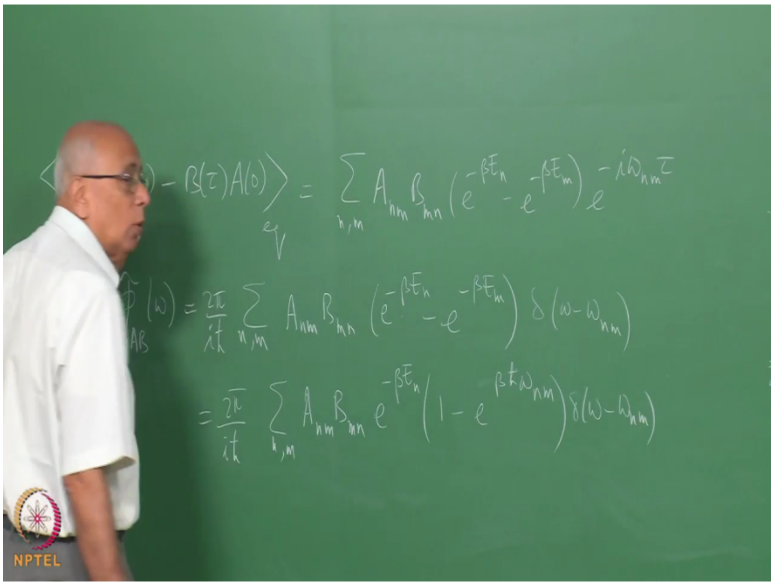

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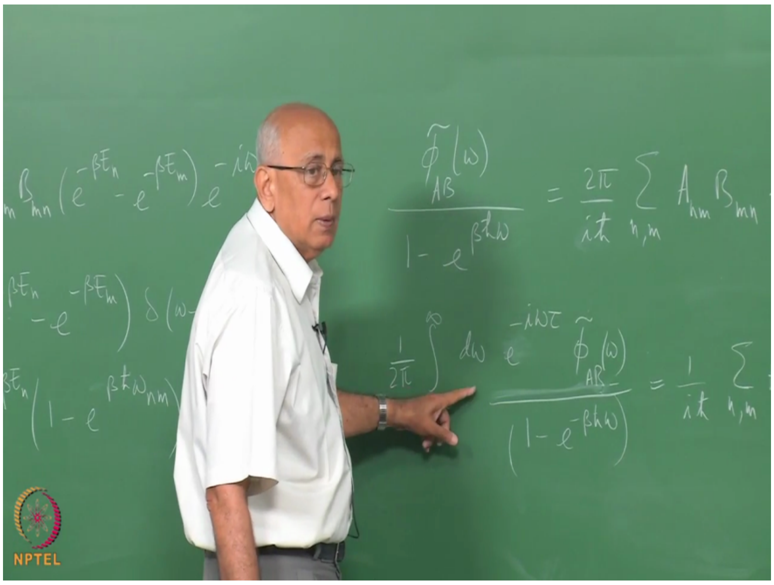

So A of 0 B of tau divided by ih cross is 1 over ih cross this garbage without that it is just this fellow, right? So it is equal to ih cross over 2 pi times this guy.

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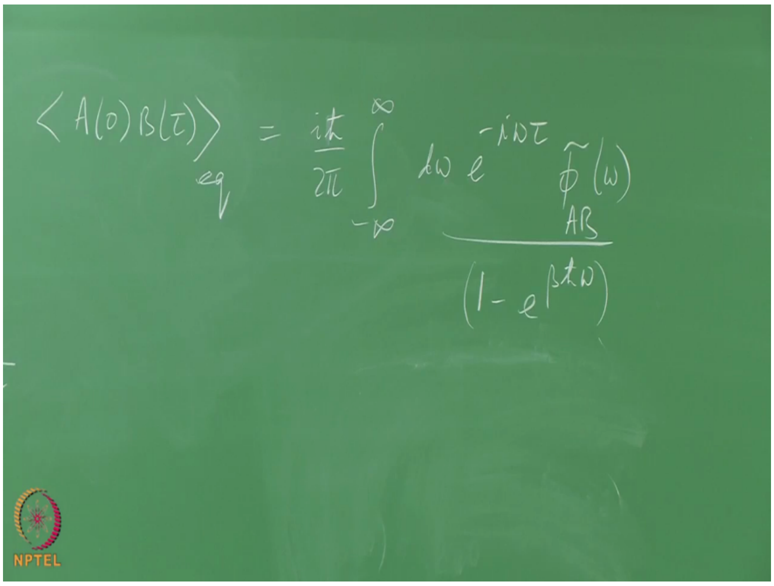

So it tells you that A of 0 B of tau alone equilibrium no commutator, alone is equal to 1 over 2 pi ih cross over 2pi d omega e to the minus i omega tau phi AB tilde of omega divided by 1 minus e to the beta h cross omega, okay. So by sleight of hand what we have discovered, now we can do this much more laboriously but what we have discovered is that while we have a nice spectral representation for the commutator we can do it for each term in the commutator except that the factor the extra factor that comes is this.

So it is the Fourier transform not of this guy but of that divided by this factor here, I am sure you can but I think it is a lot more laborious, yes because know discovering this factor is little more tricky, right?

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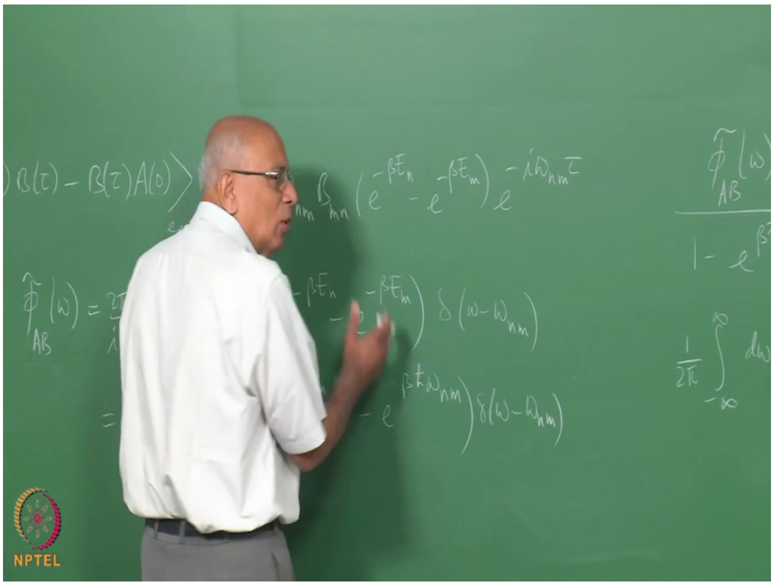

So what I did was, I exploited the fact that inside here this string is a function of n and m but I pull this fellow out the Boltzmann factor and then I replace this by the one with omega and pulled it out of the summation altogether, okay. I think it is a shortcut, now similarly for the other fellow you put the A to the minus beta in here and you need this term again you pull this out but you have to kill this term.

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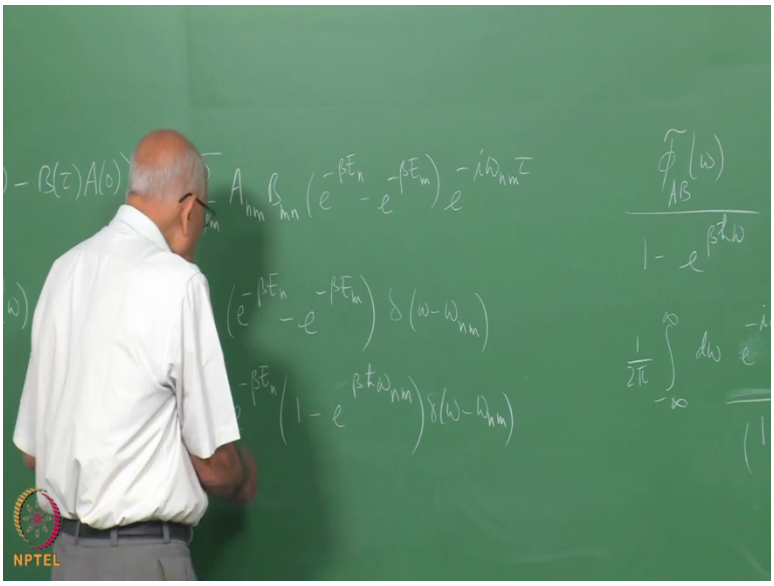

So you have to kill this and produce Em unit to multiply it by e to the beta h cross omega, right?

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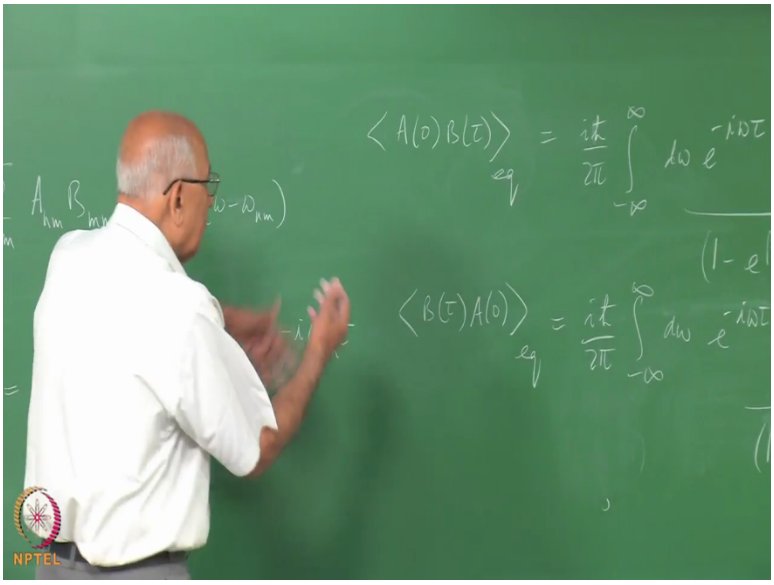

So it is clear that the b of tau A of 0 equilibrium is ih cross over 2pi and integral minus infinity to infinity d omega e to the minus i omega tau e to the beta h cross omega divided by 1 minus, so that when you subtract the 2, this factor cancels out from top and bottom and you will be back to this guy, you will be back to the representation for phi itself. So we have spectral representations for both these quantities therefore we have one for the anti-commutator, okay.

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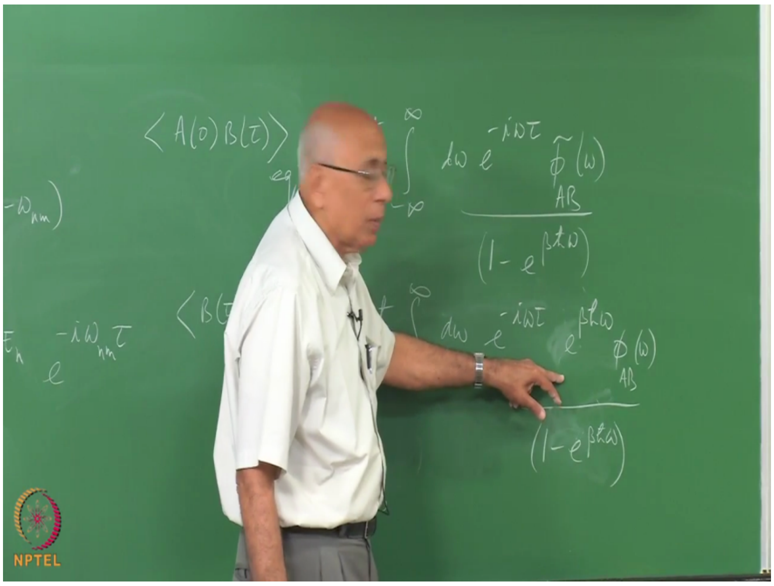

So let us see what that does? , so it says that the anti-commutator A of 0 B of tau, plus with a plus I do not want to use the curly bracket as is done sometimes because it's the poisson bracket we use that for the poisson bracket. So this fellow in equilibrium is that plus this, so is equal to ih cross by2pi integral minus infinity to infinity d omega e to the minus i omega tau and then 1 plus e to the beta h cross omega over 1 minus e to the beta h cross omega times the spectral function.

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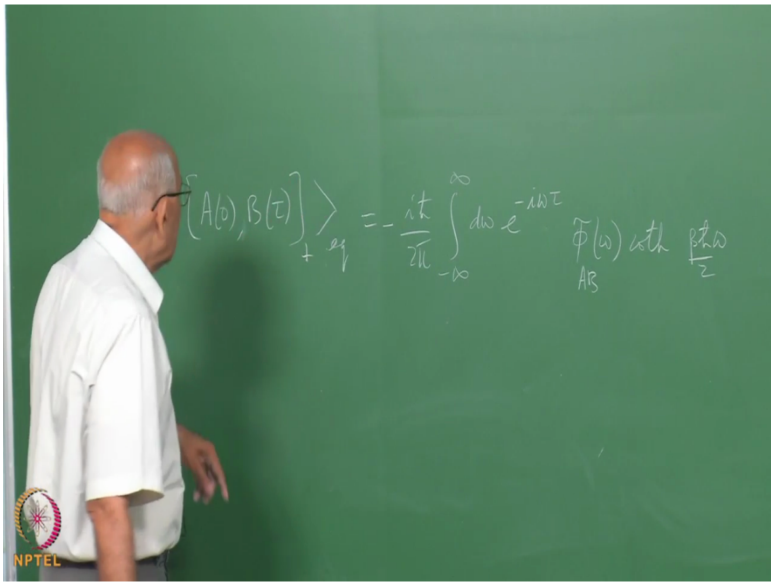

But I can pull this one out e to the half beta h cross omega then you get 2 cauch and I pull the same thing I would you get minus 2 inch, so this is equal to minus 2 is cancelled phu AB tilde of cot hyperbolic beta h cross omega over 2. So the anti-symmetric part the A of 0 B of tau the commentator had representation without this guy but the anti-commutator the symmetric part of the product has this representation.

Now there is a very neat way of we will interpret these things. This was just a little piece of algebra but we will interpret these things carefully. Does this remind you of anything? Does this remind you of any particular famous quantity?

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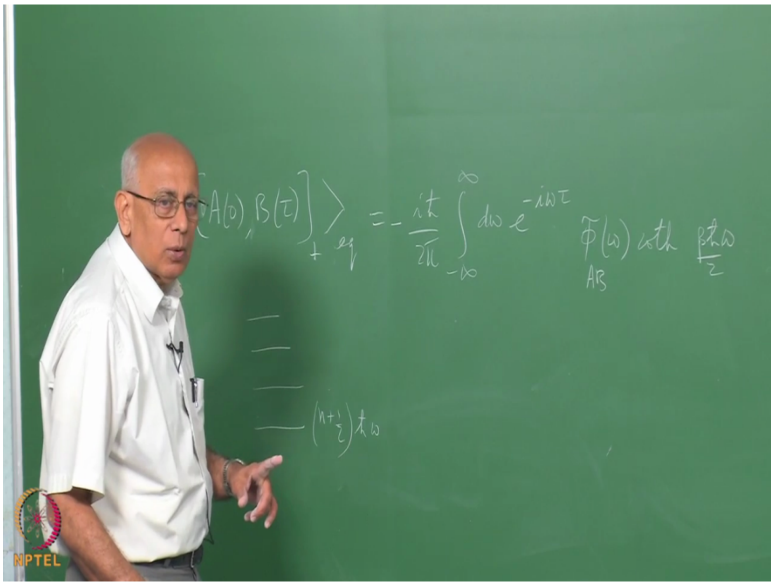

Well, even simpler than that, if you have a harmonic oscillator, so the energy levels are n plus half h cross omega, right? Let us ask what is the average energy of a harmonic oscillator, quantum oscillator with natural frequency omega at temperature beta inverse, right? So let me call this average value of h oscillator is equal to h cross omega times n plus half we have to sum it's not degenerate this thing is not degenerate.

So you have a summation n plus half e to minus beta h cross omega into n plus half divided by the same thing n equal to 0 to infinity, okay. Now look at this A to the minus half is going to go away numerator and denominator we do not have to worry about that, so this goes away and then you have n e to the is fellow divided by just this fellow, this is a geometric series. Yes or d over d beta of minus d over d beta of this guy, right?

So whatever way it is frequency that with an n up here you are going to get sine hyperbolic and without it you are going to get the constant hyperbolic over here. So you are going to get this cot hyperbolic once again. So the average energy of the harmonic oscillator, H oscillator at temperature t let me call that equal to Eg and let me put it as a function of omega for given natural frequency omega.

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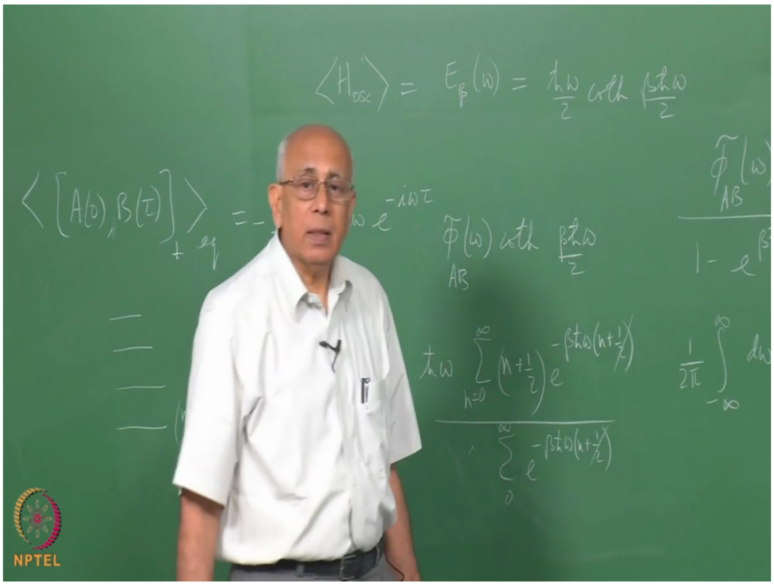

This fellow is equal to, well, what going to be the average energy at the equal to 0? Half H cross Omega it is ground state energy, so that has got to come out, it has got to be that. What happens is beta goes to infinity to cot hyperbolic 1 as beta tends to us infinity, so at absolute 0 its h cross omega over 2, that is it, okay.

What happens at t equal to infinity? What happens to this guy? What happens to cot hyperbolic? Beta H cross as beta goes to 0 it diverges, diverges like what?

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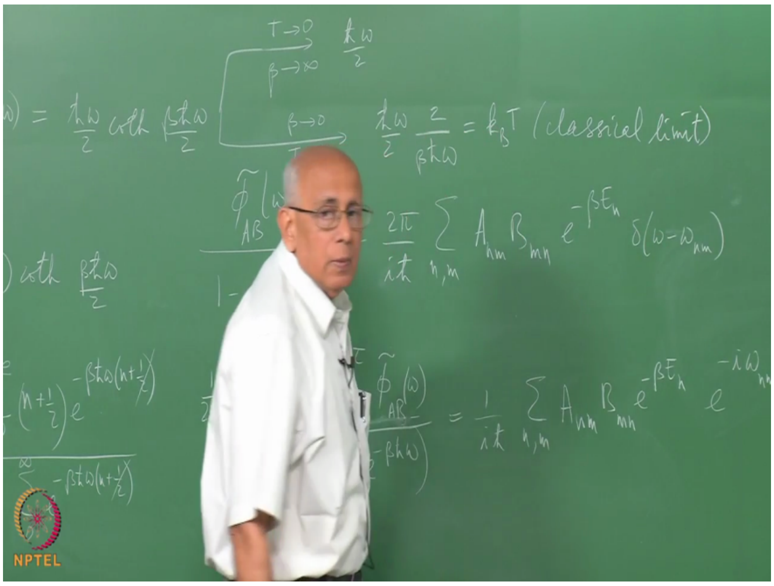

So cot hyperbolic x what does it diverges like as x goes to 0? What should it diverge like? It is sine hyperbolic over cauch, cauch has only even powers 1 plus x square etc over 2, so only the finite hyperbolic is relevant, what does sine hyperbolic x2 as x goes to 0? What does sine x do as x goes to 0? It goes to 0 like what? Like x, it goes to 0 like x, so cot sine hyperbolic also goes to 0 like x, exact like x.

So cot hyperbolic therefore x goes like 1 over x, so this leading term is going to be h cross omega over 2, 1 over x is 2 over beta h cross omega equal to k boltzman T, right? Now classically what is the average energy of an oscillator at temperature T? Half kAT because of the kinetic energy, half kAt because of the potential energy, so it is kAT, this is the dulong petit limit on whatever classical limit.

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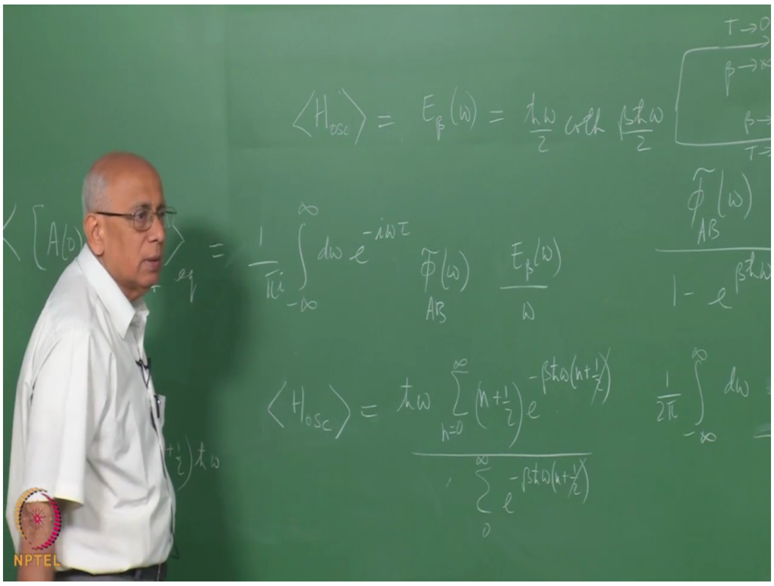

So in good shape it matches, so this is in fact a good formula therefore you can write this thing now this fellow down in terms of this E beta, you can write this cot hyperbolic as 2 over h cross omega, so this h cross goes away here and you are left with this, this is 1 over 2pi i and to goes away and that is it, okay. Sometimes this is called the fluctuation dissipation theory, we will get back to this, we will see, okay, Alright.

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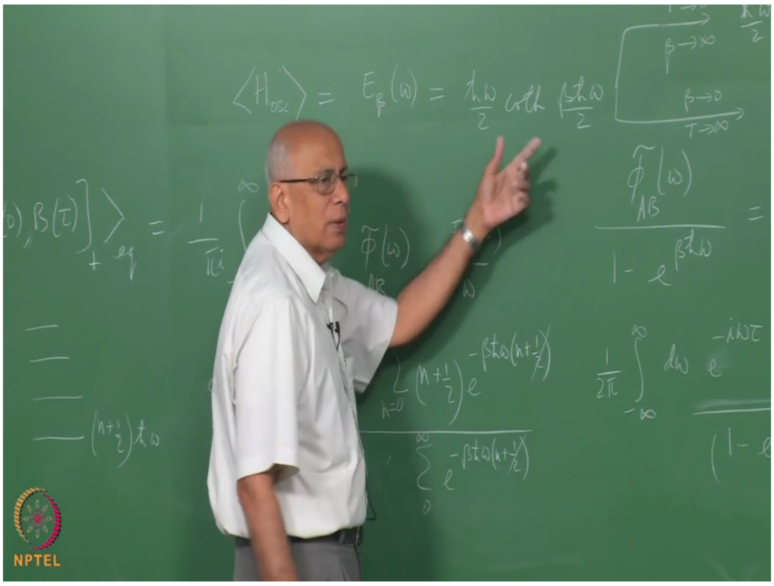

So this thing here is just shorthand for this thing here there is no oscillator we are talking about when is convenient, it is very convenient to use that expression and the crucial point is we now I have spectral representations for the product of 2 operators at different time arguments.

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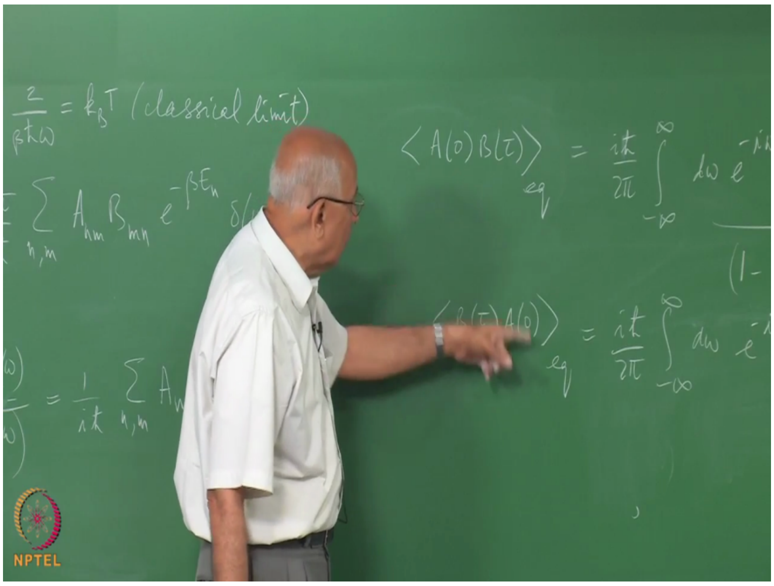

All of it in equilibrium by the way, everything is with respect to the equilibrium ensemble, okay. And from this we are going to start extracting some physics, okay. So I will stop here now.