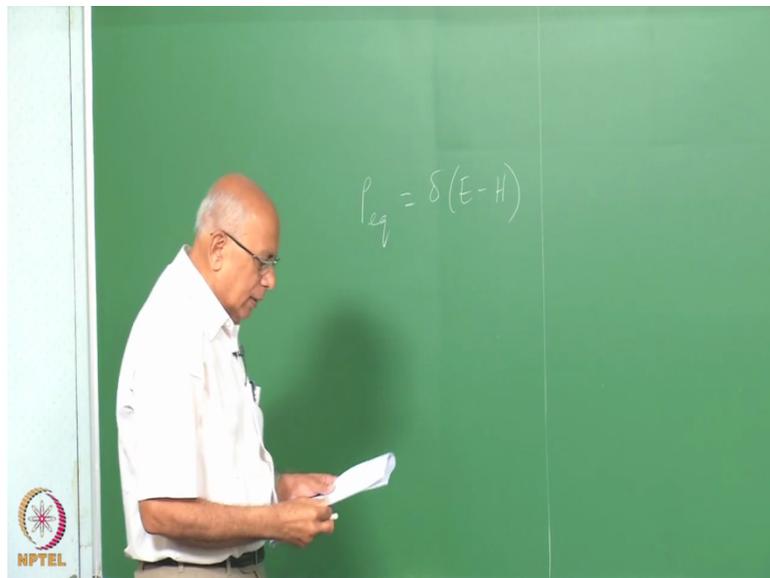


**Non Equilibrium Statistical Mechanics**  
**Prof. V Balakrishnan**  
**Department of Physics**  
**Indian Institute of Technology Madras**  
**Lecture 13**  
**Quiz 1 -questions and answers**

So today we will just discuss this quiz because I have taken a cursory look through all your answer books and I haven't yet marked them, have not read them but I thought I will do this, so that you get some idea of what this whole thing is all about and in the process I will make some side remarks, some peripheral remarks as well. So we will go through this very slowly.

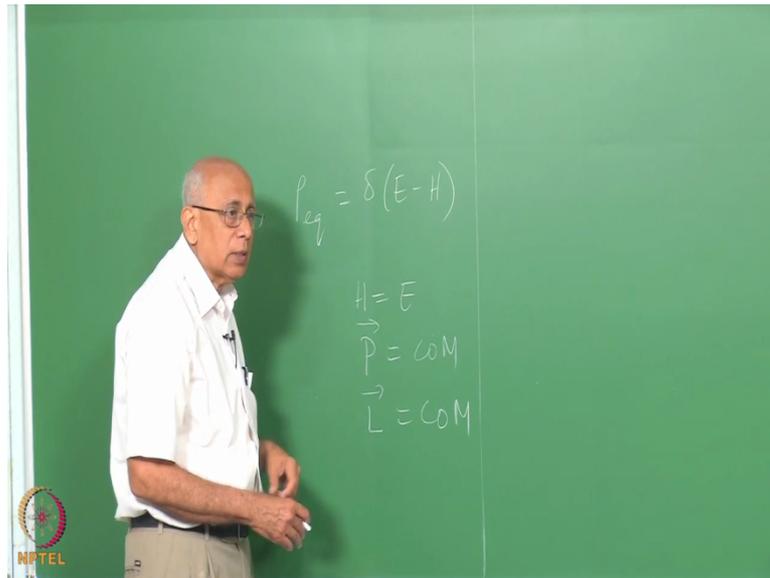
(Refer Slide Time: 0:56)



The first question said the density operator in isolated system and thermal equilibrium is  $\Delta$  of  $h$  minus  $e$ , so in the micro canonical ensemble on an isolated system thermal equilibrium the idea was through equilibrium was  $\Delta$  of  $E$  minus  $H$  the question is, is this true or false? Where is the total energy of the system? Since it is an isolated system the energy is a constant  $E$  is the constant and certainly you are on the energy shell which is what this thing is all about with some finite resolution.

So this is the density operator at least formally, formally it is so, interesting question side remarks that one can make is, we know in a classical system which has got many constants of the motion for instance if this is a system there is central force is present and no external force on the system of particles the total angular momentum of this system is constant, the total linear momentum of this system is also constant.

(Refer Slide Time: 2:22)



So strictly speaking you have access only to those microstates where not only is this true? Not only is the total energy fixed but also this is constant, a constant of the motion and this quantity is also a constant of the motion these are also called Galileon constant of the motion. So the question you should ask is why do we focus on just the energy? Why should not we say that it is the intersection of the energy surface with the surface on which this is constant and that is constant.

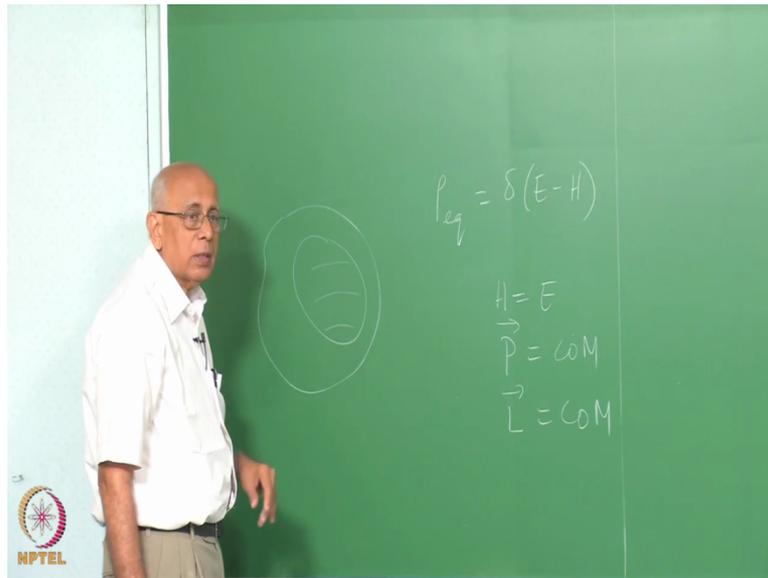
So really it is only those micro states that are accessible and not all micro-states on the energy shell, you see the point here, what you would say is the answer? And yet if you look at every book on statistical mechanics the micro canonical ensemble is just the energy shell that people worry about. How come they are not worried about the other constants of motion?

“Professor -Student conversation starts”

Student: It is a micro variable, right? I mean when you are doing your.

Professor: Why not? I mean they are now, let me draw it schematically.

(Refer Slide Time: 2:56)

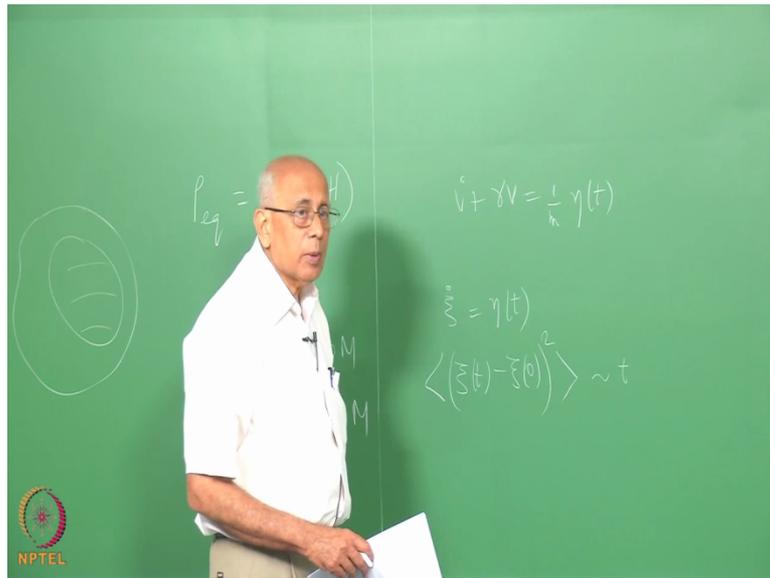


So you have this big phase space around this phase space if you fix an  $E$  there is a subspace of it on this  $E$  is constant on this surface on this hyper surface but you must also look at the intersection of this with a surface on which capital  $P$  is constant, capital  $L$  is constant and so on but you never do that you only talk about the energy hyper surface. So what do you think is the reason for that?

There are not too many such constants of the motion, basically there are just 10 Galilean constants of the motion for an arbitrary set of particles interacting by 2 body Central forces unless there are special symmetries in the problem. So the point is the answer is that when you do statistical mechanics you are talking about a system with a given state of motion.

So you are already saying the state of motion is given to you such as capital  $P$  equal to 0 for instance, you are in a state where in a system or in a frame where the total momentum is 0, so the state of motion is already prescribed to you implicitly or tacitly which is why you do not worry about the other constants of the motion, all that you worry about is the total energy because you can increase or decrease the energy by opening up the system and letting it interact again by limit, okay. So this is true but you should also be aware that the conditions under which this is so.

(Refer Slide Time: 4:42)



The next question was, each Cartesian component of the velocity of a brownian particle obeys the famous Langevin equation in 1 dimension which is  $\dot{V} + \gamma V = \frac{1}{m} \eta(t)$ , where this  $\eta(t)$  is stationary Gaussian white noise, usual white noise we are being dealing with.

Although I have not said so explicitly, it is also a mark of process we have not talked about that in detail at the moment but you have a stationary gaussian Delta correlated Mark of process that is what this noise is and the proposition is that the velocity  $v$  of  $t$  is a stationary Gaussian random process, is this true or false? It is true that Gaussianity property is transmitted beta is driving  $v$ , so this is the driving force and this is the driven variable the output variable.

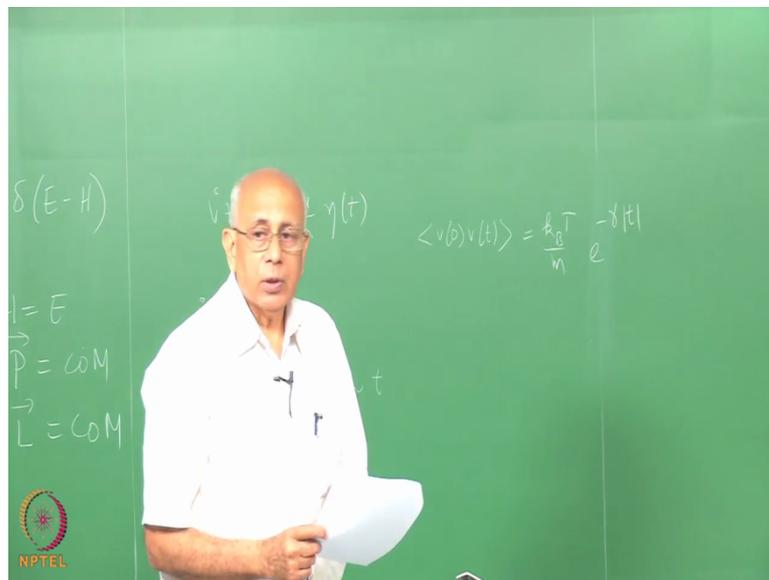
And the Gaussian nature of the probability distributions of  $\xi$  goes over into those of  $v$  as well. As for stationarity this one we saw is stationary, it is very much stationary, if you did not have the noise then you had a runaway solution for the mean square velocity and then there was not stationary at all. So this stationarity is certainly true, the presence of this ensures that you do have the stationarity.

If you did not have noise but you just had process for instance in an abstract way you have a process  $\dot{x} = \eta(t)$ , so I give you a random process  $x$  whose derivative is Gaussian white noise or  $x$  is the integral of Gaussian white noise, it is called the Wiener and the Brownian particles are  $\langle (\xi(t) - \xi(0))^2 \rangle \sim t$  (6:28) such an equation here. This process is not stationary

because what happens now is that  $\langle x^2(t) - x^2(0) \rangle$  this average given this thing here is proportional to  $t$ .

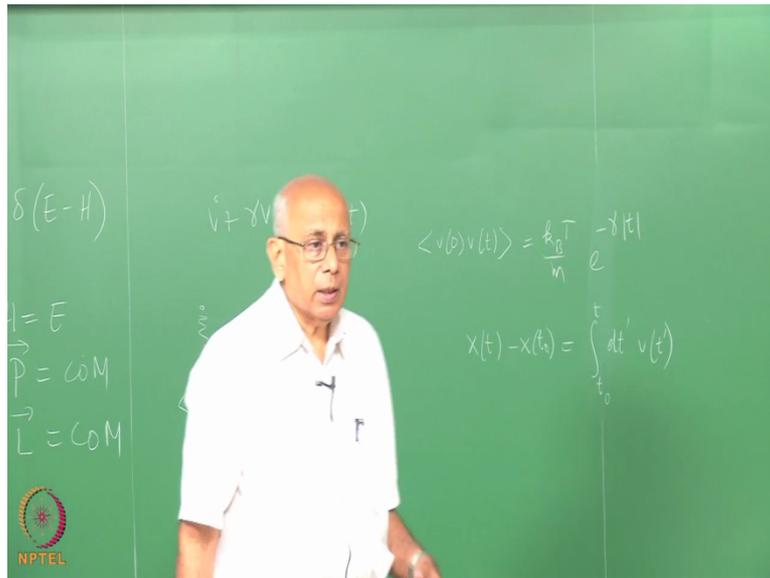
Whereas we know that if I have a process that is stationary we know that its mean square means cube all moments and so on must be at least independent of time, moreover the two-point correlation must be a function only of the time difference the three-point correlation must be a function of two-time differences and so on that is violated, if you did not have this friction term, so this introduces regularity into this system it by the way makes the  $v$  process also Gaussian makes it also a stationary process as well as a Mark off process.

(Refer Slide Time: 7:39)



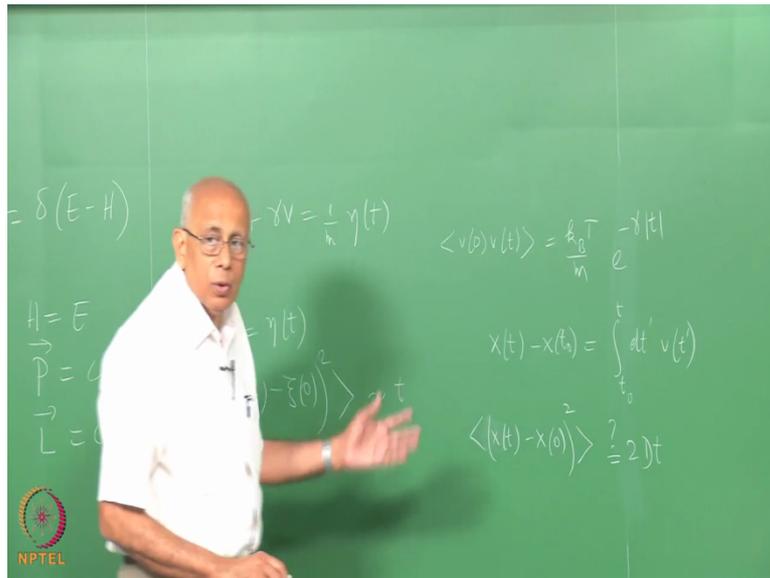
In continuation of that is that  $\langle v(t)v(0) \rangle$  correlation is a decaying exponential function of  $t$ , you know that is true because we know that  $\langle v^2(t) \rangle$  this quantity we discovered was  $k_B T/m$  that is the  $t$  equal to 0 value and it is multiplied by an exponential  $e^{-\gamma|t|}$ , so the correlation drops off on both sides, so indeed it is a decaying function exponential function of  $|t|$ .

(Refer Slide Time: 8:17)



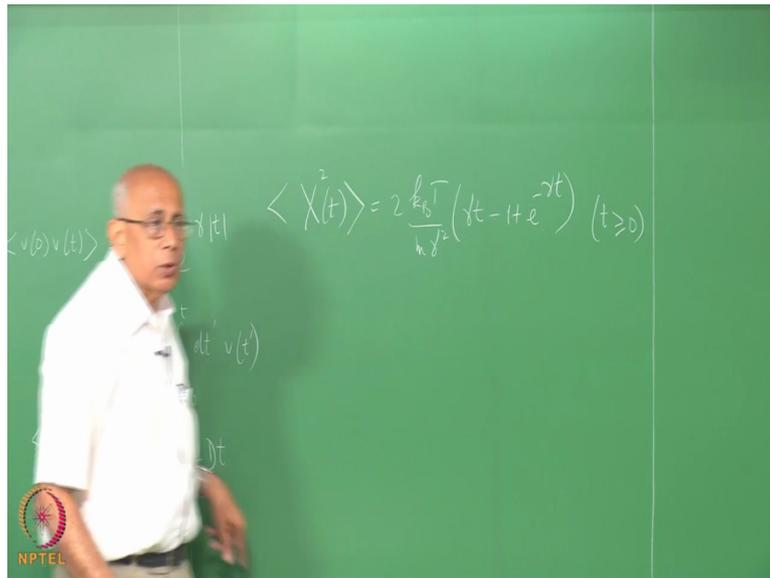
Continued the displacement of the particle  $x$  of  $t$  minus  $x$  of  $0$  is a stationary random process, so the proposition is that this quantity, this random variable integral from  $0$  to  $t$   $dt'$   $v$  of  $t'$  prime this is set supposed to be a stationary random process or more generally if you wrote  $t'$  not here this is  $t$  not, this is a stationary random process but surely this thing is a function of both  $t$  not and  $t$ , there is no guarantee that is a function of  $t$  minus  $t$  not at all, definitely not and it is in general not a stationary process. In fact its the integral of the velocity is the displacement and we know it linearly increases with time, so it is definitely not a stationary random process.

(Refer Slide Time: 9:15)



Next again for all positive  $t$  the mean square displacement is given by  $\langle x^2 \rangle = 2Dt$ , so the proposition is that in this case  $\langle (x(t) - x(0))^2 \rangle$  and the question is, is this equal to  $2Dt$ ? True or false? It is false; it is only true in the diffusion limit, right? Large, how large? Greater than  $\gamma$  inverse the timescale and the problem, we know that the exact result here is this.

(Refer Slide Time: 9:50)



So if I call that capital X's, X of t, X square of t we know this is of the form  $k_B T$  over  $m \gamma$  twice and inside you have  $m \gamma$  squared,  $\gamma t$  minus 1 plus  $e^{-\gamma t}$  this is called  $t$  greater than equal to 0. So only for  $\gamma t$  much much bigger than one, does it go to the diffusion limit? That is the diffusion regime, okay. So that was straightforward enough.

Next we have the velocity of the Brownian particle of (10:29) and charge  $q$  and an applied uniform magnetic field the (10:33) equation is given and the statement is the different Cartesian components of  $v$  are also uncorrelated to each other for  $t$  greater than equal to 0, is this true or false? It is false because they get tied up with each other due to the magnetic field which mixes of components in fact we computed this, you notice that  $V$  should have been a bold phase in the dot.

(Refer Slide Time: 10:55)

$$\langle X^2(t) \rangle = 2 \frac{k_B T}{m \gamma^2} (\gamma t - 1 + e^{-\gamma t}) \quad (t \geq 0)$$

$$\dot{\vec{v}} + \gamma \vec{v} = \omega_c (\vec{v} \times \hat{n}) + \frac{1}{m} \vec{\eta}(t)$$

$$\langle v_i(0) v_j(t) \rangle = \frac{k_B T}{m} e^{-\gamma t} \left[ n_i n_j + (\delta_{ij} - n_i n_j) (1 - \cos \omega_c t) - \epsilon_{ijk} n_k \sin \omega_c t \right]$$

So the equation is  $\dot{v} + \gamma v$  this quantity here was equal to in the cyclotron frequency  $v$  cross the direction of the magnetic field plus  $1/m$  vector value would noise white noise. In this case we know what the velocity correlation does; we know that the  $v_i(0)$ ,  $v_j(t)$  by the way the fact that it is in the magnetic field does not change the stationarity properly, velocity is still a stationary random process in fact it is still diffusive just with the modified diffusion constant.

So this quantity is  $k_B T$  over  $m$  that will appear and then  $e^{-\gamma t}$  for  $t$  greater than  $0$  and then if you recall there is this portion which comes from this part comes from solving the problem in the magnetic plus or minus I do not remember I think it is minus  $\epsilon_{ijk} n_k \sin \omega_c t$ , whatever it is, it is not proportional to  $\delta_{ij}$ , so it is clear that there are cross correlations here entirely because of the magnetic field.

(Refer Slide Time: 12:47)

$$\langle (\vec{r}(t) - \vec{r}(0))^2 \rangle = \frac{2k_B T}{m\gamma} \left( \frac{3\gamma^2 + \omega_c^2}{\gamma^2 + \omega_c^2} \right) t$$

Then for the same problem in a magnetic field the mean square displacement is a formula given for it and the statement is whether this displacement  $r$  of  $t$  minus  $r$  of  $0$  whole square this is just the dot product with itself rather this thing here is  $2k$  Boltzmann  $p$  over  $m$  gamma times  $3$  gamma square plus omega  $c$  square over gamma square plus  $(\omega_c)^2$  square  $t$ . The question is whether this is true or false? We call that what is happening here this is  $x^2$  plus  $y^2$  plus  $z^2$  if you like, if the feel this along  $z$  direction then the  $x$  and  $y$  portions get inhibited they get attenuated but this  $z$  displacement remains as before.

(Refer Slide Time: 13:35)

$$\langle (\vec{r}(t) - \vec{r}(0))^2 \rangle = \frac{2k_B T}{m\gamma} \left( \frac{3\gamma^2 + \omega_c^2}{\gamma^2 + \omega_c^2} \right) t$$

$$= \frac{2k_B T}{m\gamma} t \left( 1 + \frac{\gamma^2}{\gamma^2 + \omega_c^2} + \frac{\gamma^2}{\gamma^2 + \omega_c^2} \right)$$

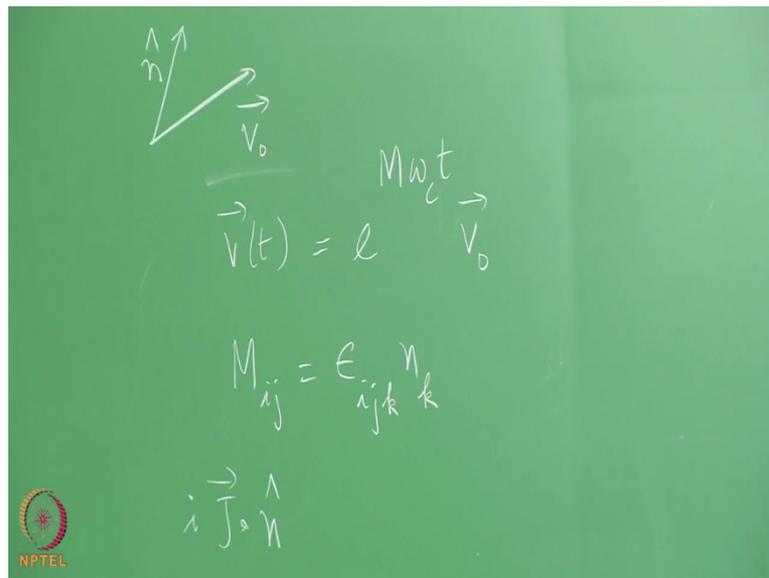
So this still remains  $2k_B T$  over  $m\gamma$  but inside you have  $t$  and then  $1 + \frac{\gamma^2}{\gamma^2 + \omega_c^2} + \frac{\gamma^2}{\gamma^2 + \omega_c^2}$  from the displacement in the  $y$  direction or  $x$  direction plus  $1$  in the  $z$  direction, so that gives you this result, okay. In the diffusion limit, once again in the diffusion limit. So all that has happened is that diffusion has been inhibited somewhat.

If you did not have a magnetic field  $\omega_c$  is  $0$  and this cancels out and gives you  $3$ ,  $3$  by  $2$  is equal to  $6$  and you indeed have asked quite goes like  $6Dt$  because  $2Dt$  is a portion between  $x$  square,  $y$  square and  $z$  square. On the other hand when  $\gamma$  is small or negligible compared to  $\omega_c$  and this becomes very very large then you still have diffusion but you will not have any motion in the  $xy$  direction at all.

That means square of displacement will actually tend to  $0$  and it will divert only along with  $z$  direction therefore it goes to  $2k_B T$  over  $m\gamma t$ . So you should check this, you should check this limits always just to make sure that you get the right answer, the correct physical answer.

Again continuing the same problem given that the initial velocity is  $\vec{v}(0) = 0$  the statement is the conditional average velocity  $\vec{v}(t)$ , conditioned upon the initial condition  $\vec{v}(0) = 0$  is a vector precessing around the direction of the magnetic field with angular frequency  $\omega_c$  the cyclotron frequency while its magnitude decreases with time like  $e^{-\gamma t}$ , true or false?

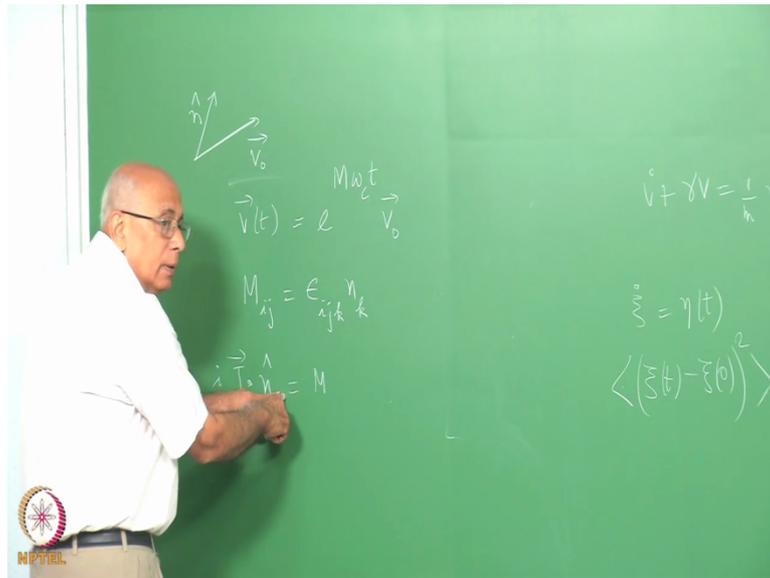
(Refer Slide Time: 15:40)



This is true, the statement is true, you solve a problem exactly there is precisely what you would expect and what you get. So the mean value  $v$  of  $t$ , we want the mean value of this thing but suppose did not have any noise at all, you did not have any thermal noise at all just had a magnetic field switched on and then you have a magnetic field in this direction  $n$  and then initial velocity of this particle  $v$  not like this.

Now what is this going to do? The magnetic field is not even energy to this particle, all it does is to change the direction of  $V$  not, so it starts processing around this guideline and what is the formula for it? It is the rotational formula, it rotates by the amount of  $\Omega ct$  in time  $t$ , so this is equal to clearly must be equal to  $e$  to the  $m \omega ct$  on  $V$  not, okay. If you did not have any friction before you took any average this is all that would happen, this is the rotational matrix, remember that  $M_{ij}$  in 3 dimensions, okay.

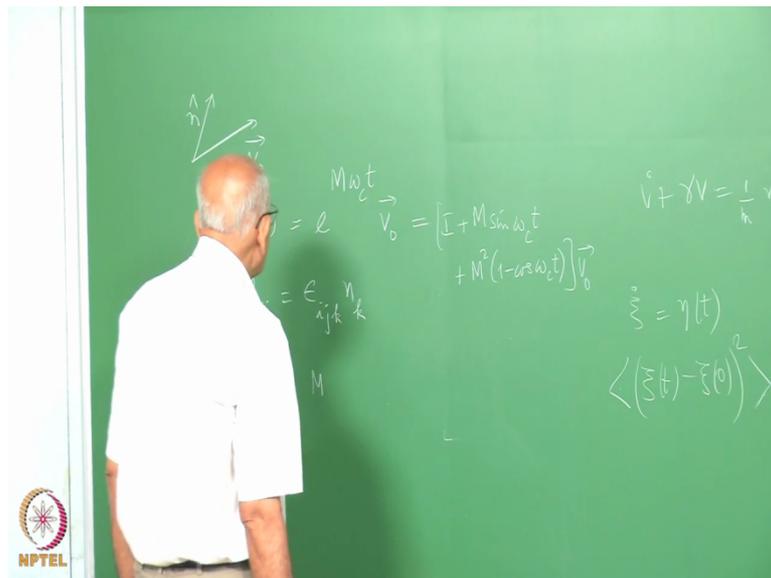
(Refer Slide Time: 17:36)



This is actually once you write the generator of rotations in 3 dimensions, so what has been written as  $i$  times  $j$  dot  $n$  is equal to this precisely what it is in 3 dimensions, I have used here for the 3 generators of rotations, you have used those 3 by 3 generators the representations, the original representations of rotations by 3 by 3 orthogonal matrices and when you do that, you end up with this answer here, this is it, the matrix side.

And then the angle through which you rotate is  $\omega t$  you exponentiate it, you end up with the finite rotation, so it is this fellow here you have to exponentiate this on right here and this is function of course of  $t$  as well as  $\omega$  not here and since we know that in this case, we know that if you square if you cube this matrix you get minus the same matrix, we have already seen that.

(Refer Slide Time: 18:07)



So this is equal to I plus M sine omega ct plus m squared 1 minus cos omega c, this guy acting on V not and you can write this down explicitly. So what it's going to be proportional to their will be a portion along in, there will be a portion along V not and a portion proportional to V not cross n, the portion along the original vector itself along V not may V not itself.

The portion along n would involve V not dot n times unit vector n and then the perpendicular portion will be V not cross n with a sine omega ct multiplying it, so this is some finite sum vector with which you can compute, right?

(Refer Slide Time: 19:08)

$$\vec{v}(t) = e^{-\gamma t} \left[ I + M \sin \omega_c t + M^2 (1 - \cos \omega_c t) \right] \vec{v}_0$$

If you took this average out here after putting in the noise what happens? What happens to this guy? All that happens is, as it is going around its being hit buffeted and it is making the average go to 0, right? So all that happens is, this is equal to  $e^{-\gamma t}$  times that. That is the only effect of the magnetic field. So this is all that happens you still have the diffusion in the velocity space you still have a mean which is going to 0, the variance which is increasing from the initial Delta function it increases still it hits the equilibrium value which is given by the Maxwell distribution finally.

(Refer Slide Time: 20:12)

So we can even write the distribution down, we can even write down what is P of v, t given V not this fellow apart from some normalization which we will write in a minute has got to be so the following, it has got to be the exponential of minus it is still a Gaussian retains that property, so it is v minus e to the m omega ct V not e to the minus gamma t, that is the mean value V bar of t squared divided by twice the variance, so it is twice k Boltzmann t 1 minus e to the minus 2 gamma t and its kt over m, so this M out here.

The normalization does not care about what this average is? Because you are going to shift this out anyway when you do the integral, so it will just be m over 2 pi k Boltzmann t 1 minus e to the minus 2 gamma t this to the power 3 half's for each dimension you get this to the power half, so that is it. Do not derive this as just said that it is a Gaussian and once I assert it is a Gaussian then if you accept that it is completely determined by its mean and its variance and that is a normalised distribution, okay. This is a three-dimensional analog of the on the (( )) (21:38) distribution but with a magnetic field present. So physically it is very appealing and it is very simple.

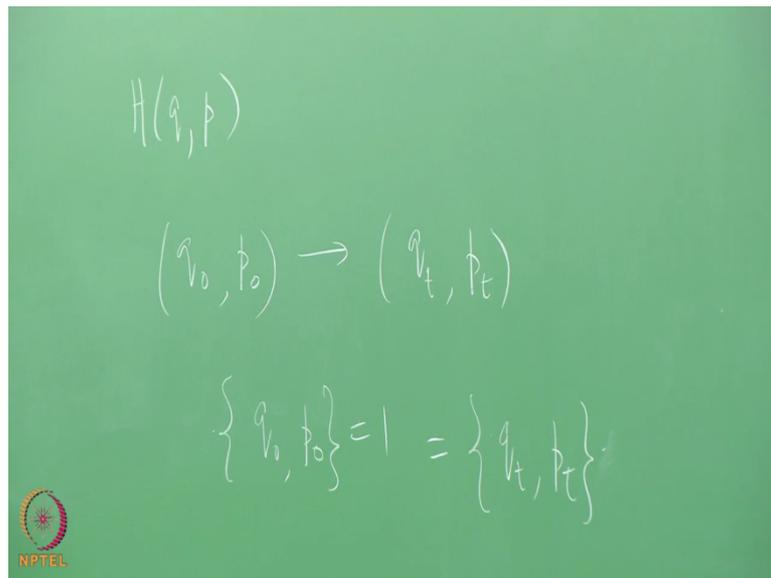
I will let some stage tried to derive and it is called the Fokker planck we will write it down, we will write this. What we will do is, what I will do is buy a shortcut I will show that every time you have stochastic differential equation for the random variable of the (( )) (22:03) you have an equation, a differential equation for the probability distribution directory. So one can solve that in principle and get this result.

Moving on next one is just a definition says consider a classical Hamiltonian system with  $n$  degrees of freedom and a given Hamiltonian and the  $L$  is the label operator, statement if  $F$  is a function of the dynamical variable such as the poisson bracket of  $f$  with  $h$  is 0 then the label operator acting on  $F$  must give you 0 identically, so this is obvious because you are already given that this is true but we know that  $L$  acting on  $F$  is equal to  $I$  times  $H$  with  $F$ .

So that is of course equal to 0 this is the definition of a label operator. What is the reason for using the  $(\cdot)$  (23:00) operator? Our reason was that the formalism looks a little simpler both classical and quantum it looks exactly the same but of course you need to exponentiate this  $(\cdot)$  (23:10) and that is not a trivial matter in general. In classical case much harder as we saw all the proves I gave were all for the quantum case because I was using the cyclic variance of the trace but if you try to do this with phase space functions then you run into you have to integrate by parts, it is a little messier to do.

So, oh! Yes it says here the next proposition for a dynamical system with Hamiltonian  $H$  of  $q, p$  the time development operator  $e$  to the ILT is unitary whether the system is classical or quantum mechanical, right? It is true, it is a unitary evolution remember that in classical mechanics in Hamiltonian mechanics, if you solve the Hamilton's equation of motion.

(Refer Slide Time: 24:03)


$$H(q, p)$$
$$(q_0, p_0) \rightarrow (q_t, p_t)$$
$$\{q_0, p_0\} = 1 = \{q_t, p_t\}$$

So you solve Hamilton's equation of motion with a given Hamiltonian and given initial conditions. So what you are doing? Is to go from  $q$  not  $P$  not at any time  $T$  you solve the Hamilton equation's of motion then along the phase trajectory you really going to  $q, t$ , right? I put subscripts but really this should be inside the bracket of this guy and for each degree of freedom, this is true.

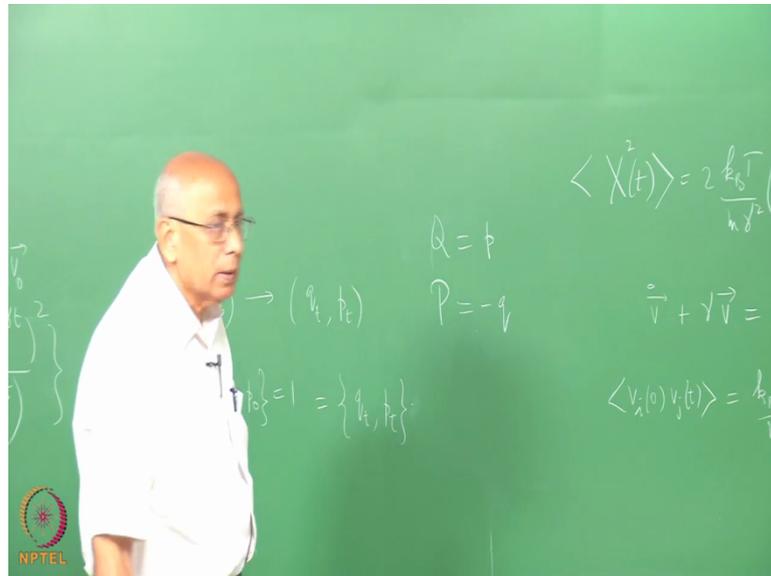
Now we know this is true  $q$  not,  $v$  not equal to 1, to start with these are canonically conjugate variables and we know that at any time  $q, t, p_3$  is also true equal to 1. So time evolution preserves the poisson bracket. It is also orientation preserving because this transformation it turns out it has what is called a symplectic transformation, a canonical transformation and it preserves orientation that is, it does not change right-handed to left-handed coordinate and so on in phase space.

So it is in fact a transformation whose which is measured preserving which is canonical etc etc, okay. I leave you to find out what is the generating function for this transformation? What you think is a generating function? Every canonical transformation has a generating function not necessarily unique generating function, for a given canonical transformation you may have more than one generating function.

What do you think is an? The Hamiltonian itself so you have to establish this, you have to establish this and you would discover of course that the equations of motion themselves are the equations which tell you how to get  $QT$  and  $PT$  from the generating function they are

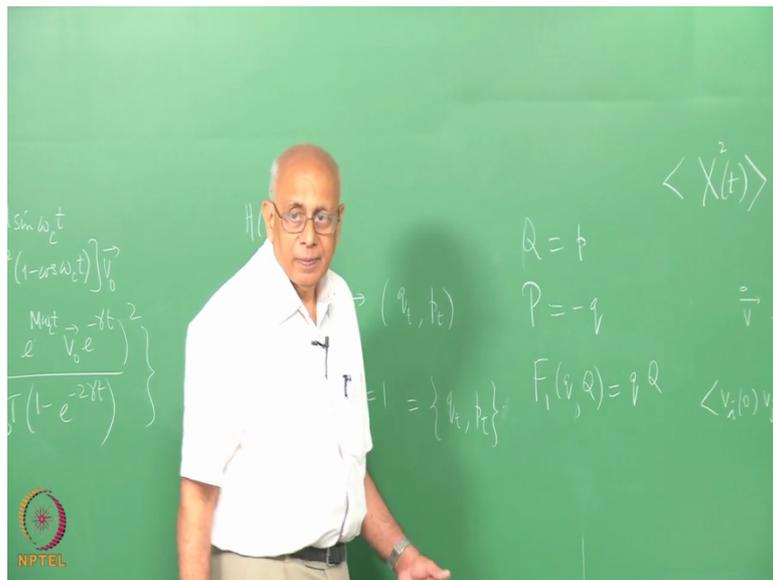
exactly the same in structure, V standard canonical transformation the simplest one which is non-trivial is as you know the one that takes you q to p.

(Refer Slide Time: 26:34)



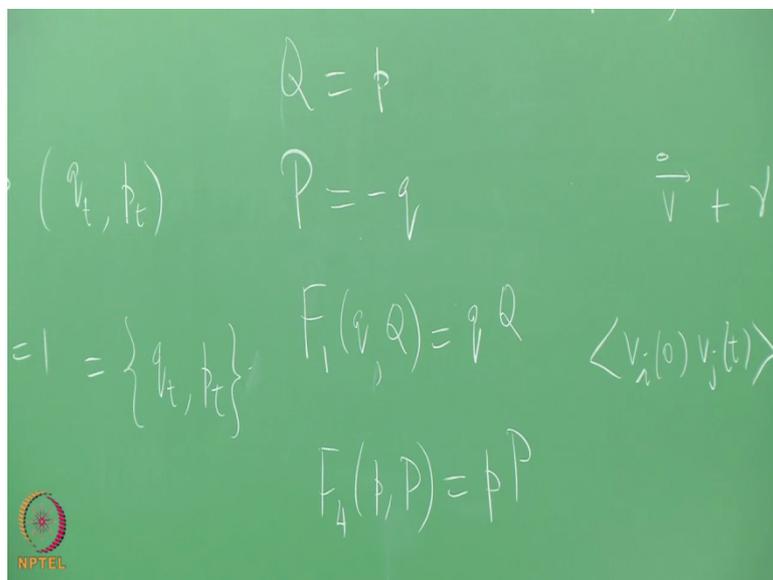
Let us write it the other way, it is the one that says Q equal to p and P equal to minus q, so the poisson bracket of this with that is minus the poisson bracket of this with this is one, the determinate of this transformation is one, so it is measure preserving and is canonical this thing here the generating function for this depends on whether you want type 1, type 2, type 3, type 4 generating function.

(Refer Slide Time: 27:21)



Are you familiar with the types of generating functions? What type would this transformation be? If I say it is a type 1 then I must have a generating function  $F_1$  which is a function of little  $q$  and capital  $Q$ , I leave you to check it if you choose this generating function you are done it generates this transformation.

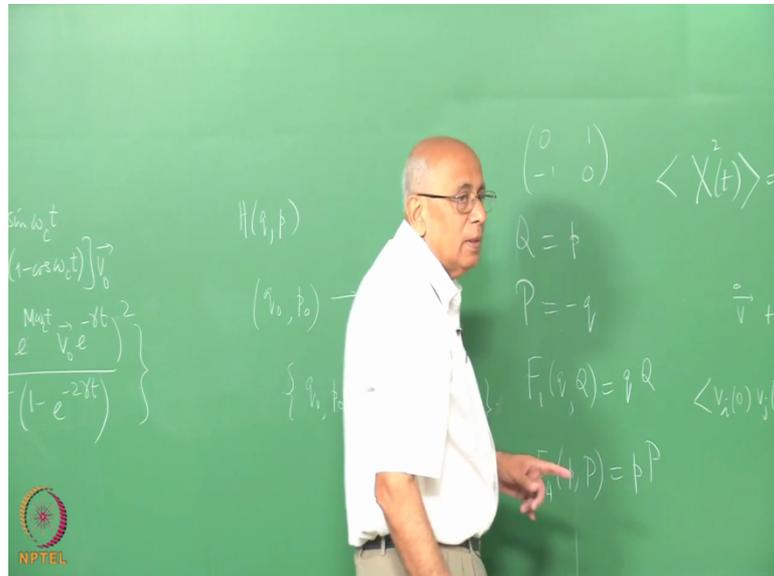
(Refer Slide Time: 27:39)



But you could also choose it as type 4 and it is a simple method to verify that also generates precisely this transformation. So the type of a canonical transformation is not uniquely specified for the transformation, okay. You may have more than one generating function for

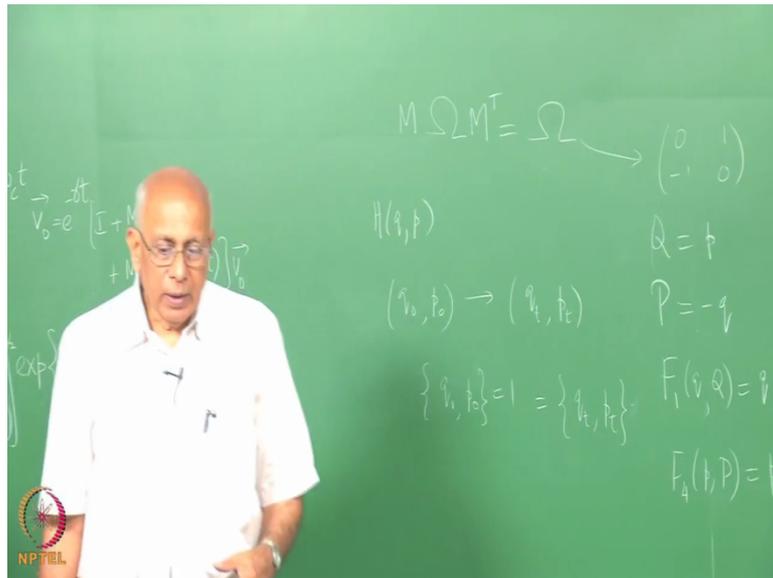
the same transformation. Now the reason I said this is a standard the basic canonical transformation, first of all it is linear, so the Jacobian is all constant some things like that.

(Refer Slide Time: 28:21)



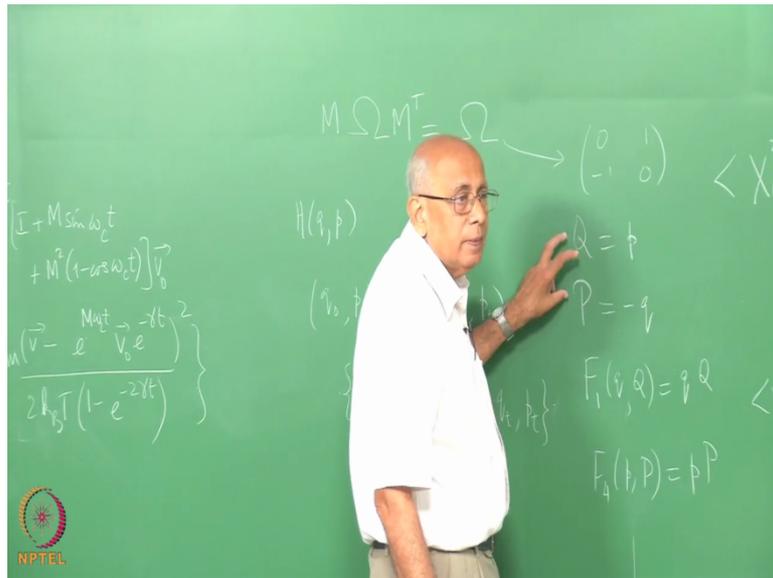
The matrix of this the Jacobian matrix is precisely this, okay. Which is the matrix that you need when you write the Hamilton equations down the form of simple gradient of something like that? The symplectic, yes, symplectic matrix itself.

(Refer Slide Time: 28:41)



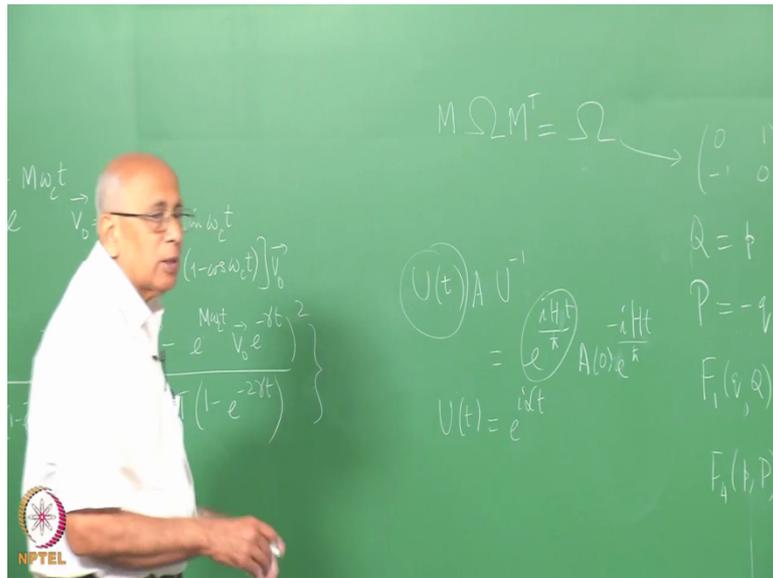
So if  $M$  is the Jacobian of any canonical transformation then  $M$  times matrix  $\Omega$  times  $M$  TransForce is equal to  $\Omega$  where  $\Omega$  is the, this matrix is there, this.  $2n$  by  $2n$  matrix with  $0$  identity minus identity  $0$  etc and other statement is, so rest the statement is that  $\Omega$  itself  $M$  equal to  $\Omega$  itself will generate will satisfy this. Now the reason why this is regarded as the fundamental canonical transformation is that there is a very deep theorem due to (I) (29:16) which says that anywhere in phase space in an  $n$  degree of freedoms, systems, phase space anywhere locally you can find a canonical which looks exactly like this.

(Refer Slide Time: 29:33)



Locally in any phase space any Hamiltonian system, so that is the significance the fact that there exist, this is the same statement as saying Suresh would say it means that there is a symplectic structure to the phase space, this fellow acts like a metric and such a transformation is possible, okay. So anyway there is a big machinery of canonical transformations.

(Refer Slide Time: 30:13)



In quantum mechanics however you talk about unitary transformations, know that when you have a time independent Hamiltonian then the time development operator  $U$  of  $t$  for a given  $t$  not this guy here this time development operator is such that when it acts on any observable this gives you  $e$  to the  $i H$  not  $t$  over  $\hbar$  cross  $A$  of  $0$ ,  $e$  to the  $i$  minus  $i H t$  in this case. So this time development operator is equal to this guy here and  $H$  is hermitian, so this is unity automatically.

So the whole idea of writing the  $(\cdot)$  (30:57) way of writing things is that you write you identify this  $U$  of  $t$  with  $e$  to the  $i L t$  whose action on any observable is to produce a conjugation with respect to this operator here. So if you like in the quantum case this  $L$  is a super operator it is acting on operators on Hilbert space and it is producing a thing like this.

Again you can show that the space of these operators on which  $L$  acts as a super operator this is a Hermitian operator that is what we just we demonstrated, right? By defining an inner product on the space of the operators and so on. Classically there is no such extra structure here this is in just as a function it acts on functions of phase space but this is a partial differential operator this fellow here and it involves exponentiation etc.

So formally writing both classical and quantum mechanics down as unitary time evolution is a very simple and compact way of dealing with  $(\cdot)$  (32:04) at least in the formal sense. So that was the purpose of the exercise there, okay.

Then the next one was the response function  $A$  of  $B$  of  $\tau$  bracket either poisson or commutator bracket but the end we are physical observables can never be negative for any  $\tau$  greater than equal to 0. So the question asked is whether this thing can be negative.

(Refer Slide Time: 32:31)

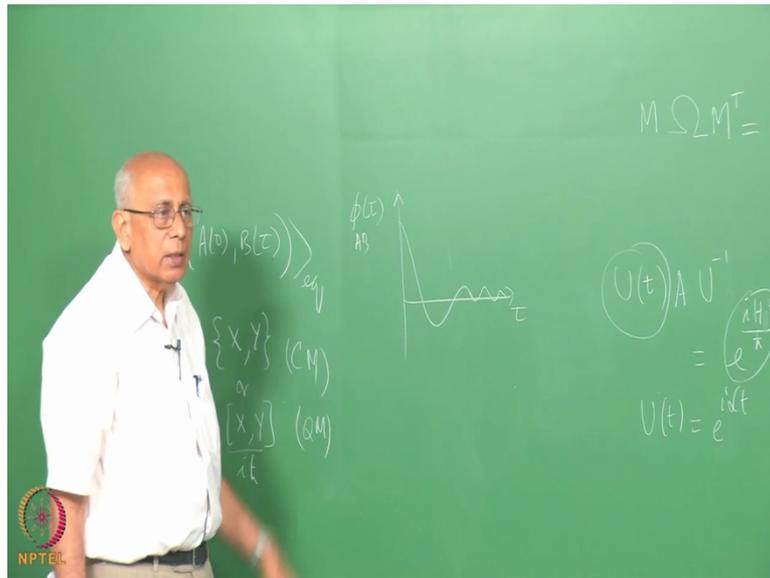
$$\langle (A(0), B(\tau)) \rangle_{eq}$$

$$(X, Y) = \begin{cases} \{X, Y\} & \text{(CM)} \\ \frac{[X, Y]}{i\hbar} & \text{(QM)} \end{cases}$$

So we are asked to find out if  $A$  of  $B$  of  $\tau$  equilibrium and recall that this thing here  $X, Y$  this stands for either  $X, Y$  or  $xy$  over it and quantum mechanics, this is classical, this is quantum mechanics and the statement asked was whether with respect to the equilibrium density operator  $e^{-\beta H}$  whether this quantity can be negative or not, for  $\tau$  greater than 0 say.

Can it be negative? We have seen that it is actually real if  $A$  and  $B$  are hermitian which is the case we are dealing with it is actually real but does it have to be negative or positive definite.

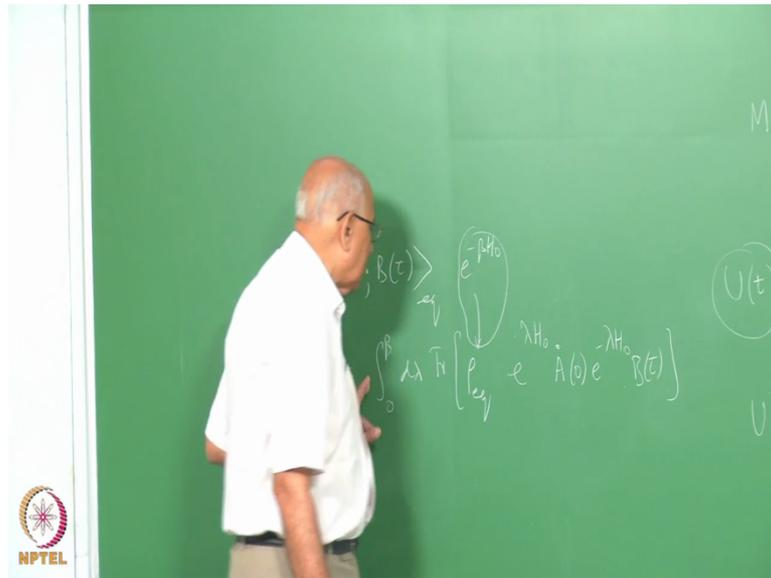
(Refer Slide Time: 33:33)



There is no such constraint that it should be positive definite it should be very very a common instance would be if you plot it as a function of  $\tau$ , if you plot it  $\phi$  of  $\tau$  or some arbitrary  $A$  and  $B$  it could go like this, we saw it is physically expected as  $\langle A(t)B \rangle$  (33:42) as  $\tau$  becomes large but it could oscillate could change in sign. Pardon me. Yes, even change the sign of  $A$  instead of  $A$  you look at minus  $A$ , so that is immediately say, so it is no such requirement on it at all, okay. In fact in the magnetic field case you know that this is there are these sines and cosines and they will of course cross the axis and go down.

Next the Cobo canonical correlation  $A \cdot 0 B$  of  $\tau$  semicolon reduces to the classical product in the classical limit and the answer is yes of course it does. So recall what we had?

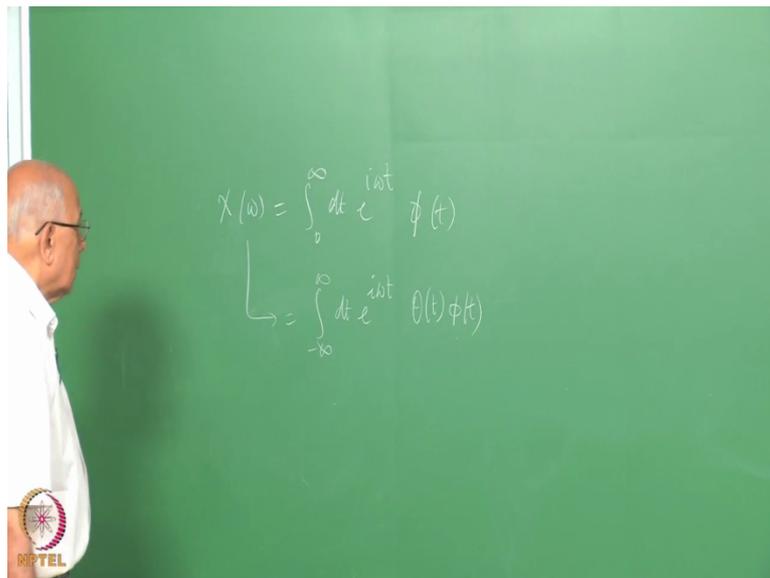
(Refer Slide Time: 34:32)



We had  $A$  of  $A$  dot of  $0$   $B$  of  $\tau$  equilibrium, if you recall this was an integral from  $0$  to  $\beta$   $d$   $\lambda$  and then a trace  $\rho$  equilibrium which was  $e$  to the minus  $\beta H$  not this fellow here times  $e$  to the  $\lambda H$  not  $A$  dot  $0$   $e$  to the minus  $\lambda H$  not  $B$  of  $\tau$  the trace of this whole product, okay. Of course in the classical case things commute this goes across here cancels the integral just gives you a factor  $\beta$  and you have the expectation value with respect to  $\rho$  equilibrium of  $A$  dot of  $0$   $B$  of  $\tau$ . So classically that semi colon is just deleted.

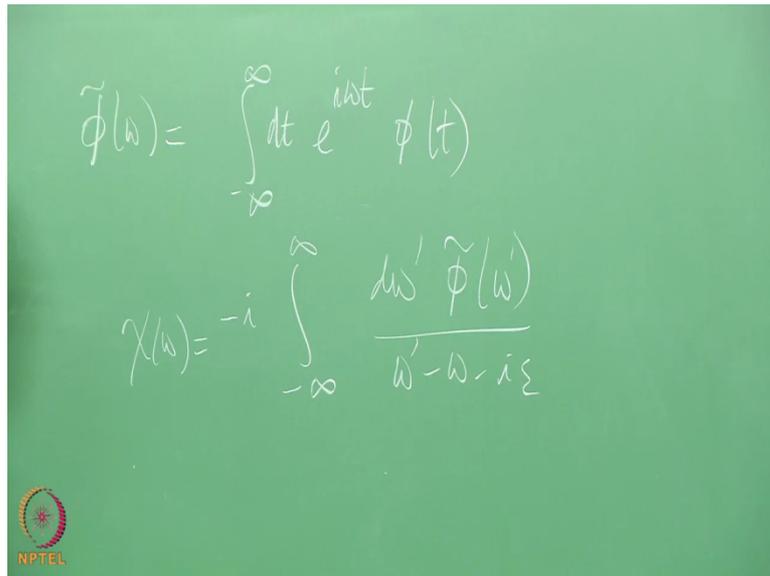
Finally the general  $i$  susceptibility is a Fourier transform of the response function with respect to the time variability, true or false? It is false, what is it the Fourier transform of green function? So it is the Fourier transform of  $\Theta$  of  $t$  times  $\phi$   $AB$  of  $t$  that is certainly true but just the introduction of this  $\theta$  makes a huge difference at once in fact there are immediately relations between as we will see the spectral function and this and let me write one of those down.

(Refer Slide Time: 36:03)



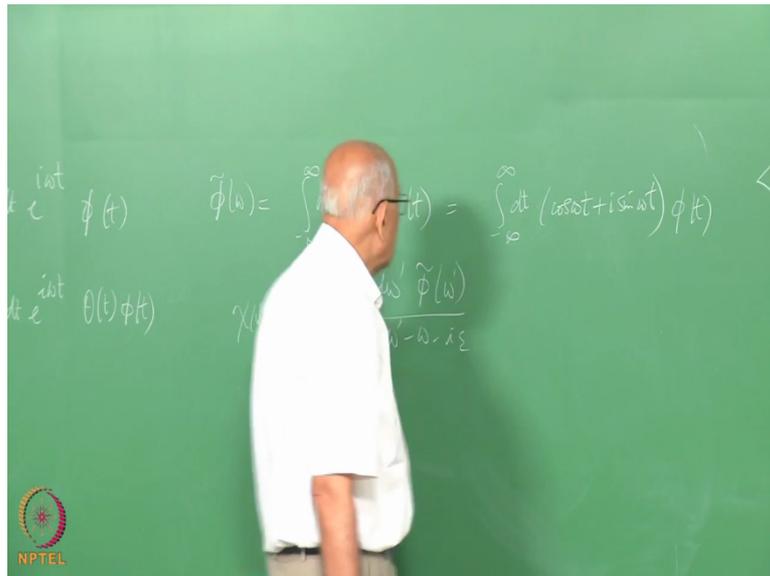
So Kai, let us forget about the AB, Kai of Omega is integral 0 to infinity, dt e to the i omega t phi of t. On the other hand this fellow here is also equal to integral minus infinity to infinity dt e to the i omega t Theta of t phi of t, this is the green function and that is the Fourier transform of that, okay. The Fourier transform of phi itself is phi tilde of Omega this fellow is integral from minus infinity to infinity dt e to the i omega of t phi of t.

(Refer Slide Time: 37:07)


$$\tilde{\phi}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \phi(t)$$
$$\chi(\omega) = -i \int_{-\infty}^{\infty} \frac{d\omega' \tilde{\phi}(\omega')}{\omega' - \omega - i\epsilon}$$

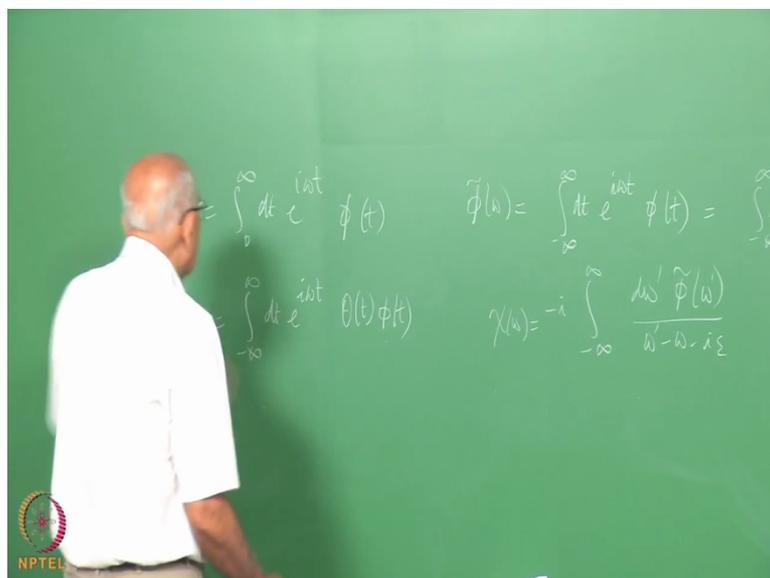
Compare these 2 there is an integral going all the way from minus infinity to 0 plus 0 to infinity here and that is missing here, so this was our spectral function for which we wrote down representations and so on. Now there is a relation between these 2, we already know it, we know that phi of omega equal to an integral minus infinity to infinity d omega prime phi tilde of omega prime over omega prime minus omega minus i epsilon in the limit as Epsilon goes to 0 from above and there is some factor here i over 2 pi or something like that, i, minus i over 2 pi or there is no, okay.

(Refer Slide Time: 38:31)



Now look at this thing here I can write it as cos plus i sine, definitely. So this could definitely be written as minus infinity to infinity dt to the cos omega t phi of t. If phi of t has a definite parity, if it is an even or odd function of t then one or the other of these 2 fellows vanishes immediately.

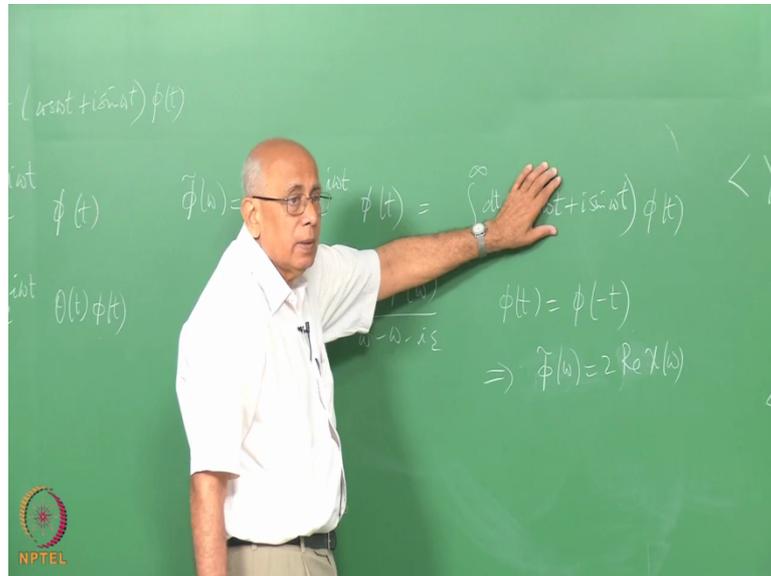
(Refer Slide Time: 38:36)



On the other hand this fellow here, if I rewrote this, this is equal to integral 0 to infinity dt cos omega t plus i sine omega t phi of t, this is a real part of Kai and that is the imaginary part of kai, after you do the integral you get the real and imaginary part. If phi of t is an even

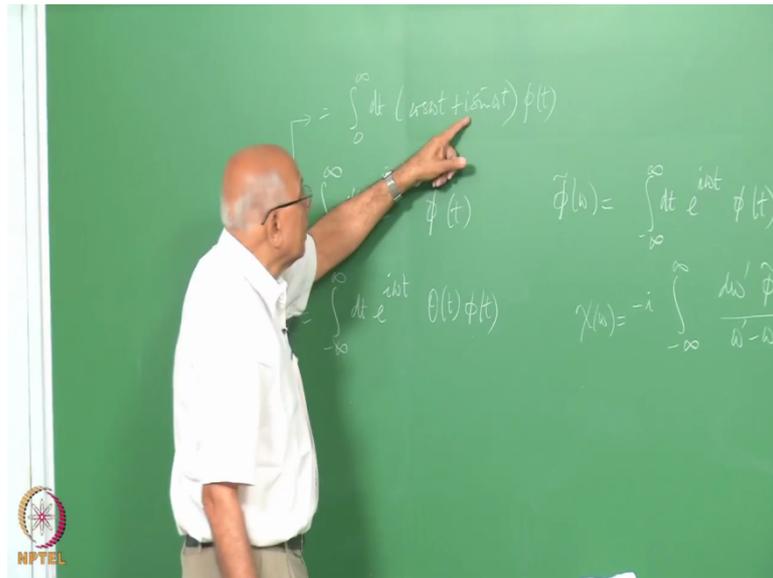
function this portion vanishes and this remain in integral becomes twice the real part, twice the integral from 0 to infinity, right?

(Refer Slide Time: 39:46)



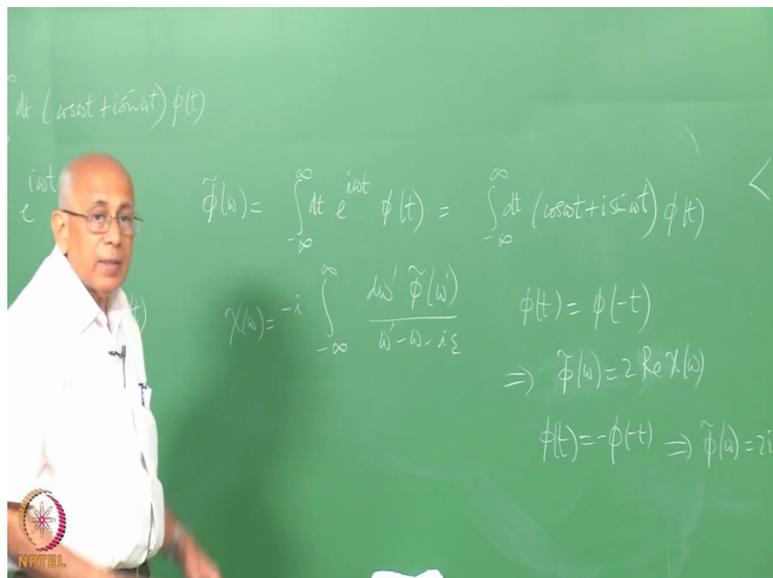
So if phi of t equal to phi of minus t will imply immediately that Kai of omega is equal to phi tilde of omega equal to twice real part of Kai of omega. Similarly if this is an odd function of t than this integral vanishes here.

(Refer Slide Time: 39:55)



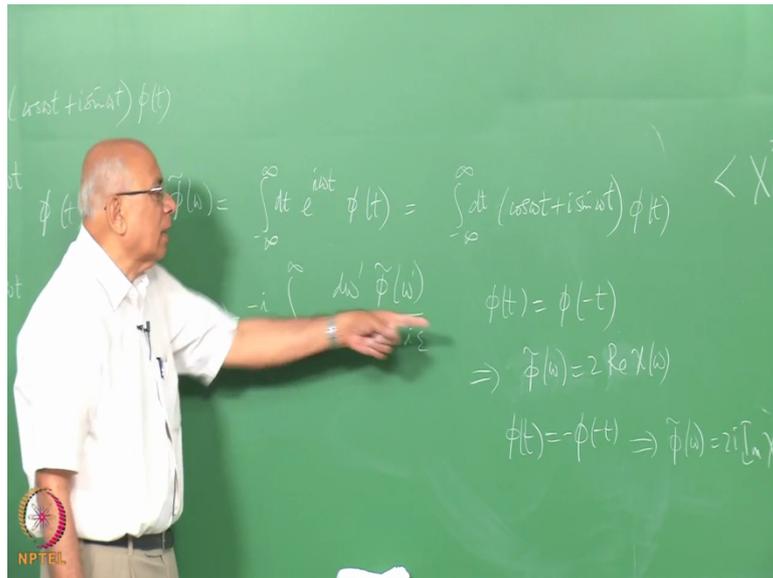
And what is left is  $i$  times this fellow here, which is twice  $2i$  times  $0$  to infinity but that is equal to  $i$  times the imaginary part here, right?

(Refer Slide Time: 40:20)



So  $\phi(t) = \phi(-t)$  with the minus sign will imply that  $\tilde{\phi}(\omega)$  equal to  $2i$  imaginary part  $\chi(\omega)$ , right?

(Refer Slide Time: 40:35)

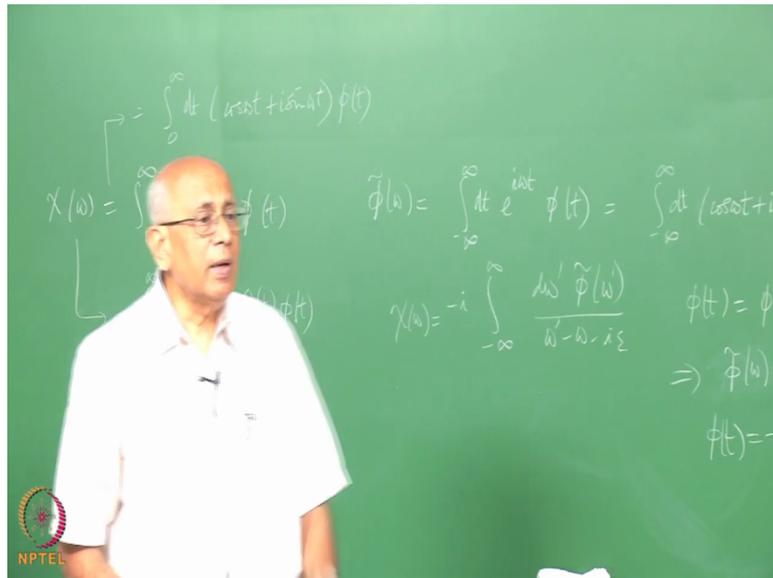


So there is another intimate relation between these 2 guys, now I leave you to take each of these cases and put it in here and look at what is going to happen. So it is starting to look as if Kai is given by, take the real case first take this even case first, it looks like Kai is given by an integral over itself, over the real part alone what is going on? That looks really weird, right?

Telling me the full susceptibility is an integral of a real part alone of this fellow but it has got to be completely consistent has not done anything wrong anywhere. Remember that this fellow  $1/\omega \pm i\pi\delta(\omega)$  over this guys is the principal value plus  $i\pi\delta$ , so if we put that in an equate real and imaginary parts will end up with a statement that the real part of Kai is equal to the real part of Kai which comes through and the imaginary part will be an integral over the real portion here which will give you the dispersion relation.

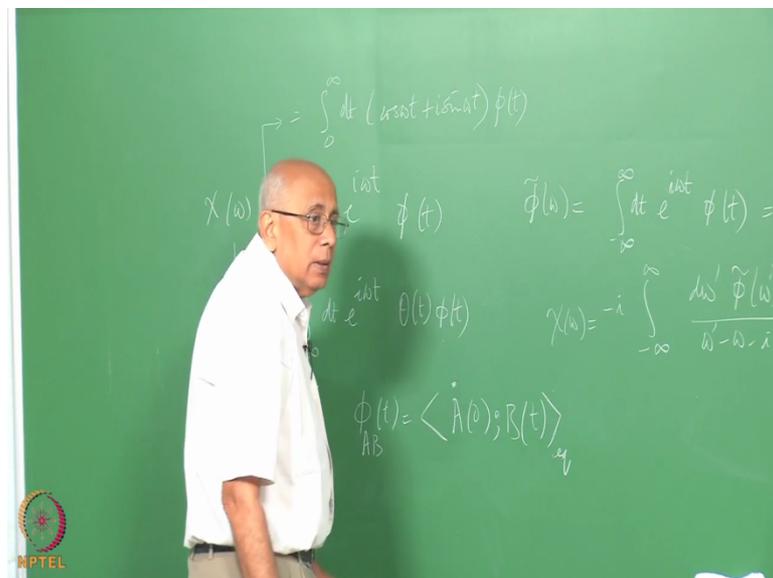
This side is in general complex, so the way to resolve the right-hand side into real and complex parts assuming this is real which by the way is true here immediately is simply to resolve this Cauchy kernel with this guy as principal value plus  $i\pi\delta$ . So it will give you an identity for the real part means the real part of Kai is equal to the real part of Kai which is an identity.

(Refer Slide Time: 42:21)



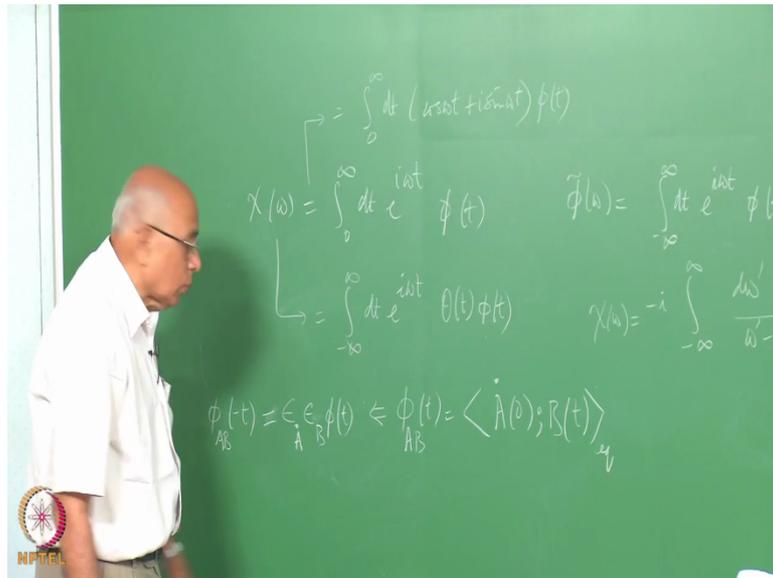
But it will also see the real part of Kai is the principal value integral of the imaginary part which is the dispersion information and the same will happen at this case as well but the question is how do I decide this?

(Refer Slide Time: 42:25)



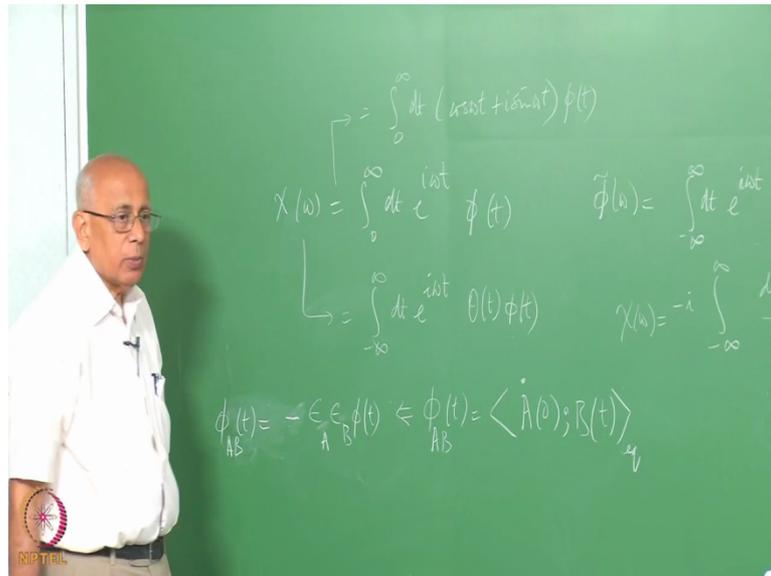
That is decided by Time reversal invariance because you see finally what you have is phi AB of t equal to A dot of 0 B of t in equilibrium. So now we are ready to talk about the time reversal property, we have computed this for various cases for t positive but now how define what happens for t negative? It depends on the time reversal properties of these guys, okay.

(Refer Slide Time: 43:49)



So this is equal to Epsilon A dot Epsilon B phi of t this will imply that phi AB of minus t is equal to this where Epsilon A dot is either plus 1 or minus 1 depending on whether A dot is invariant under times reversal or changes sign ditto for this but the time reversal, suppose A is a displacement x it has nothing to do with t, so it is time reversal properties it remains x goes to x under t goes to minus t.

(Refer Slide Time: 44:12)



But A dot is then velocity there is dx over dt and that changes sine, so in all the cases Epsilon A dot can be simplified a bit and we could write this as phi AB of t equal to minus without the dot because A and A dot are guaranteed to have opposite time reversal problem. So this is always this product with this thing here is either plus one or minus one and you can tell which one is which.

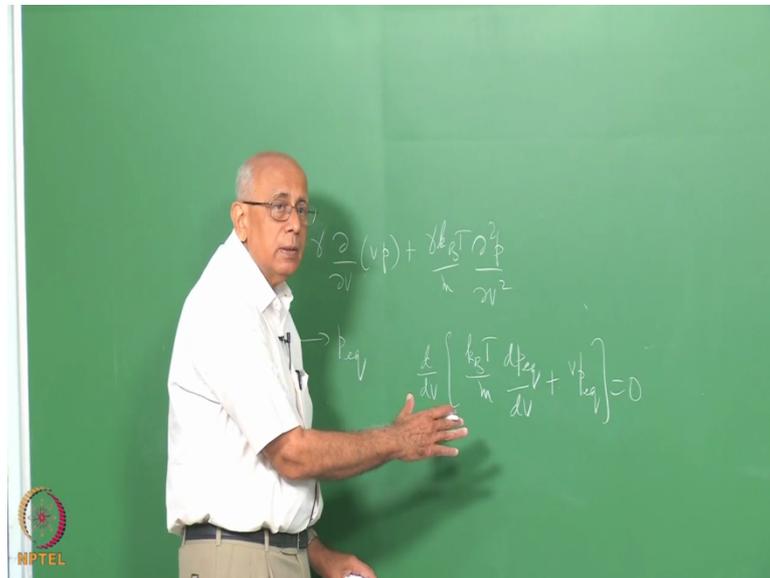
For example I apply a displacement to the Hamiltonian proportional to x the displacement the coordinate that is A is equal to x in that case, A dot is therefore v and if I am measuring v as I do in the Langevin problem that the correlation A dot B is essentially the velocity velocity correlation and you guaranty it from this, from this fellow here that in that case you are going to get a symmetric correlation which is what happened we found v of 0, v of t 0 the minus gamma mod, it is okay.

So in all cases the time reversal property of this function of these operators or dynamical variables will tell you whether it is even or odd function and therefore whether this is true or whether that is true, okay. So this is something which I had omitted to mention but we have it right here.

Next came all the fill in the blanks and the first question was of course the internal energy in terms of the partition function, sorry I forgot to write trace there it should have been trace of course. So we know the average values minus Delta over Delta (( )) (45:33) logs head that is trivial.

Then the second portion was the second question was this probability distribution for the condition of velocity? This is in fact the quarter plant equation Fokker Planck equation for the velocity, conditional density and now there is a little subtlety here,

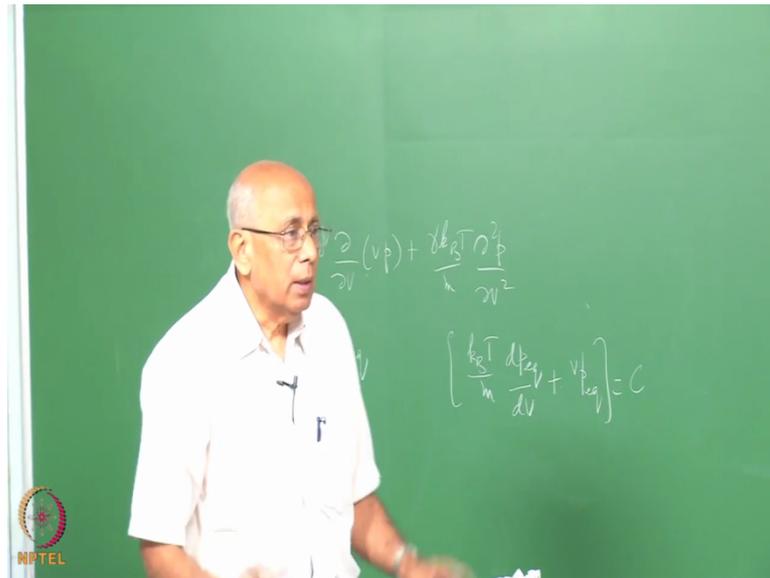
(Refer Slide Time: 46:00)



So let me rub this out. So you have delta P over delta t equal to Gamma time Delta over delta v vp plus gamma k Boltzmann t over m d 2 p over delta v by the way not surprisingly you would have guessed the fluctuation dissipation theorem as I put in here. So I get the Maxwell in distribution asymptotically. Now in equilibrium P goes to P equilibrium, this portion is 0 by definition P equilibrium has no time dependence then you have an ordinary differential equation but in second-order.

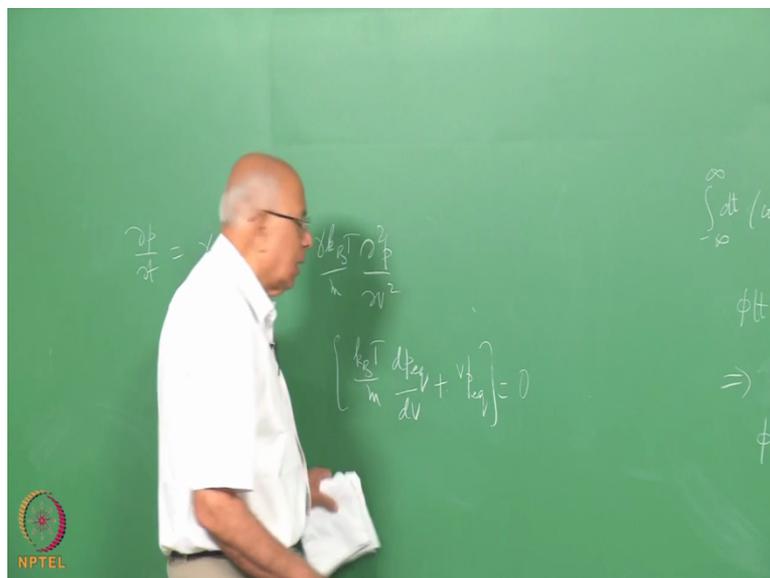
But notice there is d over dv that can be pulled out, so this will immediately imply that d over dv of kt over m dp equilibrium over dv plus vp equilibrium equal to 0 that is a second-order differential equation ordinary differential equation, what can you conclude from this?

(Refer Slide Time: 47:09)



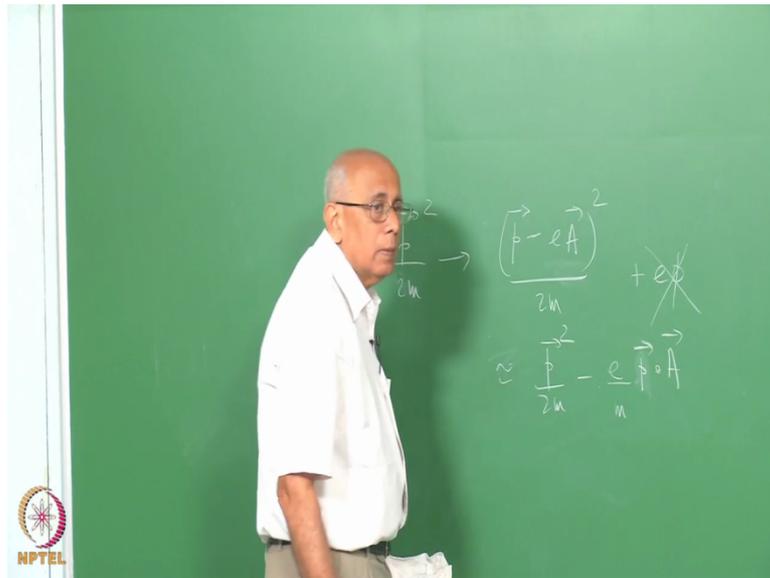
That this must be equal to a constant, it must be true at every value of  $v$  including plus minus infinity but at plus minus infinity each of these terms is 0  $P$  equilibrium manages therefore the constant is 0, therefore it is 0 for all  $v$  because it is a constant, right?

(Refer Slide Time: 47:32)



So this goes to 0 and that is a first order equation and as you can see the Maxwell in distribution is the solution. Move this constant there and then you can integrate by separating variables, okay. Alright, the next one was just a calculation of  $d$  using the integral, you need to use the fact that  $d$  is integral  $v$  of  $0$   $v$  of  $t$  for any Cartesian component, okay.

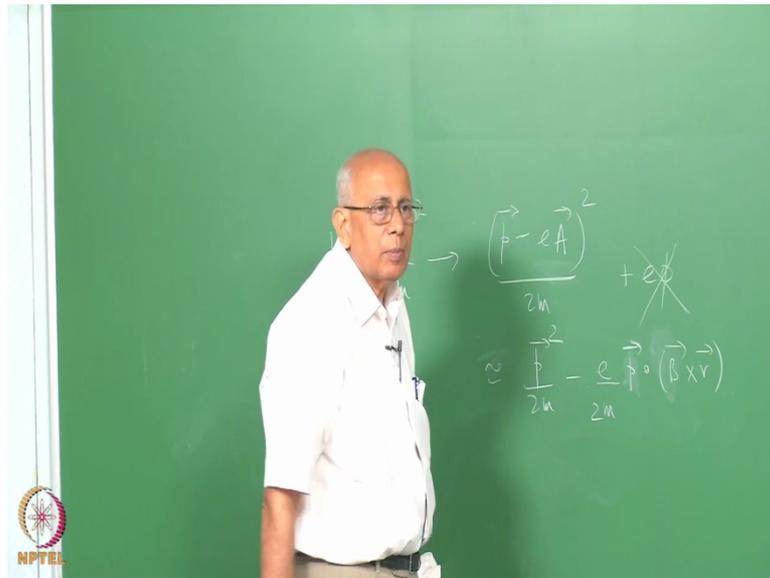
(Refer Slide Time: 48:25)



It is a trivial integral and the one with the pole at 0 this I had already mentioned earlier in class, so you just have to add this lambda over Omega your dispersion relation then the last part and let me say this is something which resume that you know already what happens in an electromagnetic field is that the Hamiltonian which is P square over 2m for a free particle goes when you have a magnetic field to P minus eA square over 2m plus of course if there is a scale of potential you have this but in a constant magnetic field you can choose that to be 0 always.

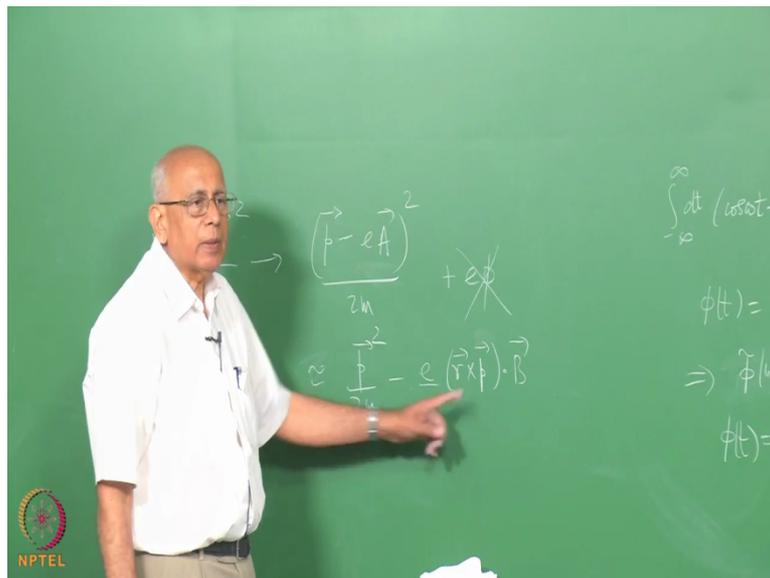
So that is your Hamiltonian and therefore to first order in the vector potential this is equal to P squared over 2m minus e over m P dot A classically but if you have a constant magnetic field you can write a simple representation on the column gauge for the magnetic field its half b cross r, the fact that b changes the time does not affect this, it has got to be a uniform magnetic field.

(Refer Slide Time: 49:38)



So this thing becomes...

(Refer Slide Time: 49:51)



And of course by the cyclic property of this triple product you can write this as B dot r cross P or you can write it as r cross p dot B but that is the angular momentum.

(Refer Slide Time: 50:06)

The image shows a green chalkboard with handwritten mathematical derivations. The first equation is  $H = \frac{\vec{p}^2}{2m}$ . This is followed by an arrow pointing to  $\frac{(\vec{p} - e\vec{A})^2}{2m} + e\phi$ , where the  $+ e\phi$  term is crossed out with a large 'X'. Below this, an approximation is shown:  $\approx \frac{\vec{p}^2}{2m} - \frac{e}{2m} \vec{L} \cdot \vec{B}$ . The  $\vec{L} \cdot \vec{B}$  term is circled. In the bottom left corner, there is a small NPTEL logo.

So this thing becomes, does this remind you of something? This is gyromagnetic ratio that's the angular momentum, so what is this equal to? It is a magnetic moment formed with by the current loop, right? That is all it is, that is how the particular respond, it has no spin, so there is no intrinsic magnetic moment. The only thing it can do is, it moves in a circle creates (()) (50:16) current and this couples to the external field that is exactly what you expect  $\mu \cdot b$  minus  $\mu \cdot b$  where  $\mu$  is the magnetic moment is the potential energy in the presence of a magnetic field.

So that is precisely what you get here, would this be correct quantum mechanically? Where would I have gone wrong? Pardon me.

“Professor -Student conversation starts”

Student: Formulation of P and A.

Professor: So I cannot write P minus A as a whole square the cost would be P dot A plus A dot P. I have to be careful about that and then you get pretty much the same. And the column gauge it does not matter, yes, exactly. So that is a further thing that it really does not matter in the column gauge. So I leave you to verify to check that out but to get expect let us.

“Professor-Student conversation ends”