Non equilibrium Statistical Mechanics
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Lecture No 02
The Langevin model (Part 1)

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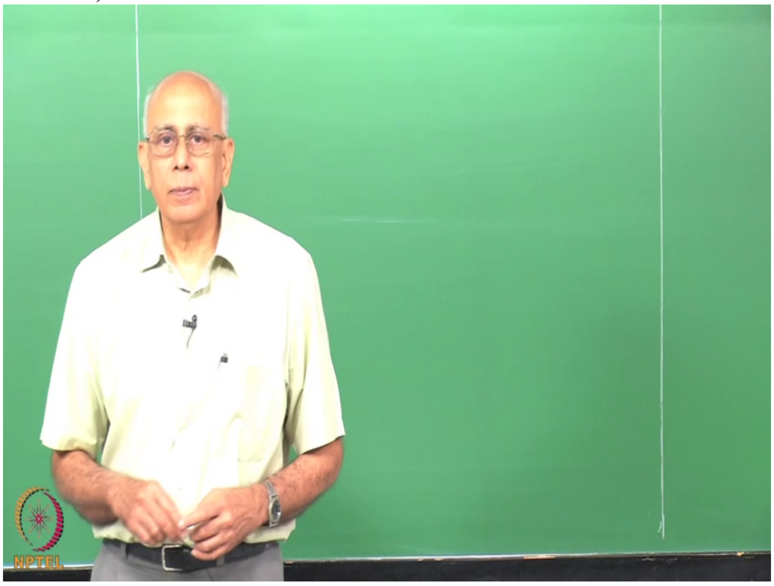

Right, so yesterday we went through very quickly, we recapitulated some aspects of equilibrium statistical mechanics, what equilibrium was all about. Today we start asking time dependent questions. And this will be the beginning of non-equilibrium statistical mechanics because you now don't have any longer the safe comfort of the fundamental postulate of statistical mechanics at the equilibrium level which is that for a given system in isolation, all accessible microstates are equally probable.

We have no such guarantee now. We are going to push and pull on a system. We are going to apply perturbations to it. We are going to move it away from equilibrium and watch what happens as the system is left alone.

Now we need a model to start with. And we will start with the simplest of models. Perhaps we will start the model where you have a fluid and it is in thermal equilibrium at a fixed temperature. The fixed number of particles, the fixed volume and it is in thermal equilibrium. If it is a gas for instance, if it is an ideal gas, then we know that the Maxwellian distribution of velocities applies and you also know that the particles are uniformly distributed throughout the volume.

We write down in equilibrium what the phase space density is for a given particle. So you can easily write down the fact that if you have this container with a whole lot of particles inside, N of them for instance and if it is an ideal gas, then we can write down the phase space density immediately. It is clear that, let me use a symbol for it, rho equilibrium and now I want the single particle phase space density, this is the probability that, probability density that the particle is at any point r inside the container and its velocity is some value v say,

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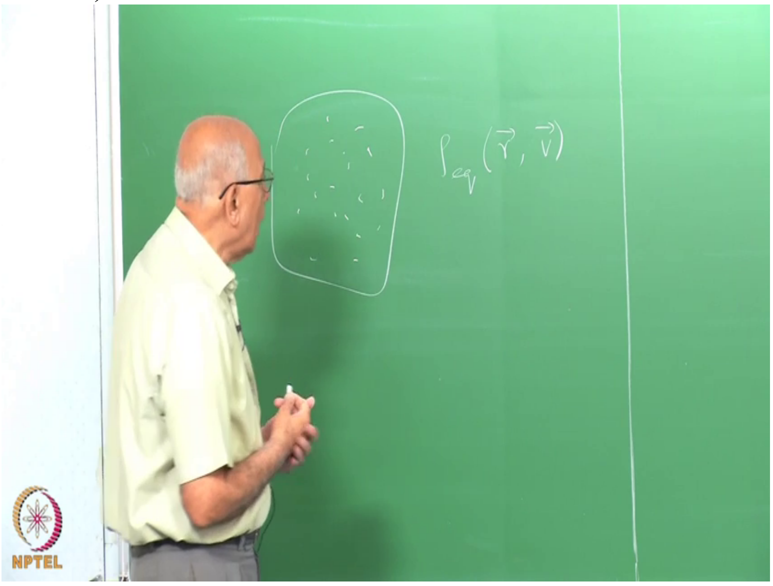

and it is in equilibrium, right.

And this is an unconditional density in the sense I don't say what happens, what the initial value of these velocity and position variables are or anything like that, I simply say I pick a particle at random and I ask what is its equilibrium phase space density, Ok. Now this is intuitively clear that equilibrium statistical mechanics of course provides an answer but it is intuitively clear what the answer is.

As far as the position variable is concerned, the density is absolutely uniform. It has got an equal probability of being anywhere in this entire volume. So this is just 1 over the volume and then there is the portion which tells you how the velocity is distributed and we know then that since the energy of this particle, if it is ideal, if it is not interacting with anything else, the energy of this particle is just its kinetic energy and the system is in equilibrium at some temperature, inverse temperature beta so this is equal to the e to the minus m v square over 2 k Boltzmann times t.

Because 1 half m v square is

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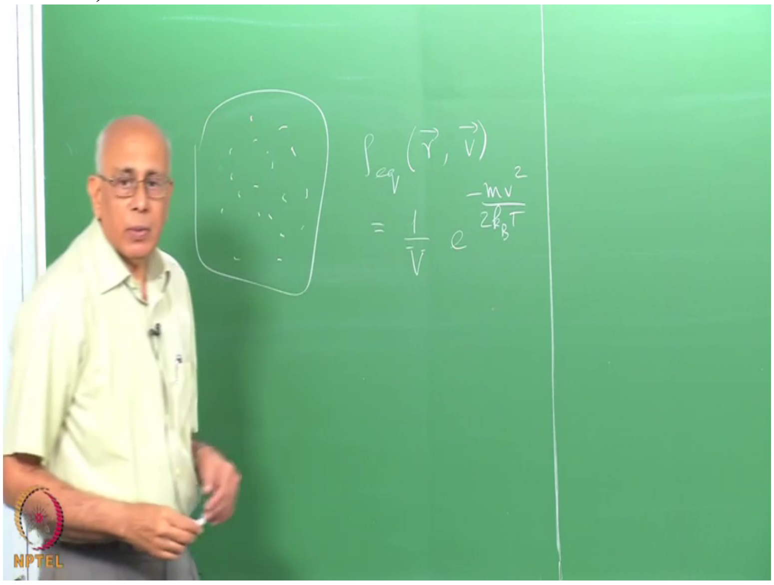

its energy, just the kinetic energy and the rules of equilibrium statistical mechanics tell us that is the density of the particles apart from a normalization factor. And of course we can write the normalization factor as well. So this is equal to 1 over v m over 2 pi k Boltzmann T and there are three of these degrees of freedom so this is 3 halves times this quantity here

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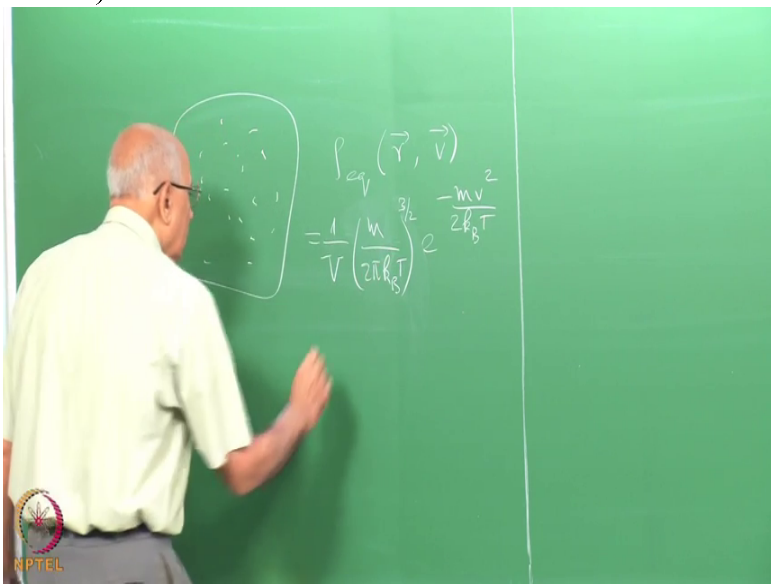

where v stands for modulus of the velocity vector.

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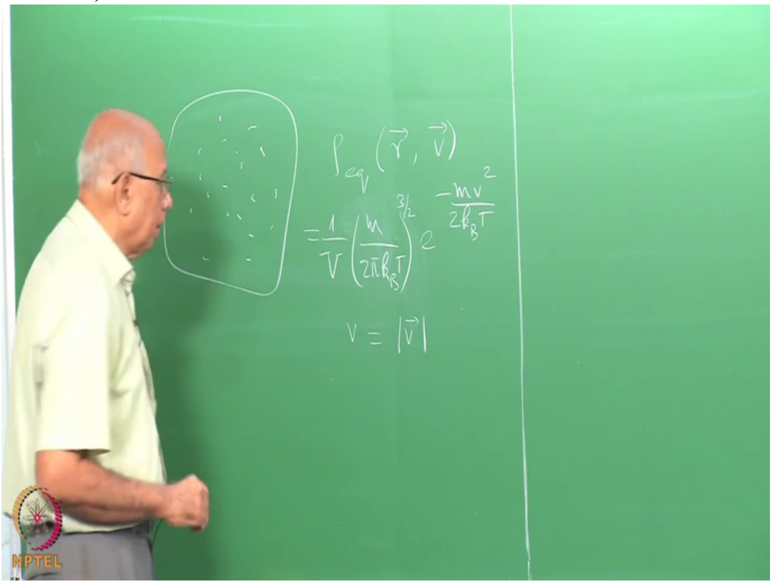

Ok

So that's the phase space density in equilibrium. But right away we can ask a more complicated question. We can ask, what happens if I take a single particle and I somehow manage to tag this particle. I am going to keep a track of it and we are working in the level of classical mechanics, so I tag this particle and I look at it by saying look, at the instant of time when I take a look at it, it has got some position r naught, some velocity v naught and then I, given that I ask what happens to it as a function of time?

Ok, so now I ask for the conditional probability density function for which I will continually, let me write it as capital, conditional probability density function, I will use the abbreviation P D F for it throughout and I ask for the conditional probability density function rho such that its position is r, its velocity is v at some time t given that it was some r naught, v naught and at time t naught. So

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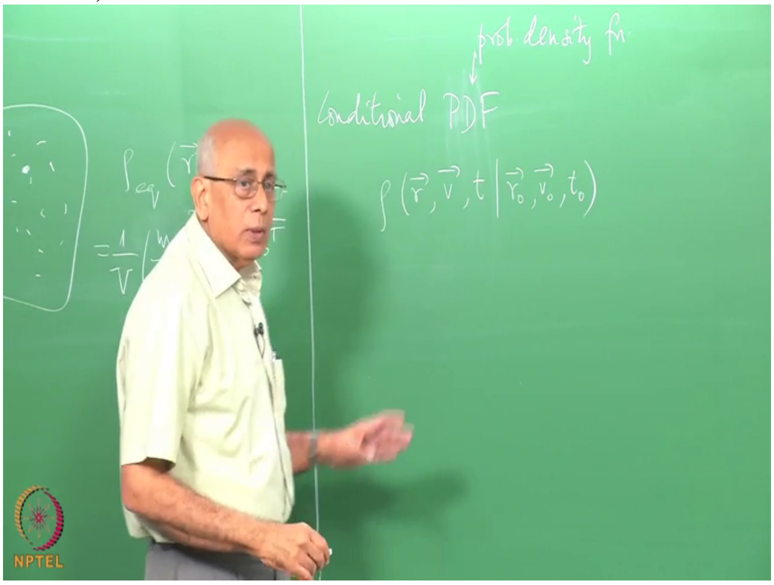

this is the conditional density and I ask what this quantity equal is to? Ok. So r naught and v naught are any arbitrary values which are allowed and I say, given that condition what is it going to do as a function of time.

Well what we do know intuitively is that time elapses, as t minus t naught tends to infinity, so I expect that if t minus t naught tends to infinity;

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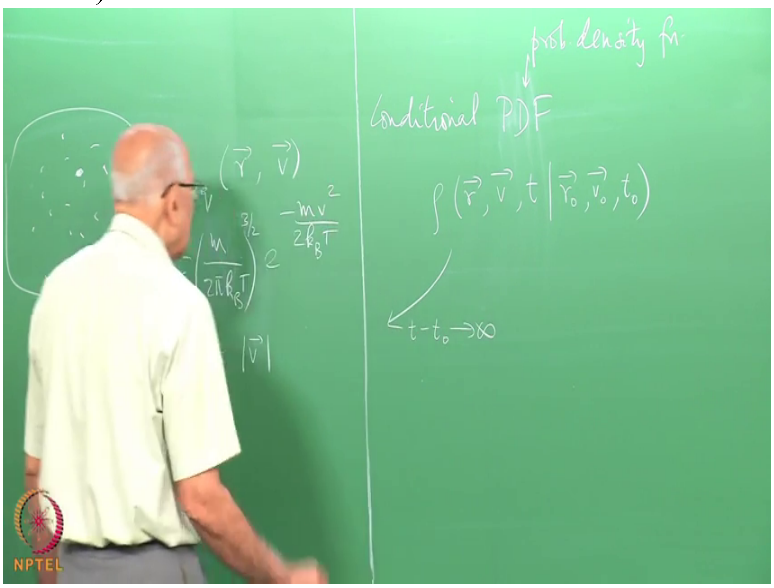

this thing will actually tend to the equilibrium density

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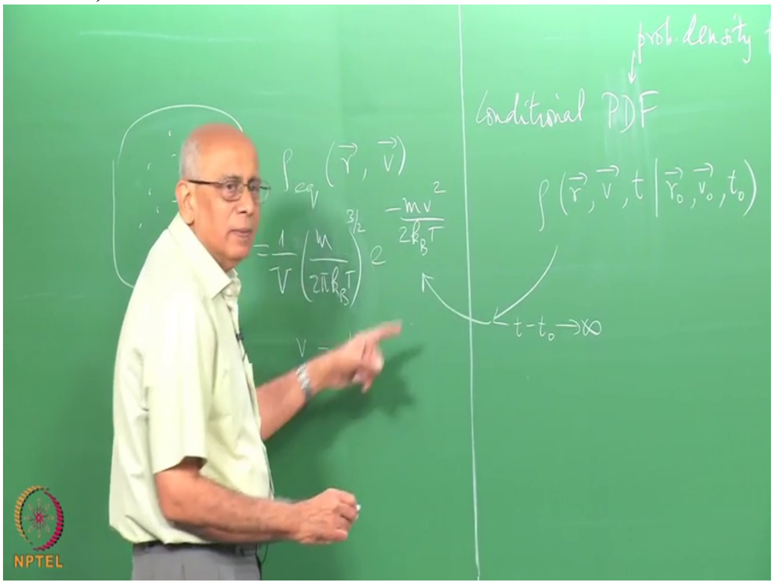

because the system is not going anywhere. It is in the equilibrium. I expect physically that , intuitively that enough time elapses since the time I measure the initial conditions, this particle will relax to equilibrium and attain the equilibrium density. It will lose memory of what its initial values were of these variables, and it will tend to this quantity here, Ok.

But the hard question is now, what is it as a function of t for arbitrary values of t and not necessarily t minus 0:06:39.7 t naught into infinity? Ok. We it is again sort of clear and we haven't established this but it is again clear that if the system is in thermal equilibrium, then it does not matter when I start this t naught. And that this whole quantity will be a function only of t minus t naught, only the elapsed time because when I start the clock is completely irrelevant since the system is already in equilibrium and the process is stationary.

So I don't really have to ask, specify any particular t naught, all I have to worry about is the difference between t and t naught, the elapsed time. So I might as well say t naught equal to zero, right? I will often do that; we will often do that assuming the system, if it is in thermal equilibrium, has no time dependency of any kind. So the time when you start the clock and measure the initial condition is irrelevant.

But the hard question is what is this function as a function of t, how does this reach this? Because I know what its value is, initially. I know what its value is, not as t minus t naught tends to infinity but as t minus t naught tends to zero.

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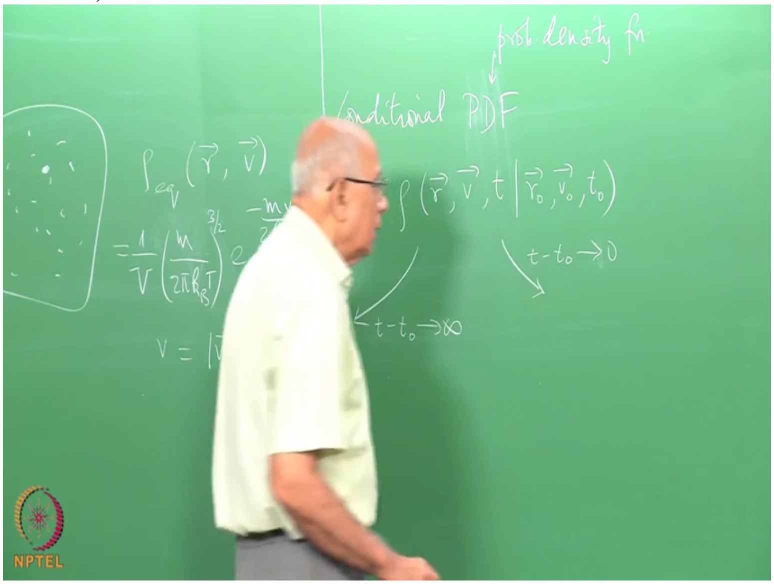

In other words, at the instant when t equal to t naught, what is its density? It is obviously equal to delta 3 of r minus r naught delta 3 of v minus v naught. Because I am telling you that the values at t naught, time t naught are these values, deterministic values.

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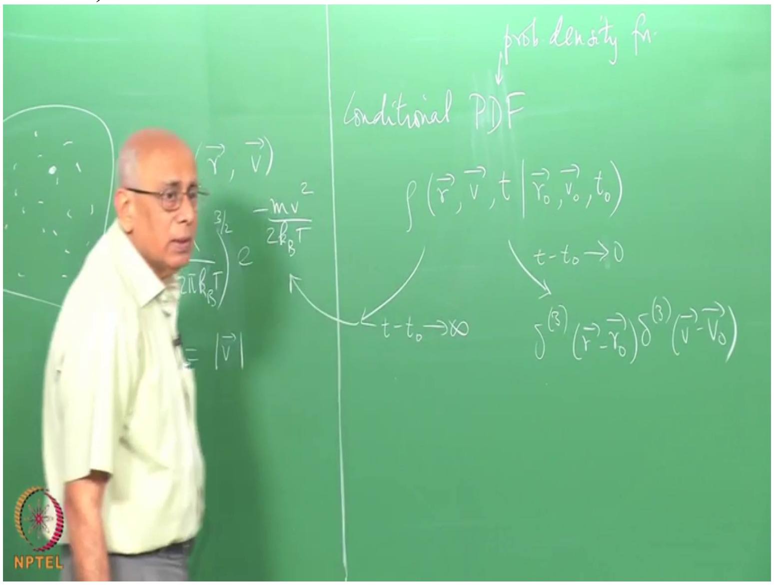

So it starts off in this very spiked way, this delta function distribution and broadens out or does something crazy, it becomes uniform in space and velocity it becomes Maxwellian with the mean value of velocity which is equal to zero. So I know the limiting cases, I know the initial conditions on it, and I know the limiting distribution but I don't know what it is in between, Ok. That is a very hard problem. It turns out; this is a very, very hard problem.

If you look at the realistic dense fluid, it is an extremely difficult problem to answer, because these particles are in interaction with each other to start with, number 1, and they are correlated with each other. So there are all kinds of correlations between the particles in such a way that you cannot write a single equation, closed equation for this variable, this density.

It gets coupled to 2 particle distributions, 3 particle distributions and so on in a well-defined hierarchy. And this hierarchy is never-ending, it is not an ending hierarchy, doesn't for a finite number of particles it will end but of course if you have an infinite number of particles in thermodynamic limit, this hierarchy is not a finite set of equations. So already you begin to see that this is a very, very hard problem to start with.

Taking into account all the possible correlations and if these are quantum mechanical objects and you have to impose for example, symmetry or anti-symmetry in the way of functions, if you say these are fermions or bosons which obey certain kinds of quantum statistics due to indistinguishibility then it becomes even more hard. It is a very hard problem in many-body theory and we are certainly not going to get towards solving this problem.

So let's look for a simpler problem to solve, a simpler model to solve where we get some insight into how time dependence appears. And we will use physical guidelines to guide us through this problem through. So let us suppose that in this fluid, in this dense fluid you have a few

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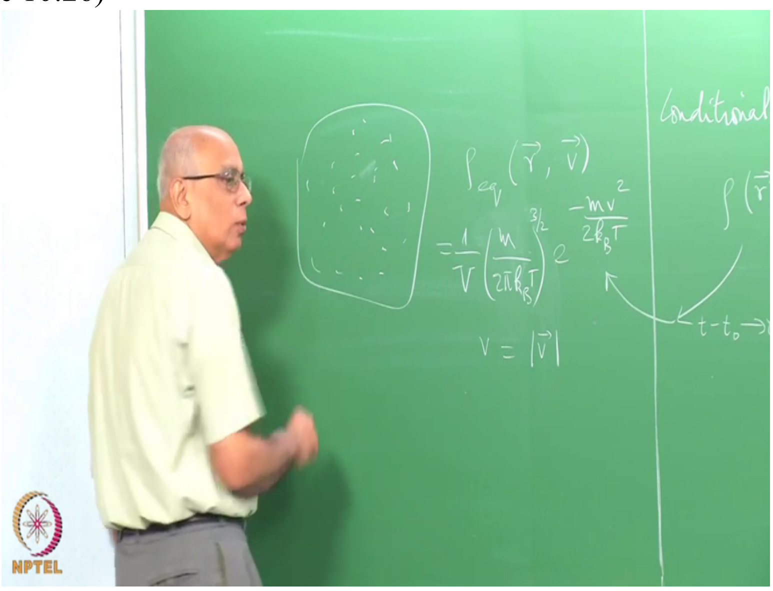

much bigger particles, a few tagged particles, colloidal size particles. So these particles are of atomic size, atomic or molecular sizes which are of the order of fractions of nano-meters but now let's put into it some objects which are minus or a little smaller than that but which are already several thousand times the size of atoms, individual atoms right?

So let's call those tagged particles, I mean, let us call those the larger particles, I will use little circles for that and let us put a dilute concentration of those things. So these are much bigger particles with individual masses which are much, much greater than m atom.

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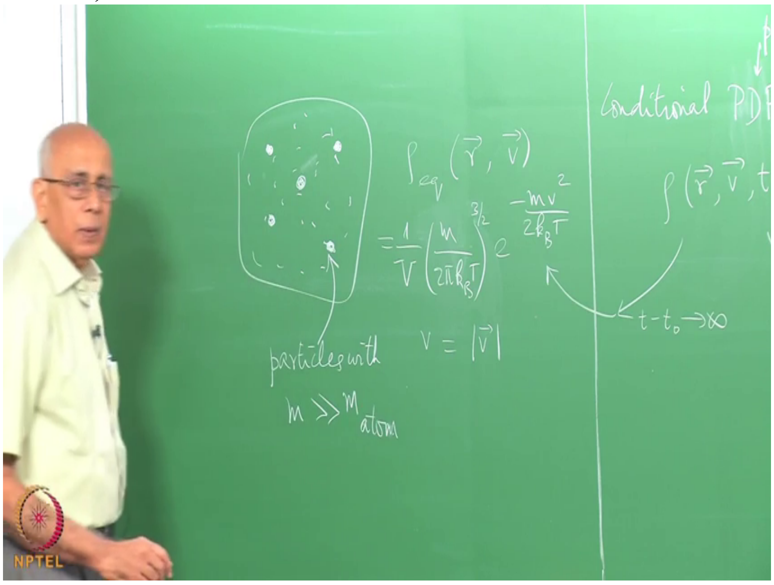

They undergo Brownian motion in this fluid. They are moved about from side to side. They are jolted about; they have very jerky motion because they are being buffeted constantly by these little tiny particles, the atoms or molecules, Ok.

We will also assume that the concentration of these objects is sufficiently small that they don't interfere with each other. So essentially we can treat each one of them in isolation. So that's the second assumption. The mass assumption will appear in a very subtle way and we will see exactly where it comes about. So this is like, for instance, in realistic cases, it would be like having pumpkins being bombarded by mustard seeds, even worse because these things, colloidal particles would be micron-sized and the other fellows are Angstrom sized, Ok. So many orders of magnitude separate them and the question is will these particles get anywhere? Obviously they are going to stay there, get bounced around etc, etc and let's see what happens to the motion of these particles here, Ok.

Now what we can do is one of several things. We could try and find out, since we want to know what the distribution in velocity in particular of these particles is, we could try and find out what the equa/equation, what the actual probability density function of the velocity does as a function of time by writing a little model for it, making some assumptions about the way in which the atoms bombard this big object.

Alternatively we could start with the equation of motion. We could guess an equation of motion using Newton's equation for it, for instance, write down this equation of motion but taking into account the random forces due to all these particles which we cannot compute, which are completely random for all practical purposes by using a stochastic equation for this particle and making suitable assumptions about the nature of the noise, Ok. So let's use that.

We will try to do both but let's write this down to start with the equation of motion and this is called The Langevin Model. It won't be apparent

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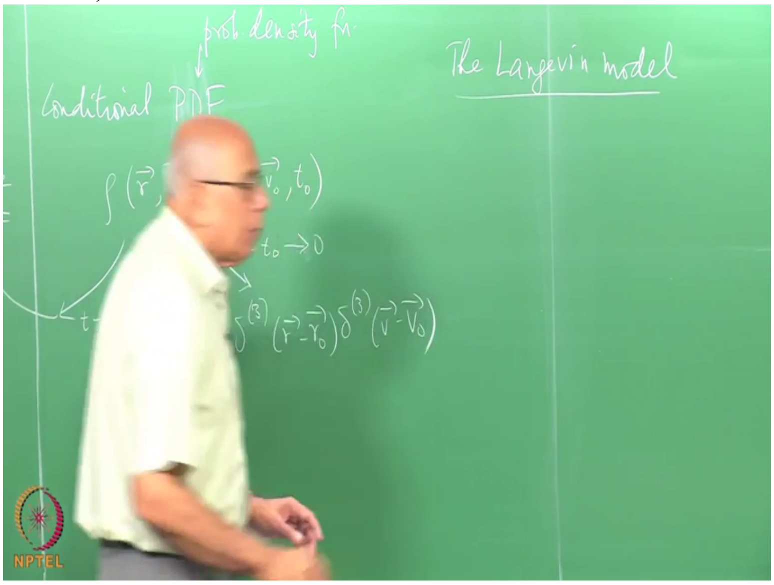

in the beginning where this assumption has gone in. That's little subtle but we will see how this figures a little later. We will run various consistency checks and we will see that you need this assumption otherwise it is not true for the reasons I mentioned earlier, namely if you are looking at the atoms themselves, and one of these particles is one of the atoms themselves then it has got all kinds of correlations with the other particles and you can't write the simple, one body phase space distribution function.

So we keep that on our mind and we now write down something for this, equation of motion for this. And let's make life very simple to start with. We will assume that this system is again in thermal equilibrium so these particles are also in equilibrium at the same temperature except that they are also uniformly dispersed. We will neglect the effect of the gravity for a moment and the velocity distribution is Maxwellian with this m here where m represents the mass of one of these particles here, one of these large particles, Ok.

So the heat bath is provided by the fluid which ultimately is in contact with the external world at some fixed temperature and these particles are in thermal equilibrium in this fluid. And their distribution function and velocity in equilibrium is the Maxwellian distribution, it isprecisely this. And in equilibrium the position is also uniform so it is precisely this with m now standing not for the atomic mass but the mass of one of these particles here. Ok, now I ask this question.

What if I start with some point and I go and I ask at t equal to zero I start somewhere, and I ask what happens as a function of t? How does it attain the Maxwellian distribution eventually? So it is exactly the same question. By little sleight of hands, instead of writing m atom I wrote this m for the large particle and this is exactly the problem we have to solve. Yeah.

(Professor – student conversation starts)
Student: The density of the larger particles are very small compared to the bath.
Professor: Yeah
Student: How do we define a temperature for such a low density matter?
Professor: A dilute gas, I can still define a temperature for a dilute gas. This is a good question. How do I define a temperature for one object? I am going to assume that its average kinetic energy defines its temperature which it does. In an ideal gas, that is precisely how temperature is defined. Temperature is a sort of wrong, is a sort of irrelevant notion that we unfortunately introduce for historical reasons. Before the nature of what heat is was known, they didn't know heat is random molecular motion, the energy of random molecular motion. Had we known that we wouldn't have used another unit called temperature at all and then introduced Boltzmann's constant to convert from one to the other? They would have just called it average energy. And that would have been the end of it. So in that sense I am going

to say that the average energy of this particle, each of these particles is 3 halves k T, Ok, right. Now I ask this question here and for that purpose, we are going to aim at that but to start with, let's do the following.

(Professor – student conversation ends)

Let's start with the equation of motion for this particle. So what is its equation of motion? It says m and for notational simplicity for the moment, we will put this in complication in a little later, for notational simplicity let's look at one Cartesian component of the velocity, x component for instance and let me just use v to simplify it, the notation. m v dot this is a given Cartesian component of v, it is a little abuse of notation because I called v the magnitude

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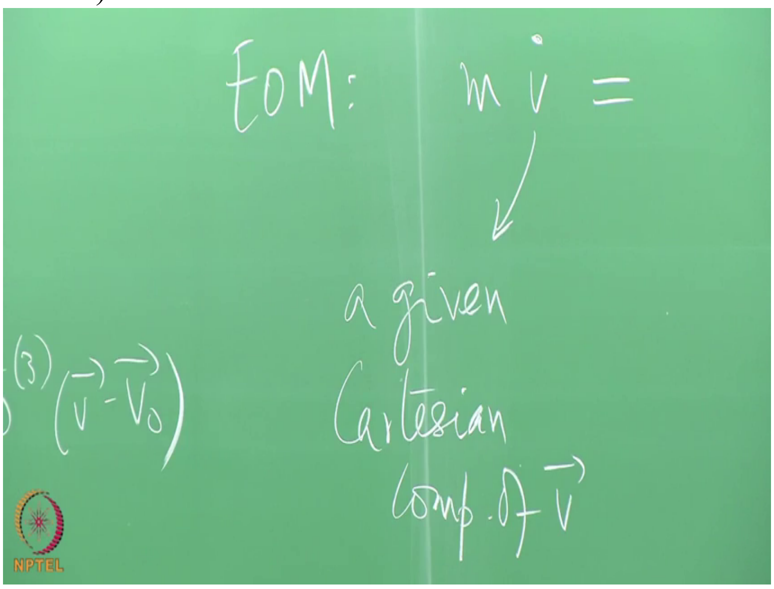

but forget about this now, I will use this, I should have, otherwise I should write v 1, v 2 or v 3, which is a nuisance.

And what is this m v dot equal to? It is equal to the force on this particle, instantaneous force on this particle which is varying as a function of time

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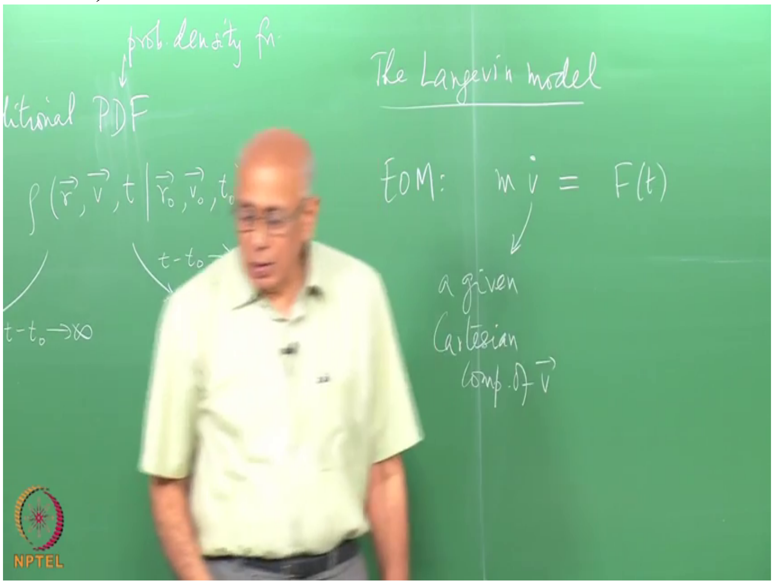

because the force is caused by the collisions of the molecules around and it is varying very rapidly and very randomly. In fact the gas in this room for instance, on the average there are about 10 collisions per picosecond or so for the molecule. So it is really happening very, very fast. Ok. And this is being buffeted by these particles very randomly in a fluctuating manner, Ok. So this is the total force and it is supposed to be random. This fellow is supposed to be random.

It's random in the sense that it is random

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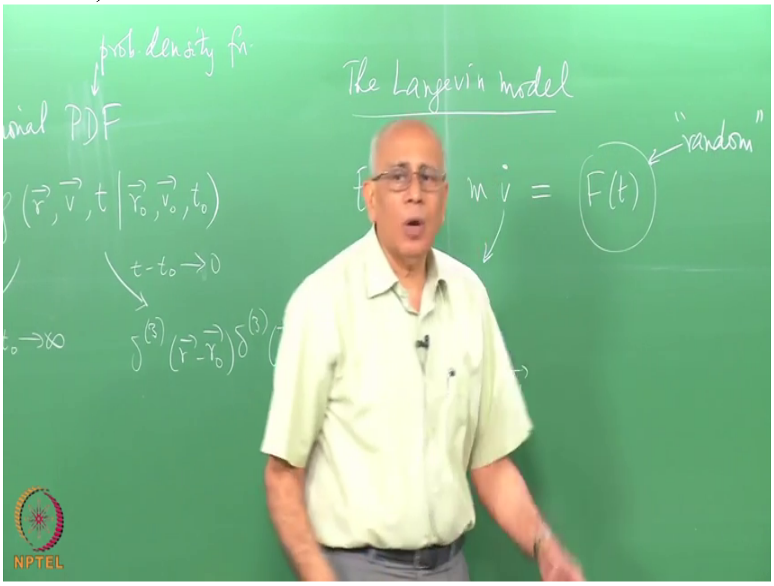

for all practical purposes. Because if I were able to actually write the equation of motion down for all the particles in the system, then of course I know where they are going, who is going to hit which other particle and so on and then there is nothing random about it in that sense. But of course, once you have a very large number of particles for all practical purposes this force is totally random here, right. I want to use the symbol for this random force. So let's write it as equal to some eta of t.

I want to use proper notation so let me write it as a quantity gamma times eta of t, where this is a constant. Well, I want to simplify this notation as much as possible so let me just write it as eta of t and we will come back to what this means, Ok.

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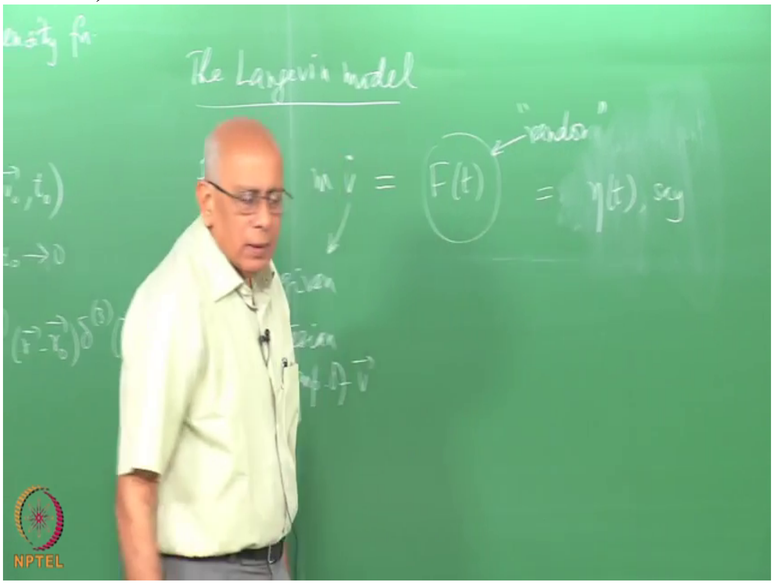

The randomness that I am going to put into it is to say that this eta of t is what is technically called a Gaussian white noise. So I will explain these terms what is meant by that as we go along but it is some random force, this kind. It has physical dimensions of force, as it stands here, Ok.

So I have a simple equation and the matter is over in the sense that I can integrate it formally. So once I integrate it, I have v of t equal to an initial value of velocity, because I want to find out this quantity here. So I am going to start by saying, to solve a different equation you need to specify an initial condition. So I am going to say at t equal to zero, the value of this velocity was of this component was some number v naught, Ok.

So v of t equal to v naught, that's the initial value plus 1 over m integral, I might as well choose the initial time t naught to be equal to zero. Set t naught equal to zero. Because as we said, as

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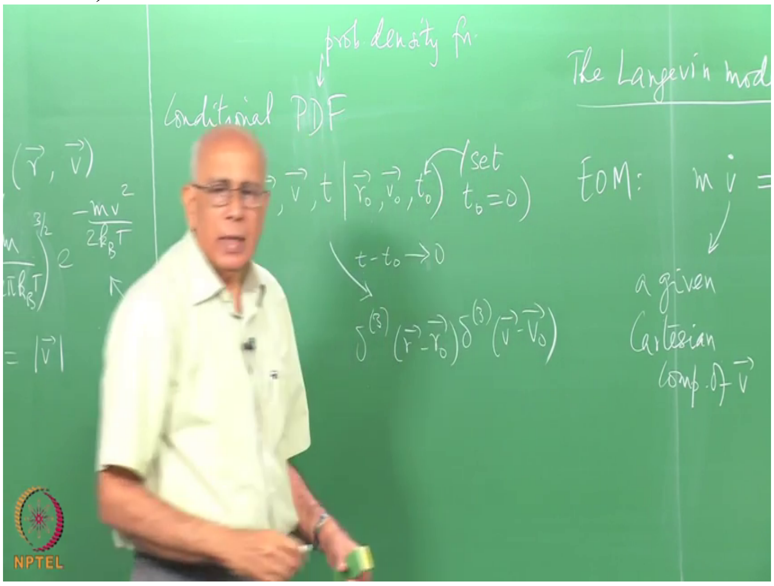

I have argued, this whole thing is in equilibrium. So doesn't matter when I start the clock. So this integral runs from zero up to time t d t prime eta of t prime.

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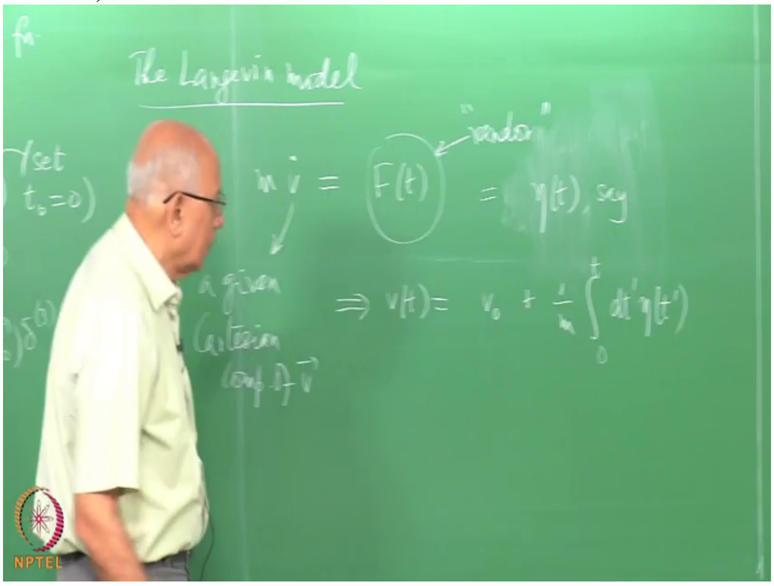

That is the formal solution to this first order differential equation. It is triviality itself and it satisfies the condition that at t equal to zero, v is v naught, here. But this is a random force. And what I want is averages. Because once I have a random variable, what I am interested in are its averages of various kinds, averaged over all realizations of this force. So all the force histories that are possible, and each time there is a different history you get a different equation.

So really this equation looks very trivial but it is actually infinite number of equations. Because each time the noise has a different kind of fluctuation or realization, you have a fresh equation really because it is a different function, eta of t. But we would like to average over all realizations of this noise.

Now we got to be a little cautious. What do I mean by averaging over realizations of the noise? What, what's the input variable here? Well, we will do this averaging in two steps. When I want any quantity which is an average of referring to this particle's dynamical variables, such as its velocity or its mean square velocity and so on, I have to tell you what am I averaging over. Not only should I average over all realizations of this noise, but I should also average over all possible initial conditions. Because there is no reason why I should have chosen v naught as the initial value. I could have chosen something else as the initial value.

So there is a double average involved here. First an average over a, for a given v naught, you average over all realizations of the noise for the given initial condition and then you average over all possible initial conditions as well. So I am going to use overhead bar for conditional averages, whatever is inside here, for conditional averages for a given v naught. And I am going to use this for a complete average, for a given v naught over, over realizations of eta of t, complete average over all v naught as well, Ok.

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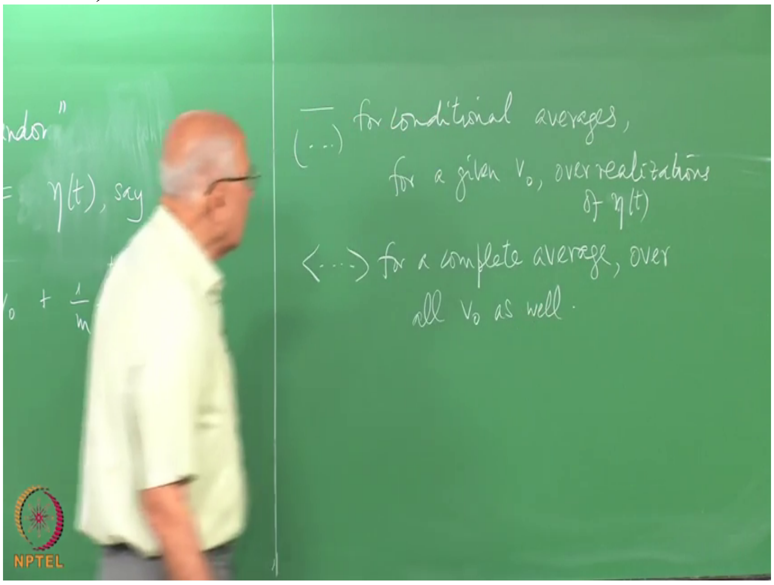

So we will do average in 2 steps. First we average over, start with a given v naught, so we look at the ensemble of these particles such that the v naught is given and we repeat this experiment with different eta of t each time, take the average and after that we will average over the initial velocity as well, Ok. Now implicit in this is the fact that these averages should commute with each other. Whichever order I do it, I should get the same final answer.

And that is more or less obvious with little subtle assumptions involved here, first of all averaging is an arithmetic averaging, it is just adding numbers and addition is always commutative. But more than that there is a deep assumption here that whatever is the fate of this particle doesn't affect the bath, the heat bath. So the assumption is the heat bath's properties do not change as a consequence of the motion of these particles. That system remains in thermal equilibrium at temperature T, Ok. So this noise, its statistical properties are not affected by what an individual Brownian particle is doing, Ok. So that's the physical assumption when you have to make sure that that's really satisfied before this model become realistic. So given that let's take the average over this.

So what is v of t equal to? There is nothing to average here, because this bar is for a given v naught, so this is a deterministic number and you get just a v naught plus 1 over m, the average of this integral, Ok but an integration is a summation and the average is also a additive operation right, arithmetic average so, this is equal to integral zero to t d t prime eta of t.

So notice how carefully

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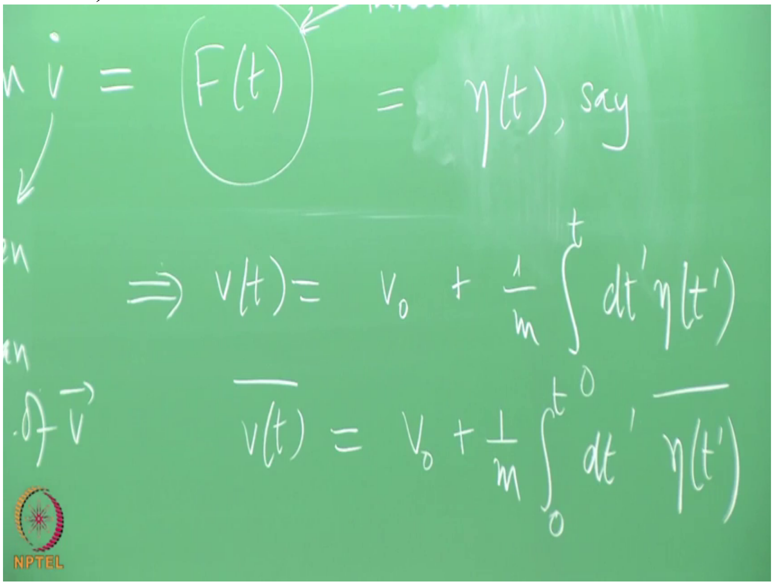

we are proceeding step by step so we know what the assumptions are at every stage. So every one of these operations has to be justified. So you agree that this is indeed the average value of the velocity but now I argue saying this particle is not going anywhere. It is staying inside the container and it is hit as much from the front as from the back and the average value of this force, it is very reasonable to assume, is zero. The average force exerted on this Brownian particle by all other particles, is on the average, zero because its average velocity is in fact zero, Ok.

So we will make the assumption that eta of t average which indeed is equal to eta of t as well because even if you change all the initial conditions it is still true; this is equal to zero.

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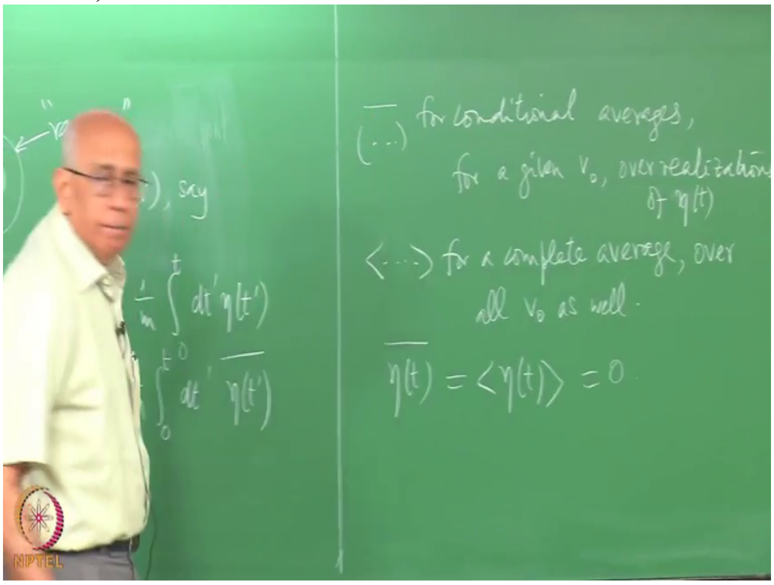

So as far as the properties of eta are concerned, it doesn't care what the Brownian particles are doing and its average value is zero. That is the first thing, that's the mean; it's the noise with zero mean, Ok. So this term vanishes and this is equal to v naught, yeah.

(Professor – student conversation starts)

Student: Sir, is realization equivalent to direction, I mean like

Professor: No, no, no, realization is if I plot this eta of t which is the x component of the force, if I plot this eta of t versus t, this might be one realization of the noise.

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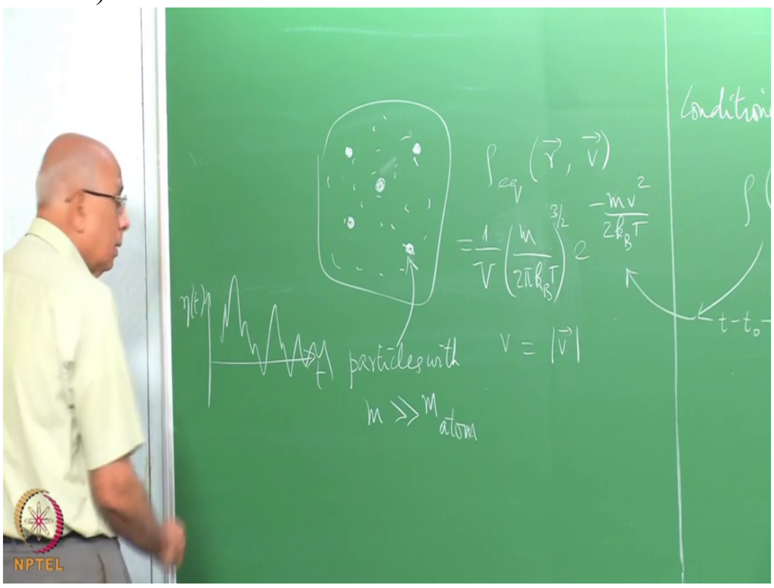

But it could equally well have been this. It could have

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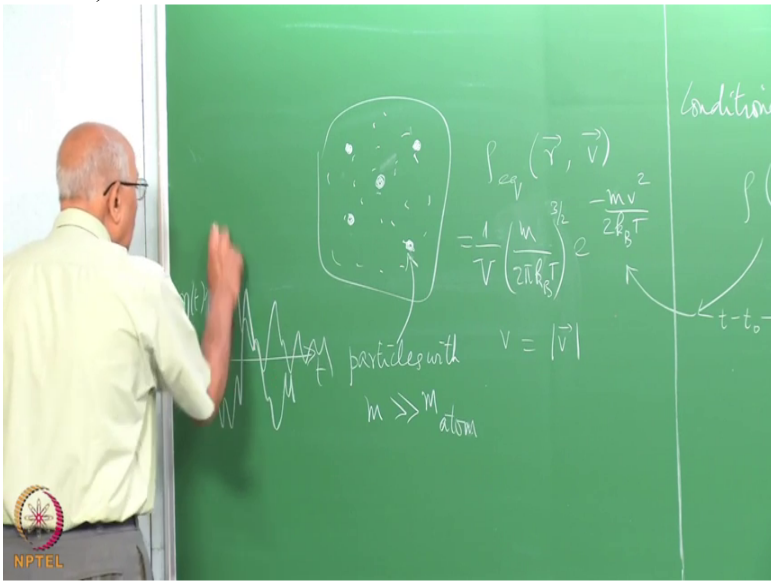

been this.

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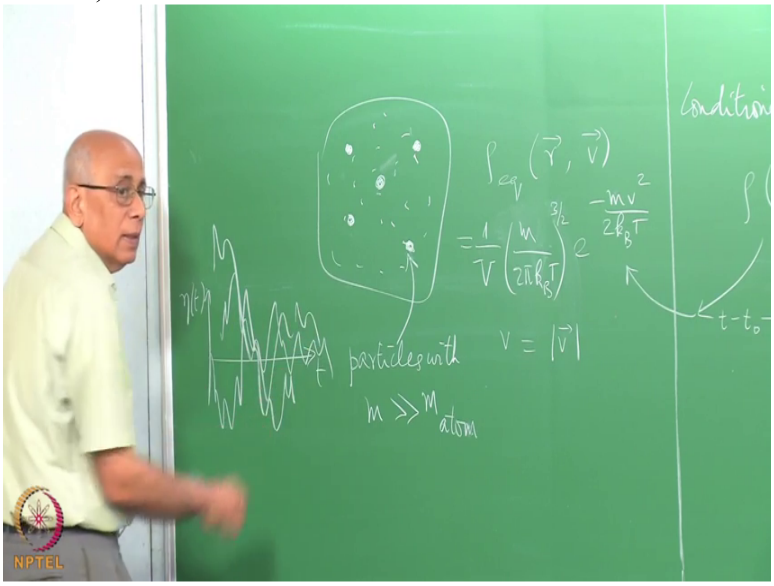

So I am going to average over all these realizations.

Student: Why should it be 0:28:10.6

Professor: Pardon me?

Student: Why should it be zero?

Professor: Average, average, on the average. Because if it were not zero, this particle would move systematically in some direction. So it is clear, on the average it is zero. These are not; these fellows are not going anywhere. They have a fluctuation about their mean position but the mean itself is zero to start with, Ok.

(Professor – student conversation ends)

We have already said that these Brownian particles are in thermal equilibrium and their mean value is zero completely. We are not going out of thermal equilibrium. We are just saying, I focus on a particular particle and look at its initial condition and ask for conditional averages, subject to the condition that this system is still in thermal equilibrium, right?

So we are asking a time dependent question because we chose an initial condition that breaks the fact that this velocity is zero on the average. It starts with some v naught and I ask what is it doing. Or to put it yet another way, in pictures let us do that, if I plot the velocity distribution, because the position is irrelevant here, that remains uniformly distributed throughout, but if I look at this rho of v t given v naught, this is the quantity I really want for this tagged particle and I plot v here,

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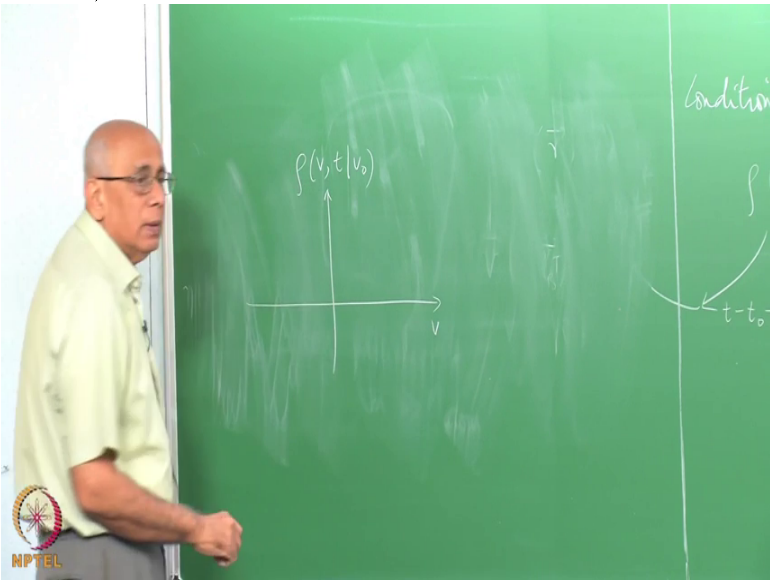

then at t equal to zero it is starting with a delta function at v naught. So it is clear that this is the distribution where this is v naught.

It is starting

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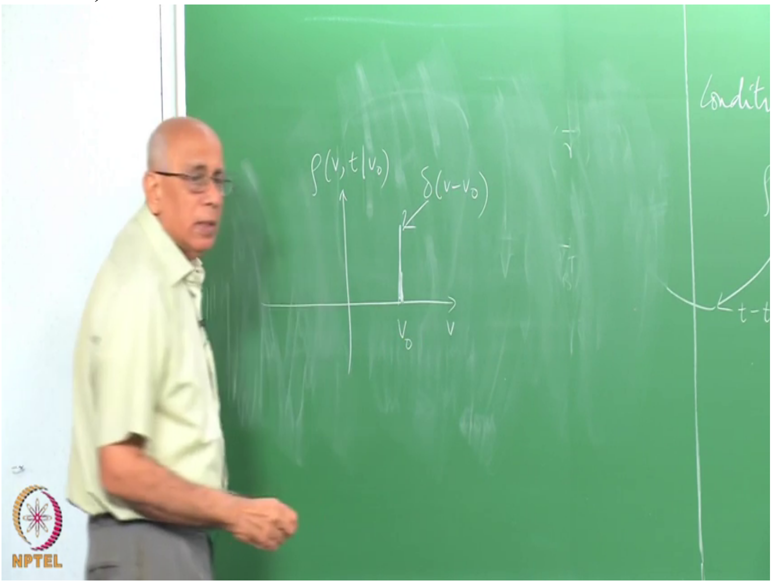

with a normalized delta function as the distribution. And as t becomes infinite the value of this distribution here becomes independent of the initial condition. It loses memory and it gets into the Maxwellian distribution. So it is finally like this. And the

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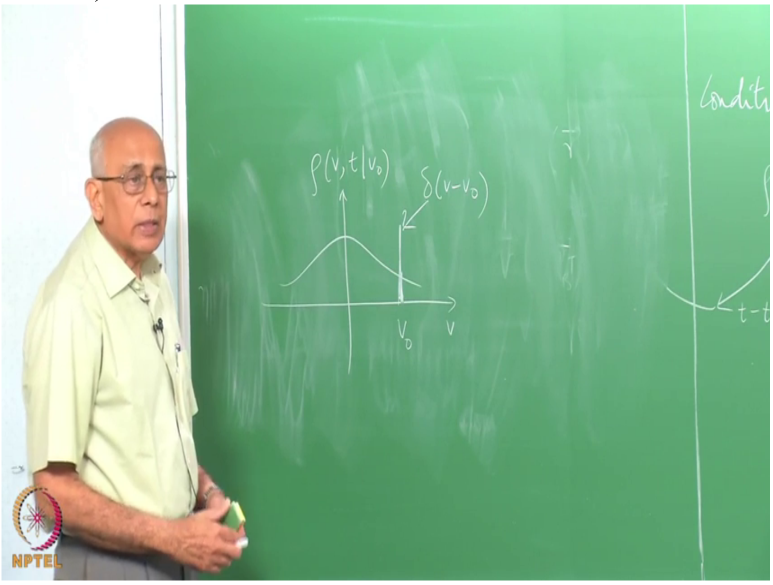

question we are asking is how does a distribution managed to start with a delta function there and end up with a Maxwellian here as t goes to infinity. So this is the distribution, this is at t equal to zero and this is at t tending to infinity.

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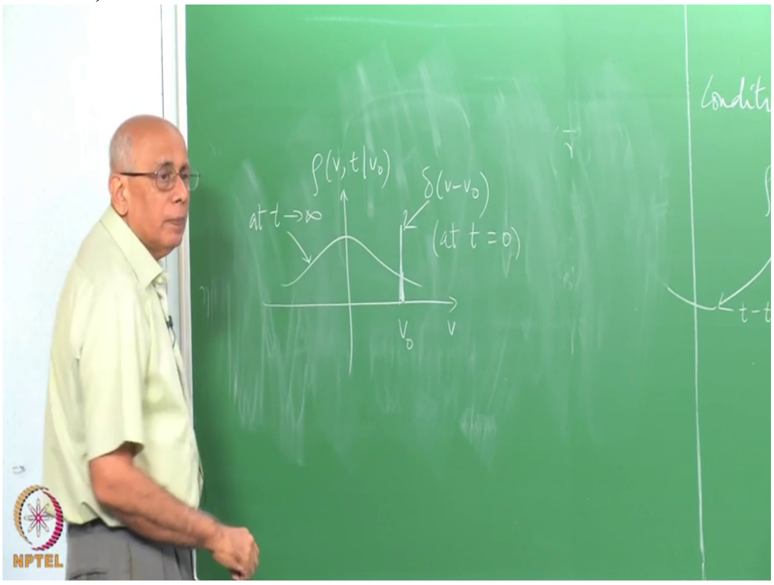

So that's the question we are really trying to answer. How does this distribution do this? What does it do in between?

Not very surprisingly you will discover that this mean value starts drifting to the left until at infinity, it becomes zero here. But in the meantime it is also broadening because this has zero width and this has the width dependent on the temperature, k T over m, square root of. So that's the kind of question we are trying to answer. But we are doing it through the equation of motion.

So we will first get information on the mean, the mean square, the correlation function and so on and then work backwards using that information to try to get the functional form for this quantity here. And perhaps you will writing equation down for it and may be even solve it. So this was the first step here. Now the next thing to do is to ask what happens if I average over initial conditions as well. So we can do that right away. We have t...

(Professor – student conversation starts)

Student: Is that the problem 0:31:40.0 we had 0:31:41.4 wanted v naught to be zero, right?

Professor: Pardon me?

Student: Average will go to zero eventually, right?

Professor: Yeah.

Student: Then this is not working, I think.

Professor: No, no, it will, it will work, you will see. This will work because now I am going to ask what is the average value, if I now average over all initial conditions, Ok. But remember this particle was in equilibrium. So we know the following is true. We know that rho equilibrium of v, equilibrium distribution is the Maxwellian distribution.

(Professor – student conversation ends)

So we know that this is equal to m over 2 pi k Boltzmann T to the power half, this is one dimension, one component only so it is just a power half, e to the minus m v square over 2 k Boltzmann T. One component v is, denotes so that is the reason for the half here instead of the 3 halves.

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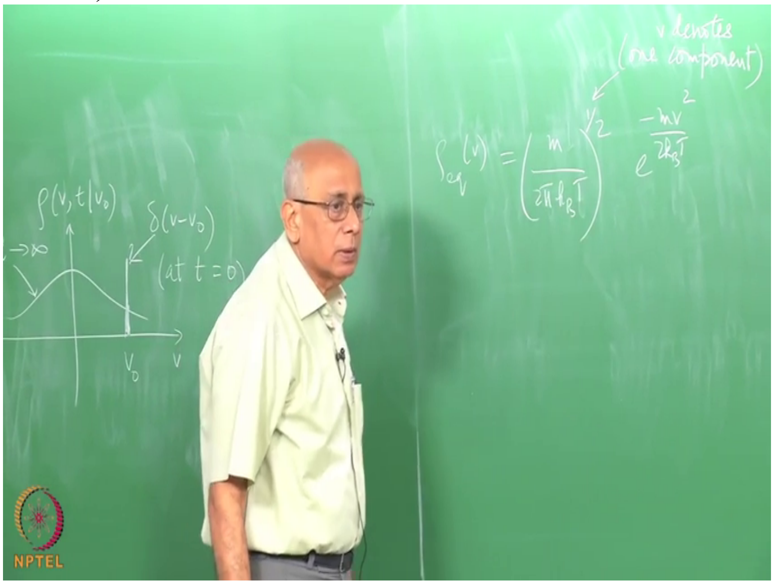

So that's the Gaussian symmetric about the point zero. So if I now do this, this v of t, this is equal to integral from minus infinity to infinity d v naught times v naught which is this quantity here multiplied by rho equilibrium of v naught,

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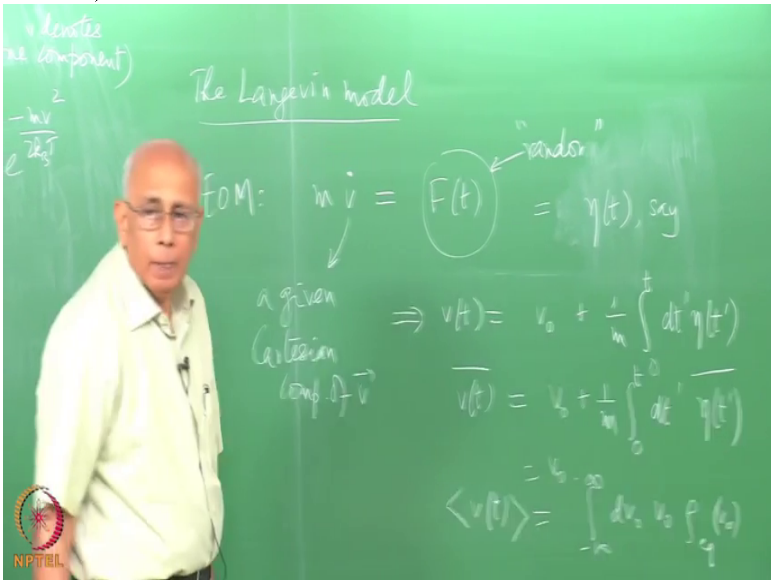

Ok. And what's the value of that integral?

(Professor – student conversation starts)

Student: Zero

Professor: It's zero and why is that so?

Student: Odd function 0:33:21.4

Professor: Yeah because this is an odd function and that's an even function, this distribution so it vanishes, which is completely 0:33:28.7 consistent.

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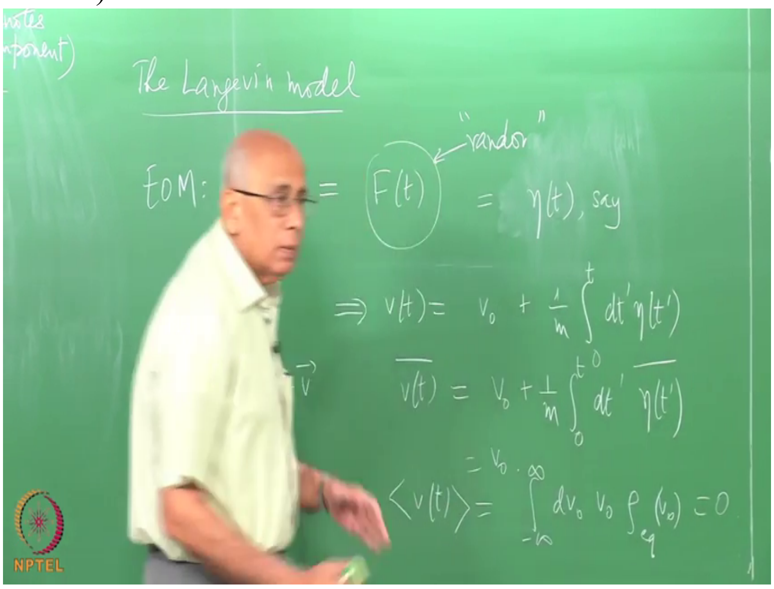

We know that the average value has to be zero in equilibrium. And it remains zero at all times. So we are completely Ok because at no time, it is actually moving off anywhere or anything like that, the full average.
(Professor – student conversation ends)

The conditional average will of course start at v naught at t equal to zero and perhaps drift towards this, but the full average, since the system is in thermal equilibrium; the velocity is a stationary random process. The mean value cannot depend on time. Because then it is not a stationary process, Ok. The mean, the mean square, mean cube none of them can depend on time, no moments and we must check that.

So you agree so far that this has been perfectly alright. In other words what this has tested is that this assumption is not leading to any contradiction so far, it is a physical assumption and seems to have worked. Now let's find the mean square and see what happens.

So the next step is to ask what happens to v squared of t. This is equal to, I take this quantity and I square it, so I get v naught square plus 2 over m times v naught integral zero to t E t prime eta of t prime. So I take this integral and multiply it by v naught, twice that plus the term which is 1 over m square and integral, now let's get rid of this prime notation and write something sensible, zero to t d t 1 integral zero to t d t 2 eta of t 1 eta of t 2.

That is the value of the square, because it is a definite integral, I really have to use 2 symbols of integration when I want to square this term, Ok, right. Now let's take the average, conditional average. So this implies that this quantity, this thing here, there is

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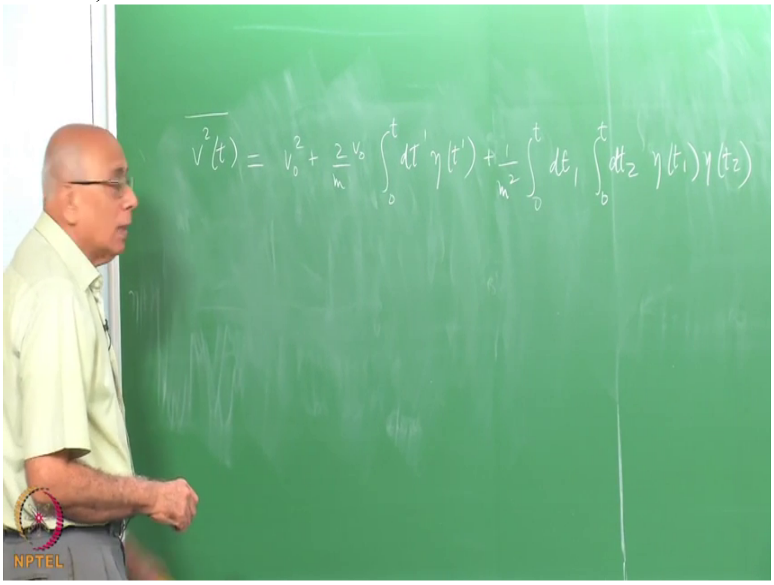

nothing to average over here because it is given, v naught square is given and I average over this, nothing to average here, average is over eta but that average is zero because this averages to zero.

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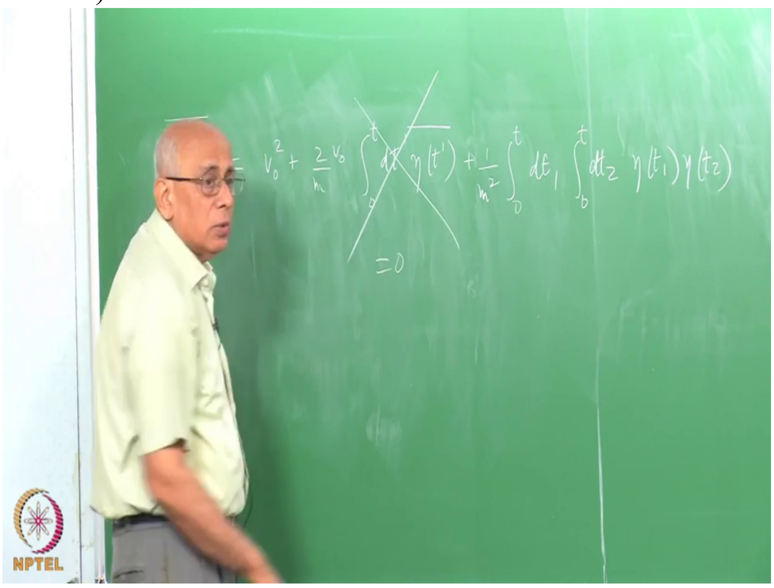

And then inside I have this average.

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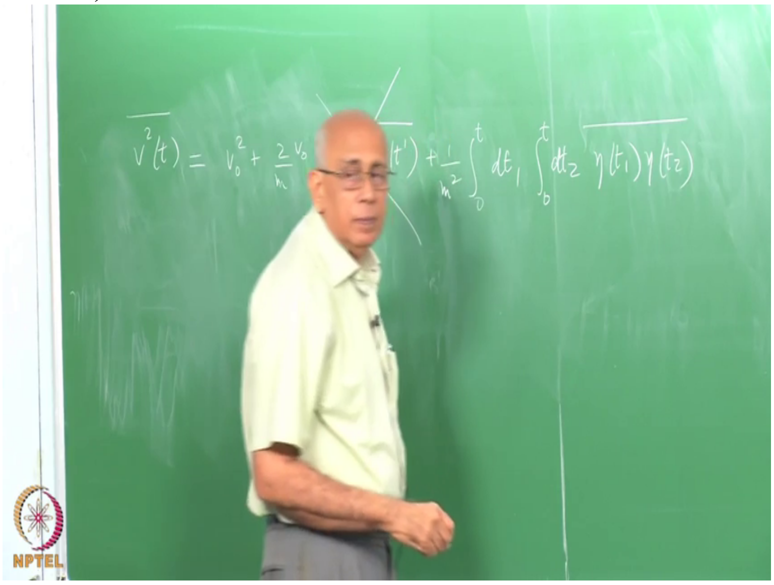

So now we need a model. I need to know what is eta of t 1, eta of t 2 average, we know by our assumption that the bath is not affected by this particle that this is really the same as eta of t 1 eta of t 2 is the question, Ok. Now here is where the physics has to come in, Ok and this is why I said this is applicable to a particle whose mass is much, much larger than the mass of the molecules.

So the statement is that this noise which is the individual molecules hitting this particle, Ok, is completely uncorrelated. In other words what hits it at time t 1 is very different from what hits it at t 2. They have nothing to do with each other at all. So this thing here which is telling you how much of memory sticks on here, is essentially zero if t 1 is not equal to t 2, correct? This memory would in fact drop exponentially and it would drop like a characteristic time there would be of the order of the mean time between collisions. That's of the order of the picosecond. But we are looking at much longer time scales. So this is effectively a white noise. That is the whole point about delta correlated white noises, two noises which is delta correlated so it is proportional to delta of t 1 minus t 2 which has the wrong dimensions because

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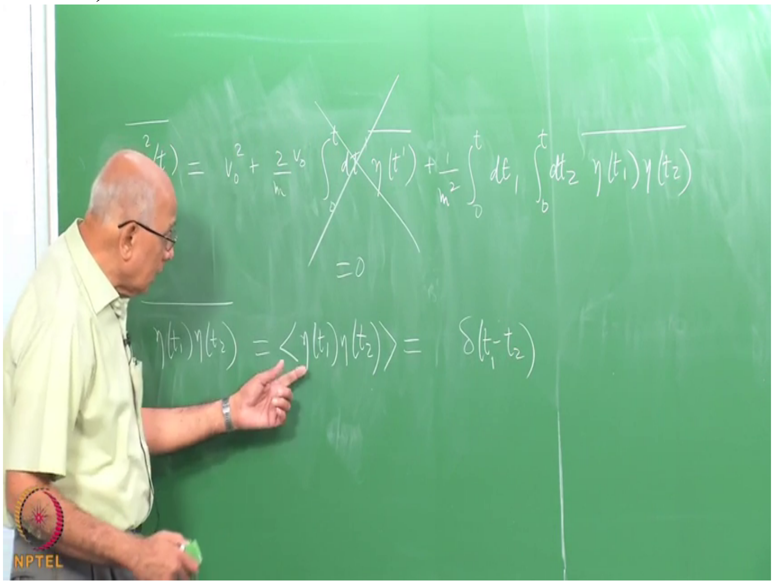

this is square of the force, so you need to fix the dimensionality, what is the dimensionality of this quantity,

(Professor – student conversation starts)

Student: 1 by t

Professor: 1 over time, so if I put a constant gamma here, this is a constant, which tells you in some sense the strength of this force.

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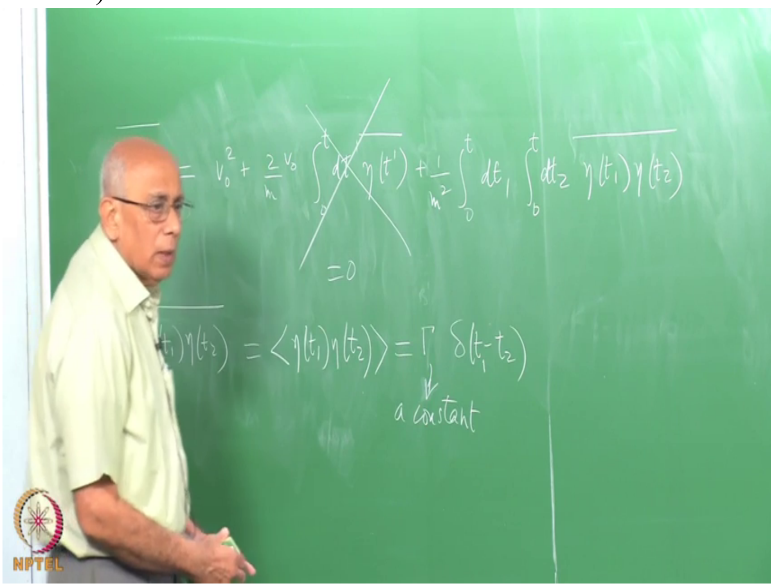

The larger gamma is, the stronger the force, right. So this why I called it a white noise. We will come to the technical definition of white noise little later but it is something which has a flat power spectrum, essentially a delta correlated noise.

(Professor – student conversation ends)

We need to make additional technical assumptions about what sort of, this is very nice for the correlation function but if you give me a noise, a stochastic process, not only should I tell you all its mean values, I should also tell you all its correlations and infinite number of correlations at different time and I should tell you the shape of the probability density functions for this random process. Not just one time, but 2 times, 3 times etc, all the joint probabilities I have to tell you completely.

We will make the simple assumption that they are all Gaussians, Ok. Because we invoke at this stage the central limit theorem which says if you have a large number of f x which are independent of each other and each of them has a finite variance and a finite mean, then when you add them all up in some linear combination, the resultant distribution is a Gaussian. That is very roughly speaking, the central limit theorem of statistics. We will invoke it when the time comes.

But right now, we need just this assumption about the correlation. Notice that this is a function only of t 1 minus t 2, what 0:39:40.5. It is also a symmetric function of t 1 and t 2 doesn't matter which came first. So this is the one assumption that I have been talking about. Delta correlated noise, stationary noise;

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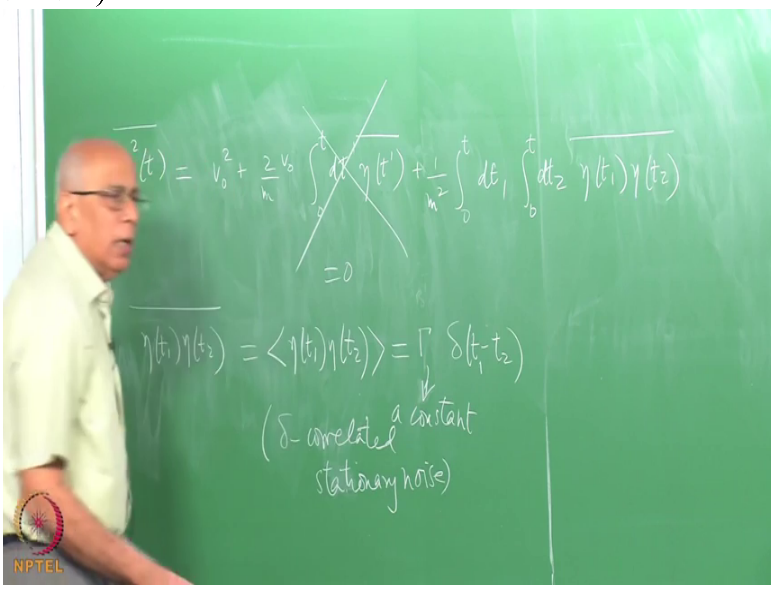

stationary because its statistical properties don't change as a function of time. So all these called the average value, zero, this is the function only of the time difference, the three point function would be a function only of two time differences and so on. The absolute origin of time doesn't matter.Ok

So let us put this into that and see what happens. So I put that in, this implies that v square of t averages v naught square plus 1 over m square and I have to do this integral, the gamma comes out and

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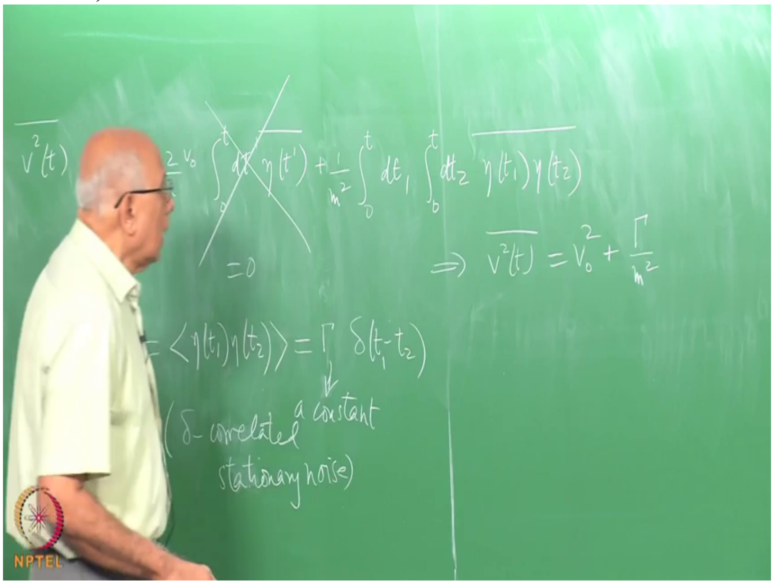

I have to do a delta function integral inside here, Ok. But the delta function just says; replace t 2 by t 1, right. And you have to be careful here again, because if I plot t 1 here and t 2 here, the integral runs from zero to t, in each of the variables and that's the line, the 45 degree line is a line on which t 1 is equal

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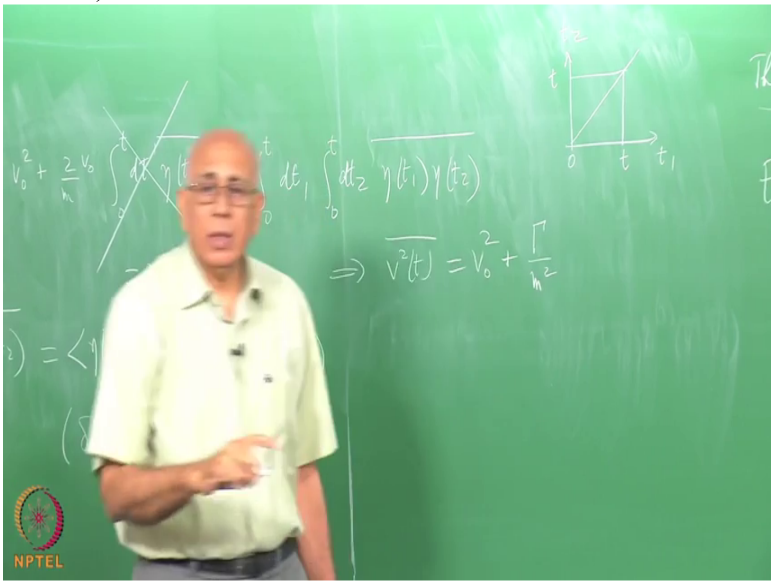

to t 2.

And now if I do the t 1 t 2 integration first, it means I fix the value of t 1 and I integrate in t 2 from zero to t and the delta function fires here. I go to the next value of t 1 and the delta function fires here etc.

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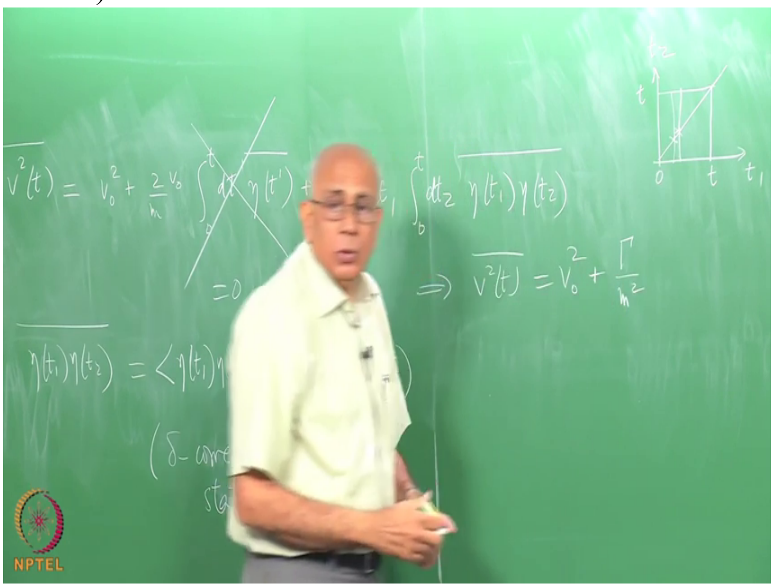

So it is clear that through the range of t 1 from zero to t, there is delta function fires for every value. So I can close my eyes and remove t 2 and put t 1 wherever it appears, right.

And of course, there is nothing to put. There is no t 1 here, it is just a delta function which goes to 1 and I get an integral zero to t d t 1,

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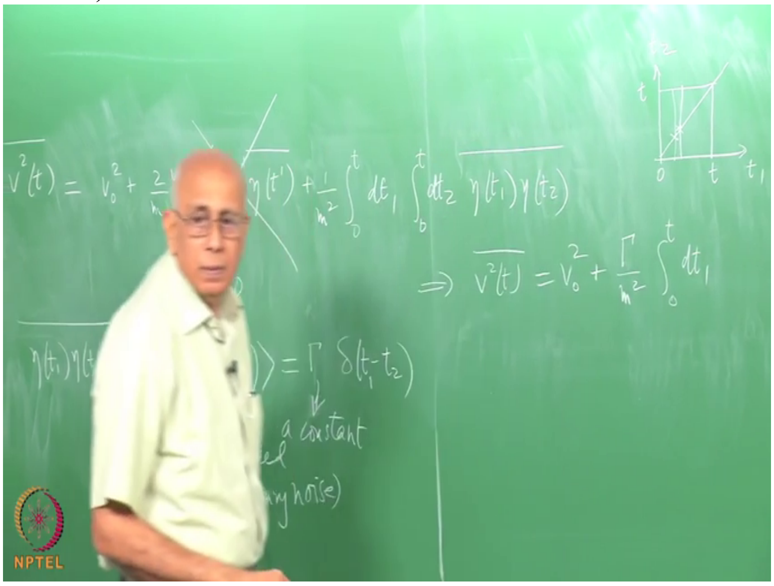

Ok which is v naught square plus gamma over m square t.

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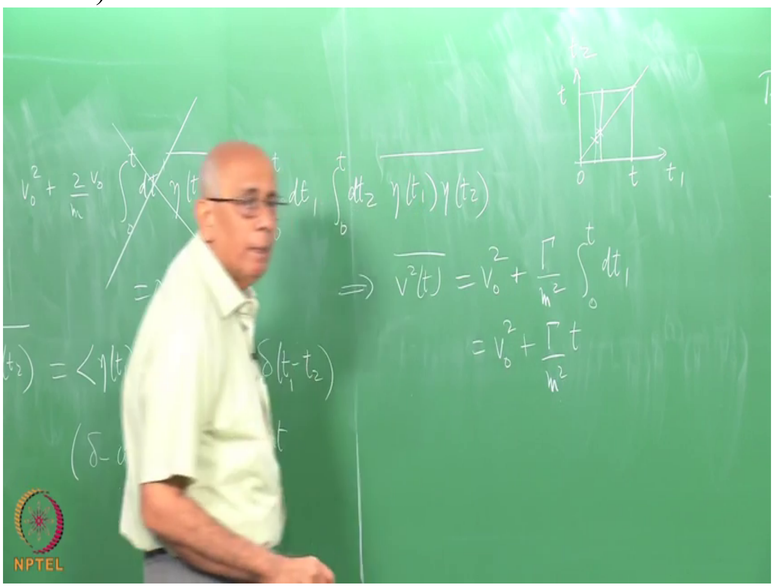

Very bad news, because this is now telling you that for this initial condition, this fellow is actually increasing with time linearly. And now if I average and do this, v square of t, this is equal to an average over v naught square which is just a mean square value of the velocity over the Maxwellian and that is k T over m, plus gamma t over m square, there is nothing, there is no v naught dependence here

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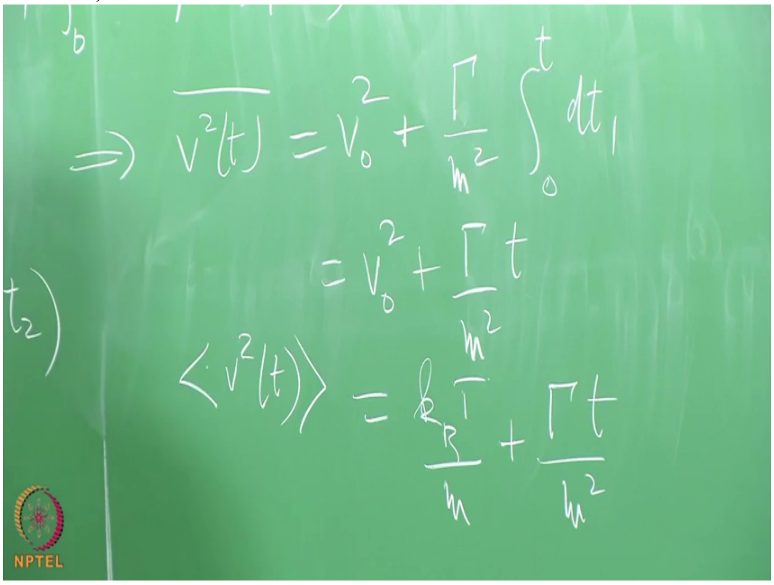

so the average value remains where it is and it is this thing here and it is completely unphysical.

Because it says if you leave this beaker of water alone, put a colloidal particle in it, then its energy, particle's energy will spontaneously increase till it becomes infinite 0:43:03.0 as t tends to infinity. So it is actually taking energy from all the molecules and reaching infinite temperature or energy if you like Ok, which is wrong. It is just plain wrong.

So this is completely wrong, incorrect.

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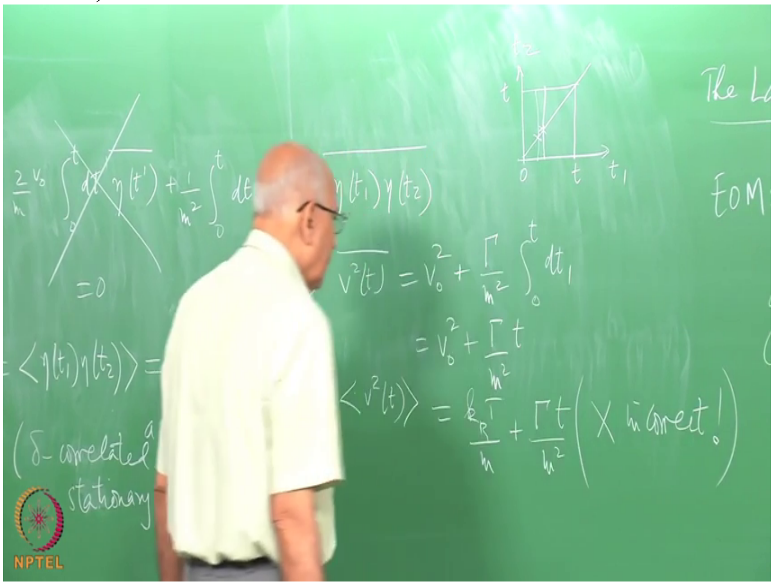

What do you think has gone wrong? Since this is 0:43:41.4 incorrect, it is clear that some assumption made there is wrong, one or more assumptions. So what assumption do you think is wrong? We will eliminate it one by one. What assumption do you think is wrong?

One possibility is that this is not correct, a very strong possibility that this is not right. This is really not doing this at all but it's got some exponential correlation. It is a finite time. It cannot be, there is no such thing in real life as delta correlated noise because at some correlation time, no matter how small it can never be mathematically zero, right? So that is the first step. So let's do that.

Let's say that this quantity is not that at all but it is some, some other constant k times e to the minus t over tau, e to the minus mod t 1 minus t 2 over tau. That's a symmetric function. It is stationary and so on,

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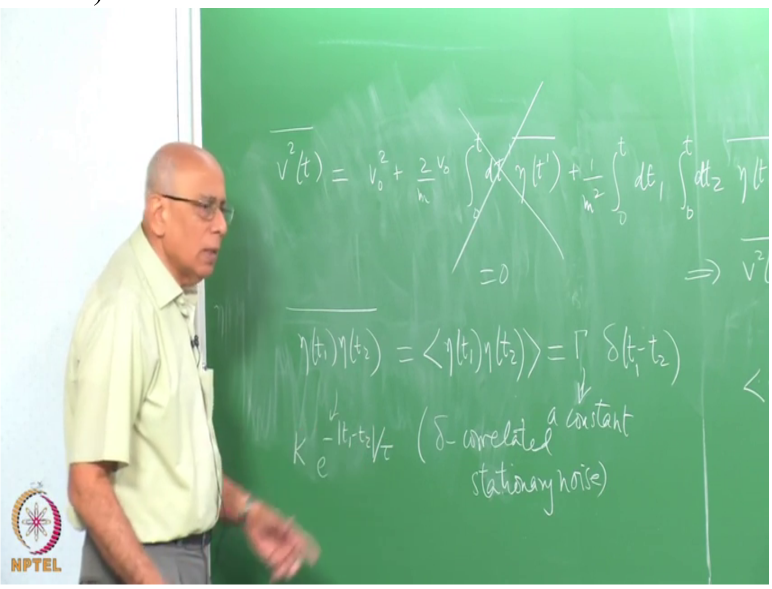

so we could say, good, we will put this here. So this integral is not so easy, instead of a delta function you have got to put this here into it. I leave you to check that you can do this integral once again now; it is a very reasonable assumption to make. It is an exponentially decaying function instead of just a delta function.

And one can say, alright. Let me do that integral now and see what happens. A little more hard work because you have to do both integrals, t 1 and t 2 but I leave you to check that you will again run into exactly the same problem. This won't quite be, there would be a little more complicated expression but there is no doubt that eventually you will end up with something that increases with t and doesn't stay in equilibrium, Ok. So check that the incorrectness of this model is not due to the assumption that this noise is delta correlated. Even a finite correlation time will still produce the same thing, Ok. So that's an exercise for you to check out. But it still does.

So that, that’s out. That explanation is ruled out. What is the other possibility? What are the possibilities there? Would you say Newton's equation is wrong? A classical particle has to satisfy Newton's equation. Would you say the fact that the mean value of the velocity, the noise is zero is wrong? That's not because that will just remove the mean value of the velocity, itself will not be correct if...Ok. So we have ruled out all the other possibilities. So what do you think is wrong?

(Professor – student conversation starts)
Student: If the particle is moving in the fluid, it will probably have a drag...
Professor: Yeah, so there are subtle effects like that. There is a back flow, there is all kind of complications like that there are many, many such effects. There is a reaction on the particles definitely. There is certainly a backflow and a reaction on the bath particles, that's not taken into account here. But that's not the reason in this case. One can take into account in some fashion but it is not.
(Professor – student conversation ends)

But the other statement you made, that there is a drag on this is certainly a place to pause and give some thought to it. How does this drag show up in this model? How will it show up? Well, imagine this particle, I am the particle and it is one dimension motion, and I move this way and constantly being buffeted on both sides by molecules. What happens if I move relative to these particles in one particular direction? What happens when you walk in the rain? And the rain is coming straight down and you walk? Where do you get wetter, in the front or at the back?

(Professor – student conversation starts)
Student: In the front. 0:47:39.1

Professor: Front. Certainly what happens is when you move in a crowd, there is more particles hitting you per unit time from the front than from the back, right. And they impede your motion. You turn around and walk in the other direction. There are more particles hitting you from this side and they impede your motion. That is what you call viscous drag. That is precisely it.

(Professor – student conversation ends)

So there is a part of this random force which is actually dependent on the motion of the particle itself. That force disappears if the particle had zero velocity instantaneously. The moment it starts having a velocity, there is a drag on it, a viscous drag right. So it means that model is incomplete, this force, this random force has really got two components. So there is systematic, eta systematic of t, and eta truly random, let us put it in quotation marks.

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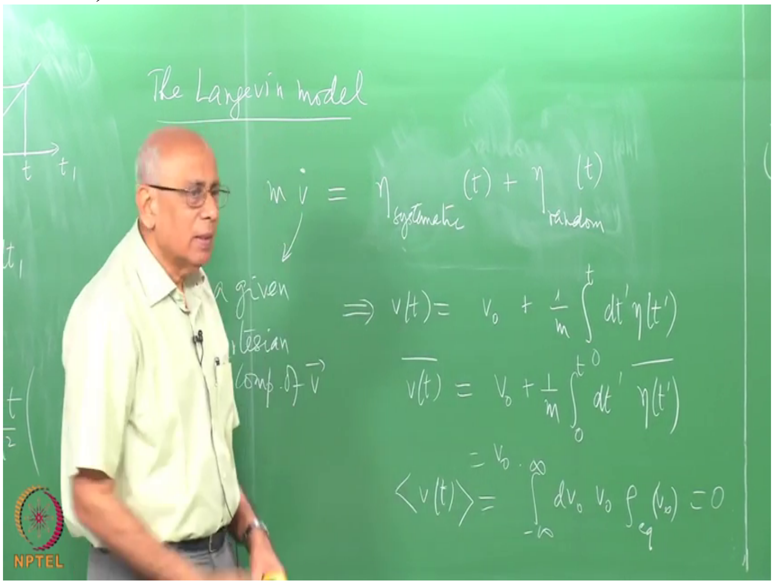

This is acting like noise but this depends on the state of motion of the particle itself, Ok. And what is the simplest model of viscosity, the linear model?

(Professor – student conversation starts)

Student: Two times 0:48:53.3

Professor: Proportional to its velocity. So it is clear that what we have to do is to leave this as the white noise out here, but this quantity here is in direction opposite to the motion of the particle, multiplied by some constant gamma and then v of t itself, right. I want this gamma to have dimensions of time inverse, so let us put an m here.

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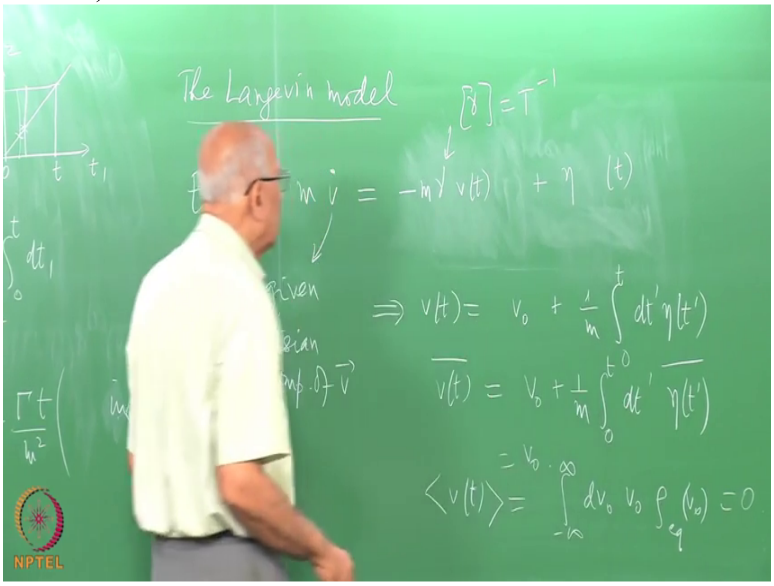

Yeah

Student: Sir

Professor: Yeah

Student: Talking at molecular level, what is this drag force like? Already we…

Professor: This is a much bigger particle, right. What you call viscosity is the internal friction in the fluid which any given fluid layer sees due to the other particles in the fluid, right. So we are now adopting an extremely simple naive view of viscosity as being simply being proportional to the velocity to start with. But we will see if this can be refined, it should be refined but that's the zeroth order guess.

(Professor – student conversation ends)

Eventually I have this vague feeling somewhere that this quantity, this force, this gamma, this constant gamma will get related in some mysterious fashion to the viscosity of the fluid. That's what I would expect. Because that's what measures the level of viscous drag, drag forces on objects in the fluid, right?

(Professor – student conversation starts)

Student: Viscous is like the molecular level and at molecular level 0:50:25.1 is it like some kind of...

Professor: But this object is much bigger than a given molecule.

Student: There is some kind of particle attraction...

Professor: No it is much bigger than the molecules like when you calculate Reynolds Number to tell you when turbulence sets in, etc, the viscosity plays a role because you put a big circular obstacle or spherical obstacle or whatever inside a fluid and then you measure what the drag on it is. So that's one of the reasons I said this particle we are talking about is tens or thousands of times bigger than the molecules. So it is not at the molecular level. But the manifestation of that will come from the property of the fluid which is its viscosity.
(Professor – student conversation ends)

And yes, it is a hard problem to calculate what the coefficient of viscosity is from the molecular level. But that's the standard problem in many-body theory. There are computations for it; I might even mention some of them later. So this is the model we are going to put in here. I will stop here today since we have run out of time. But once you put this in and make the same assumptions about eta of t, we go exactly the same calculations.
Let me just write down just the first step in it.

The solution of course is v naught e to the minus gamma t here because there is an integrating factor

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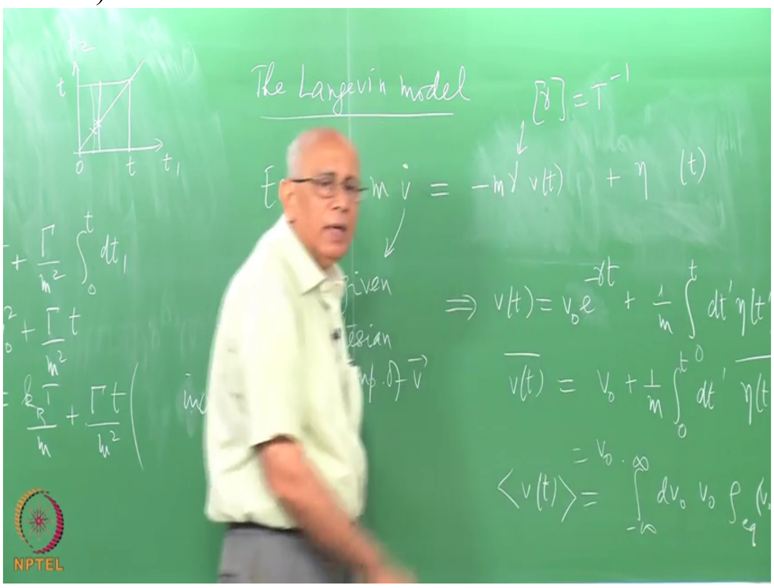

which is e to the gamma t. So I put it to the right hand side. You get this, plus you no longer have this simpler solution. So you have plus 1 over m integral zero to t d t prime e to the minus gamma t minus t prime eta of t prime. So that's

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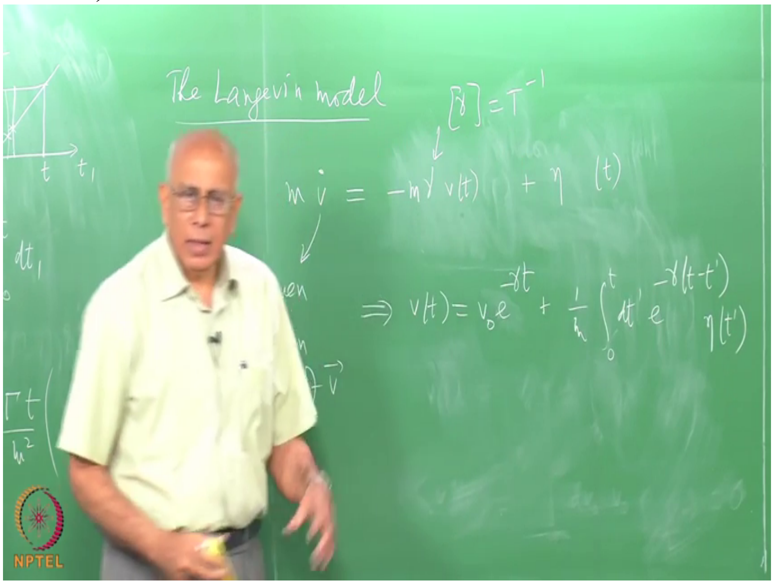

the solution and I request you to find out now what the mean value is, first the conditional mean and after that the complete mean and then similarly what the mean square value is, first the conditional mean square and then the full mean square value. We take it from that point.