Nonequilibrium Statistical Mechanics
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Lecture No 04
The Langevin model (Part 3)

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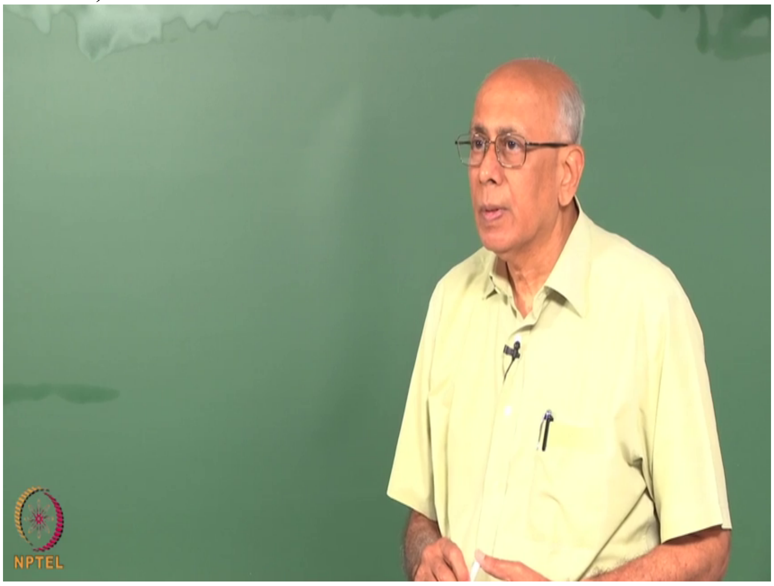

So let's resume our discussion of the velocity process for Brownian particle in a fluid. And just to recapitulate very quickly what we discovered, we found that when the particle obeys the Langevin equation then its velocity process, this random process driven by white noise, Gaussian white noise is exponentially correlated.

So we discover that this quantity v of t naught, v of t naught plus t was a function only of time difference t between these 2 arguments and this was essentially equal to k B T over m e to the minus gamma t in this fashion. So I might as well set

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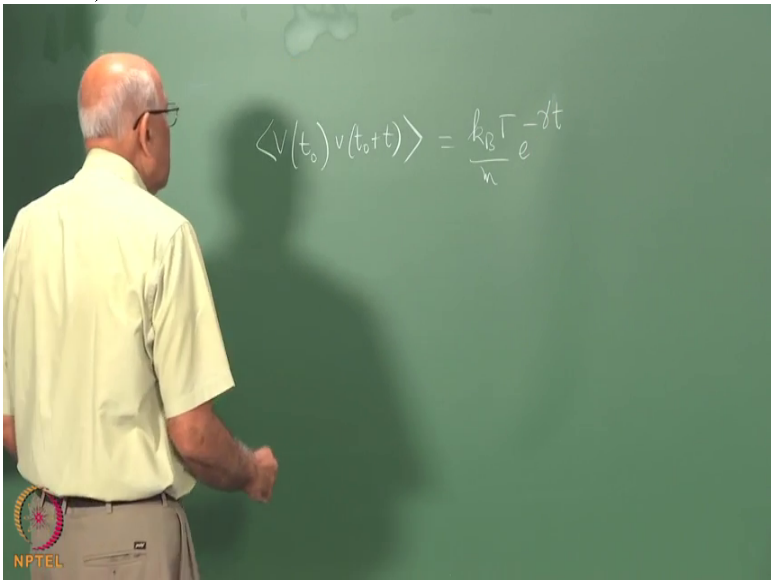

t naught equal to zero and write it as v of zero v of t equal to k B T over n e to the minus gamma t.

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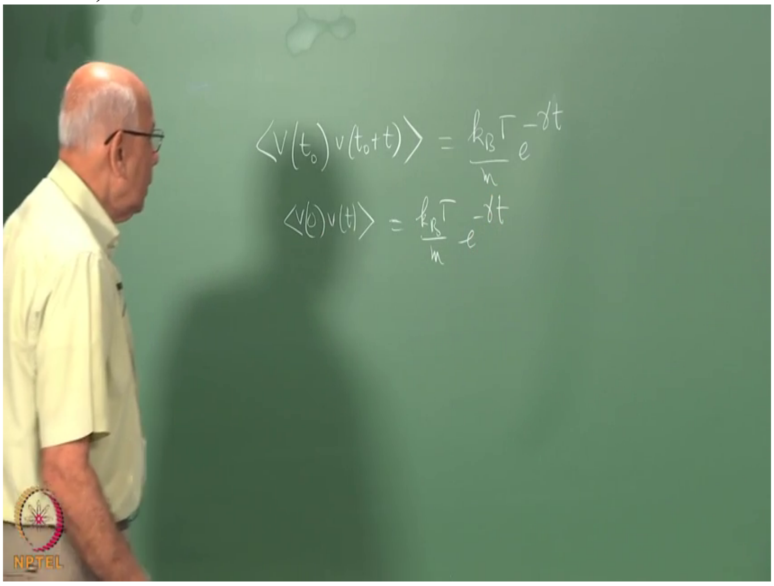

Now we also saw, I am not sure if we proved this but we also saw using stationarity that this very trivially implies, if I subtract minus t from each of these arguments, this also implies that v of minus t v of zero, I set t to minus t here is going to give us modulus there. So in general, it is clear that this quantity satisfies this expression,

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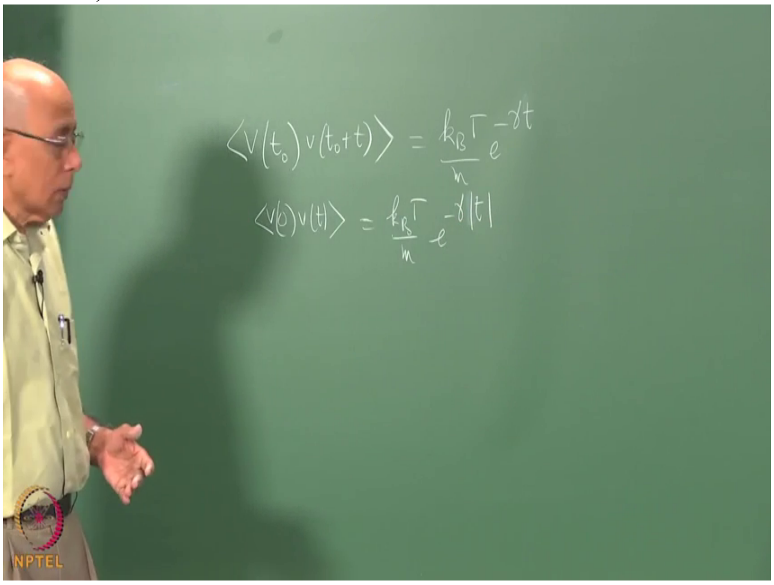

Ok.

So it is a symmetric function in t and it dies down exponentially on either side of the t axis, Ok, in equilibrium. We further that as a consequence of this, by the way this implies that there is a time scale in the problem, gamma inverse which we could actually estimate by using the fact that we put this particle in a fluid with viscosity eta for instance and it has a radius r, then we saw that m times gamma was equal to 6 pi r eta where this is the viscosity of the fluid and this is the mass of the particle

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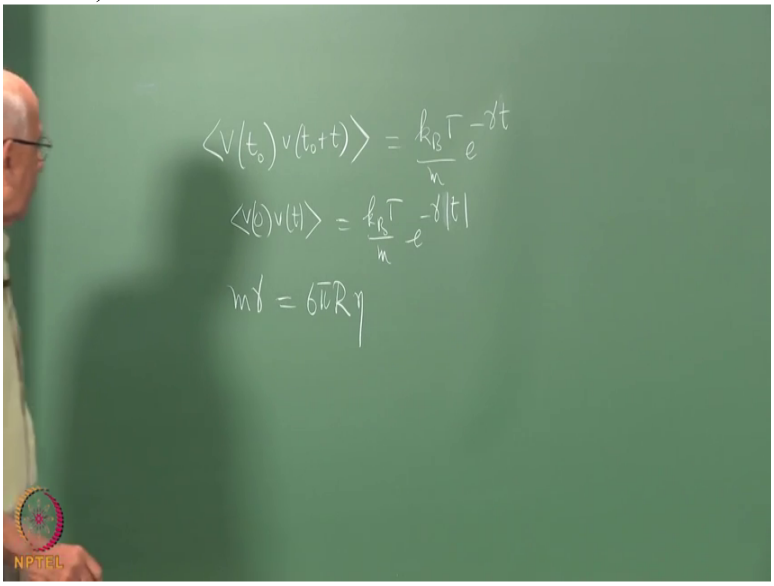

and if you estimate this mass to be of the order of 10 to the minus 15 kilograms, gamma turns out to be of the order of 10 to the minus 6 or 10 to the minus 7 second inverse, so gamma inverse turns out to be about 10 to the 6 or 10 to the 7, r micron sized particle 10 to the minus 6, eta is 10 to the minus 3 in SI units, Standard International units, newton second per meter square or something like that.

Then we discovered that there is a time scale in the problem which is of the order of microseconds or tens of microseconds and we must compare it to the other time scales in the problem. The other time scale we have is actual interaction time between molecules and that is of the order of 10 to the minus 15 seconds or less and then there is a time scale between collisions of particles. That is of the order of picoseconds or less and this time scale is another 6 orders of magnitude higher.

Now of course you can consider times much, much greater than gamma inverse and that's the diffusion regime in which the mean square displacement of the particle goes linearly in time with the diffusion constant, this coefficient D given by k T over m gamma;

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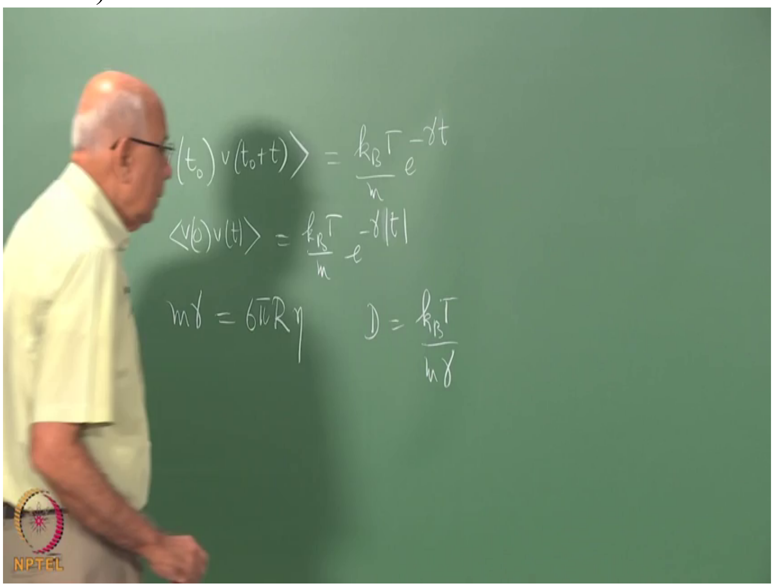

the diffusion coefficient of this massive particle in the fluid, not of individual molecules.

We also discovered as a consequence of this expression, we could actually write down what the displacement is, the mean square displacement is, and we found that if you define an X of t to be equal to little x of t minus x of zero and you computed the

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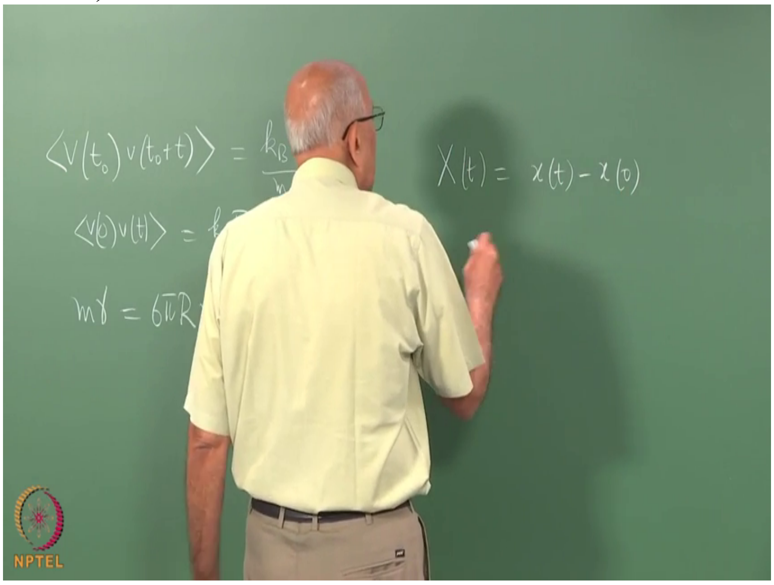

mean square value of this quantity X squared of t, not the conditional mean but the actual mean of this quantity, computed the full equilibrium average value of this quantity, then this turned out to be k B T over m gamma square times gamma t minus 1 plus e to the minus gamma t.

That was the exact expression and all we needed was to use the fact that the position is the integral of the velocity and that's it. So with that we immediately got an expression which went like this. This of course goes for gamma t much, much greater than 1 to twice d t where d is given by this expression

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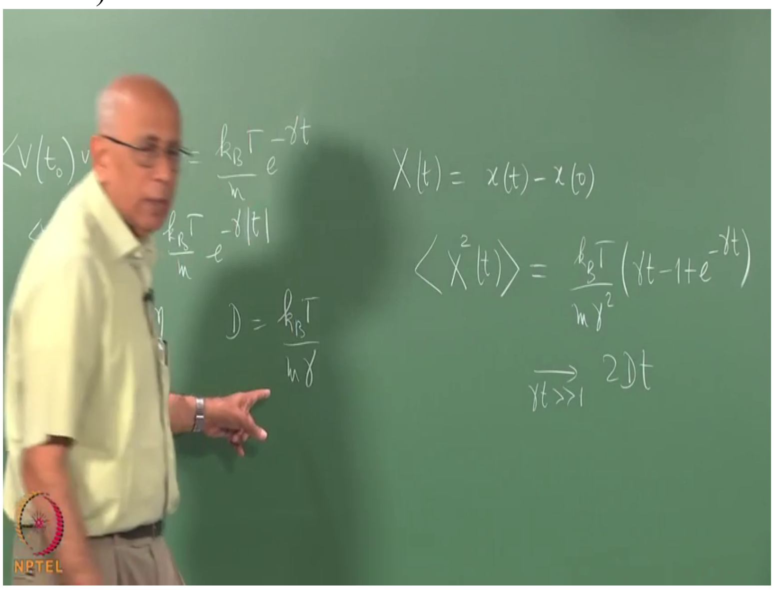

here. In other words that's the diffusion regime.

But for all times it is exactly equal to this, in this model as far as this model goes. Now you can ask further questions of this. You could ask what does this quantity itself do for instance and what's its average value and so on. I am going to leave this as an exercise, just one step, first step for instance if you compute what is X bar of t, this is the conditional average, the conditional average for a given v naught and a given x of zero, then this is easy to find.

Notice that a simple integration immediately gives you x of t is equal to an integral from zero to t d t 1 v of t 1,

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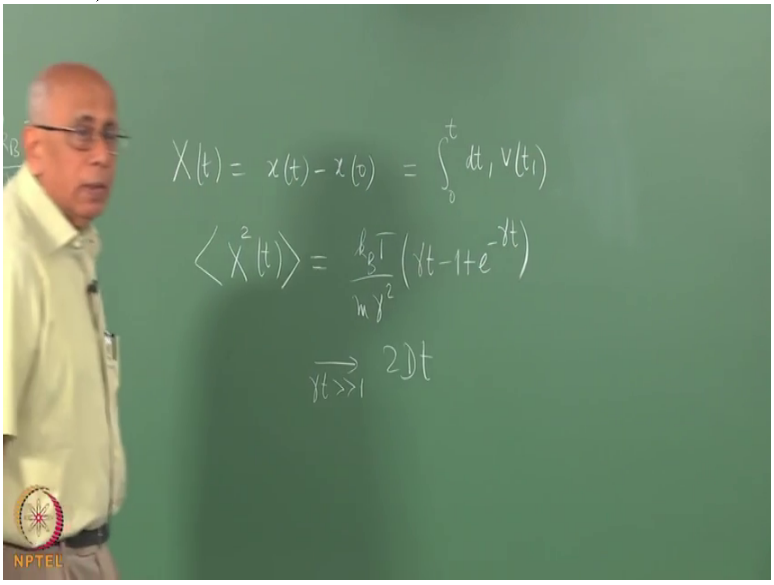

and we know what v of t 1 does, the conditional average, this quantity v of t 1 bar is equal to v naught e to the minus gamma t plus the portion that depends on

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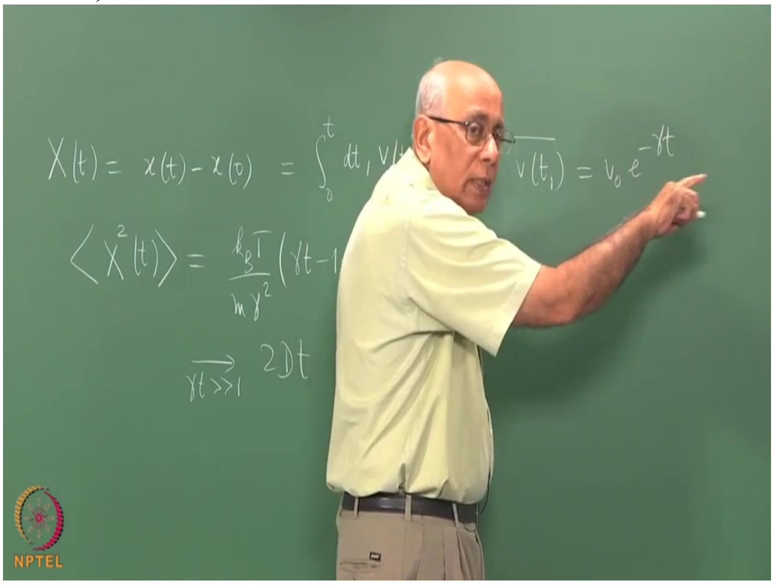

the initial, depends on the random force, the eta and that averages to zero.

So if I compute this integral here, this thing becomes equal to, all that I need to do is to plug this in, v naught over gamma 1 minus e to the minus gamma t. All I have done is to substitute

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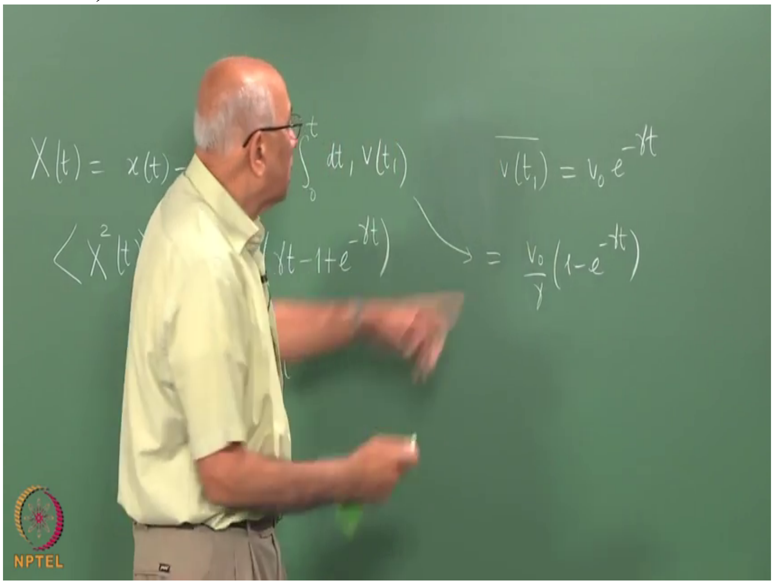

this expression here and compute it here and this is equal to X bar of t.

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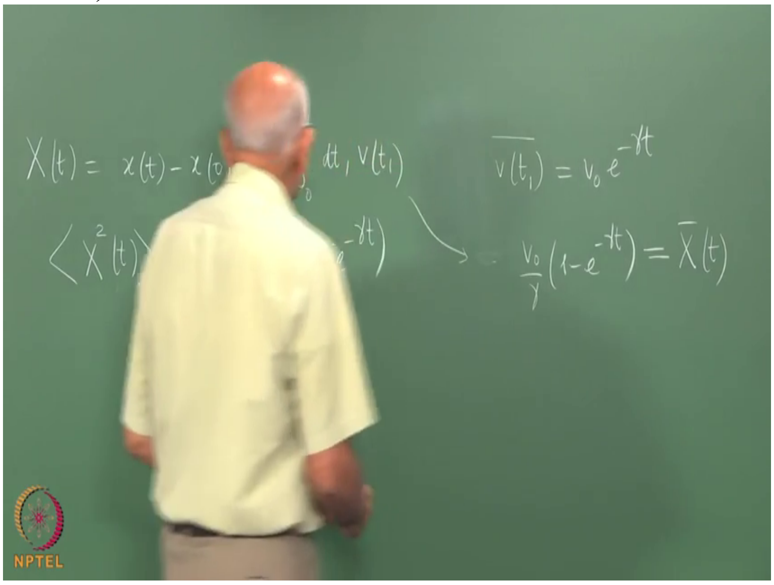

So the average value, conditional average of the displacement is this quantity here, Ok.

Of course if I take a full average now over v naught, it will vanish as it should. The displacement should vanish. Having got this, you can now ask what's the variance of this quantity. Not of this quantity itself but the deviation of this quantity from its mean. So the natural definition of delta X of t, capital X of t would of course be X of t minus the average value, the conditional average of X of t.

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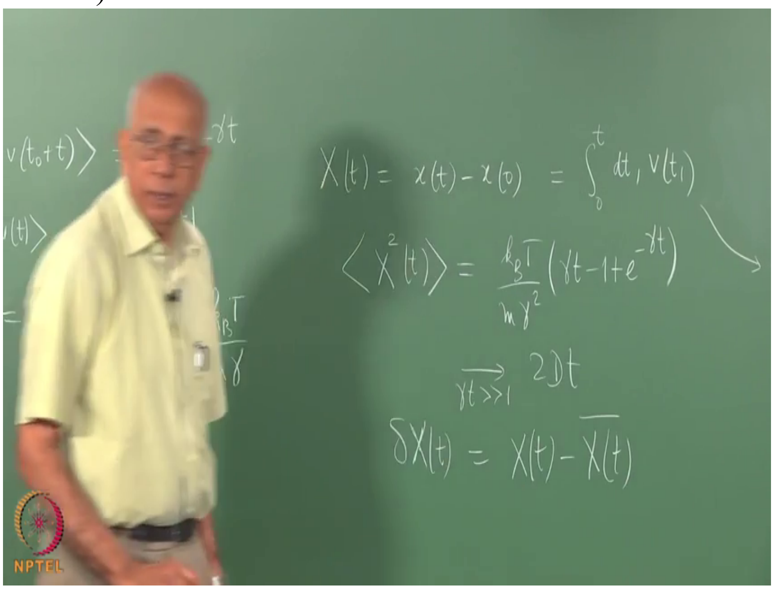

That's obviously the natural definition of the deviation from the mean of the displacement, not the position but the displacement itself.

And then one can ask what is delta X of t whole square, the full average? You have to take the quantity, square it in the usual way and take the full average. If you use this fact, what we need is information about this X bar of t obviously in this expression. We use that information in, then it is not hard to show that this becomes equal to d over gamma times, oh incidentally, we could also have written this as d over gamma times gamma t minus 1 plus gamma e to the minus gamma t, I would substitute d equal to k T over m gamma here.

So if I do the same thing here for this variance, then this is equal to, this turns out to be equal to, not sure if I remember this expression completely but let's see if I can mentally write this out, 2 gamma t minus 3 plus 4 e to the minus gamma t, yeah I remember that part of it, minus e to the minus 2 gamma t which comes from squaring this fellow, Ok.

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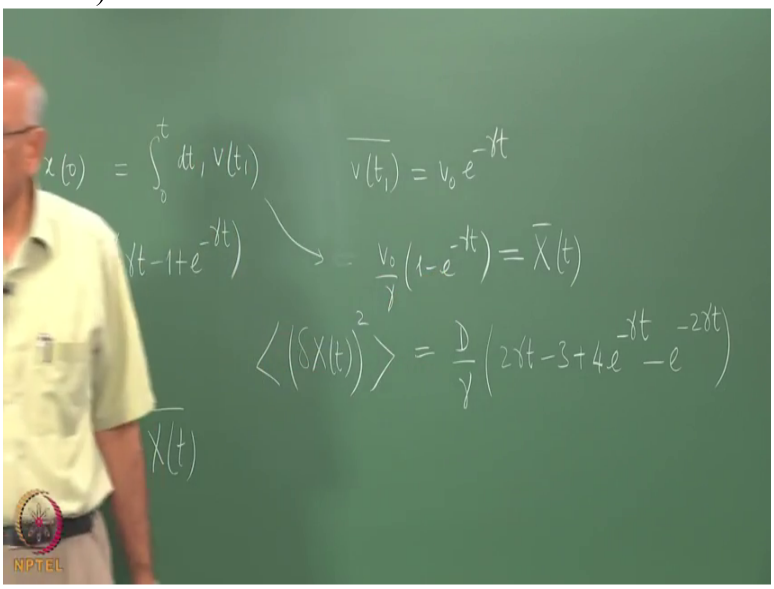

So you get some expression like that for the variance of this displacement itself.

Of course as t tends to infinity, this will go to 2 d t as it should, Ok. So if you are interested in the displacement rather than the velocity, we have this expression here. Now what's interesting is that there is no simple equation as there will be for the velocity process, there will be some kind of equation. We will talk about this equation. We shall give the distribution and probability of the conditional density, the conditional, probability density of the velocity, we are going to write that down shortly but there is no such equation for this.

However the very fact that the velocity is just, the position is the integral of the velocity helps you to find these things, these quantities here. You could in fact go on to find delta X of t 1, delta X of t, delta X of t prime, it is a messy expression of some kind. So we can play with this, find all these moments explicitly.

But let's come back here, backtrack a little bit and say alright this is very nice, can we say something about the probability density of v, the actual distribution of this velocity as a function of time? The conditional distribution. Starting from the fact that it, t equals to zero, it is some delta function v naught and in t tends to infinity, it should go to the Maxwellian distribution. Can we write this distribution down?

We are going to do that a little later when I show you that there is a correspondence between the Langevin equation for the variable itself and an equation called the Fokker-Planck equation for the conditional probability density. There is a complete one-to-one correspondence in certain cases and we will exploit that. But right now I want to write the answer down and introduce you to this distribution which you would have seen in other context perhaps but let me show you what this distribution is. We can simply write it down in this particular case and it is as follows.

So remember what we know about velocity. We know it is a stationary process in equilibrium because it is a function of t alone. In fact you can show that it is stationary in the strict sense, in other words, all its densities, joint densities are independent of the origin of time you can shift to time. At this level it is only the correlation, the two point correlation that has been shown to be so but this is true for all its joint distributions.

We know for instance, that v of t average is v naught e to the minus gamma t, the conditional average

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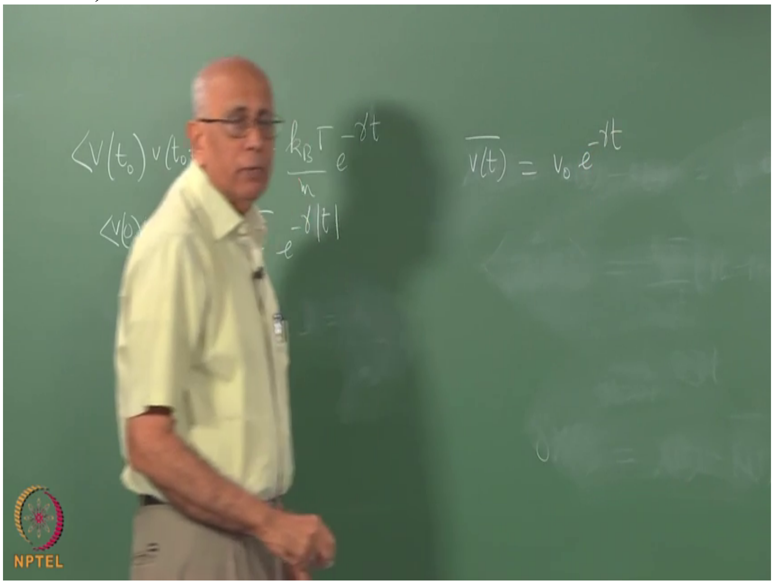

for a given v naught. We know that v square of t average; we had an expression for this quantity. We know that it is v naught square, 1 minus e to the minus 2 gamma t.

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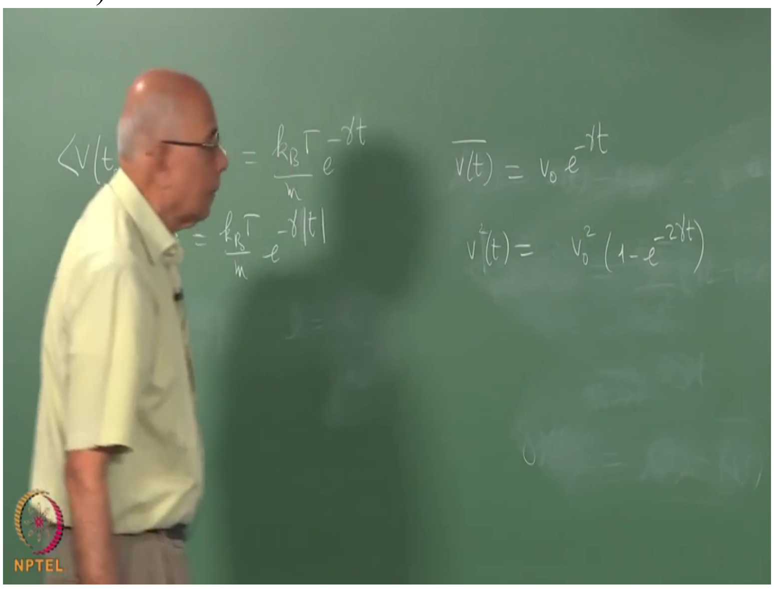

If I take its, sorry, this average, if I square, if I take the average with respect to v naught, there was an extra term here, you have to remind me what this term is, there was an extra term which also had this plus…

What was the actual expression we found out, otherwise I have to go back and start

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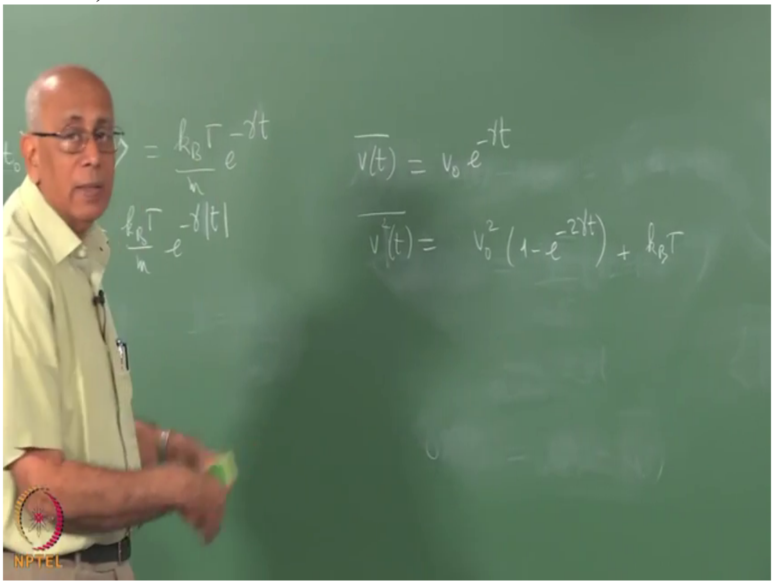

working out the algebra. What was the actual expression? As t tends to infinity, so perhaps this was correct. Average of v naught square is k B T over m. So that's Ok,

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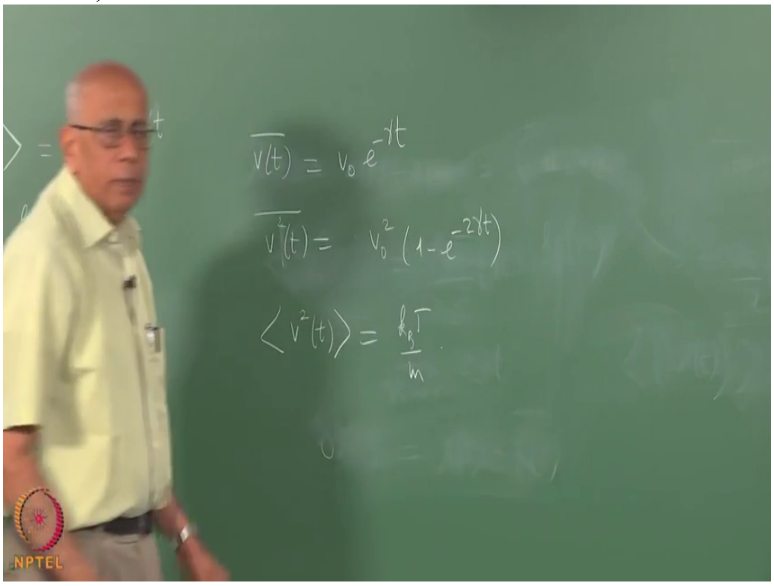

that's what it was explicitly, Ok, right? But we also put in, I am a little unhappy

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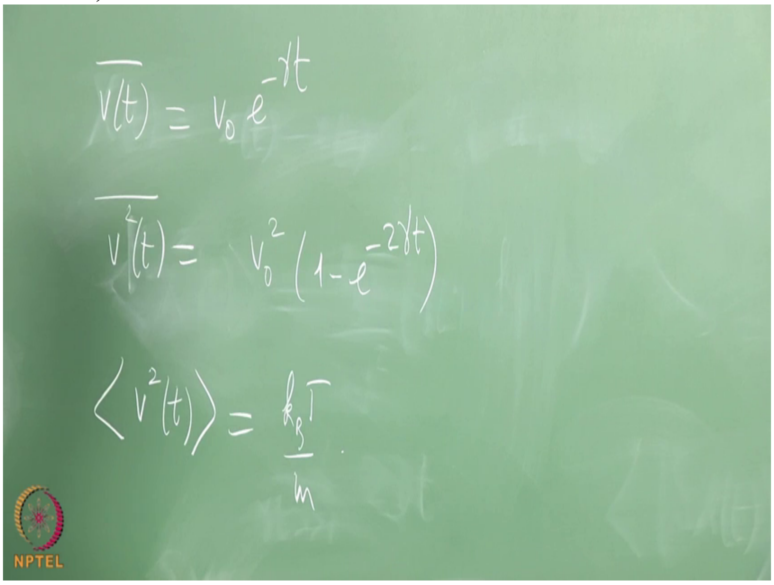

about this, what I would like to know, what I would like to do is write down what is the variance of this quantity, the conditional variance. What was the actual expression for this quantity? Is this correct as it stands?

(Professor – student conversation starts)

Student: No, there was a plus gamma like capital gamma and...

Professor: Yes

Student: We have 2 terms one involving

Professor: Yes

Student: It was v naught square minus gamma upon 2 m square gamma times e power minus 2 gamma t

Professor: v naught square

Student: minus

Professor: v naught square e to the minus 2 gamma t

Student: Minus, yeah, plus

Professor: plus

Student: Capital gamma upon 2 m gamma square, m square gamma into 1 minus

Professor: 2 m square gamma

Student: No v naught square in that

Professor: No v naught square, yeah

Student: Gamma upon 2 m square gamma into times 1 minus e power minus 2 gamma

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Professor: Good, that's it. So this is equal to, we wrote this as, by the way this quantity we know there is a fluctuation dissipation relation so it k T over m. So it is k Boltzmann T over m plus v naught squared minus k Boltzmann T over m e to the minus 2 gamma t, good.

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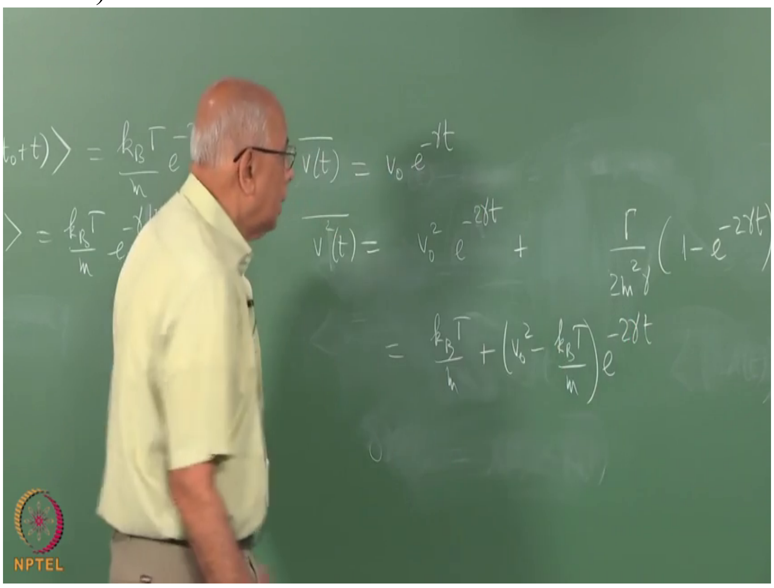

So that was the expression. So let's kill this and this was v squared of t average, exactly, exactly.

(Professor – student conversation ends)

Now we argued

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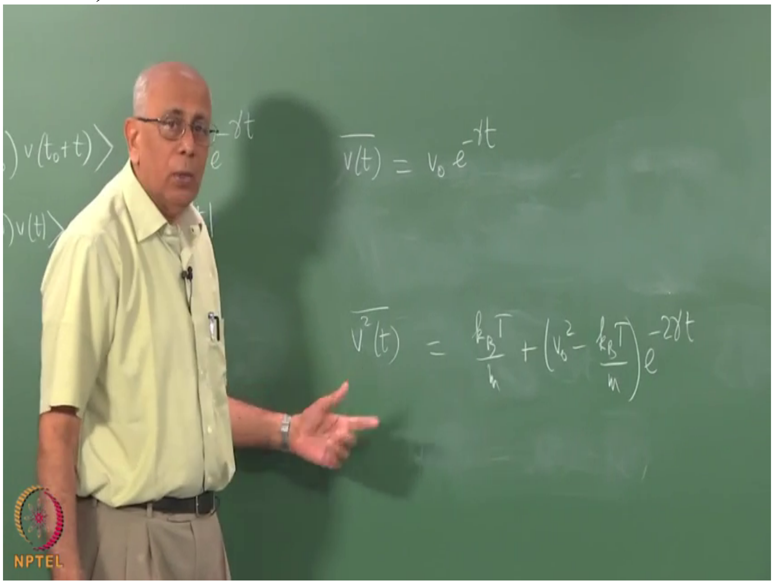

that if you let t go to infinity for a fixed t naught to start with, for a fixed origin on time, then this term goes away and it reaches the equilibrium value. On the other hand if you average this quantity with respect to the Maxwellian distribution in v naught then this gives you a k T over m and that kills this and there is nothing to average here, so it remains k T over m. This was our consistency condition, right.

So now given these two, we can compute what's v squared of t minus v of t average squared, this is equal to conditional variance of v and what is this equal to? What we need

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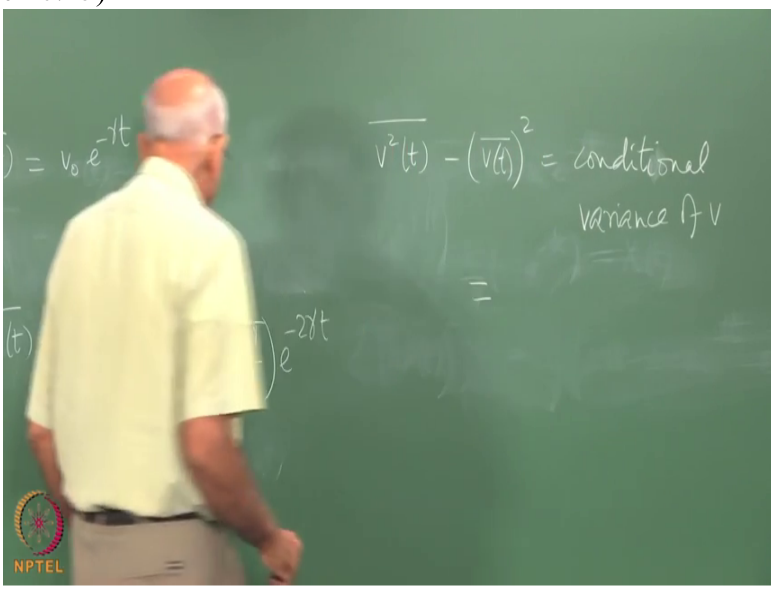

to do is take this and subtract from this square of this quantity and that kills this term here. So this is equal to k Boltzmann t over m 1 minus e to the minus 2 gamma t,

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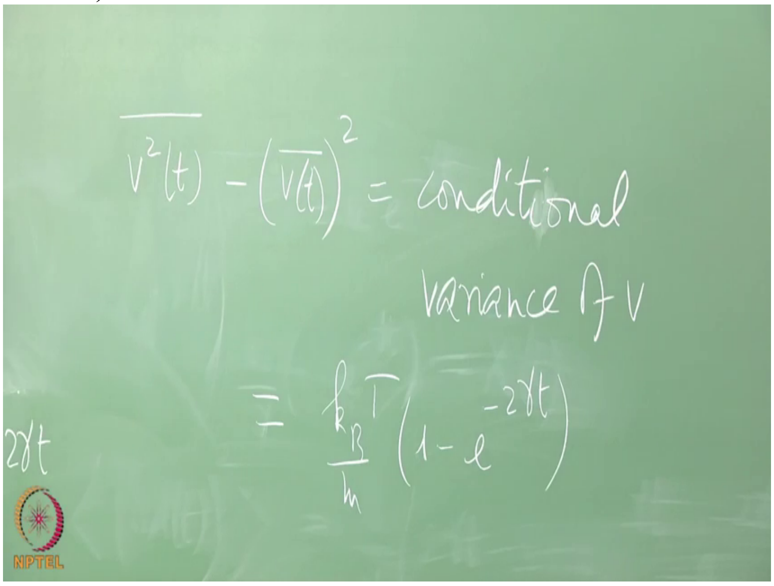

Ok.

So we have the conditional mean and we got the conditional variance. Now if, and this is a big if, this process is a Gaussian and remains Gaussian at all times, we know what t equal to infinity, it’s a Gaussian, it is the Maxwellian distribution, right? If it remains Gaussian at all times, then we can actually write the distribution down and what distribution would that be? It's the conditional probability density so, p of v t given v naught, this is the conditional P D F of velocity. It is conditioned upon this specific initial condition, starts with the delta function v equal to v naught. As t tends to infinity, it goes to the Maxwell distribution in v and now the question is what is it actually equal to?

Well, if it is a Gaussian, if it is a Gaussian, then mean and variance determine the distribution completely. A Gaussian is determined by its mean and variance completely, right? So if that is so, then apart from normalization factor, if is a Gaussian, we have to show this but we will do so later on, then p of v t v naught is actually equal to, apart from a normalization factor, e to the power minus v minus v naught, e to the minus gamma t the whole square, that is the Gaussian up there, divided by twice the variance, so it is minus m over twice k Boltzmann t 1 minus e to the minus 2 gamma t, that's the exponential

And all we have to do is to normalize this exponential which is m over 2 pi k Boltzmann T 1 minus e to the minus 2 gamma t to the power half exponential of this whole thing in bracket, so let me write down neatly, this is exponential of minus m v minus v naught e to the minus gamma t whole square over k Boltzmann T twice k Boltzmann T 1 minus e to the minus 2 gamma t 0:19:22.0.

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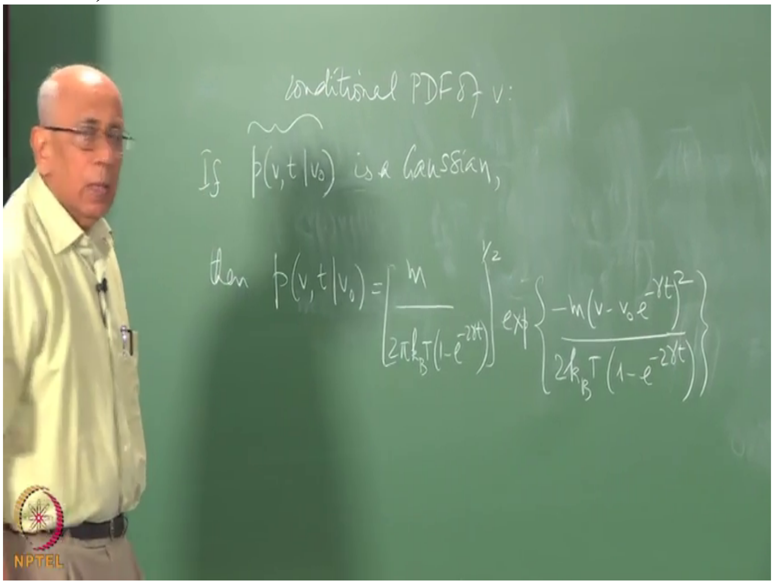

That tells you that this distribution in v, p of v t v naught, starts with the delta function v naught, at any intermediate time, it looks like this, a peak at this point

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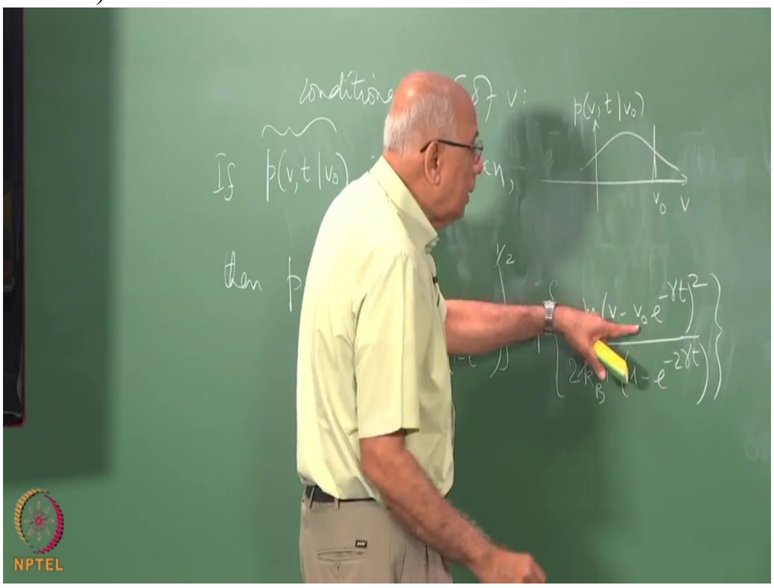

v naught e to the

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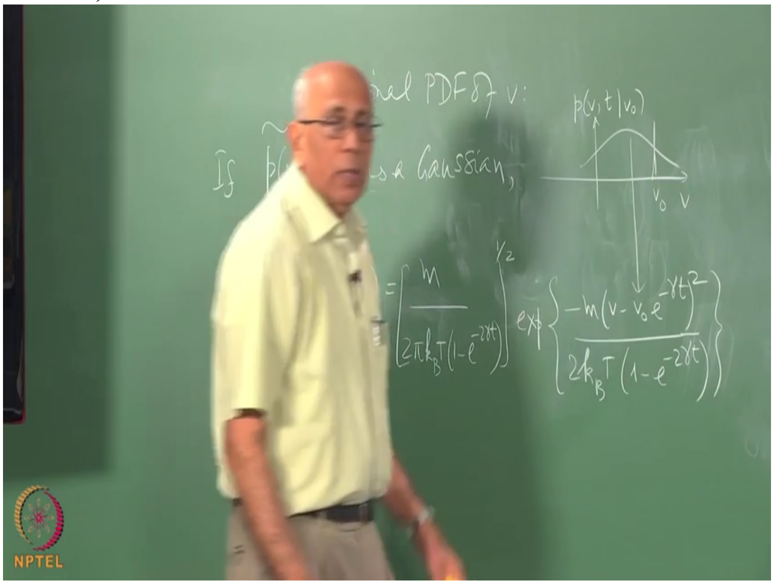

minus gamma t and the width that's growing all the time because as t increases, this quantity decreases till at t equal to infinity it reaches its value of 2 k T, largest value of 2 k T, twice the variance and then it becomes a symmetrical Gaussian up here 0:20:08.0, so it eventually ends up with this at t equal to infinity.

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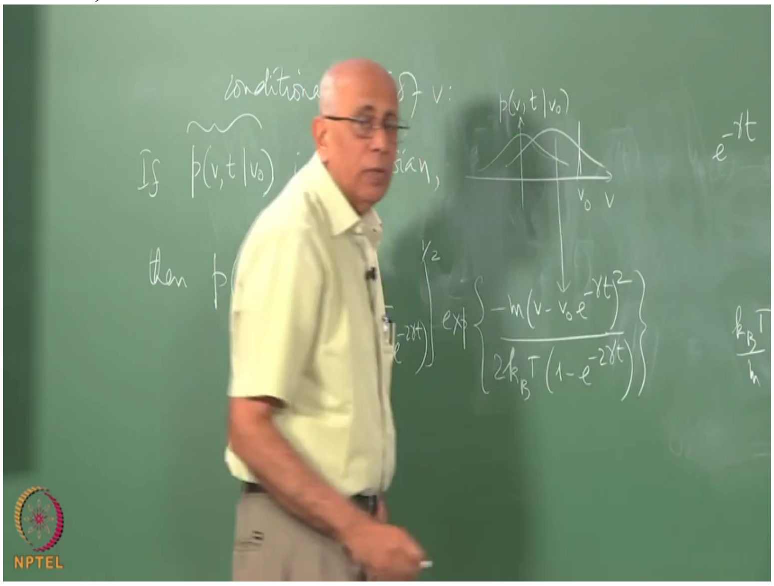

This is called the Ornstein, Ornstein-Uhlenbeck probability density function,

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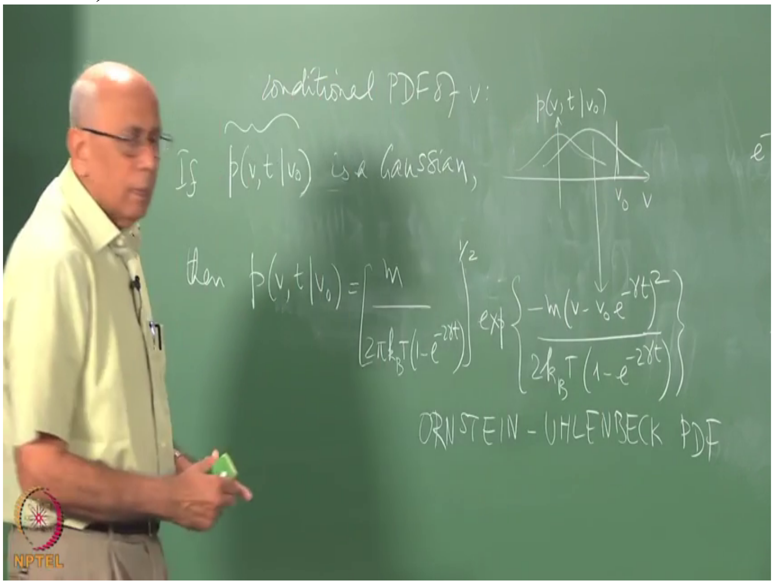

Ok.

And the general statement, which I made as a statement is that, if you have a continuous stationary Gaussian Markov process then it is exponentially correlated and then it looks like this in general. We wrote this for the velocity based on the Langevin equation and the assumption that it remains a Gaussian but this is in fact the Gauss Markov process, prototypical Gauss Markov process, Ok.

So with statement in place and I tell you it is Markov then all moments are known, everything is known about it completely. Later we will; a little later we will derive the Fokker Planck equation or at least justify the Fokker Planck equation from which this, of which this is going to be the solution, appropriate solution, Ok

(Professor – student conversation starts)

Student: For that initial condition...

Professor: For that given initial condition, yes, absolutely. So it is essentially telling you, how does the probability density function itself relax to the equilibrium value. So that is the crucial point about this. Ok, having done that and talked a little bit about the displacement, let's do the following. The next question to ask, the natural question to say, if you put this Langevin model little further then we also need to be able to say what is the joint distribution of the position and the velocity in phase space? Or the position and the momentum.

(Professor – student conversation ends)

But I am not going to do that right now because it is a lot easier to do that in terms of the distribution function itself for which I would need something called the Fokker Planck equation corresponding to that 2-dimensional process, so its, I haven't justified that yet, we haven't come to that yet, so meanwhile before we do that, we are going to do a lot of other things. So let me keep that in abeyance for the moment because it will become easier to understand later on and go back now and look at a three-dimensional case just to show you that the velocity correlation function can actually mix up different components of the velocity if, for instance you have a magnetic field.

So let us look at this very simple problem, so actually quite a simple problem of a Langevin particle in a magnetic field. That problem too can be solved quite exactly, a constant magnetic field. And I want to look at the simplest case

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where this particle is placed in a constant magnetic field in this fluid and everything else remains exactly the same. Again I say this model which is the Langevin model for the particle, I write its equation of motion but this time including the Lorentz force on the particle, the v cross B force, Ok.

So the mass is m, the particle mass equal to m, charge equal to q and the magnetic field applied is some B which is in some arbitrary direction defined by some unit vector n, Ok.

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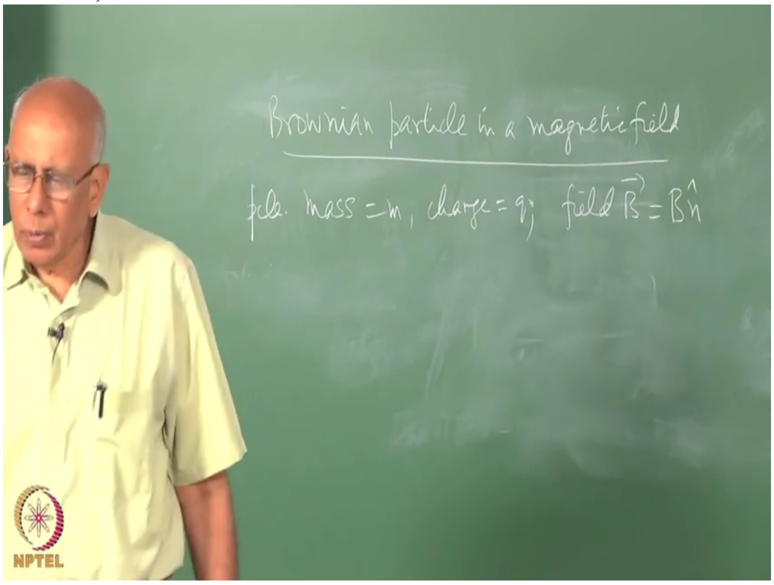

We could, without loss of generality take this n to be along the z direction, there is no reason to. Let's just look at it for arbitrary n, a little more algebra but it is helpful to separate than the transverse and the longitudinal components easily, Ok.

Now I am going to cut this story short and do it in the following way. We will use physical arguments here to make certain assumptions which are actually justifiable completely, rigorously. First of all, fluid is in thermal equilibrium at temperature T, Ok. Now this particle, all the other assumptions in the absence of the field continue to hold good. So the distribution of velocity of this particle in equilibrium is not going to be different from the Maxwellian.

In thermal equilibrium nothing happens because the magnetic field does no work on this particle at all. It doesn't change its energy and if doesn't change its energy, it remains in the canonical ensemble; the equilibrium distribution is still going to be exactly the Maxwellian distribution. On the other hand, if I start with some given initial velocity v naught in some arbitrary direction, then there is a question as to how it relaxes to this equilibrium distribution. How do the components, different components relax?

We will continue to assume without or with some intuition that the velocity remains a stationary process. The different Cartesian components of the velocity may be correlated, we don't know yet. We are going to find this correlation. So let's compute this correlation function directly. And let's do in the case of the magnetic field assuming that the system remains in thermal equilibrium and moreover this velocity is a stationary process. This is all we need.

Then we could have computed, in the absence of the field, by a slight shortcut, let me do that with the presence of the field and you will see that how this calculation goes. So the Langevin equation that I write for it is m times, let's look at some given Cartesian component j of t, v j dot of t. j is one of the Cartesian components, runs over 1,2,3, Ok. This is equal to minus m gamma v j of t, the same gamma, I assume the fluid is isotropic, gamma depends on the viscosity of the fluid, it is completely isotropic, exactly the same in all Cartesian components. And then there is a portion, there is a random force as usual, but there is also a term which is the v cross B term. So there is a q times epsilon j k l v k B l which is n l but let's put B outside. I assume

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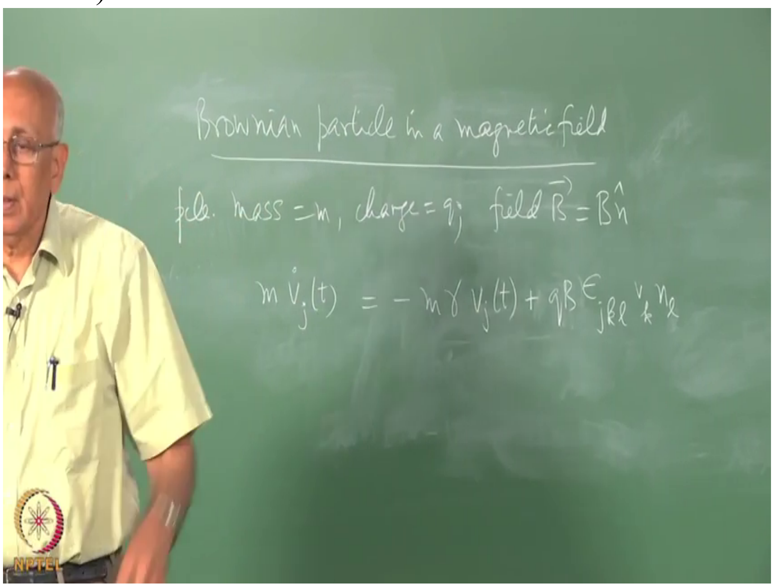

you are familiar with the index notation and with this epsilon symbol,

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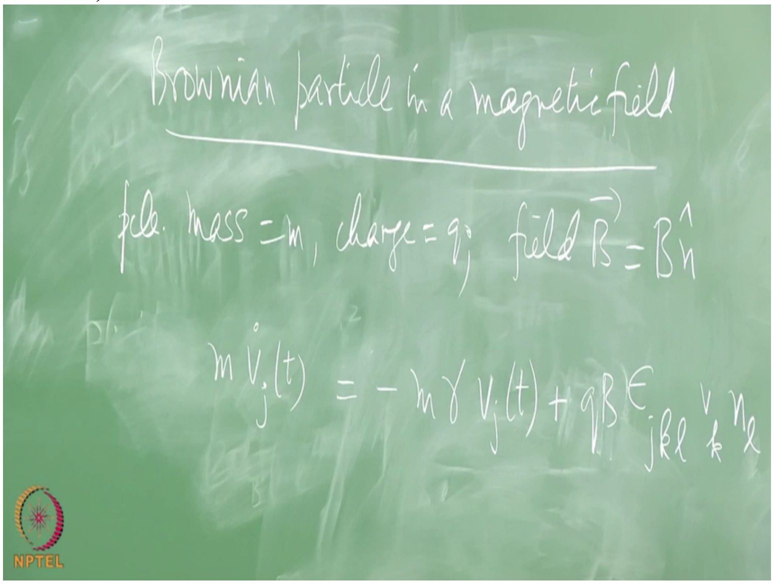

which is a short way of writing the cross product, v cross B.

This quantity is equal to plus 1 if j, k, l are in the order 1, 2, 3. Or permuted, cyclic permutations there are minus 1, if they are not and any two indices are equal,

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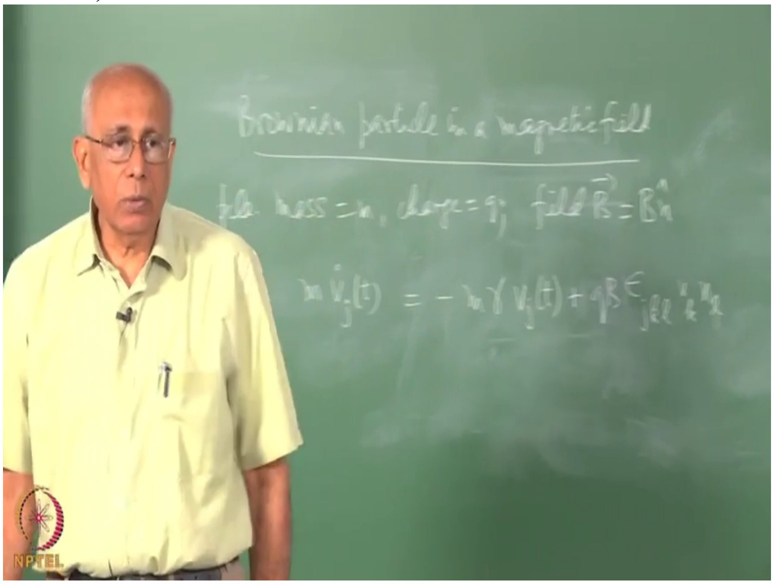

it is equal to zero, right. So the technical way of saying it is epsilon j k l is plus 1, if j, k, l is an even permutation of 1, 2, 3 in natural order, minus 1 if it is not permutation and zero in all other cases, Ok.

Plus it is the force here now, which is eta j of t. It is a vector force so I write this j curve on it. And let's as usual divide by m, so it this is 1 over m, you have q B over m, this fashion, this goes off, this goes off.

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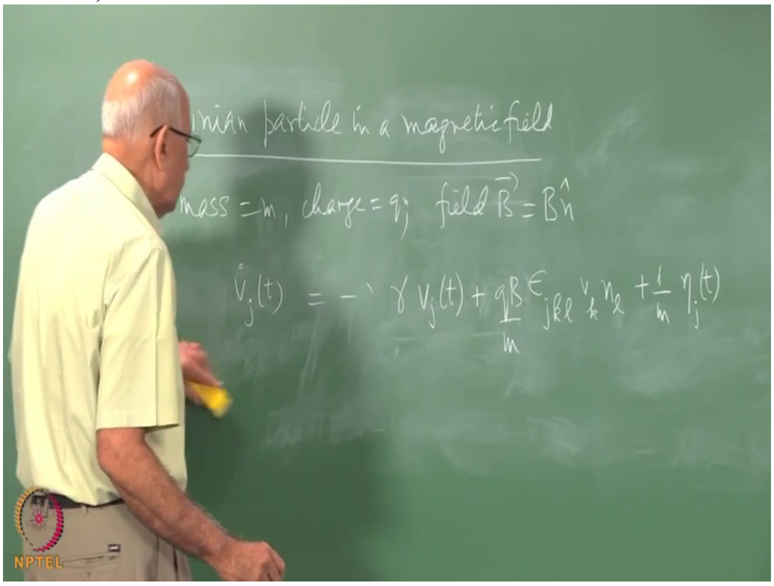

It is convenient to write this as minus gamma v j of t minus, this quantity q B over m has a physical interpretation. It is a quantity of dimensions frequency or inverse time same as gamma. That's dimensionless, this is dimensionless, that's got dimensions velocity, now what do you call this quantity?

It’s a cyclotron frequency. So omega c equal to cyclotron frequency q B over m. So let's write this as minus omega c m epsilon k j l n l v k, v k is the function of t, of course plus 1 over m eta j of t. And let me define a matrix. Let us define

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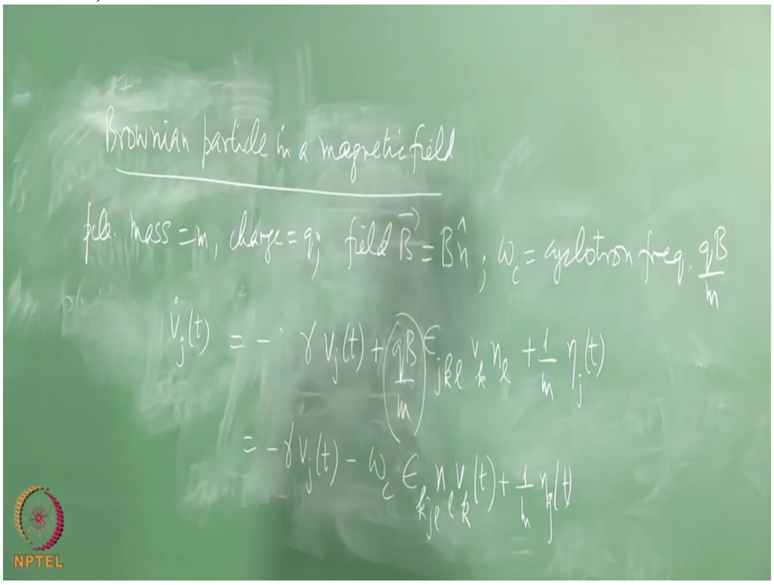

a tensor of rank 2, you can write it as a matrix if you like. Let's define M, define M k j l to be equal to epsilon k j l times n l. l is contracted, so sorry, this

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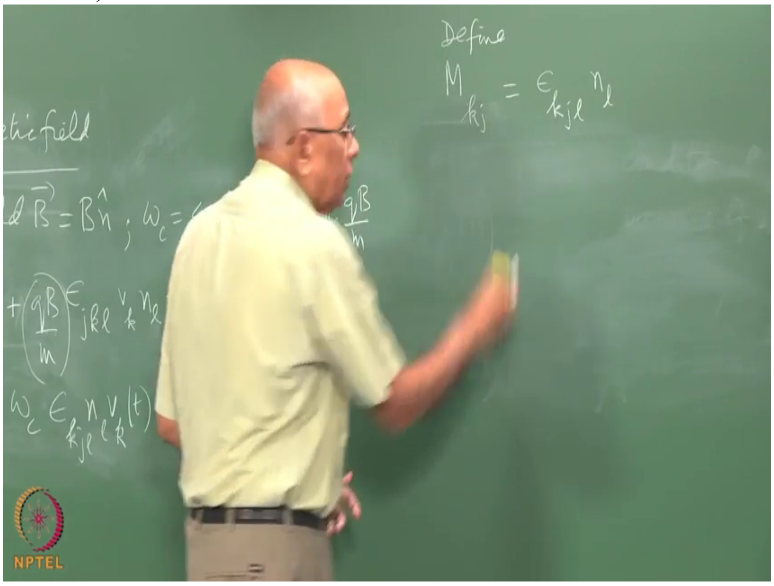

this cannot be, M k j.

So the k jth element of this tensor of rank 2, or matrix, 3 by 3 matrix is defined to be k, j, l and m. Therefore I can remove this and write this as M j k times v k.

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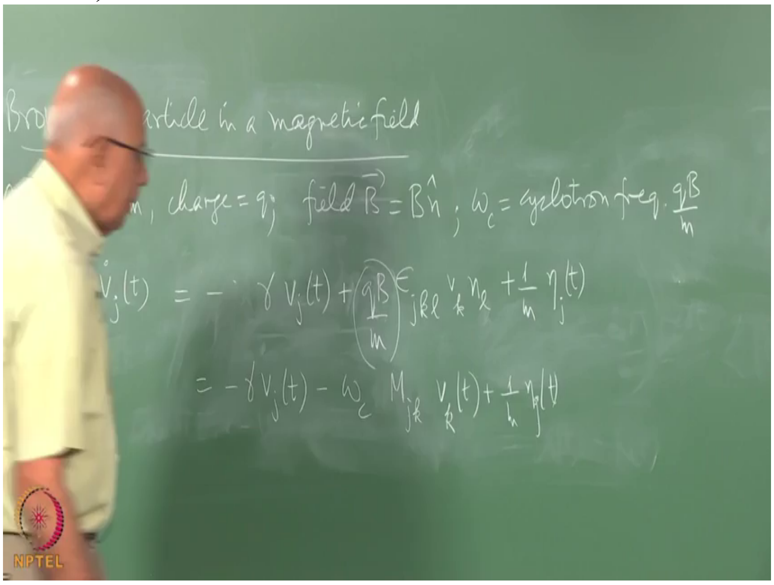

Now to find the correlation function we assumed that the velocity, we are going to assume the velocity is stationary process. Then a quick way of finding the correlation function is to write, let's pre-multiply both sides by v i of zero, v j and take average, equilibrium average.

We can go through the rigmarole of solving this equation, taking conditional average and then taking full averages etc, showing it stationary and so on. Let's cut all that short. Just multiply by v i of zero. t is greater than zero here. v j dot of t equal to whatever. This is equal to minus gamma and then I go ahead and take averages, v i of zero, v j of t minus omega c, average value of v i of zero, v k of t times m j k, notice that m is a constant matrix. All its elements are constants.

Plus average value of v i of zero eta j of t 1 over m. But this is zero by causality because for all t greater than zero, this thing is not, vanishes identically for all t greater than zero by causality. For all t greater than zero, this thing here vanishes because the effect cannot precede the cause, Ok. What the random force does at some time t greater than zero cannot affect what the velocity was at t before zero. So that's it, this equation here.

Now unlike the previous case where you had the correlation function, now you got a correlation matrix because there is these symbols, i, j, indices i j etc. So let's define C i j of t to be equal to v i of zero, v j of t. In fact, let's do the following. We know that asymptotically, asymptotically if i is equal to j, this quantity here is going to die down exponentially. And at t equal to zero, it is going to start with k T over m, the average value. It is going to start with average value of v naught square which is k T over m.

So let us divide by k T by m. We will define a normalized

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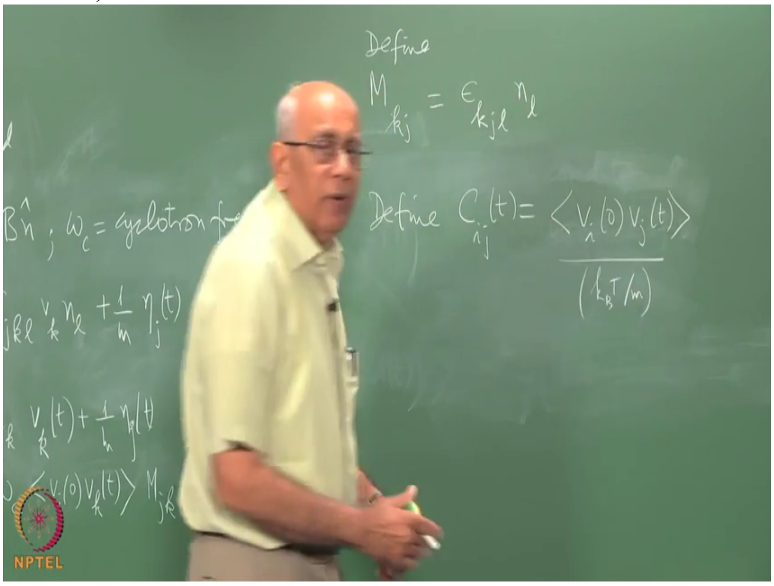

correlation matrix by dividing by this asymptotically, this initial value k T over m. So

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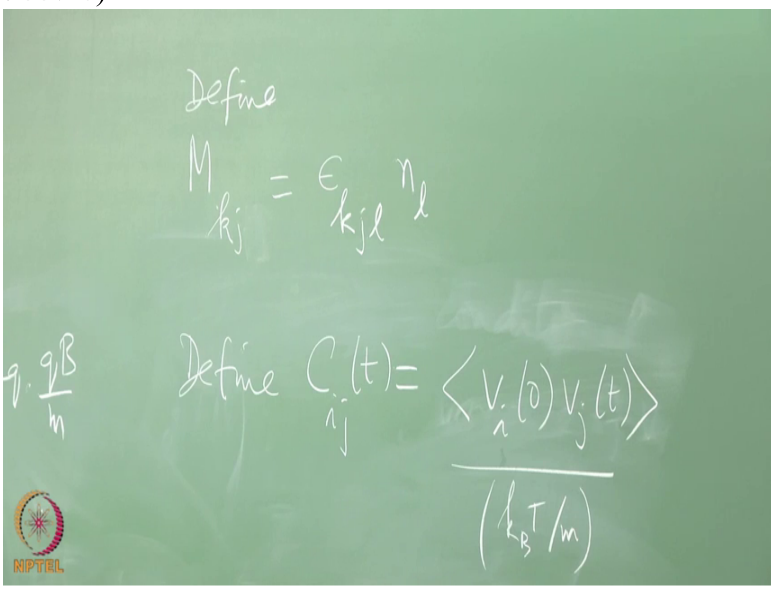

C i j of zero is equal to 1, by definition. So let's keep that in mind. If i is not equal to j, then these two are uncorrelated at t equal to, at the same time, but if i is equal to j then you just get v squared,

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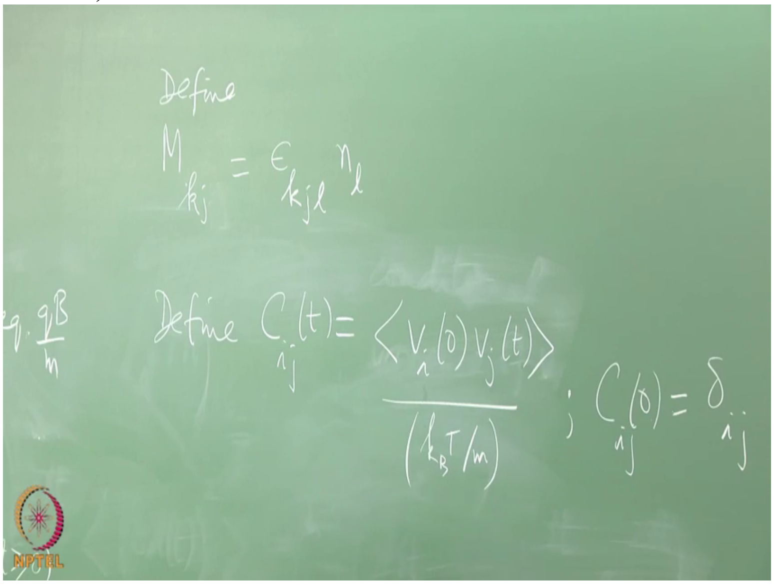

one component and that is equal to k T over m, the average value.

So if I write this C of zero, C of t as a matrix, call it some matrix with component C i j, then at t equal to zero the matrix is the unit matrix. That's the delta function is just, these are just the elements of the unit matrix. So that's useful thing to know. So now we can solve this equation. We can solve this equation because it simply says d over d t, C i j of t is equal to minus gamma C i j of t minus omega c M, we should be careful with commutation, M i k, C i k, of t, M j k. Is that correct?

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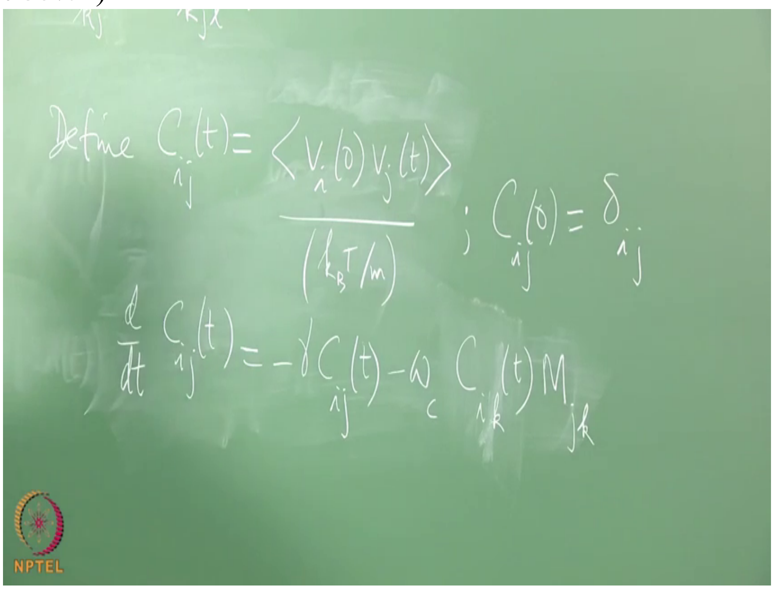

(Professor – student conversation starts)

Student: M k j

Professor: I am sorry, we had M j k.

Student: It is M k j.

Professor: What happened here? Did I define...?

Student: You flipped it to change the sign

Professor: I flipped to change the sign and then I brought this...

Student: You can change your definition of M k j

Professor: I should do that.

Student: If you want...

Professor: I should really do that properly, j k l is Ok, n l

Student: So you just define that as M j k; because there is no error otherwise.

Professor: Yeah, there is no error so let's, did I get this right?

Student: Yeah

Professor: This was correct, this part is Ok. So this is M k j, Oh yeah, oh yeah, yeah! I wrote this term, sorry, I wrote this term as minus omega C epsilon K j l v k and I define M k j as epsilon k j l n l. So this fellow here

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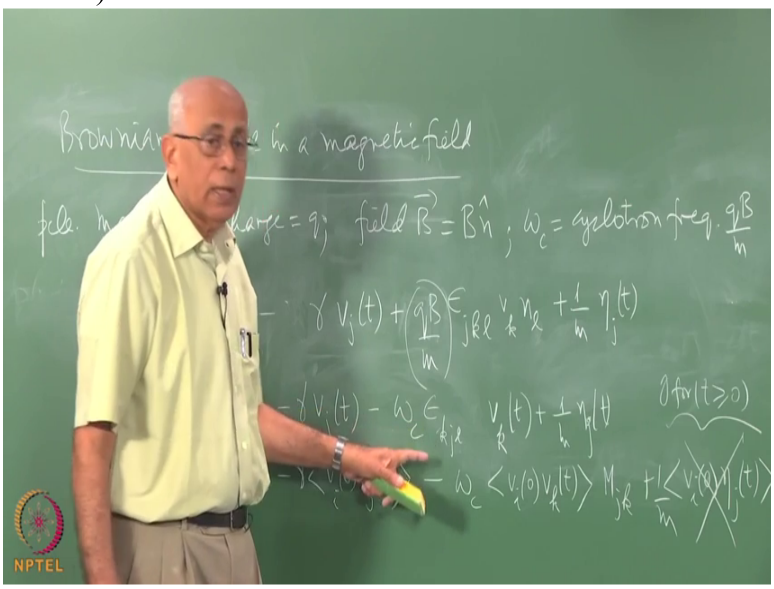

was an M k j.

Student: Yeah.

Professor: M k j, that's what it was. And this is M k j. You could do it

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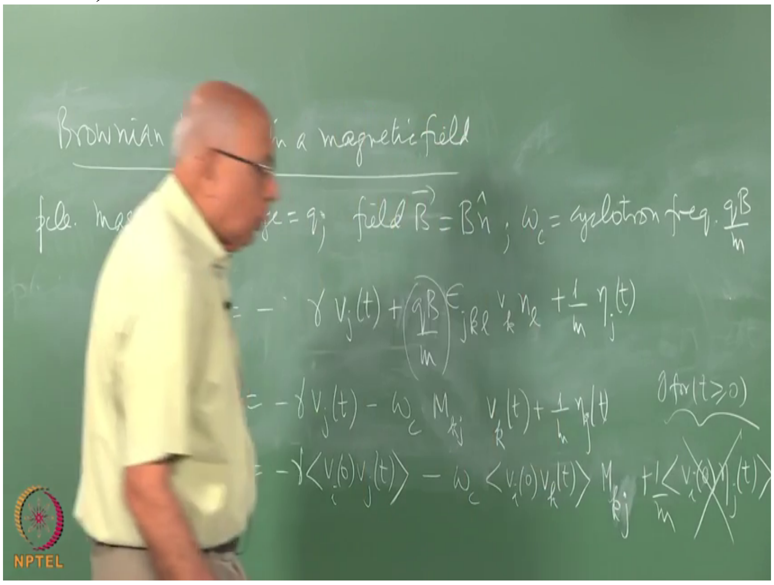

by defining it in any way you like

Student: But the last one is M k j.

Professor: But now it is consistent, yeah. This is therefore M k j, thank you, Ok. Or in matrix form,

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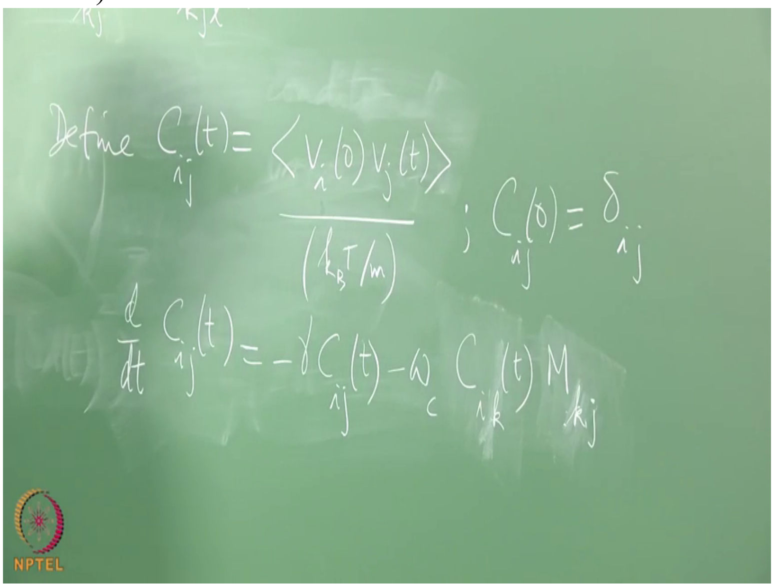

this is the same as saying d over d t C of t where this is a matrix, C of t is a correlation matrix is equal to minus gamma times the unit matrix plus omega C times the matrix M, is that correct...no, no, no C times the whole thing, so C times, yeah minus C times gamma times unit matrix plus omega C times the M matrix. Yeah now we are in good shape.

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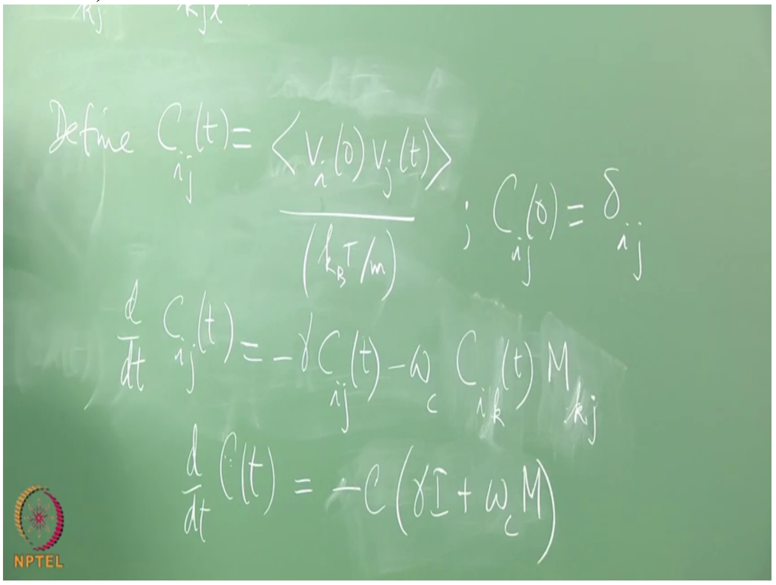

Student: Is there a reason to having on the right side?

Professor: You should either have it on the left or right, that's all. Otherwise it doesn't matter at all. But I should be careful where I put this C, where I write the solution. So this is minus C of t times this fellow. This is

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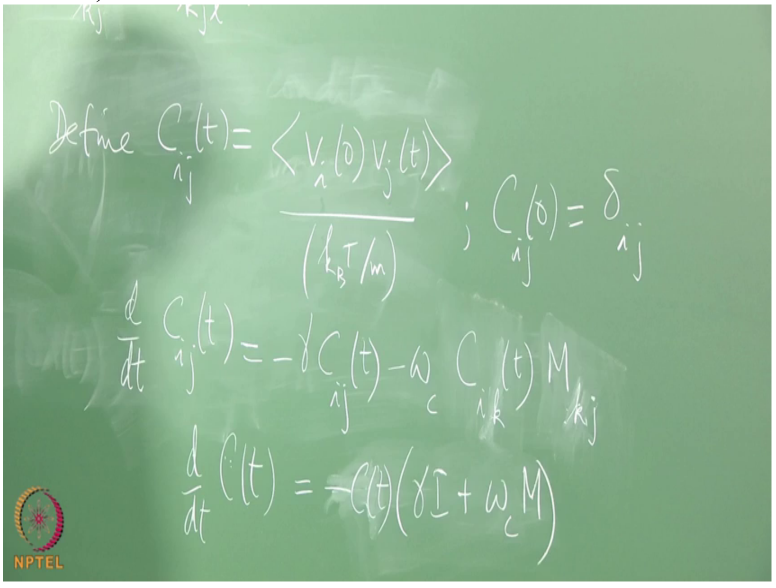

a matrix, M is a matrix; this is a unit matrix. This is a matrix equation. But this is a constant matrix. There is no time dependence here, this fellow here.

So this immediately implies that the solution is C of t is equal to e to the power minus, is equal to C of zero times e to the power minus gamma times unit matrix plus omega C times M times t.

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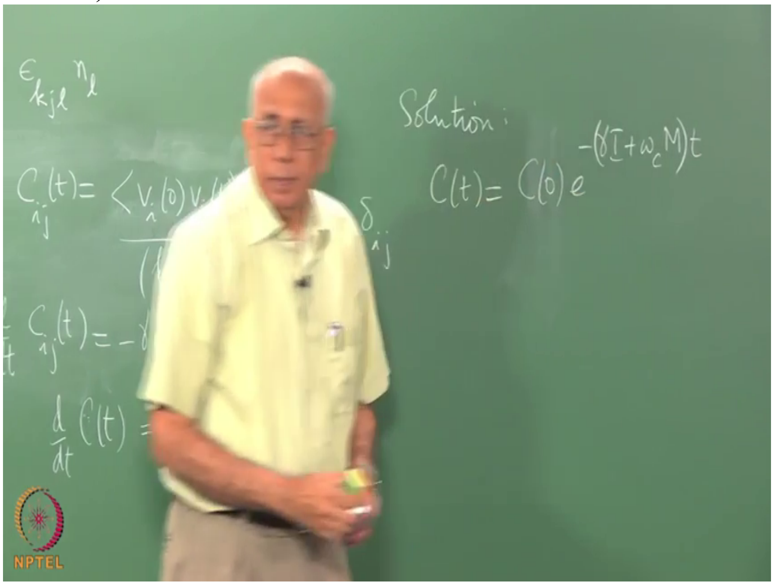

I have to be consistent. This C is on the left of this thing here. So on the solution too, it is on the left. In the present case it doesn't matter. Why is that?

Student: C of zero is

Professor: C of zero is the identity matrix. It commutes with everything, so we don't really care. But it is just good discipline. It may not always be the case so we should just be careful doing that. So that's the solution for C and all you got to do is to read off this matrix. But you have the problem of exponentiating this.

(Professor – student conversation ends)

So by the way, since this is equal to the identity matrix, the whole thing is equal to, this implies C of t, implies C of t equal to e to the minus gamma t times e to the minus omega c, minus M omega c t.

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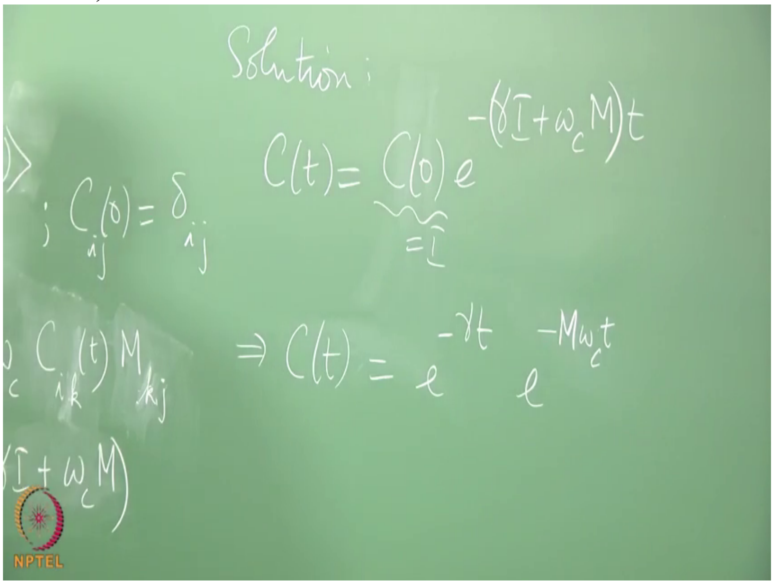

So we have to find the exponential of M times the constant. That's all we have to do, and then the problem is solved. Now how do we go about doing that?

This is a 3 by 3 matrix. If it were a 2 by 2 matrix we could write it in the Pauli basis, in terms of Pauli matrices and you can read off what the exponential is, right? But it is a 3 by 3 matrix. What should we do then? Yeah, there are several tricks to do this. One of them could be the following. We could take this matrix M. It is a 3 by 3 matrix, right? Now it is clear that the exponential of a 3 by 3 matrix cannot, you have to; you should be able to sum this thing reasonably if this has got some physical meaning and so on, but writing down an explicit formula may not be all that easy.

You can write this exponential down because it's characteristic equation after all must be a third order polynomial in M, which means that M cubed can be written in terms of the identity matrix M and M square. Therefore M 4 can be written in terms of these fellows and so on and so forth. But there will be a pain in the neck to try to combine the coefficients and to compute what it is. Not doable in general, but this matrix is so simple that it is possible to do it.

Another way to do this would be to find its eigenvalues, therefore write its characteristic equation down, the secular equation and replace lambda by the matrix itself, by the Cayley-Hamilton theorem and then may be one can find out what M cubed is in an easy way. But there is even an easier way. This is a rotation matrix. I hope you recognize it is a rotation matrix.

So M squared k j equal to M k j equal to epsilon k j l n l this is unit vector's component, so M squared k j is equal to epsilon, it is equal to M k, k r M r j whre r is another index.

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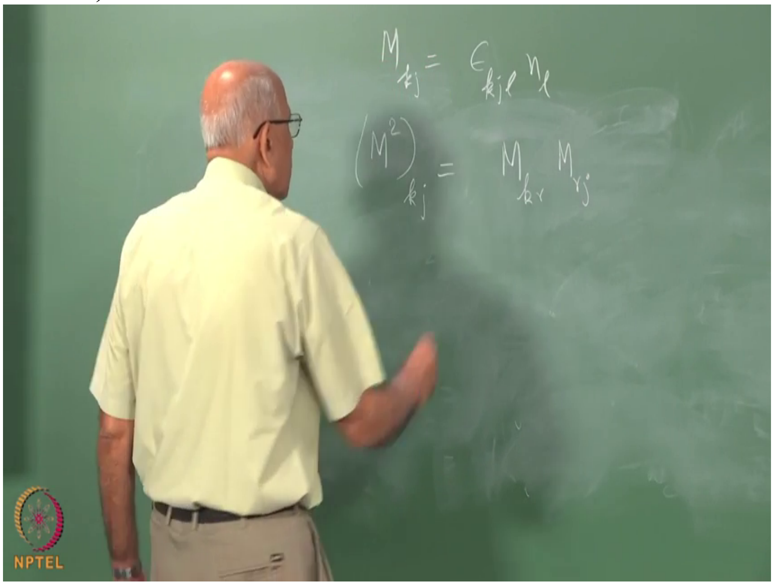

So this is equal to epsilon k r l n l epsilon r j s n s.

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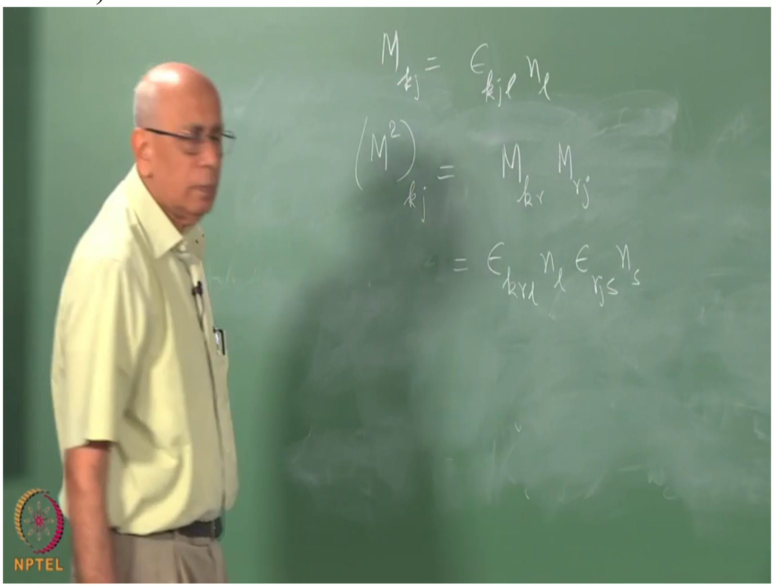

That's what it is, right? So this is equal to epsilon k r l, epsilon j r s, n l n s with a minus sign. I flip this once here

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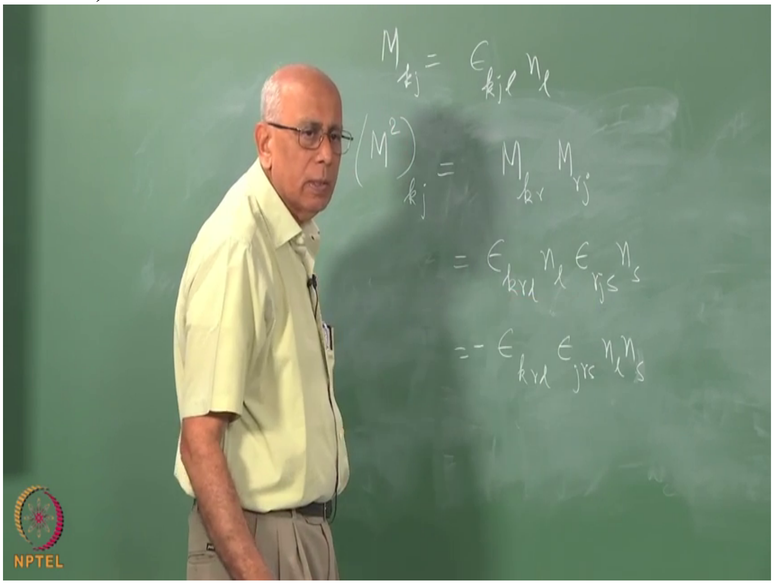

and then I use this identity, well-known identity when you take this epsilon symbol and you contract one of the symbols in the same position, then it is just the product of delta functions so this is equal to minus of delta k j, delta, no what did I do, no, no, no, this is equal to minus epsilon r k l, epsilon r j s, n l, n s. So this is equal to the delta function of these 2 fellows, k j, delta function of l s minus delta function of k with s, delta function of l with j acting on n l, n s which is equal to what?

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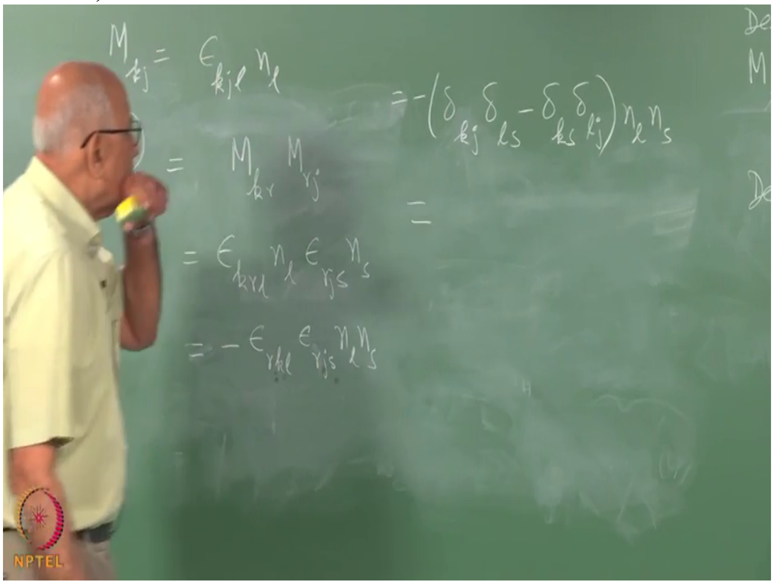

The first term, you have a delta k j, delta l s n s is n l, n l which is equal to 1, it's a unit vector and another term is plus, wherever l appears, replace with j, wherever s appears, replace with k. So n j, n k. So it is just n j, n k. You got the 0:44:25.3 the k j elements, so let's write it symmetrically, n k n j minus delta k j.

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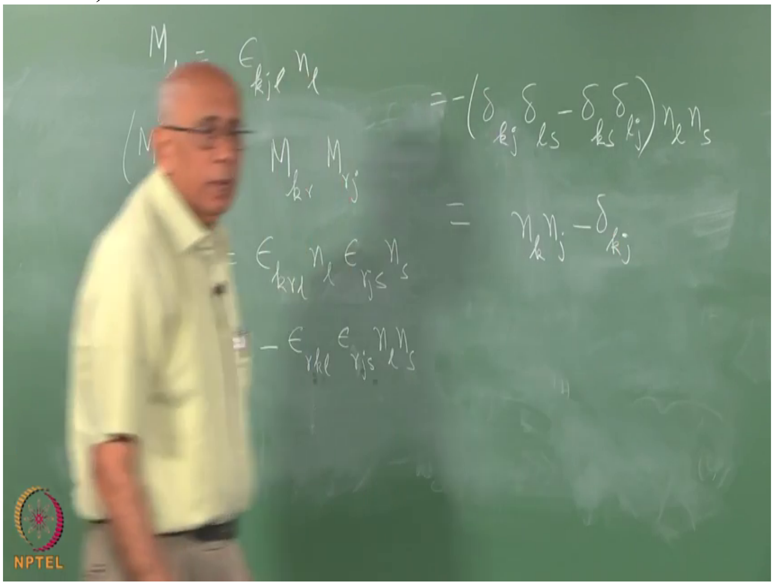

That's the square.

(Professor – student conversation starts)

Student: Aren't we done once you say it's a rotational matrix because....

Professor: How many people know that it's a rotation matrix? They are not going to believe you or me (laugh) .It's a rotation matrix, we know. What do you think its eigenvalues are? It is a rotational matrix in 3 dimensions. And it's got; it is rotation about the direction l, the index l, right? So it must, it is clear that n l must be an eigenvector of this matrix with eigenvalue equal to 1, got to be so if it is rotational matrix.

(Professor – student conversation ends)

Then there are 2 other eigenvalues. Can either of them be real or must they be imaginary? Well, suppose it's real. Then this means, if this eigenvalue is real, then there is a direction in space which is also left invariant by this rotation. But in the 3-dimensional rotation, there can be only one axis that can at best be left invariant, right? So the other two eigenvalues must be complex.

It is a rotational matrix. So this matrix is unitary, it is orthogonal; the elements are real therefore it is ortho, unitary matrix with real elements. It is an orthogonal matrix. Because it is an unitary matrix, all its eigenvalues must lie on the unit circle. 1 is already an eigenvalue. Minus 1 is not an eigenvalue. Ok, why is that? Why is that?

(Professor – student conversation starts)

Student: Three dimensional 0:46:21.5 is not

Professor: Yeah, if the product of all the 3 eigenvalues must be equal to the determinant of this matrix which must be plus 1, so a proper rotation, right? So if minus 1 appears as an eigenvalue, it must appear second time too because 1 is already an eigenvalue, right. So it must be a repeated eigenvalue, Ok. It also means that there is again a real eigenvector. Real eigenvalue will imply, I leave you to figure out why minus 1 cannot appear as an eigenvalue? So the only other possibility, some e to the i theta appears and e to the minus i theta

Student: 2 minus 1s.

Professor: Yeah? They have given arguments as to why 2 minus 1s don't appear here for a real rotation matrix in this case, in this case in 3-dimensional rotation. So the only other possibility is a pair of complex conjugate roots which lie on the unit circle. In this case, there will be pi over 2, minus pi over 2; either the i pi over 2, it will be e to the minus i pi over 2.

(Professor – student conversation ends)

Look at it this way. Once you have this direction n l, regard that as a z direction, then rotation about it is rotation in the x y plane which is given by matrix of the form cos theta, sin theta, minus sin theta, cos theta and it's eigenvalues are e to the plus, minus i theta. So that's how it is, in this case. Anyway we are going discover the same thing in... So this is M squared k j. So implies M cubed k j therefore equal to M squared k r M r j and that's equal to what, M squared k r is n k, n r minus delta k r times epsilon r j l n l.

What does that work out to? What is the first term?

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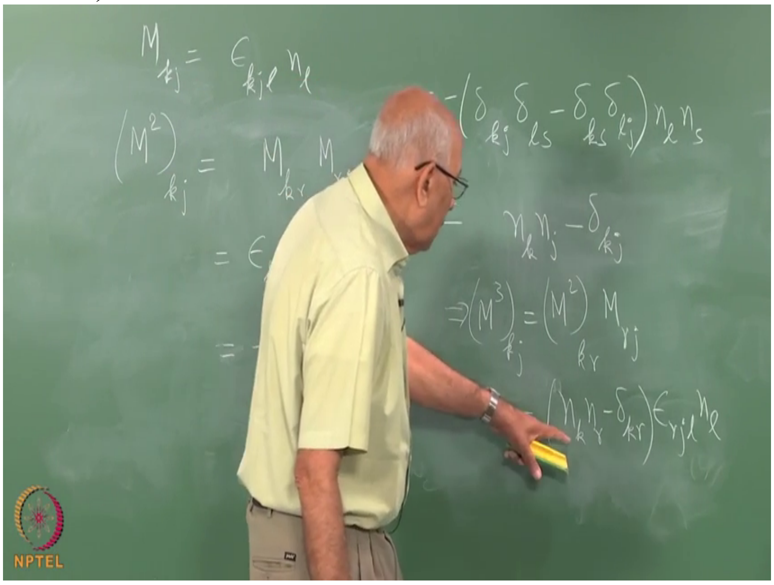

n k n r n l epsilon r j l

(Professor – student conversation starts)

Student: Zero

Professor: Why is it zero?

Student:

Professor: It is symmetric in r and l, n r n l but there is epsilon here which is anti-symmetric in the two, so the first term is zero. So the second term tells you that M cubed k j equal to, the second term is a delta where this is replaced here, so it is epsilon k j l n l minus M k j, minus M k j.

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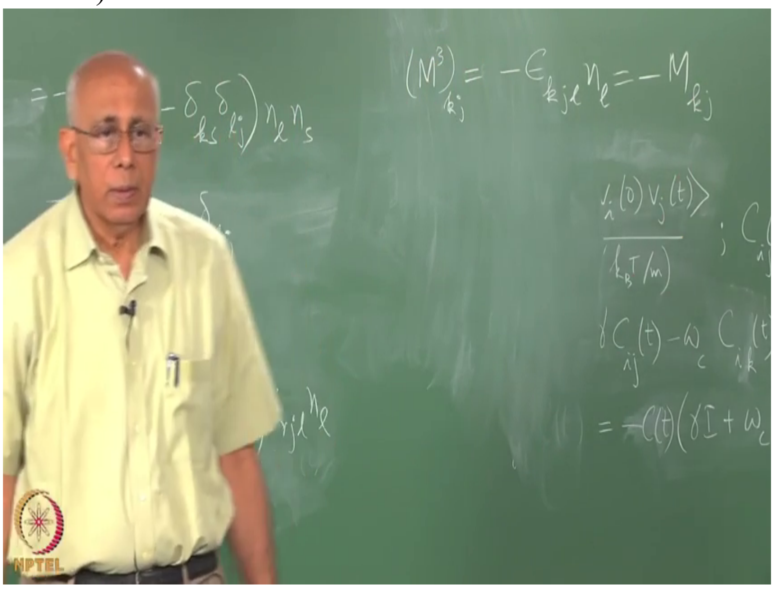

So this implies that M cubed equal to minus M,

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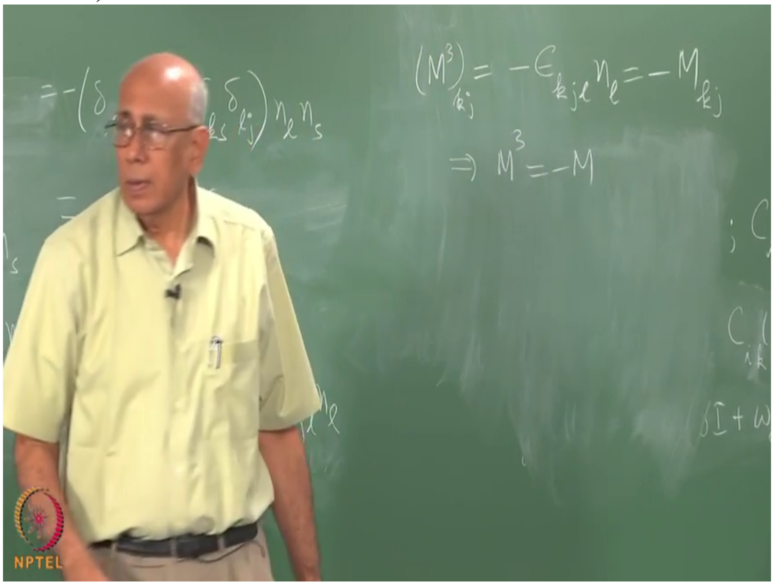

that's very simple.

(Professor – student conversation ends)

By the way that also tells you the characteristic equation right away, if the Cayley-Hamilton equation would be M times M squared plus I times M equal to zero,

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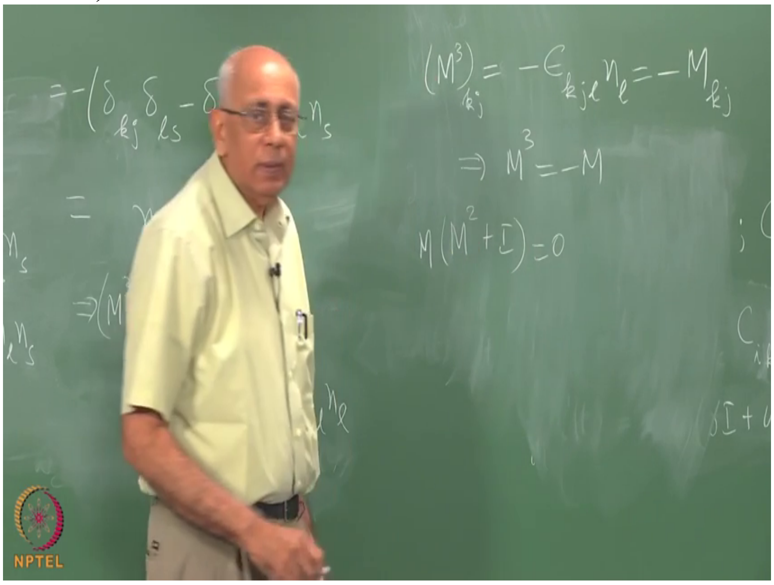

that is the Cayley-Hamilton equation for this case because it is characteristic equation where you replace the eigenvalue by the matrix. By the way this is the statement that M cubed is minus M. Once I write it like this, it means that lambda squared plus 1 times lambda equal to zero which means lambda is equal to, you have your 3 eigenvalues in this problem, Ok, alright, once...yeah?

Once we have this, the exponential is very easy. So now let's go back and do what's the exponential, this case and now we can do this very fast. So this says e to the minus M omega C t is equal to I minus M omega C t plus M squared over 2 factorial omega C t whole square minus M cubed over 3 factorial omega C t cube plus M 4 over 4 factorial omega C t to the power 4 minus dot dot dot dot.

This is equal to I,

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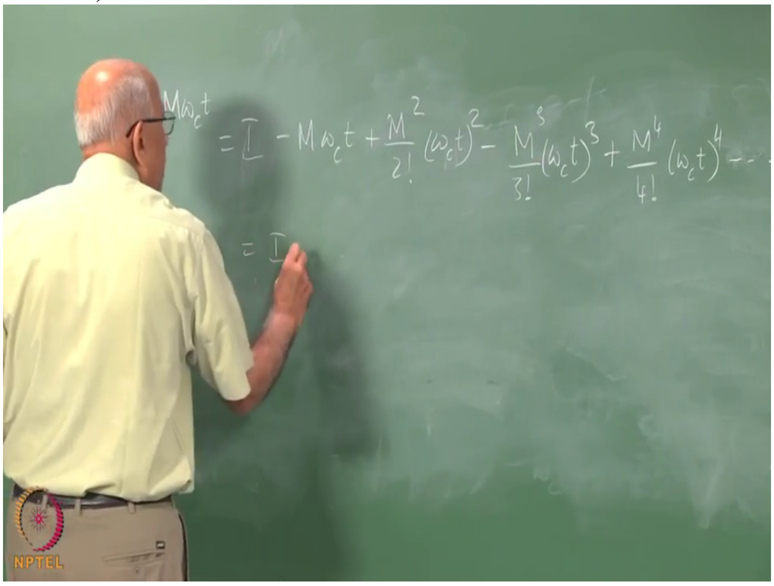

let us collect all these terms together, minus M omega C t, that is this portion and then M cubed, but M cubed is minus M, so this becomes a plus out here, so this gives you M times omega C t and this becomes a plus, so this has to be a minus out there. That term is going to keep going in this fashion and then you have to deal with this fellow.

Plus M squared over 2 factorial omega C t whole squared plus M 4 and what is M 4, it is equal to M times M cubed, but M cubed is minus M, so this is minus omega C t to the power 4 over 4 factorial plus dot dot dot, this keeps going this way.

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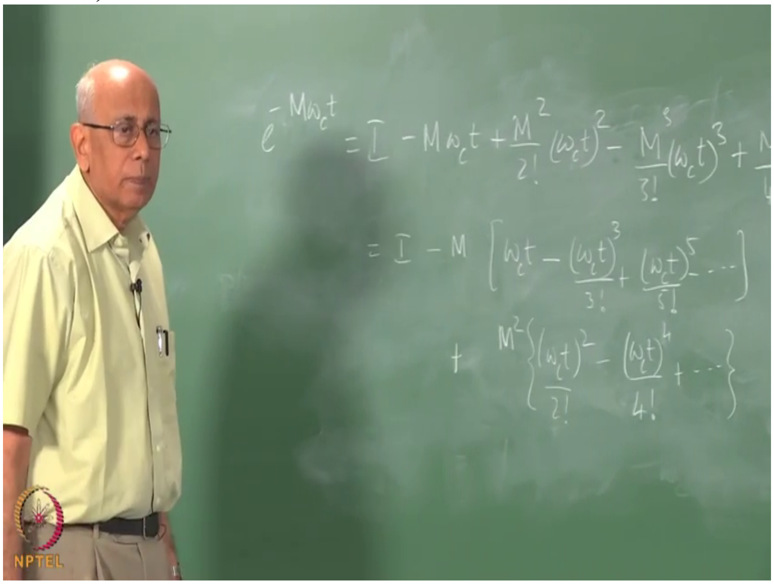

If I had a 1 here, then this would be a cosine. So let us add and subtract a 1.This came with a plus sign right? So let's put a minus 1 here, and put a plus 1, this fashion.

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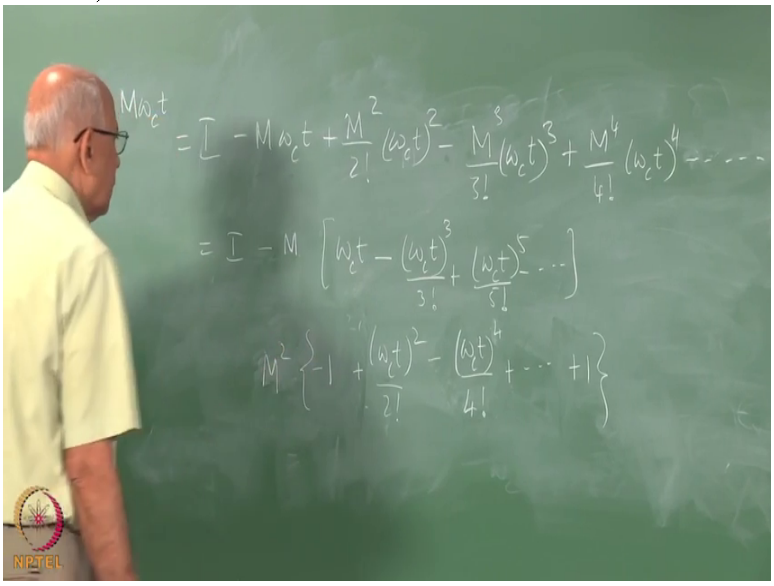

This fellow is minus cosine of omega C t and there was a 1 here. That's the identity matrix in this. So we have done the job. This here now, is equal to I plus 1 minus cos omega C t M squared, but before let's write the M term first, I minus M sine omega C t plus M square, 1 minus cos omega C t, that's the final answer.

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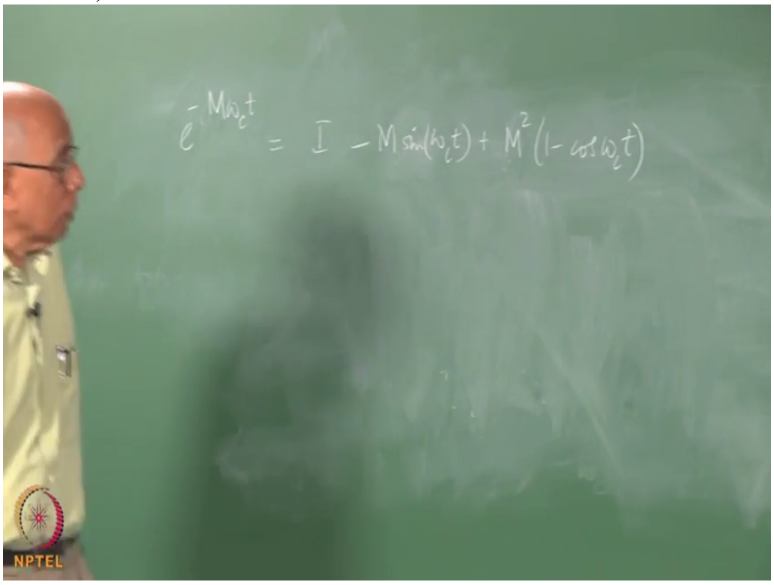

Therefore the correlation matrix itself, the normalized correlation matrix itself C of t equal to e to the minus gamma t times this. And notice

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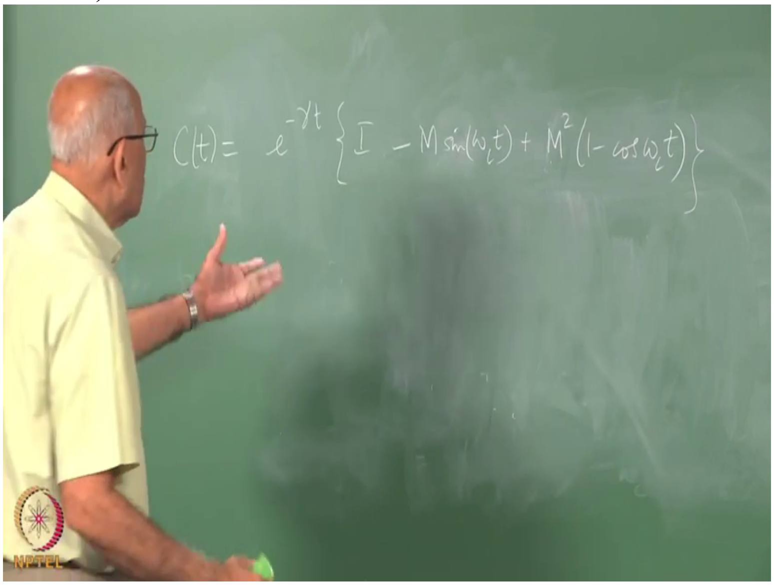

as t goes to zero, this disappears, that disappears, you are left with this, times the unit matrix. This is 1, Ok, right. So let me stop here since we have run out of time, but let's take it from this point onwards. Now I request to write down what C i j is. It will of course start with the e to the minus gamma t and then you have to write whatever is inside. What do you get from here?

(Professor – student conversation starts)

Student: delta i j

Professor: delta i j. What is this? epsilon i j l or i, j, k if you like, n, k, sin omega c plus m squared but remember we have a formula for the components of M squared, this fellow here was M i n j minus delta i j, 1 minus cos omega c t. This delta i j will cancel

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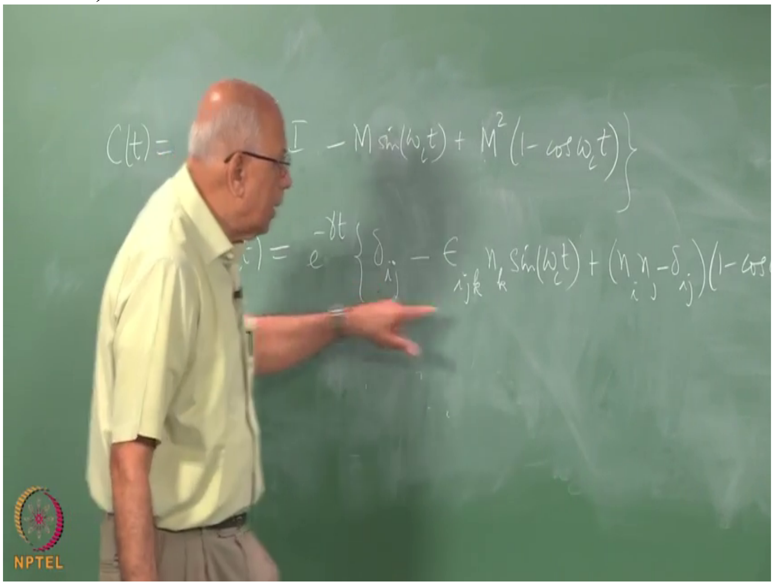

against that delta i j. This n i n j will sit as it is here, and there is a delta i j which also multiplies this. So what is this equal to?

(Professor – student conversation ends)

We can also write this as e to the minus gamma t n i n j, that's the first term and then, so there is plus, correct me if I am wrong here, delta i j, well, work this out explicitly, I don't want to make a mistake in writing this expression, but you notice there is a portion which is odd in time and a portion which is even in time. We will interpret this. We will interpret what this whole thing is, all this for t greater than zero, Ok.

So there is certainly a part which mixes up the component's velocity, this thing scrambles up here and we will interpret each of these terms, Ok. So we start up with expression next time and see where this gets. We will also try to see what happens when t becomes less than zero. We can write it down from here using physical arguments. We will do this. Then the next step would be to use the Kubo formula to get the diffusion tensor. So we do that and see what the transverse and longitudinal diffusion coefficients are, after which we will take up linear response theory and we will come back to this once you studied what the general formulism is, a little bit. So we may stop here now.