Nonequilibrium Statistical Mechanics
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Lecture No 05
The Langevin model (Part 4)

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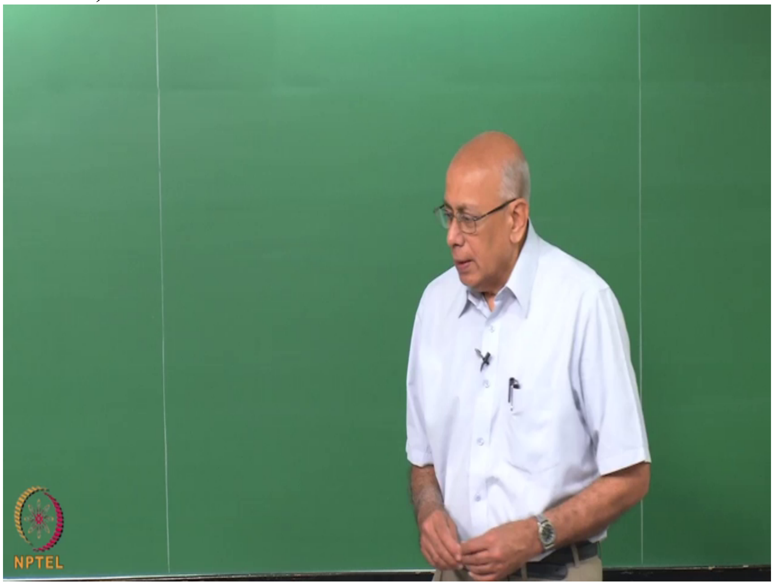

So we were in the process of examining the velocity auto-correlation function for a Brownian particle moving in a constant magnetic field, a uniform constant magnetic field. And if you recall, our final answer said that this quantity which I call

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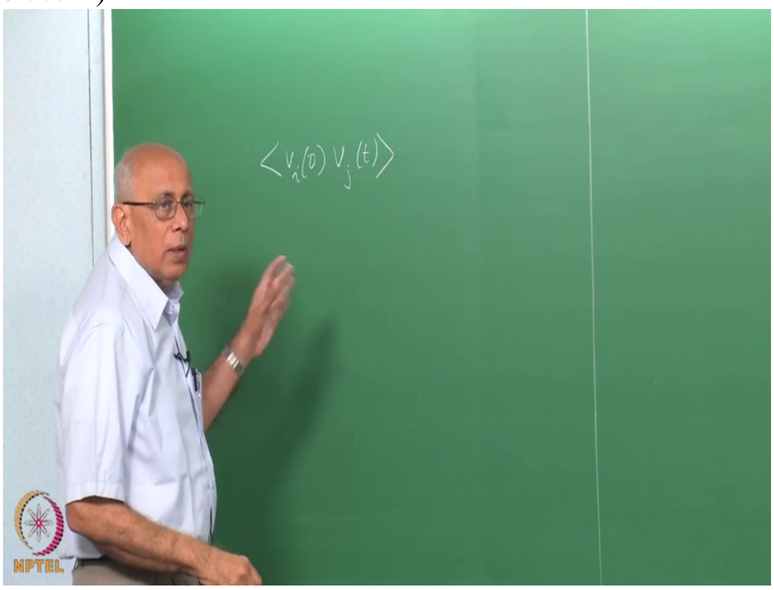

the correlation function apart from normalization, I multiply it with what happens at t equal to zero, this thing here is k T over m, then we have got a complicated expression for it here inside.

There was of course damping factor, so e to minus gamma t and then that gets multiplied for a field B, which was B times some unit vector n.

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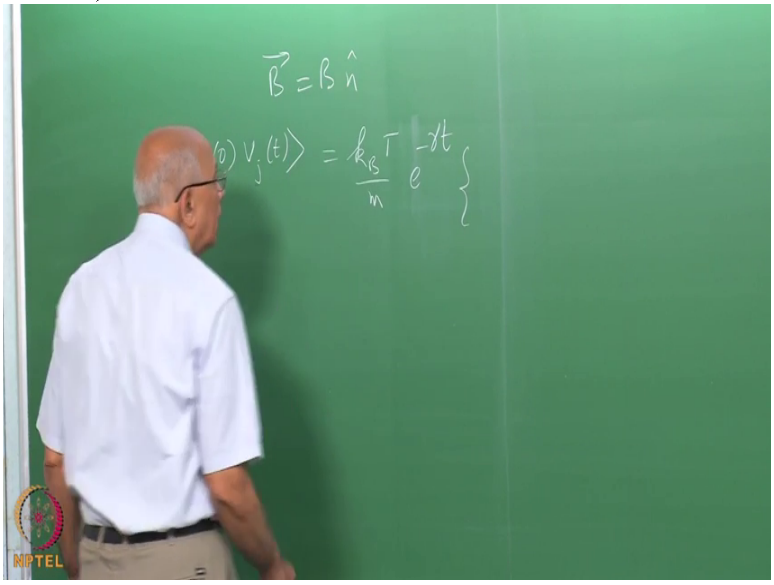

This gets multiplied by n i n j plus delta i j minus n i n j cos omega c t where omega c is the cyclotron frequency, q B over m,

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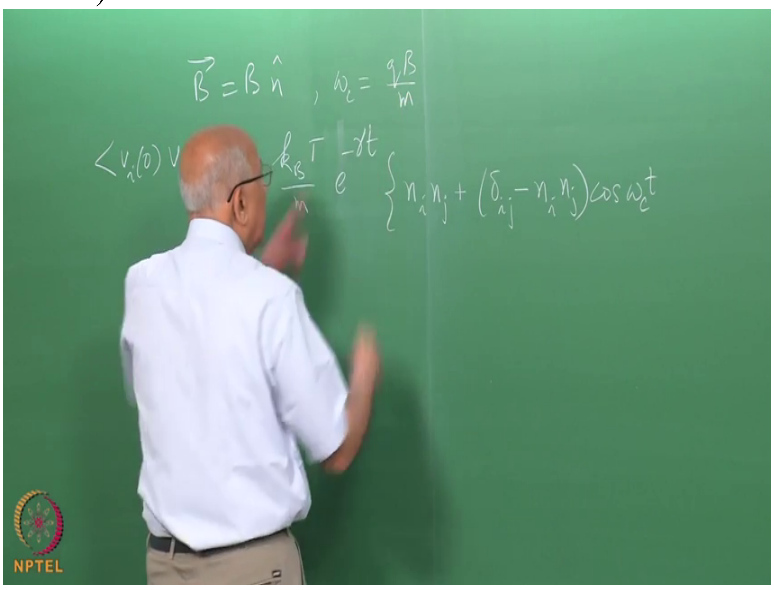

q being the charge of the particle, so there was the second term minus a third term which is epsilon i j k n k sin omega c t. And this was true for greater than zero, equal to zero. This is the expression we derived.

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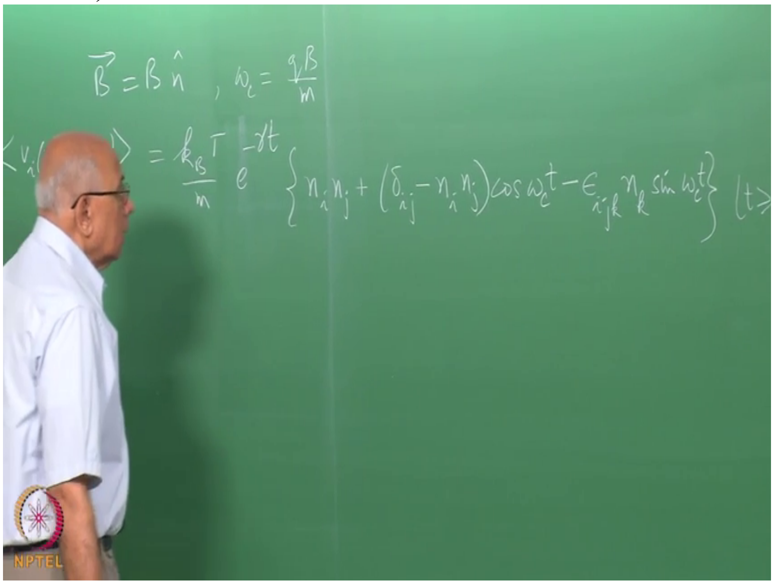

So if you check I rearrange some of the terms and then after simplification, this is the expression you get, Ok. Now the first thing you notice about it is that gamma does not appear anywhere here at all. It appears only here. So the effect of dissipation is taken care of entirely by this factor exactly as in the field free case. The moment you have a field switched on, you have this expression. Of course if you switch it off, you go back to just this expression with delta i j because this is zero, that is zero, this is zero identically and you end up with just the original expression as before.

Now we would like to find out what happens for negative values of t? We derived for positive values. We would also like to examine what does it do for negative values of t? Now recall that in the field free case, we had v i of zero, v j of t in equilibrium, this was equal to k Boltzmann T over m e to the minus gamma modulus of t.

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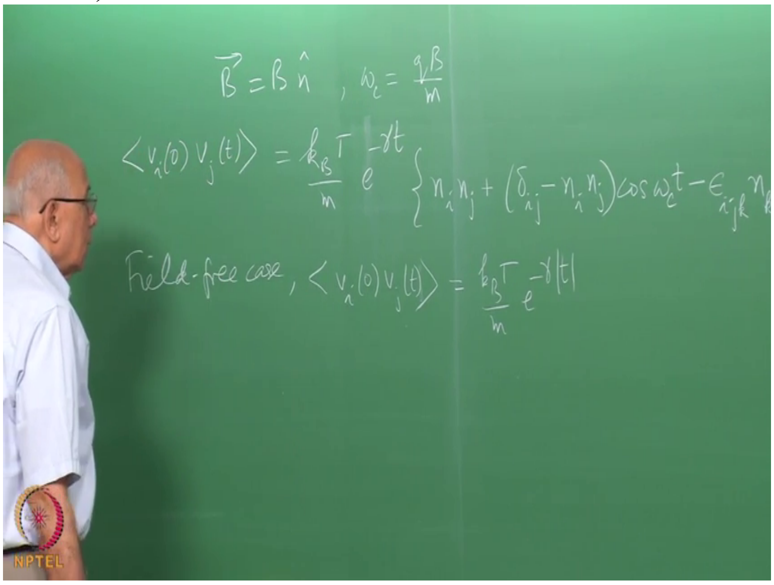

The way we derive this, this thing here is by pointing out that this must be an even function and the way to get the evenness of this or oddness property whatever, the symmetric property of this, is to put in, if you like time reversal and ask what the whole thing does under time reversal exploiting stationarity.

So if you recall in the field free one-dimensional case, it started by saying v of zero, v of t in equilibrium, since it is a stationary process, so equal to implied by stationarity of the random process v, this was equal to v of minus t, v of zero.

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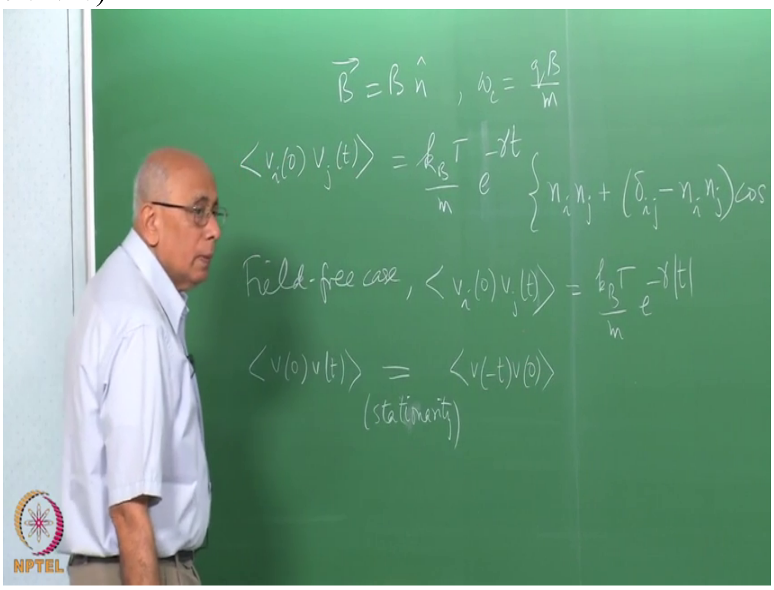

(Professor – student conversation starts)

Student: In the earlier formula there was delta i j

Professor: There should be delta i j, thank you. So in the one-dimensional case I said that the origin of time does not matter. So I subtract t from each of these arguments and I end up with this expression here. This immediately of course says, that since these are commuting variables, this immediately says that this is a symmetric function of t. That's the reason we got hold of e to the minus gamma modulus t, yeah.

Student: But for field free case, if we derive from the first formula, we will have a cos term in 0:04:49.6, entirely cos over here.

Professor: n is zero in that case, I mean there is no n.

Student: omega c is there?

Professor: This is gone; omega c is zero, of course, right. And this goes away, this vanishes. So I want you to appreciate that we are looking at what happens at t negative, not by doing another calculation but simply arguing that this is the stationary random process. So I can subtract any number I like from the argument of the whole function, from all the time arguments.

(Professor – student conversation ends)

When I do that it becomes an even function of t, Ok. So the argument was it is k T over m, e to the minus gamma modulus of t using stationarity. We can do pretty much the same sort of thing and this term will become modulus t here. But let's do this systematically. Let's ask what happens to this in the general case.

So in general, I already mentioned that even in the presence of the magnetic field, the velocity continues to be a stationary random process because there is no energy being given to it; there is no dissipation involved with the magnetic field or anything like that, Ok. So if you grant that, then it is immediately clear that in general, v i of zero, v j of t, if I call this quantity, let me call this equal to phi i j of t. The reason I am calling it phi is because when I divided this by its value at t equal to zero, I call that C i j of t. I don't want to use the same symbol,

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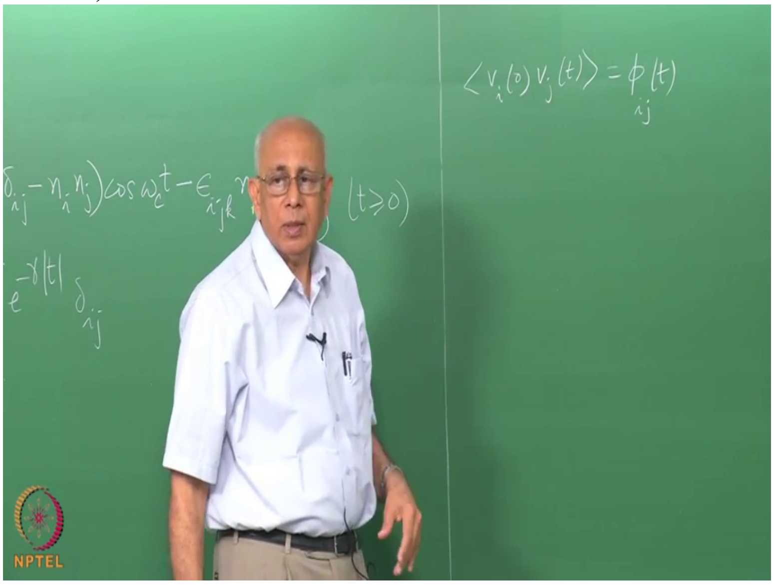

phi i j is...

So this is equal to v i of minus t v j of zero by stationarity. I subtract t from both sides, right. But this is equal to v j of zero v i of minus t,

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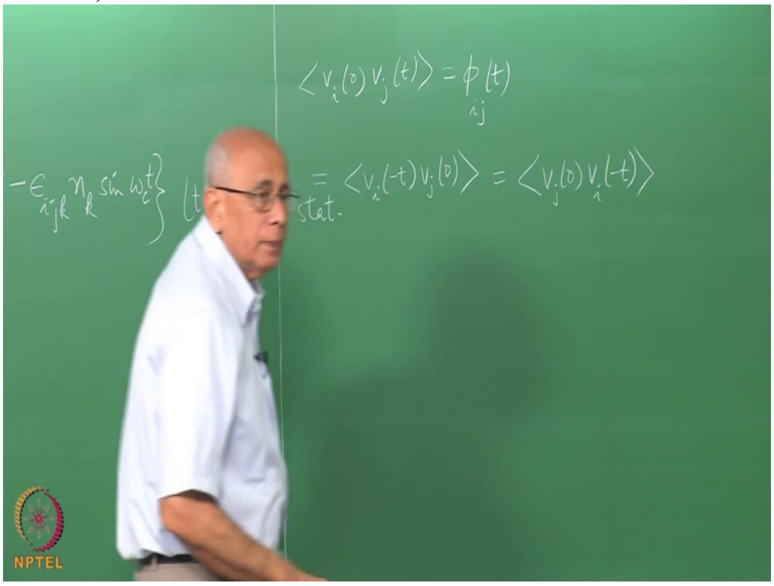

which is equal to phi j i of minus t, Ok. Because these indices get interchanged which did not happen in 1-dimensional case. So this tells us that this correlation function C of t, this matrix C that we computed yesterday is such that it is equal to C transpose minus t

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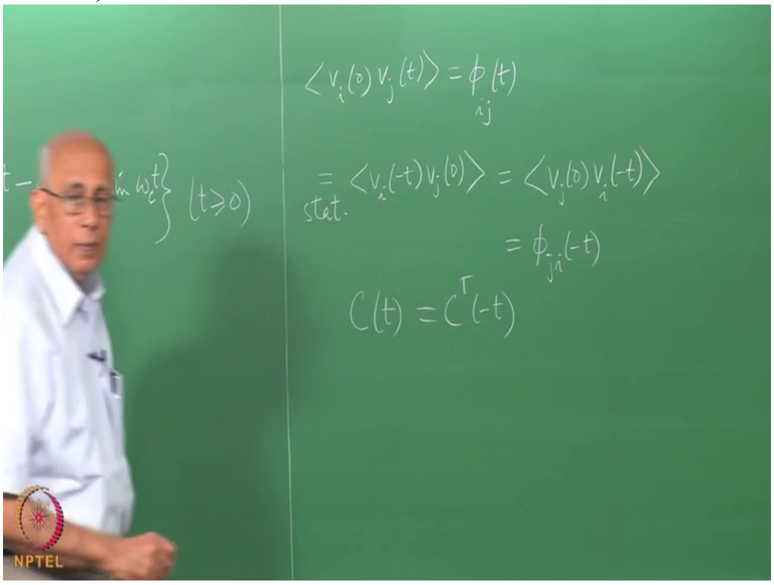

because of this property. It becomes transpose and then the argument becomes minus t, right? So it immediately follows whether I use phi or C, doesn't matter, they just differ over a multiplicative constant k T over m. So this immediately follows that C i j of t plus C j i of t, this is the even part of the tensors of C i j of t divided by 2, of course. The minus part is the odd part of this tensor. So given

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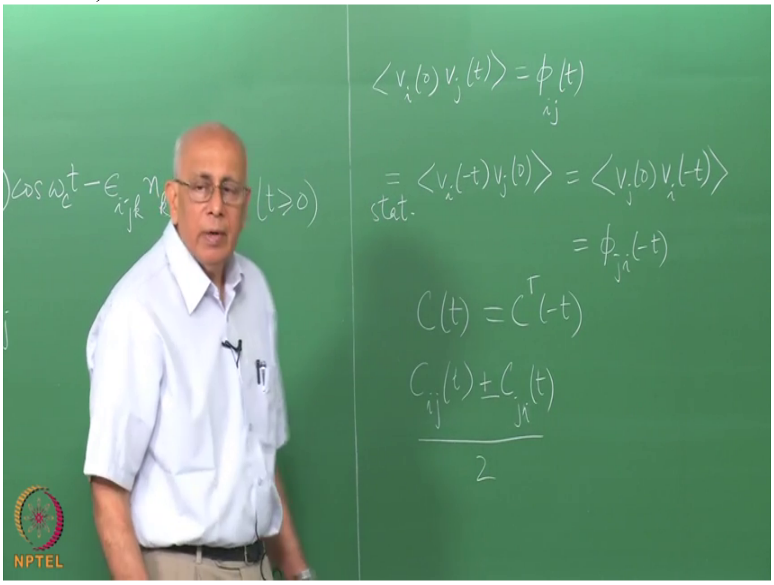

any second rank tensor t i j, I can write t i j plus t j i over 2, that is the even part and the odd part, the anti-symmetric part is t i j minus t j i over 2.

So this is the symmetric part of the tensor correlation tensor, this is the anti-symmetric part. But by this property this is equal to C i j of t plus or minus C i j of minus t, over 2,

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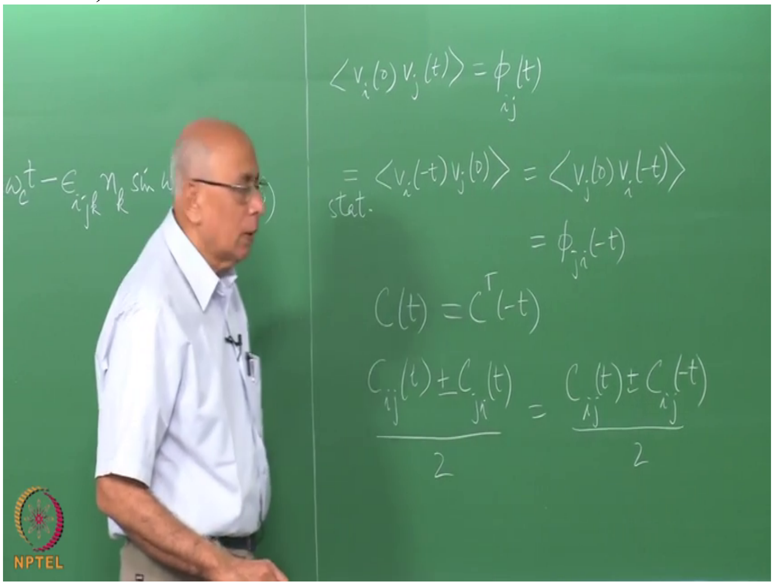

using this property. It follows therefore that this correlation tensor C i j of t is such that it's symmetric part is an even function of t, where there is an even function of t, and its anti-symmetric part is an odd function of t. That's a general property.

As soon as you have a correlation matrix for some random variable and it is stationary, it follows that the even part of the correlation tensor, the symmetric part of the correlation tensor is an even function of the argument and the anti-symmetric part is an odd function of the argument. We will use this property later on, Ok

(Professor – student conversation starts)
Student: And it does not require detail that…
Professor: This doesn't require you know what the function is at all. I have only used stationarity at that end over there. We will use this property. It is a crucial one. We will use this symmetry property. But you can see how this is, how it actually is tallying with what goes on here. We need to write down what this thing is for t less than zero and let's write it down in the following way.
(Professor – student conversation ends)

What does this do, for this t less than zero, less than equal to zero, v i of zero v j of t is equal to, none of this gets changed k T over m, e to the minus gamma modulus t, you have to put a mod here exactly as in the field free case, multiplied by whatever is inside here is going to be the time reversed value of whatever is in the bracket for t greater than zero. So you have to reverse time, from t to minus t, Ok. And what happens if you do that?

You get n i n j plus delta i j minus n i n j cos omega c t and then what do I get? The next term, it is not just setting t to minus t.

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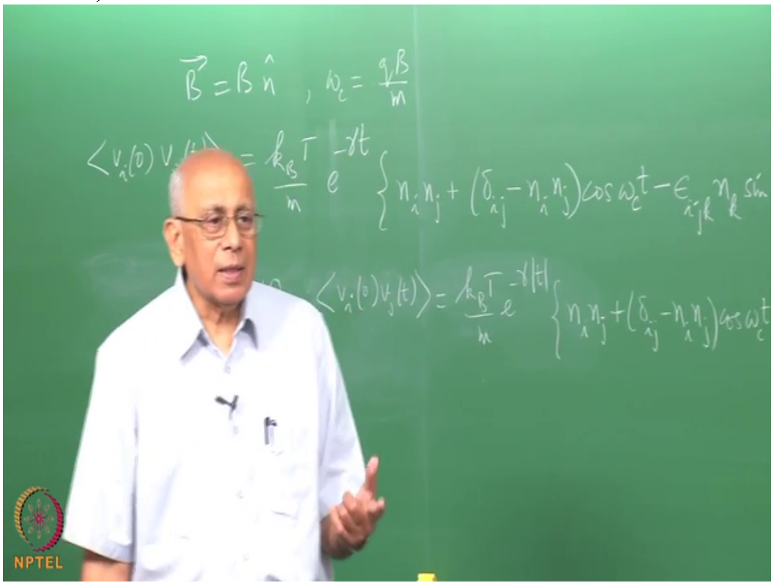

That's time reversal. But when I reverse time and let the system run backwards I should also change the sign of the magnetic field. It is an externally applied magnetic field. So on the time reversal; I have to change its sign as well. You can see this happening even in Newton's equation for a charged particle.

If you look at what the Lorentz force does, the equation is F equal to d B over d t equal to q times v cross B. This is an external applied field.

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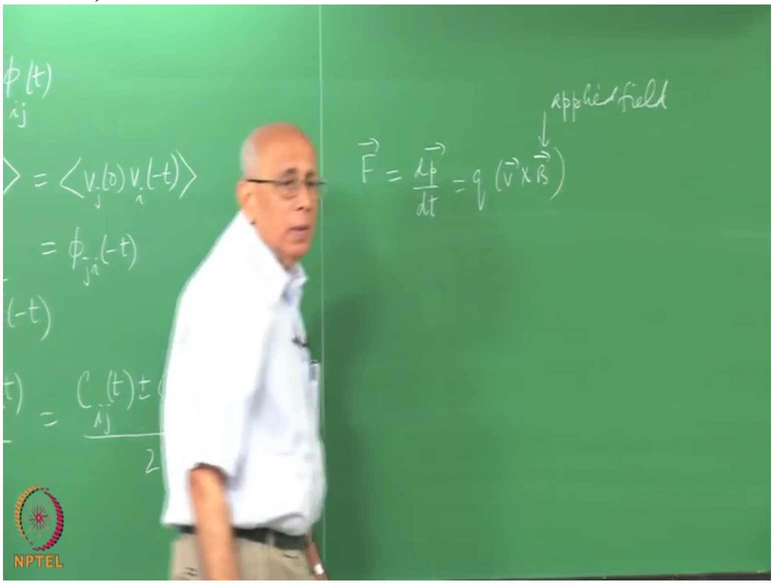

Now I make the time reversal transformation. t goes to minus t, then p goes to minus p because this is m d r over d t. And r doesn't change, position but the momentum changes sign. Whatever was going in this direction now goes in the backward direction, right? So this changes sign, this changes sign. Therefore this does not change sign d B over d t.

And if the equation has to be the same under time reversal invariance, in other words we impose the fact that Newton's equation for charged particle is invariant under time reversal. This is an imposition from outside. If you impose that condition, then since v changes sign, B must change sign, Ok. So does the electric field change sign? No, if you put in electric field also, it is q times E, that doesn't change sign because this side doesn't change sign.

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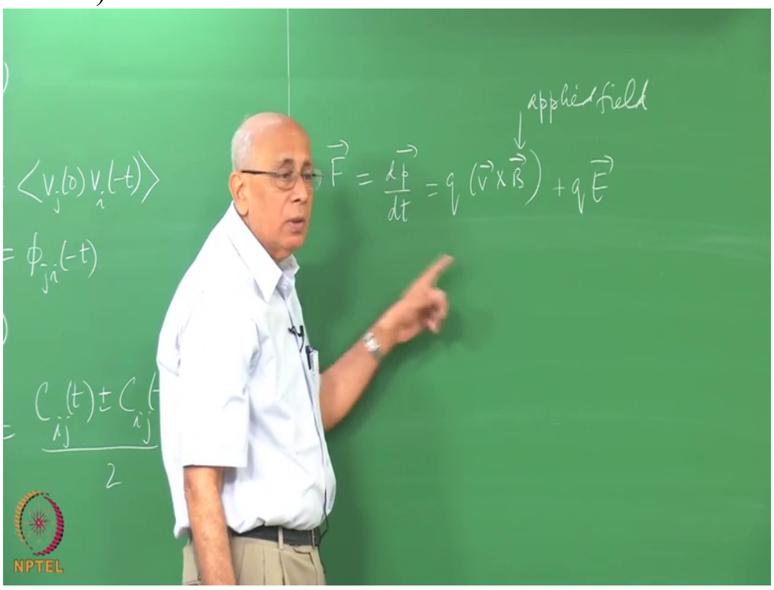

So this cannot change sign under time reversal. But this will change sign. B will change sign. You can kind of, physically understand it by saying in heuristic terms; look finally every magnetic field is produced by some current loop of some kind. If there is time reversal, then that current flows in opposite direction and it produces the field in the opposite direction, Ok? So B must go to minus B which means that n k must go to minus n k. So under time reversal, goes to minus n sub k.

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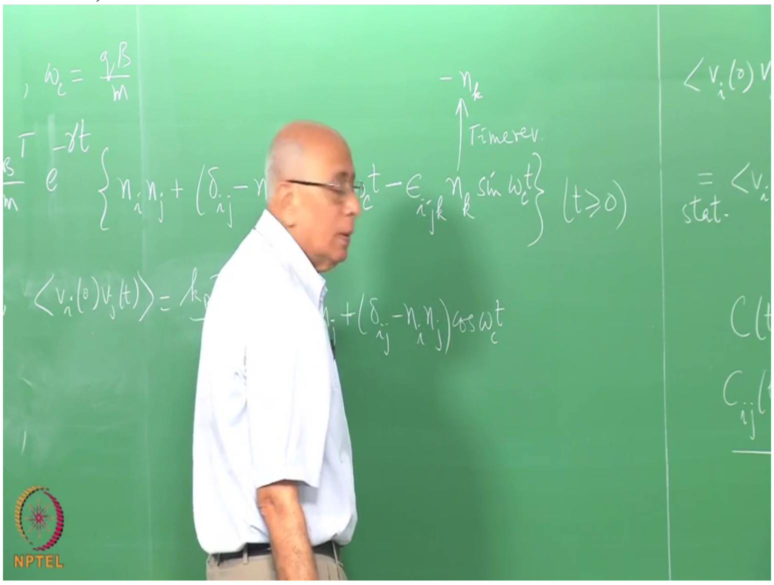

So this term remains minus epsilon i j k n k sin omega c t.

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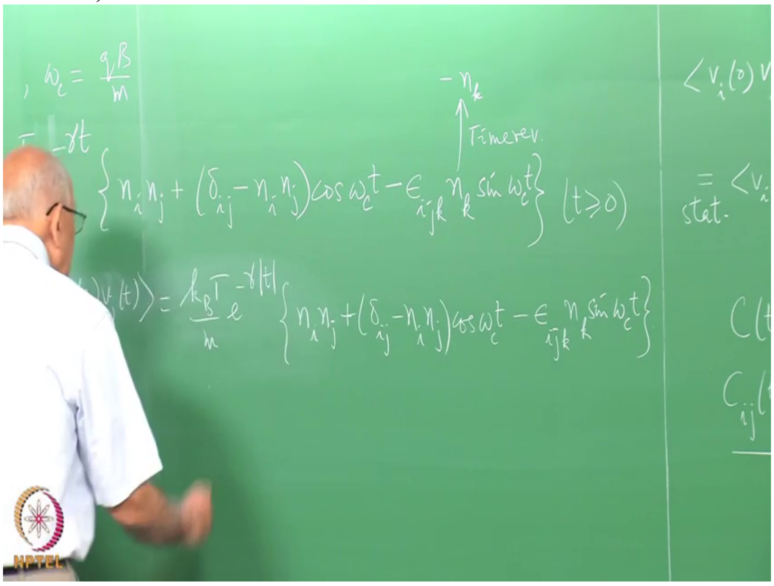

And this expression is true for all t.

We have taken care of this here for negative t.

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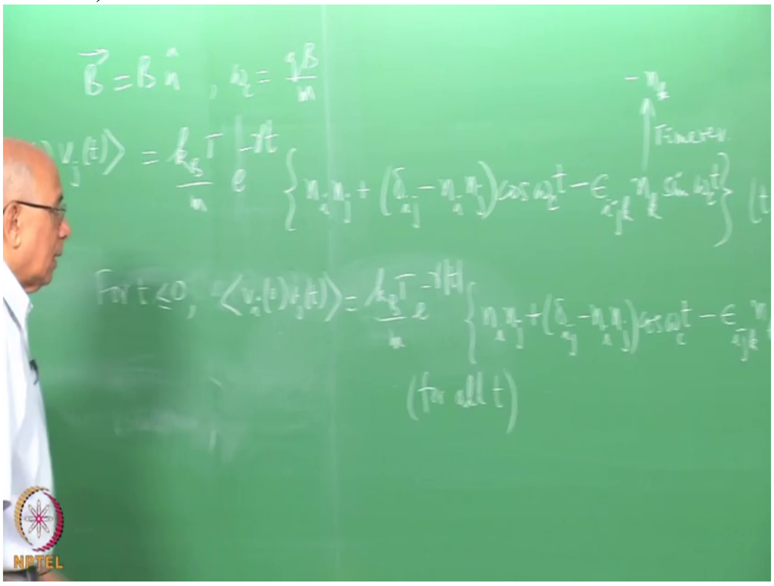

So that's the exact expression for the correlation function for all t. And now you can verify explicitly that this property is satisfied. So check out that the symmetric parts of the tensor is in even function of t and the anti-symmetric portion is an odd function of t. That appears by inspection because this tensor, the symmetric part comes from here, here and here. This part is anti-symmetric in i and j. That's an odd function of t. This part is the symmetric part of the tensor and that's an even function of t, Ok.

If that did not happen, I would really be in deep trouble, Ok, worry about what's going on. So this gives you a check on what the t reversal properties are. It helps. That symmetry is valid, it is applicable here too. It's a general statement. So it better be true here too. Now given this, the next step is, well, we can proceed in many directions, but the next step we could do is the following.

We saw that for a single free particle in one dimension, we saw the diffusion coefficient got related, imposition got related to the velocity auto-correlation. We saw in fact, in that case, we saw that x of t minus x of zero whole square went asymptotically very large t to 2 d t. And we got an expression for this d, k T over m gamma in the, in this Langevin model but we saw that from first principles, if I just took

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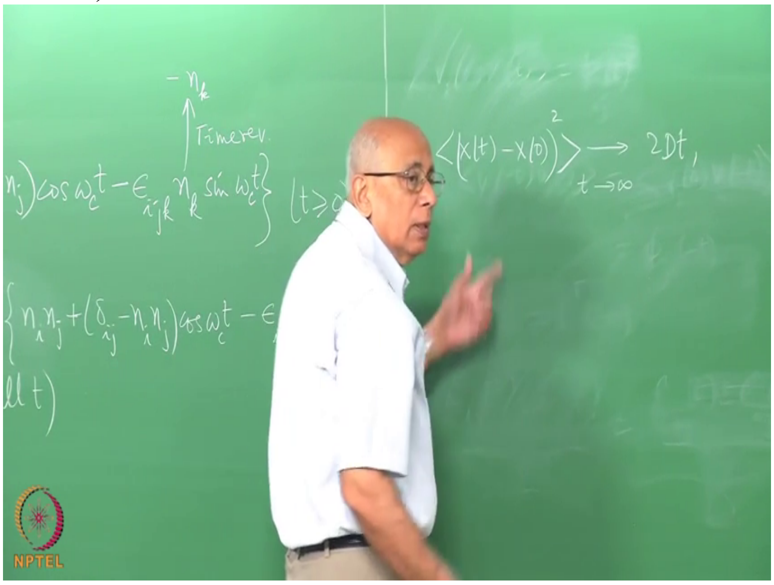

displacement to be the integral of the velocity and then impose the fact that velocity is a stationary process, I ended with a statement that D was equal to integral from zero to infinity, d t v of zero v of t. The equilibrium autocorrelation function

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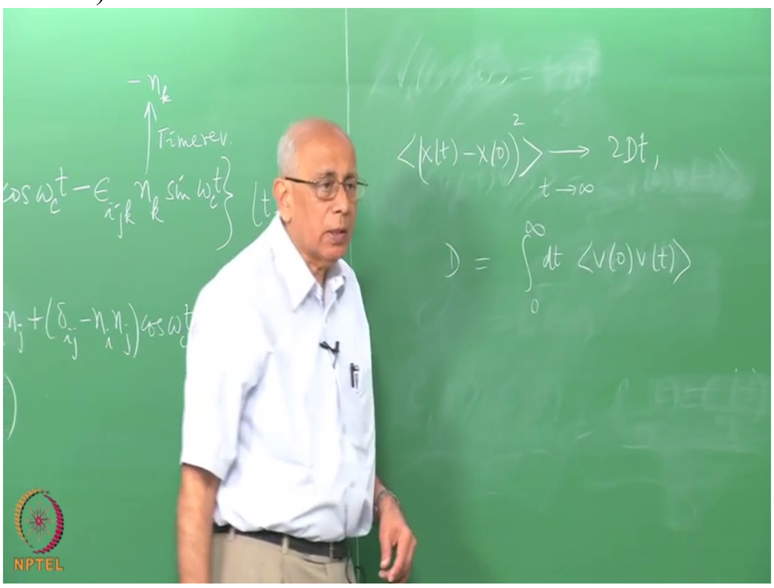

of velocity. So we got this explicit formula here.

Now the question is what happens now in this problem? What would happen in this case? Well you can kind of see intuitively that the portion that is not going to, that's going to be unaffected would be along the direction of the field, along the vector n because there is no magnetic force in the direction at all but in the perpendicular or transverse directions there is a force which tends to make this particle go in loops, go around the direction of the field in cyclotron orbits. So it is diffusing, it is being kicked around but every time it is being kicked around, it is still trying to curve back on itself, Ok.

So I would expect the diffusion coefficient to be less in the longitudinal, more in the longitudinal direction unaffected from the free particle case and in the transverse directions, I had expected to be a little smaller. The fact that it diffuses; there is no question because this integral exists because of this factor and these are just oscillatory terms here, Ok.

So the question is what is the generalization of this formula, this is the famous Kubo Green formula, a special case of it

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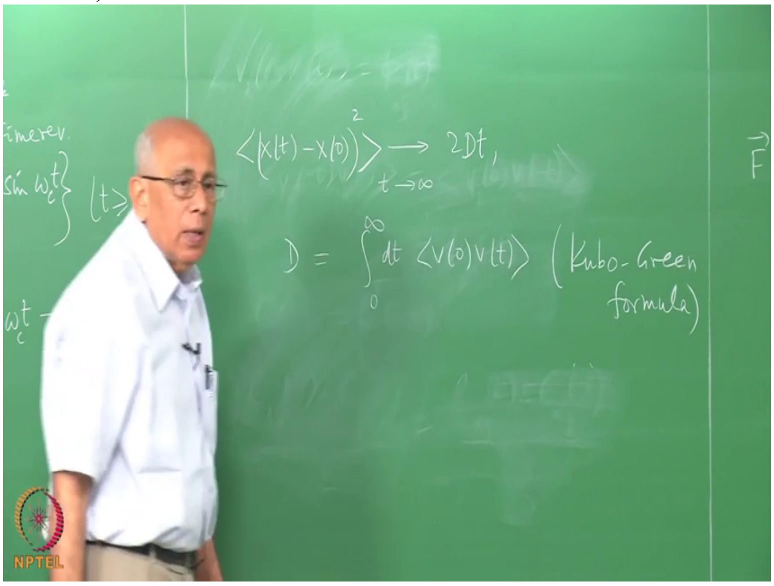

and when we do linear response theory in

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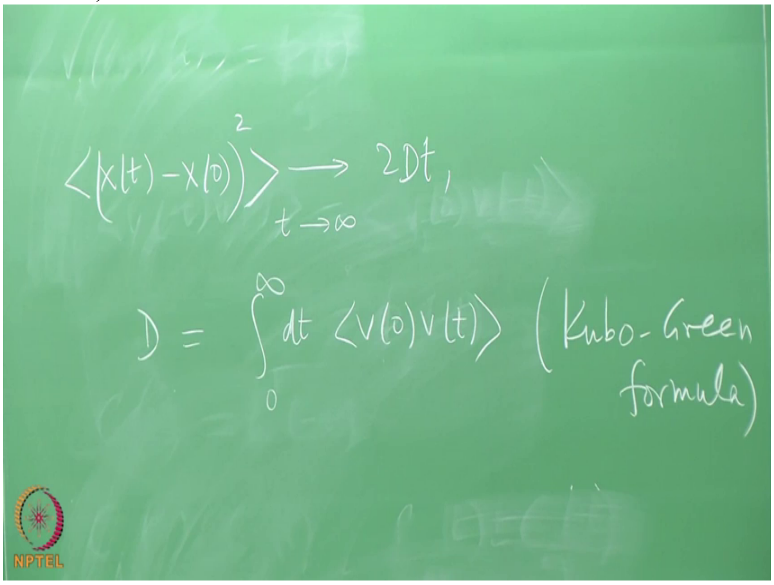

some detail, we are going to work this formula out, we are going to explicitly prove a much more general version of this formula for all kinds of susceptibilities or response functions. But let me state the result here.

What happens now is that diffusion becomes a diffusion tensor, the coefficient is a set of coefficients, diffusion tensor denoted by D i j, Ok, because I also have to tell you where does this fellow come from, what does this D i j look like? And it comes from the fact that the probability density in position obeys the analog of the diffusion equation, little more complicated than free diffusion and that involves the set of coefficients which are summarized in this diffusion tensor here.

We will do this when we write the general formulism down the linear response theory we will come back, we will revisit this problem. But the answer can be written down here and you can see from physics in it, 0:18:24.3 so we can see, this tensor is defined as the symmetric part, so it is an half D t phi i j of the plus phi j I of t, where phi is the auto-correlation.

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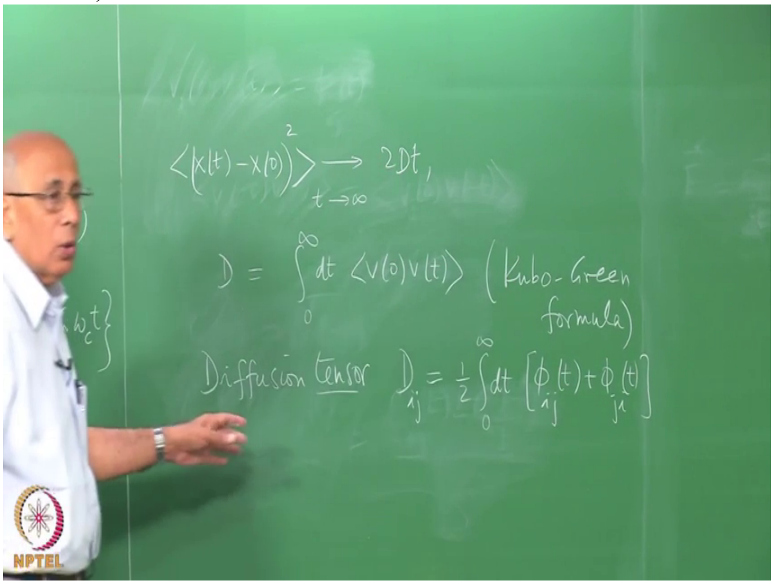

So this fellow here stands for v i of zero, v j of t. We can therefore compute it; we can go back here and compute it. We need only the symmetric part of this tensor therefore this doesn't contribute at all and so only this portion would contribute here. And this is an easy integral to do. First of all, this term is immediately obvious, it is e to the minus gamma t, that's just 1 over gamma. This term, e to the minus gamma t cos omega t which is gamma divided by omega square plus gamma square, omega square plus gamma square. That's it. So we can write the answer down explicitly, right

And it turns out, D i j, this thing here is equal to k B T over m gamma as before multiplied by, that portion remains as it is, n i n j plus delta i j minus n i n j gamma square over gamma square. So that's the answer. As I said this won't contribute at all because it is the anti-symmetric part of tensor and does not contribute.

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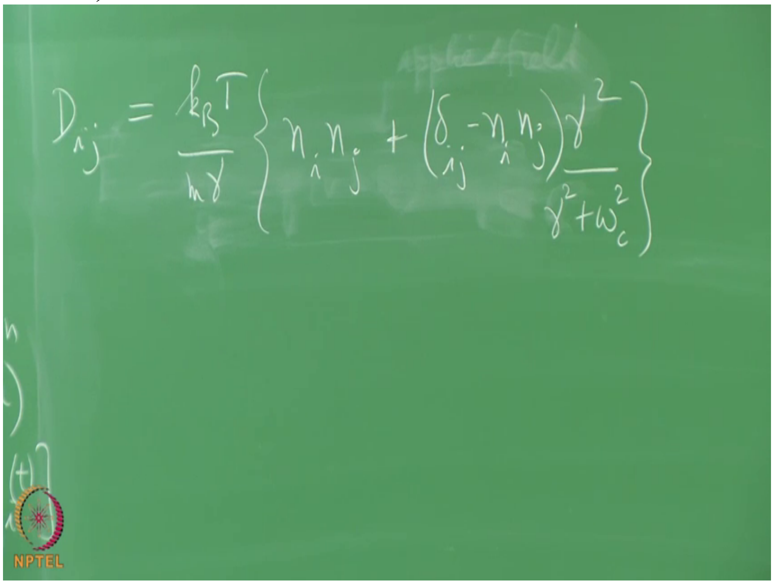

Now can you interpret this?

For instance you can see directly what is going to happen. For instance, suppose n was equal to zero zero 1, so the field is in the z direction. And we have the x-y plane. There is no force in the x-y plane; sorry there is no force in the z direction because the field is in the z direction. Then n i, the only term that contributes, they are the diagonal terms that you can see, and now what will happen if it's 3, d 3 3, that's going to have a contribution 1 from here. And this portion cancels out and it is the original diffusion constant.

On the other hand if you look at 1 1 for example, in this case, then this term is zero, doesn't contribute, that portion is zero, this gives you 1 and it gives you gamma squared over gamma squared plus omega c squared. So the diffusion coefficient, the longitudinal part equal to k Boltzmann T over m gamma as before, but the D in the transverse direction is equal to D longitudinal multiplied by this term. So it is therefore

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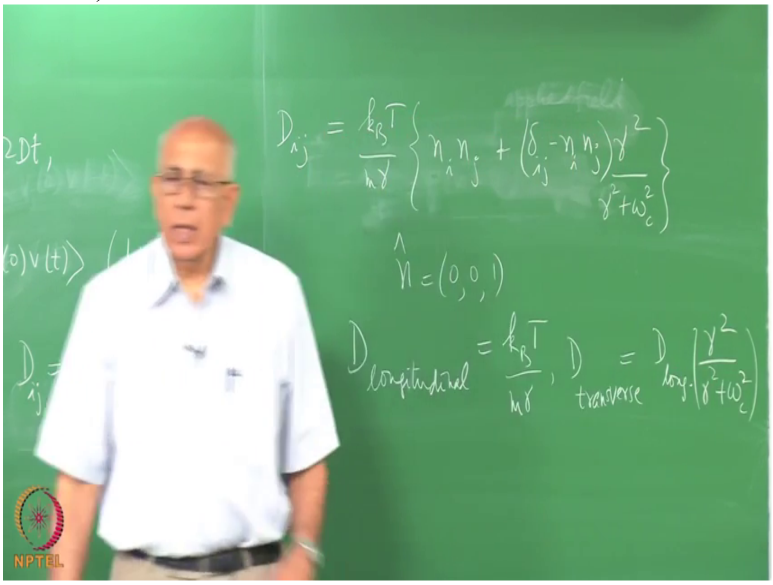

attenuated. It is decreased.

If omega c becomes much larger

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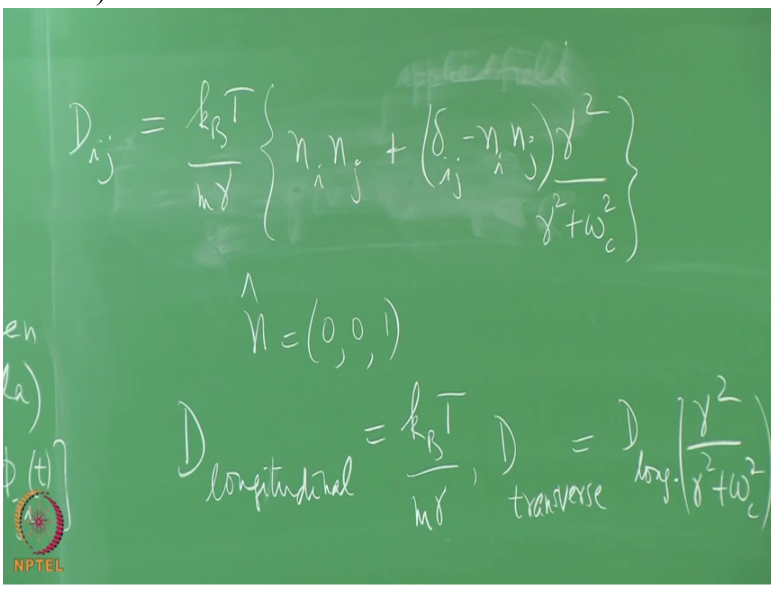

than gamma square, then you can see it decreases by a factor of gamma square over omega c square, Ok. That's exactly what this says. You don't have to go to a special case like this. This thing here is a projector in the direction of n and that thing there is 1 minus the projector, Ok. So this is, you know from ordinary vector...

(Professor – student conversation starts)

Student: 0:22:46.3

Professor: Pardon me

Student: Projection onto the transverse direction?

Professor: It is the projection on the transverse direction because well, all you have to do to verify it is multiply both sides by, contract it with n j or something like that. And it immediately tells you D i j n j just has n i here because n j n j is 1 when you sum and this is obvious what you have here, Ok.

(Professor – student conversation ends)

So you know, when you do elementary vector algebra in 3 dimensions, you learn about dot product and the cross product between 2 vectors and so on, but there is also a tensor product of 2 vectors but you don't write anything in-between. That is called a diadic in ancient literature, just another word for tensor of rank 2, but when they did vector analysis; people used this term throughout 0:23:43.9 in the beginning.

So this quantity here is such that it is a 2 headed object,

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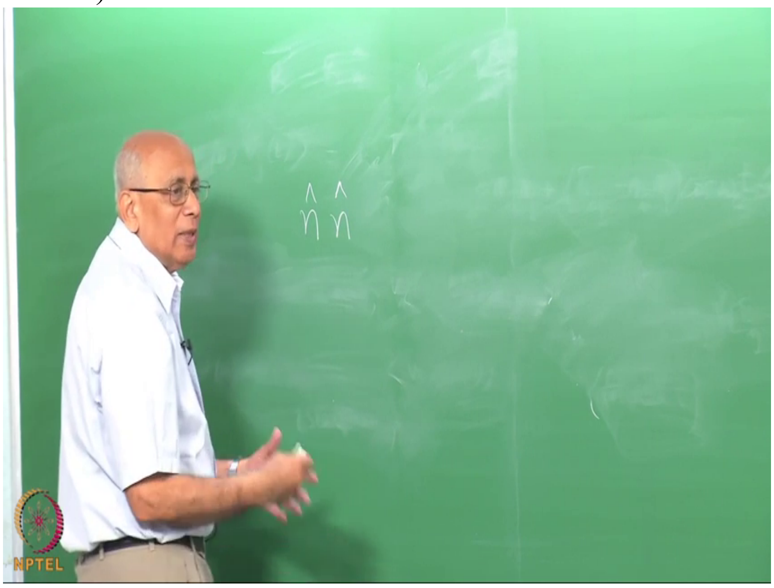

it is such that no matter what vector you operate this on, whether from the left or the right, you produce a component of the vector in the direction of n. Because you could take this vector and dot with a, then there is a component of a along the unit vector n, multiplied by the unit vector n, so it gives how much of that vector points along the direction of n. So you have an arbitrary vector a and this is your unit vector n and this fellow is actually measuring this, this quantity is measured

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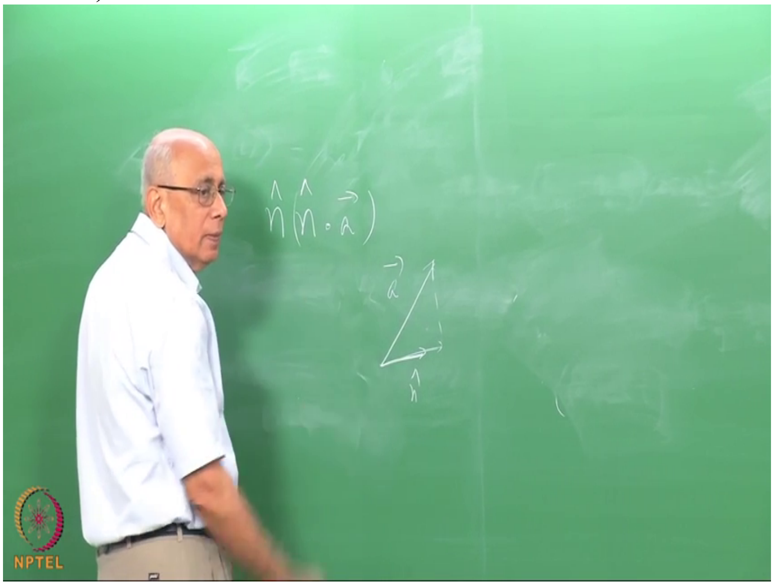

here, right?

So this is the projector, it is the projection operator n n. If you took 3 orthogonal directions and projected them out, then you get the identity operator because when you apply that to any vector, you have taken all the 3 orthogonal components of this vector and added them up, so you get the original vector itself, right?

If for instance you took this, e x, e x plus e y, e y plus e z, e z that's the projection operator which when applied to any vector will give you the vector itself. So what should this be? This should be equal to the identity operator.

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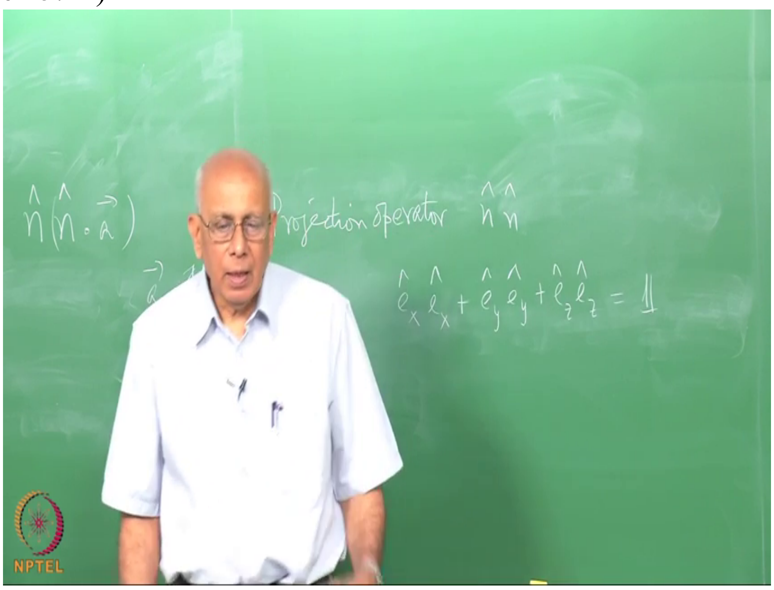

In any linear space you sum up all the projection operators and you get the identity operator. This is like saying that if I have an abstract space with eigenvectors, with an orthogonal basis phi n phi n over n, this is equal to the identity operator. In Dirac notation this is the way it is written.

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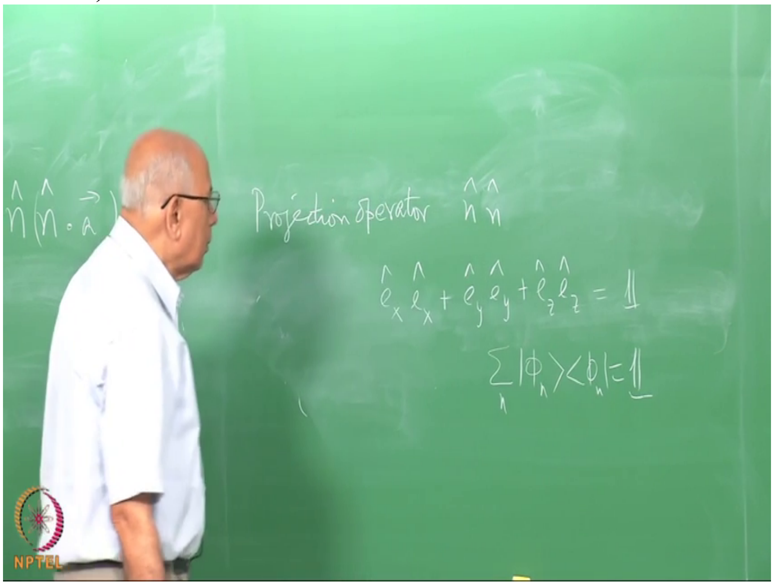

But it is the same statement out here.

So it is clear that written in tensor form, this fellow is being written as n i n j in tensor form.

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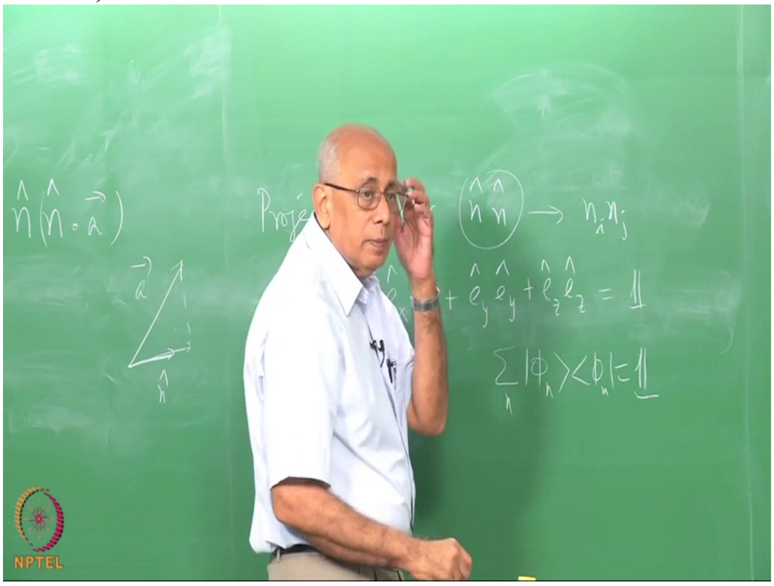

And the complementary part of it, if you for example, take n to be e x, the rest of it is this fellow which is 1 minus this guy here, so 1 minus n n is the projection in the plane perpendicular to n of any vector, the transverse components which you may further resolve into 2 orthogonal components, but it doesn't matter. This is the complement. This multiplied by that must be zero.

When you project in some direction and when you project in the orthogonal direction, when you operate the two, it must be zero. So this fellow written in tensor form is of course delta i j minus n i n j. So that's what we have been doing all along. So this part is a longitudinal part, this is the transverse part. Now it is crystal clear

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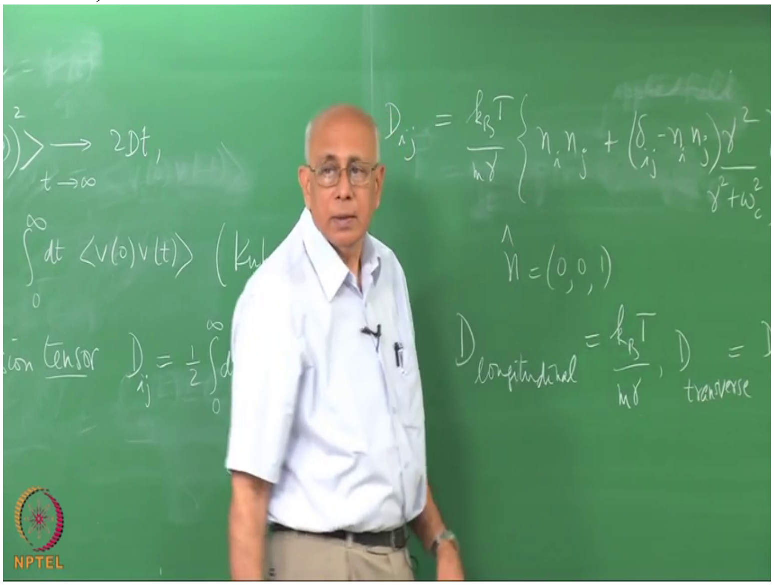

immediately. So this is the longitudinal part, and this guy here is the transverse part of this tensor,

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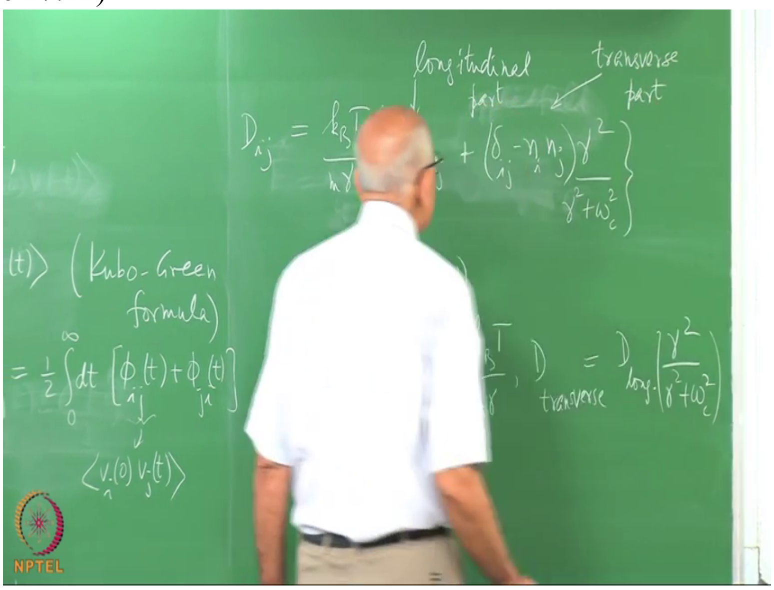

So in 3-D free particle, free particle, free Brownian particle namely no, for this fellow the conditional density v at time t given an initial velocity v zero, this is just the generalization of the Ornstein-Uhlenbeck distribution written component-wise and multiplied together, three Gaussians and you end up with m over 2 pi k Boltzmann T, 1 minus, you have minus 2 gamma t, that is how the variance goes, this whole thing to the power 3 halves, exponential of minus m into v minus v naught vector e to the minus gamma t whole squared, that is how the mean drifts to the origin. There is a vector here, divided by 2 k Boltzmann T times this quantity for the variance.

That's the 3-dimensional Ornstein-Uhlenbeck distribution, Ok. Now the question is what is this in the presence of a field?

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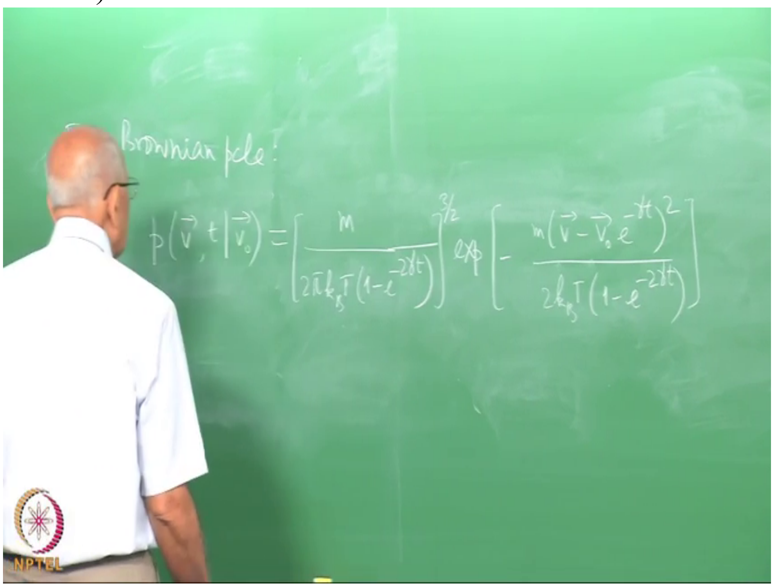

What would this be?

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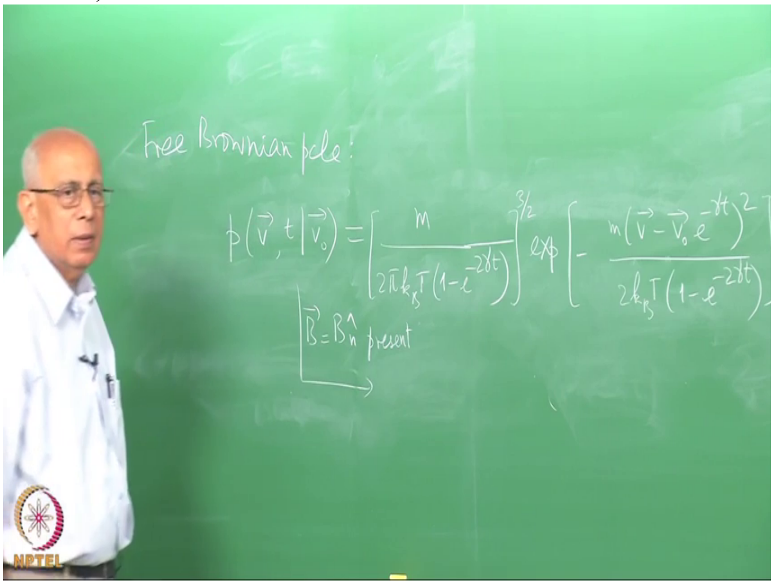

I am already telling you that this remains a Gaussian, that the asymptotic distribution is still the Maxwellian, that the dissipation is taken care of entirely in this factor gamma t; that this will not change. This doesn't change. None of this changes. How does the field show up? What will it do?

(Professor – student conversation starts)

Student: k B T by m … 0:30:32.4

Professor: So think about this in this fashion, whatever be v naught, this distribution is finally going to go with this kind of square, Gaussian in this fashion here. So when you start with some vector, this velocity, and as t tends to infinity, the average velocity is going to shrink to zero. This is the mean, instantaneous mean for the given v naught. So clearly this vector is reducing in length due to dissipation.

That feature 0:31:10.4 is still going to be true, right but as it reduces in length due to collisions, this mean value, what else will it do? It will rotate round the direction of the field, Ok. And how does it do so?

Student: omega c

Professor: So it will rotate with a cyclotron frequency about the direction of the field, right? And how do you implement that? I already wrote down an expression when we derived this correlation function. I already told you that we exponentiated the generator of this rotation matrix which was m omega c t and that is how it relaxed and that gave you terms proportional to cos omega c t, sin omega c t etc. So in the presence of the field exactly the same thing goes

through and this is now intuitably clear. Whatever I am going to write down will be intuitably clear.
(Professor – student conversation ends)

p is present then p of v t v naught is equal to the same thing but you don't get this here. You get a certain u here which will of course depend on t and v naught and then there is e to the minus gamma t. That's the effect of the dissipation,

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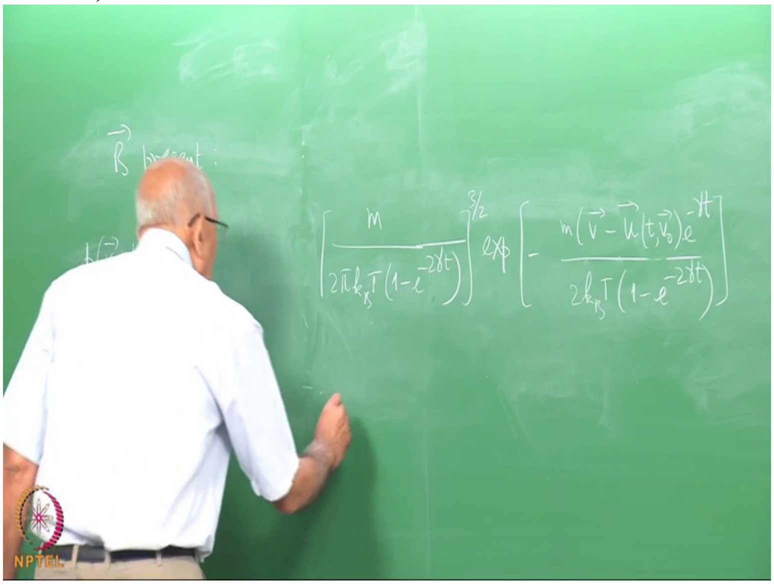

Ok. And this u of t v naught, at any instance of time, it is rotating round the direction of the field. It starts at v naught at t equal to zero and rotates round, precesses round along the direction of the field.

So that comes about by e to the power M omega c t acting on v naught. Take this to be a column vector and take this rotational matrix and since it is time dependent, there is a t dependence here and that's it. That will tell you how,

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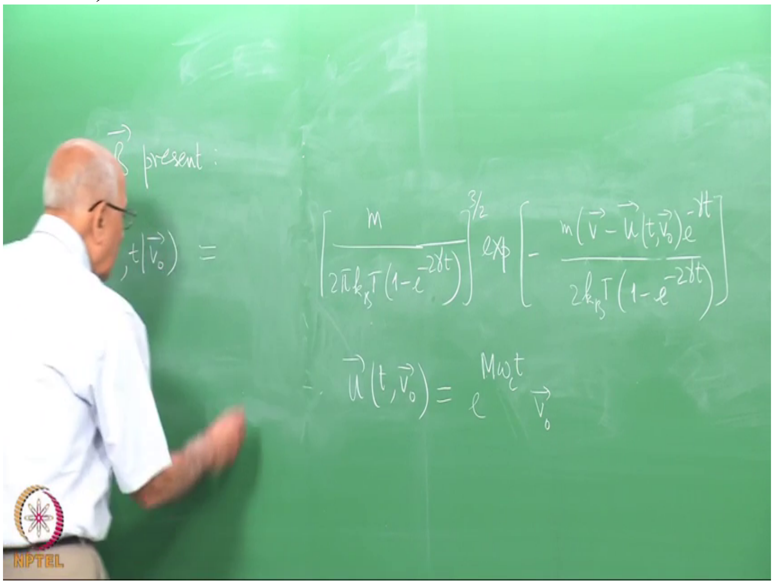

if you started with v naught, this vector and this is the direction of the field, how this vector precesses around it. This is what this

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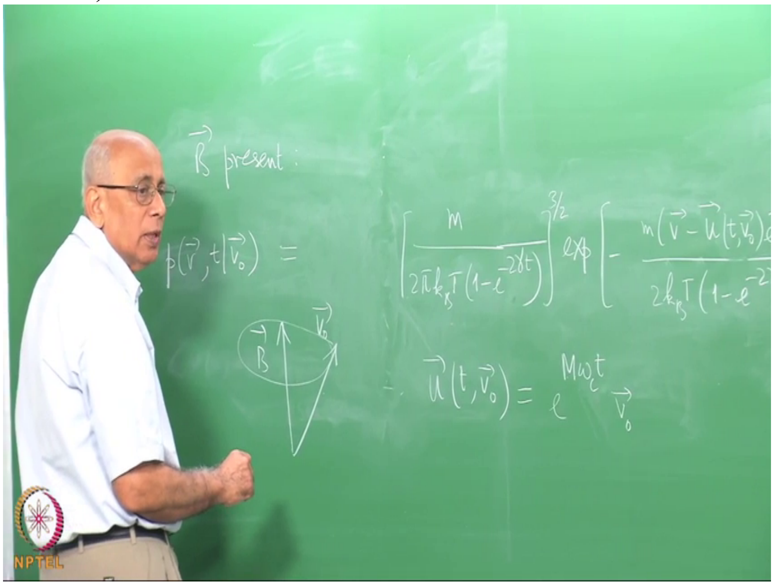

portion does.

Simultaneously its length is coming down according to this factor. So it is this thing here squared, and that's the answer.

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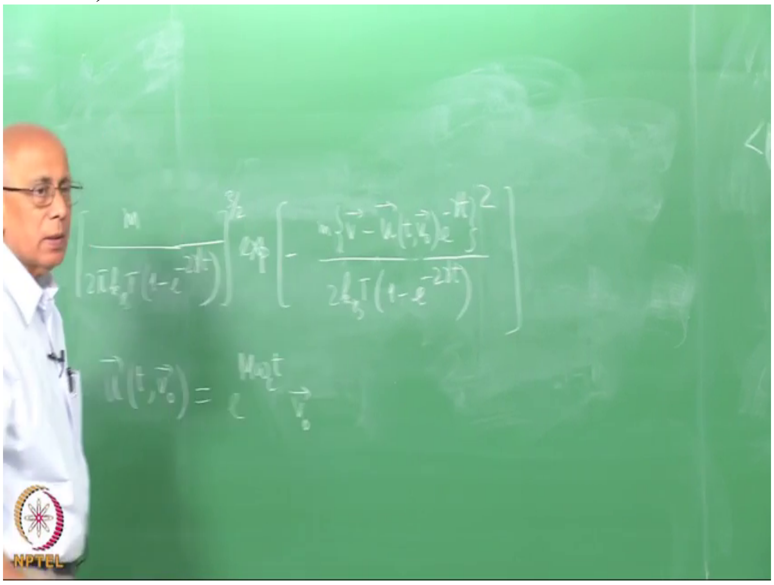

But we can write this down, because remember M cube was minus M, so the exponential can be computed and not surprisingly this is equal to the identity operator plus M sin omega c t plus M squared cos omega c t acting on v zero 0:34:35.0, Ok.

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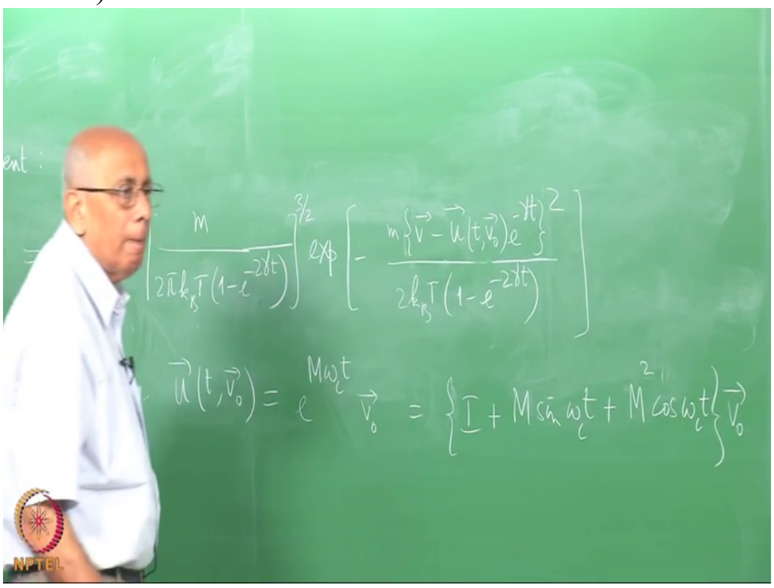

So that's what, and you can work this out, I leave you to figure out, simplify this, and write down what it is. I am not 100% sure about the factor here plus or minus but you can check this out, I believe this is M 0:34:59.0 but you can check this out explicitly. Is it 1 minus omega c t? I think so.

(Professor – student conversation starts)

Student: 1 minus cos omega t

Professor: Yeah it is 1 minus cos omega c t, that's right, for the same reason as before.

Student: i minus n, minus n sign, minus sign

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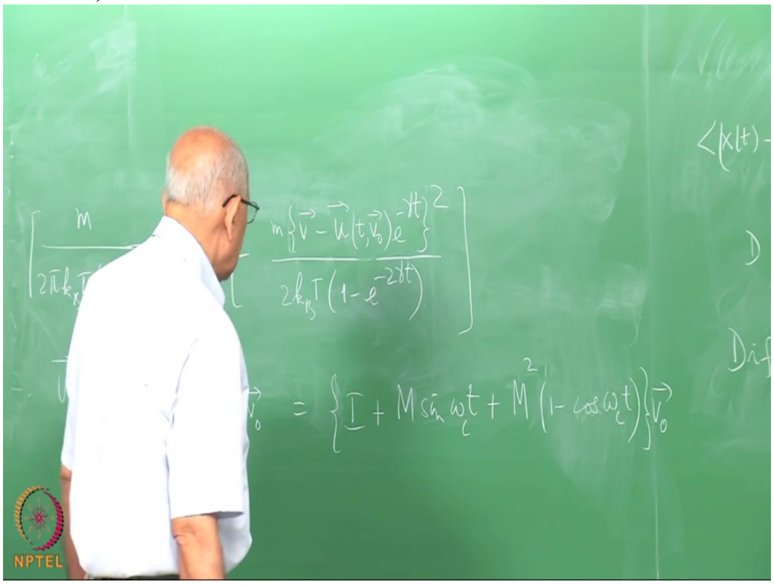

Professor: No, M cubed is minus M so that brings in the minus.

Student: e to power minus m omega t.

Professor: Whether this is plus or minus?

Student: That was minus

Professor: This was a minus? Check this out

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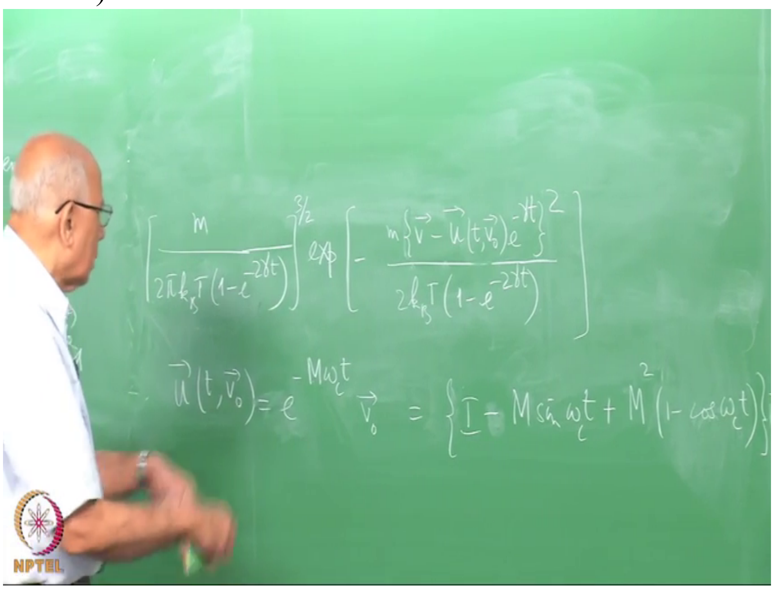

explicitly but this is physically clear what is happening. This is the interpretation and that's the way the Ornstein-Uhlenbeck distribution gets modified. As t tends to infinity, you can see that this goes away and you are back to the Maxwellian. So this is a very, very, very appealing physical picture that in the presence of the field, the velocity keeps doing this but because of the particles colliding against it, it damps out to an average value of zero while it is, so it is some kind of helical motion which goes to zero, Ok.
(Professor – student conversation ends)

We haven't yet written down the differential equation of which this is a solution. We do that. We will have a general formulism to write it down and we will be able to write it down in the presence of the magnetic field. It is not very hard, quite straight-forward so we will do that eventually. So we will stop here with this. In fact we will stop here with the Langevin model itself and now start with the formalism of linear response theory so that we can handle these questions much more generally even without a specific equation of motion like the Langevin model.

So we will start now our study of linear response and again I have to say what our target is. We start by assuming that, so our problem is the following. The general class of problems is the following. We start by saying that we have some system which is described by Hamiltonian,

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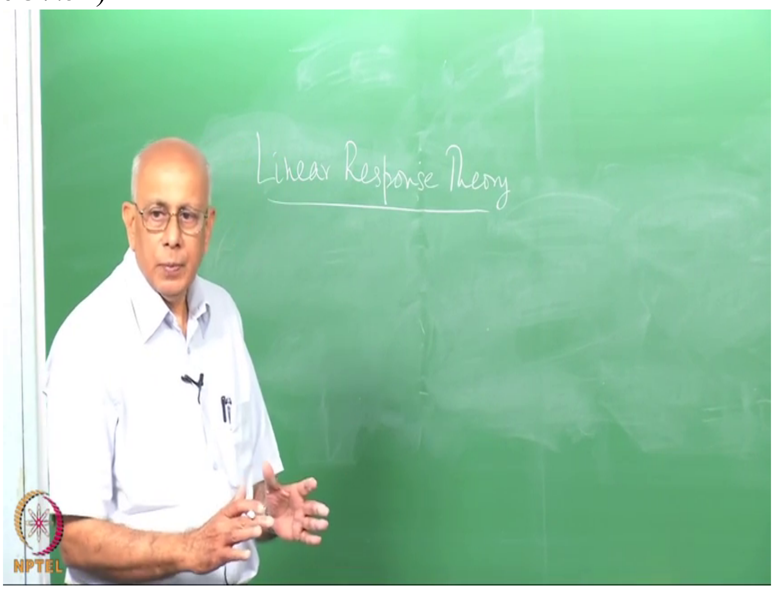

which is time independent and the system is in thermal equilibrium at a temperature beta in contact with the heat bath. So the system consists of, this is described by some Hamiltonian H naught, unperturbed Hamiltonian and it is a function of some dynamical variables, qs and ps. We will

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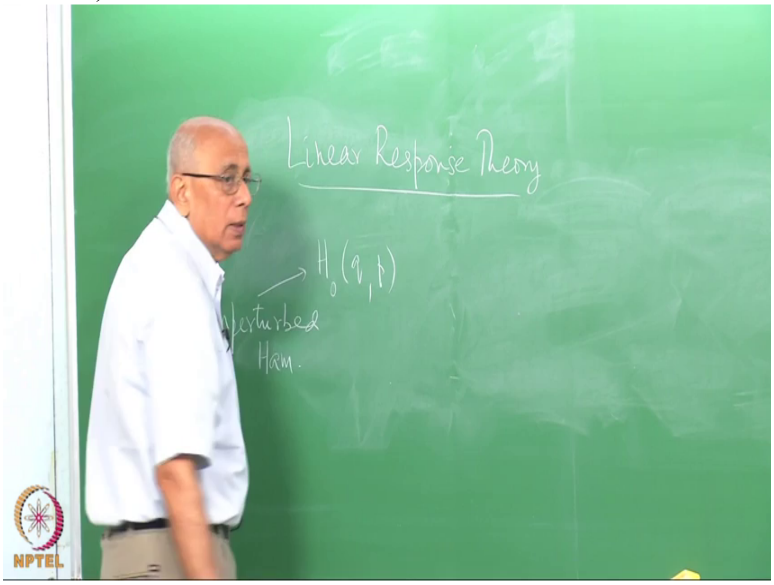

also look at the quantum case simultaneously. Whenever there is a quantum case coming up, I will say so explicitly. But we will look at both these simultaneously because there is a formalism which applies to both of them. The only difficulty is in quantum mechanics, you know that different observables are represented by operators and some Hilbert space and these operators don't necessarily commute with each other. And the whole essence of quantum mechanics is in the non-commutativity of this whole business. Capturing that by any classical manipulation is not possible in any simple way at all. So this is intrinsic quantumness, if you like, the non-commutativity and we have to use operators to describe that, Ok.

We will take adequate precautions for that. But to the extent possible, we will develop formulisms in the matched way, and the way to do this is to say, in classical mechanics, we would write down Hamilton's equations of motion and then we deal with Poisson brackets and so on, in quantum mechanics we write down the Heisenberg equations of motion or observables directly and you deal with commutators instead of Poisson brackets, Ok. As opposed to the usual Schrodinger equation where you write down an equation of motion for the wave function itself, for the state vector itself, that's the so-called passive picture.

But when you do classical dynamics, you hardly ever do that. You hardly ever say in classical mechanics, when you are looking at the particle or a body moving, you don't talk about the distribution of probability density in phase space or anything like that. You write directly the dynamical variables and write their equation of motion and all, the active picture.

In quantum mechanics, the conventional way of doing it using the Schrodinger equation is to go and look at the passive picture. So you make a statement about the way the state vector evolves and the state vector is supposed to give you probability densities and so on with some further manipulations. So you are making the statement about how the distribution evolves and you say the dynamical variables themselves, the averages are computed with respect to that changing distribution. That's the passive picture which is very natural in quantum mechanics but it is very artificial in classical mechanics. But these are completely equivalent to each other as we will see as we go on. So we will mostly use the Heisenberg picture in quantum mechanics or the corresponding dynamical evolution by Hamilton's equations in classical mechanics.

So the general problem I have is the following. You have an unperturbed Hamiltonian. But this system is now in contact with the heat bath at a fixed temperature and is in thermal equilibrium. So physical quantities are evaluated, average values of physical quantities like some, let's call it some observable B which is in general the function of the qs and ps of the system, it would have any number of degrees of freedom. This collectively denotes all the generalized coordinates, all the generalized momenta, conjugate momenta, the average value in equilibrium, to avoid confusion let me well necessarily write this outside, this is equal to, in the canonical ensemble, it's equal to formally trace of a density matrix through equilibrium B divided by trace of rho equilibrium. This is the average value in equilibrium.

I presume you are familiar with this formula. This is equilibrium statistical mechanics. Is everybody familiar with this, comfortable with this? You could ask what's meant by trace. Of course if I write the usual quantum mechanical sense where I write finite matrices for these traces, for these operators then it is very clear, you take the diagonal elements and sum them up. But what do we mean by it classically?

What I mean by this

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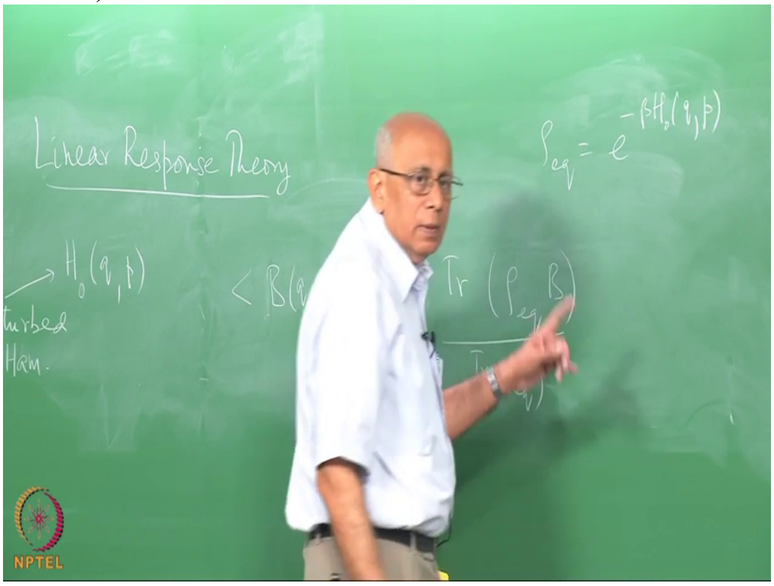

is this rho equilibrium is e to the minus beta Hamiltonian of q and p. That is the equilibrium density matrix, density operator and this stands for integral d q over integral d p over all the qs and ps, over all of phase space

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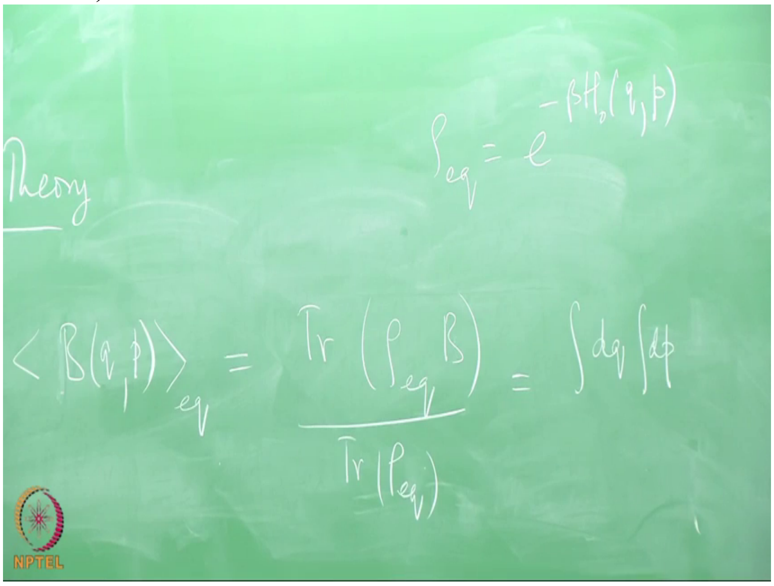

times B of q p e to the minus beta the Hamiltonian H naught of q p divided by this fellow here is d q integral d p e to the minus beta H naught of q and p.

This is the normalization factor, average, statistical

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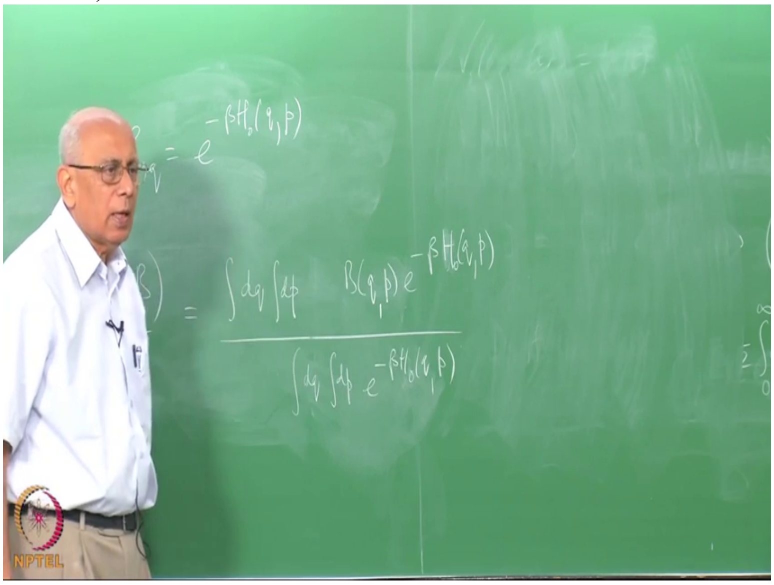

average and the idea is that in the canonical ensemble the weight factor

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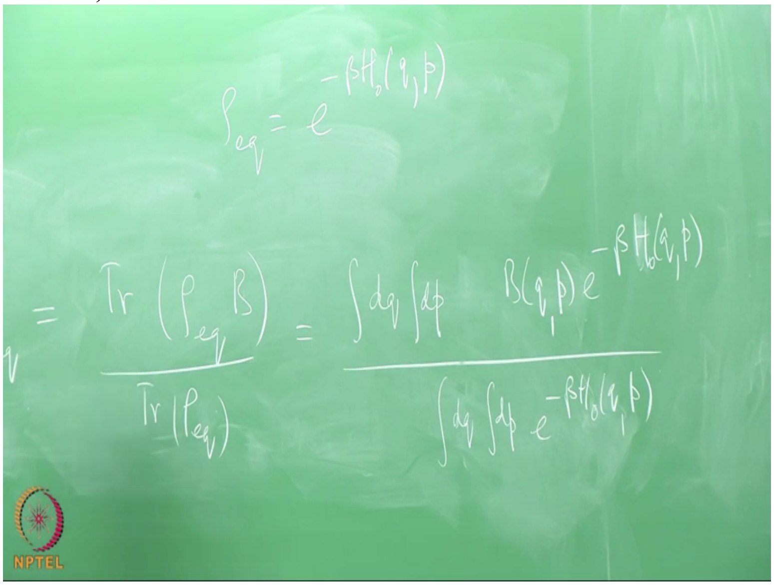

in free space is e to the minus that Hamiltonian over k T. beta will always stand for 1 over k Boltzmann T, the inverse temperature always. I will try not to use beta for any dynamical or any other variable or parameter,

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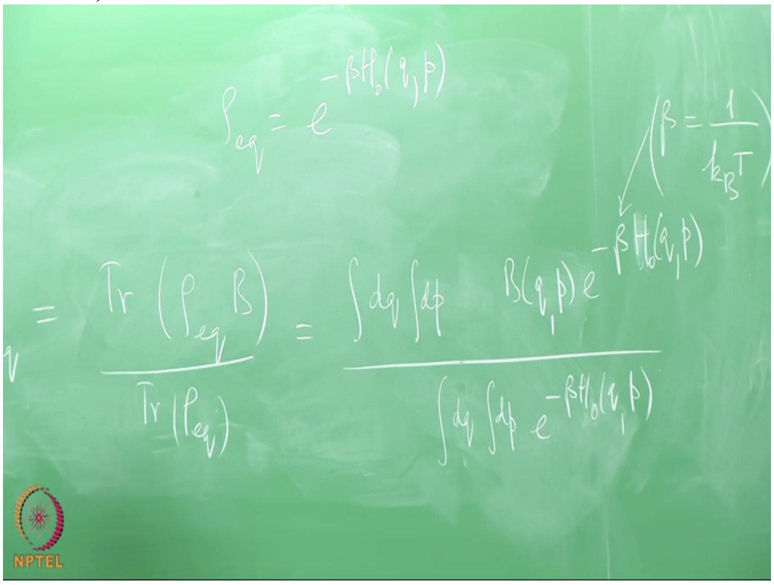

Ok.

So this is what is meant by the trace in the classical case. All integral or all phase space this fellow here, now this term, this fellow here is just in fact the normalization factor 0:44:02.4 for the probability.

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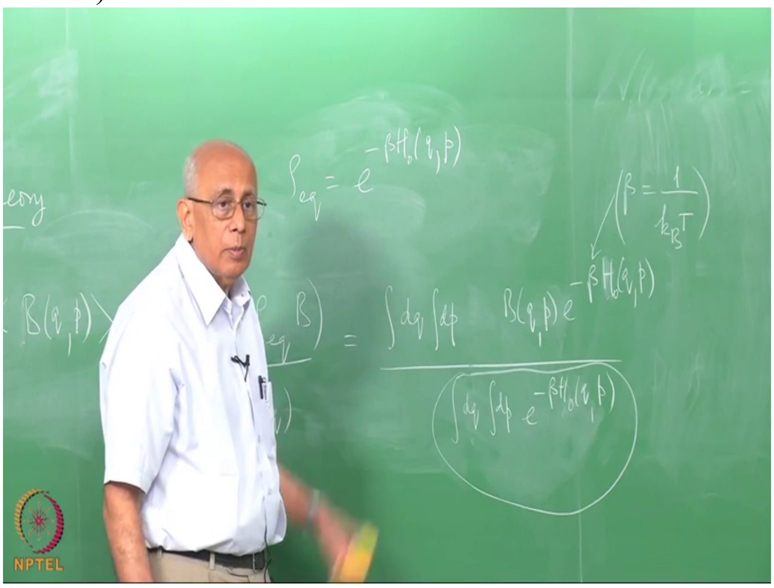

So you could 0:44:05.0 in the density operator by saying this divided by this number here, is in fact my probability distribution. Then it is a normalized probability density function. There is a name for this.

What do you call this in equilibrium statistical mechanics? It is the canonical partition function, this fellow here, this integral, is Z canonical.

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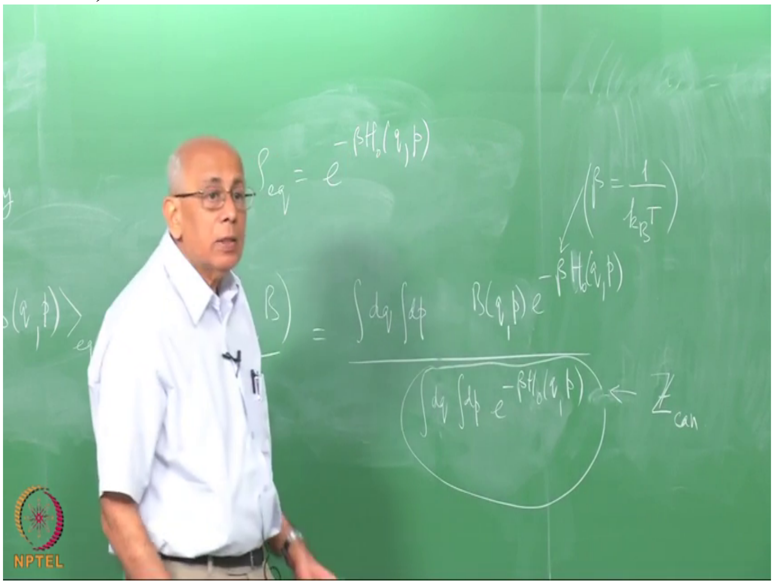

It is not a function of qs and ps because they are integrated over. It is a function of the temperature, this parameter. So putting a system in contact with the heat bath drives fluctuations into it and we don't need to know what this heat bath is actually made up of. We don't need to know the details, what are the degrees of freedom and so on. The entire ignorance of heat bath is subsumed in a single parameter called the temperature.

So this is the canonical, of course if you do this in a finite volume and things like that with a fixed number of particles then it is a function of those variables as well, microscopic variables. But we are going to look at the case where I put this equal to 1, so I put this trace rho, I am going to put trace, from now on I take trace rho equal to 1.

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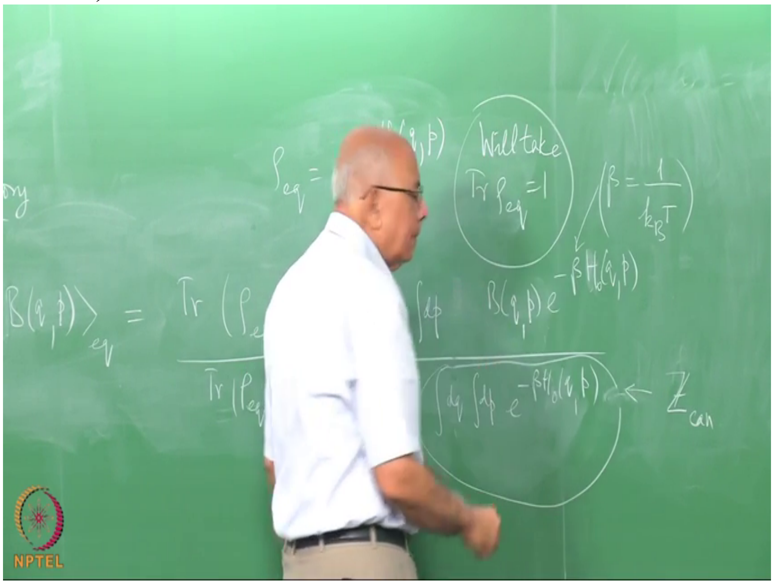

I will redefine my density operator in such a way, if this is divided by that number so that the whole thing is traced out to 1, Ok.

Now remember that when we do quantum mechanics, I am not assuming that the system is in any one pure state. So when it is in finite temperature, you cannot associate with it in general, your state namely state vectors and Hilbert space. You can only associate a statistical weight to it and that's given by the partition function Ok, by this, the density operators. So this is what we are going to do. So this is what it is in equilibrium; and now for the problem.

The problem is we are going to say this fellow gets perturbed, the perturbed Hamiltonian is some H of q. p and possibly t which will in general be H naught of q and p plus a perturbation which I am going to regard as small in some sense and it involves some operator A of q p times the time-dependent c number force, so F external of t, then we explicitly say it is an applied force here. And A is some dynamical variable pertaining to this system to which this force couples, through which force is coupled to this system, system couples with the external force, Ok.

Now you could ask, why this minus sign? Suppose it were a mechanical force, right, then the force on the object is F external of t. Then I associate a quote unquote a potential with it which is minus x times this F external if it is one-dimensional motion. Then minus d over d x of this fellow is supposed to give me the force and of course that will give me F external. And this term has dimensions of an energy, quote unquote a potential energy even though there is a time dependent force here.

So to keep track of that, I have a minus sign here, no other reason. And to take care of the fact that this could be a very general kind of force, not necessarily a mechanical force coupling to the displacement, I have a form like this in general. So A refers to the, of course there could be several forces, maybe I have A i, F of i, that is a generalization which is trivially taken care of.

So this is the general form

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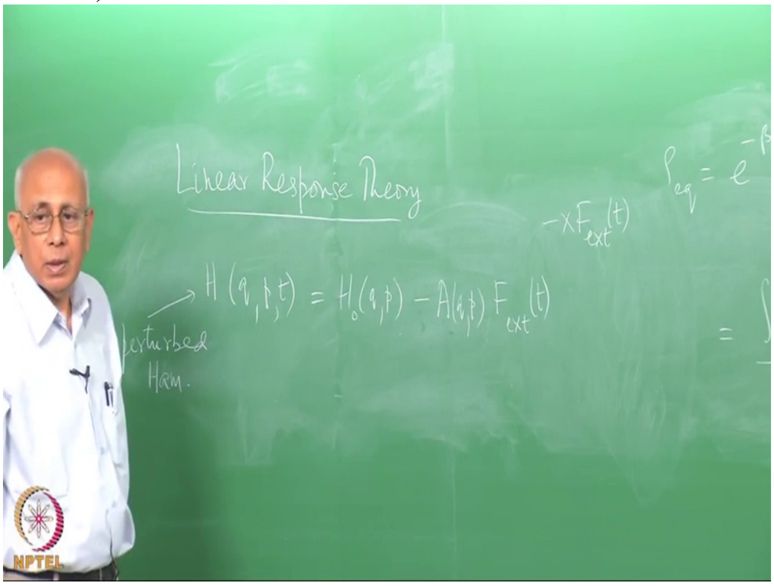

which we have but in some physically measurable sense this is supposed to be small compared to that and now I want to know what happens to averages. So I take any other quantity B and I ask B equal to what? This will of course be a function of t.

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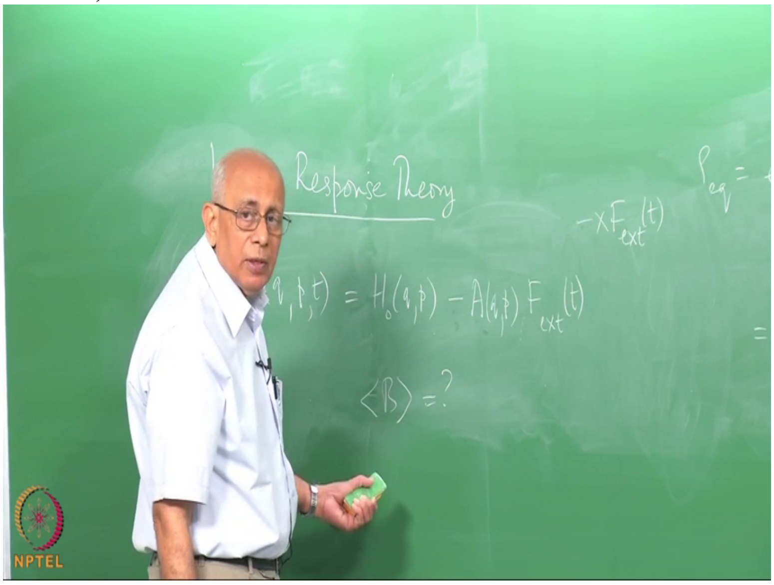

So I would like to know what function of t it is. So in general, this fellow is going to be of the form B equal to B in equilibrium which is what it would have been using this rule, yeah, plus a delta B which is going to be a function of t, some average value and the whole point is to find this.

So this is our target. We will choose all kinds

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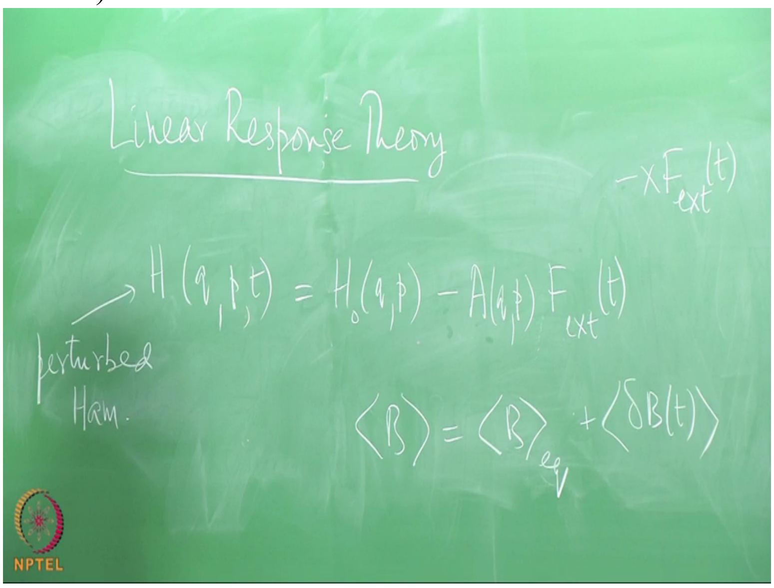

of As here, all kinds of Bs here. B could be A itself. You could ask what happens to A itself. So that's the general problem. And we are going to work to first order in this perturbation, so everything will be to first order in this external force, and then the assumption is, if this is very small, first order term alone, then this is infinitesimal or first order alone which is why I put a delta here. That's a rationale of this, Ok.

And the target is to find this under very general conditions. This could be classical, this could be quantum mechanical, this could be horribly complicated; we don't care. We are going to try to find the formulism to tell me what this quantity is, Ok. So here onwards that's our target to do this, so let's see where it takes us. Ok.